W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Jul 19, 2016 – 01:25 AM EDT

PDB ID	:	4ZIW
Title	:	Crystal structure of AcrB deletion mutant in P21 space group
Authors	:	Ababou, A.; Koronakis, V.
Deposited on	:	2015-04-28
Resolution	:	3.40 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
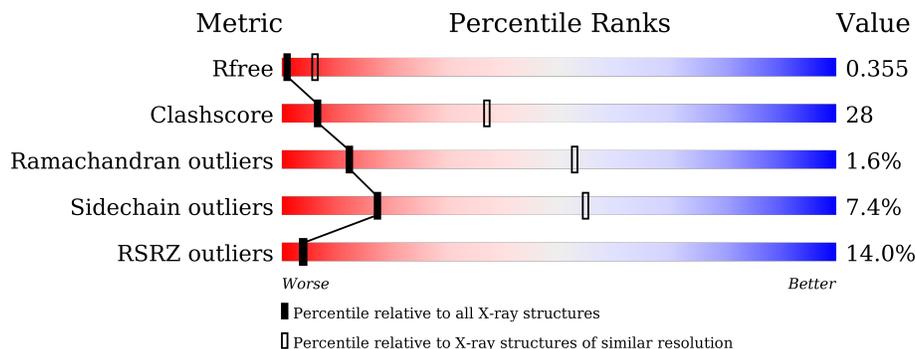
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1044	12% / 47% / 47% / 5% •
1	B	1044	10% / 50% / 45% / •
1	C	1044	12% / 47% / 47% / 5% •
1	D	1044	16% / 44% / 50% / 5% ••
1	E	1044	17% / 47% / 47% / 5% •
1	F	1044	17% / 46% / 48% / 5% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	LMT	B	2000	-	-	-	X
2	LMT	D	2000	X	-	-	-
2	LMT	E	1101	X	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 47532 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1038	Total 7893	C 5072	N 1306	O 1472	S 43	0	0	0
1	B	1039	Total 7900	C 5076	N 1307	O 1474	S 43	0	0	0
1	C	1035	Total 7867	C 5057	N 1299	O 1468	S 43	0	0	0
1	D	1038	Total 7893	C 5072	N 1306	O 1472	S 43	0	0	0
1	E	1037	Total 7883	C 5066	N 1303	O 1471	S 43	0	0	0
1	F	1037	Total 7883	C 5066	N 1303	O 1471	S 43	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	615	GLY	PHE	engineered mutation	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	PHE	deletion	UNP P31224
A	?	-	ALA	deletion	UNP P31224
A	?	-	GLY	deletion	UNP P31224
A	?	-	ARG	deletion	UNP P31224
B	615	GLY	PHE	engineered mutation	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	PHE	deletion	UNP P31224
B	?	-	ALA	deletion	UNP P31224
B	?	-	GLY	deletion	UNP P31224
B	?	-	ARG	deletion	UNP P31224
C	615	GLY	PHE	engineered mutation	UNP P31224
C	?	-	GLY	deletion	UNP P31224
C	?	-	PHE	deletion	UNP P31224
C	?	-	ALA	deletion	UNP P31224
C	?	-	GLY	deletion	UNP P31224

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ARG	deletion	UNP P31224
D	615	GLY	PHE	engineered mutation	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	PHE	deletion	UNP P31224
D	?	-	ALA	deletion	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	ARG	deletion	UNP P31224
E	615	GLY	PHE	engineered mutation	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	PHE	deletion	UNP P31224
E	?	-	ALA	deletion	UNP P31224
E	?	-	GLY	deletion	UNP P31224
E	?	-	ARG	deletion	UNP P31224
F	615	GLY	PHE	engineered mutation	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	PHE	deletion	UNP P31224
F	?	-	ALA	deletion	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	ARG	deletion	UNP P31224

- Molecule 2 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).
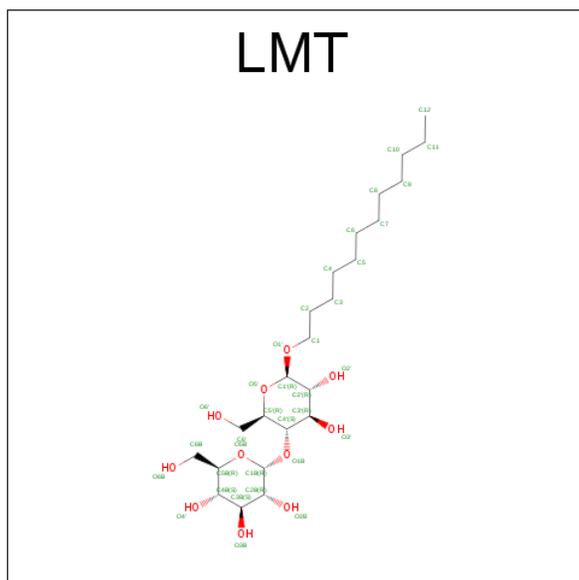
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	35	24	11	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 35	C 24	O 11	0	0
2	C	1	Total 35	C 24	O 11	0	0
2	D	1	Total 35	C 24	O 11	0	0
2	E	1	Total 35	C 24	O 11	0	0
2	F	1	Total 35	C 24	O 11	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ni 1	0	0
3	C	1	Total 1	Ni 1	0	0
3	E	1	Total 1	Ni 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Multidrug efflux pump subunit AcrB
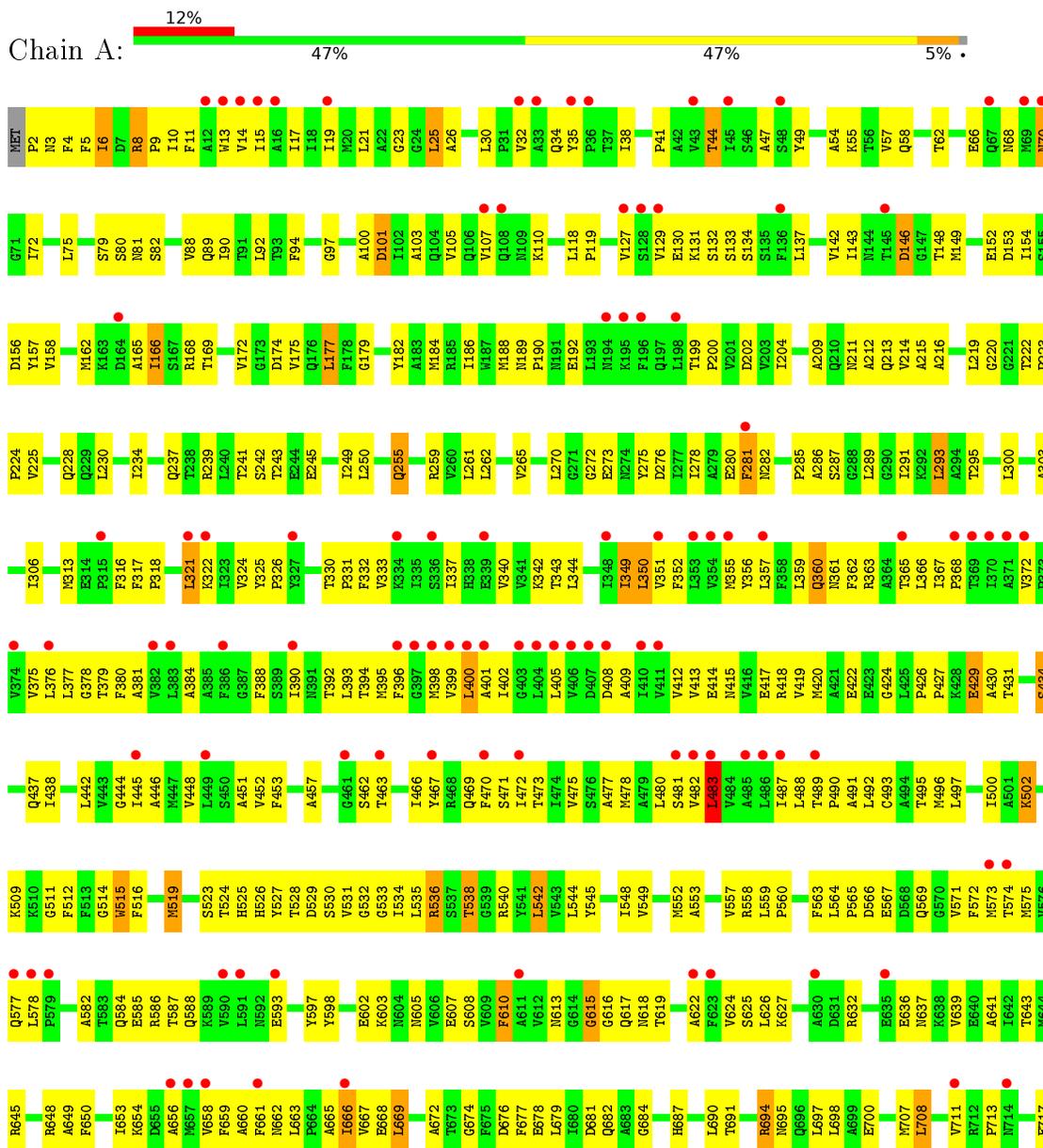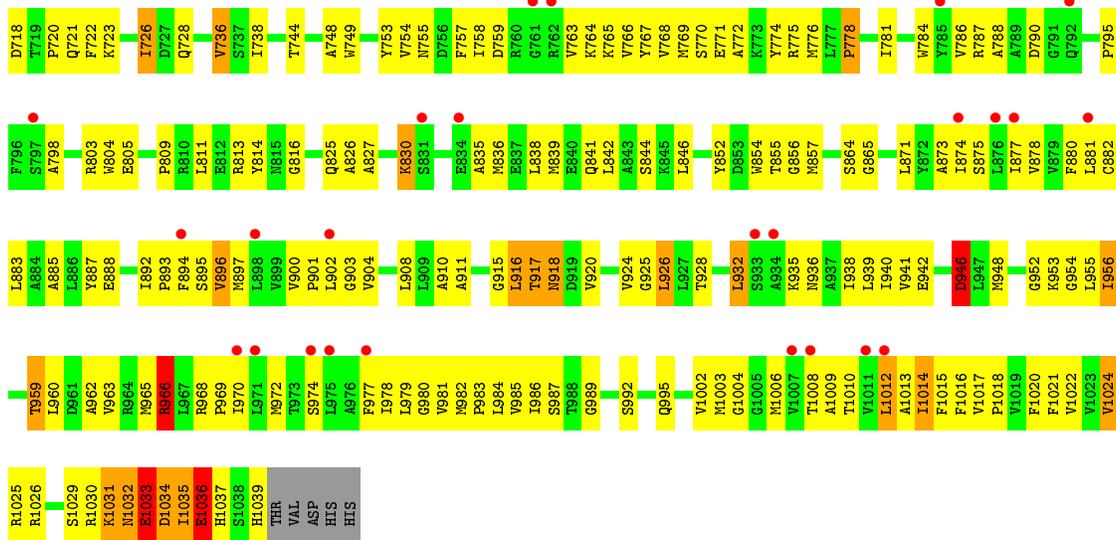
• Molecule 1: Multidrug efflux pump subunit AcrB

Chain B:

10%

50% 45%

• Molecule 1: Multidrug efflux pump subunit AcrB

Chain C:

• Molecule 1: Multidrug efflux pump subunit AcrB

Chain D:
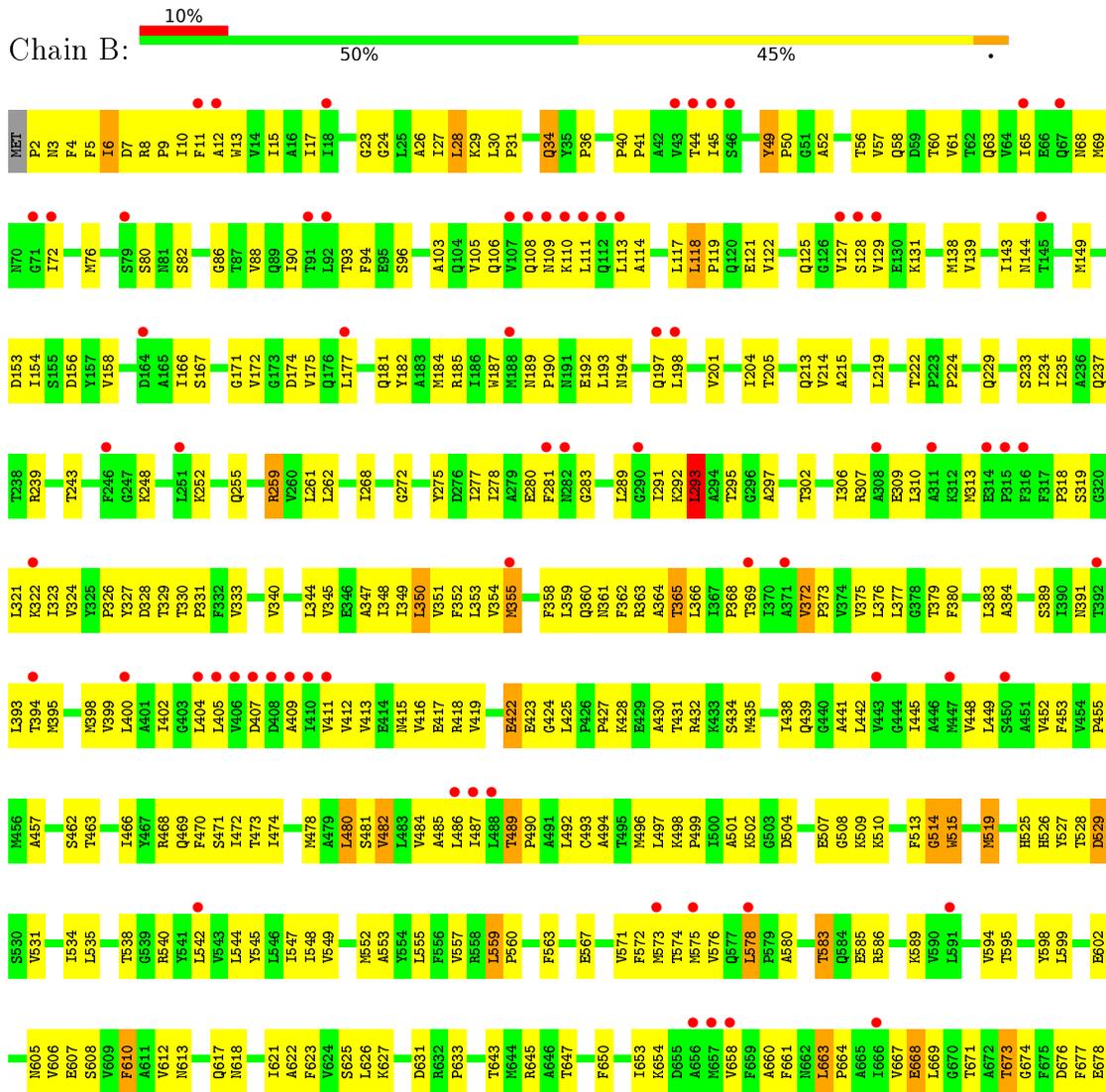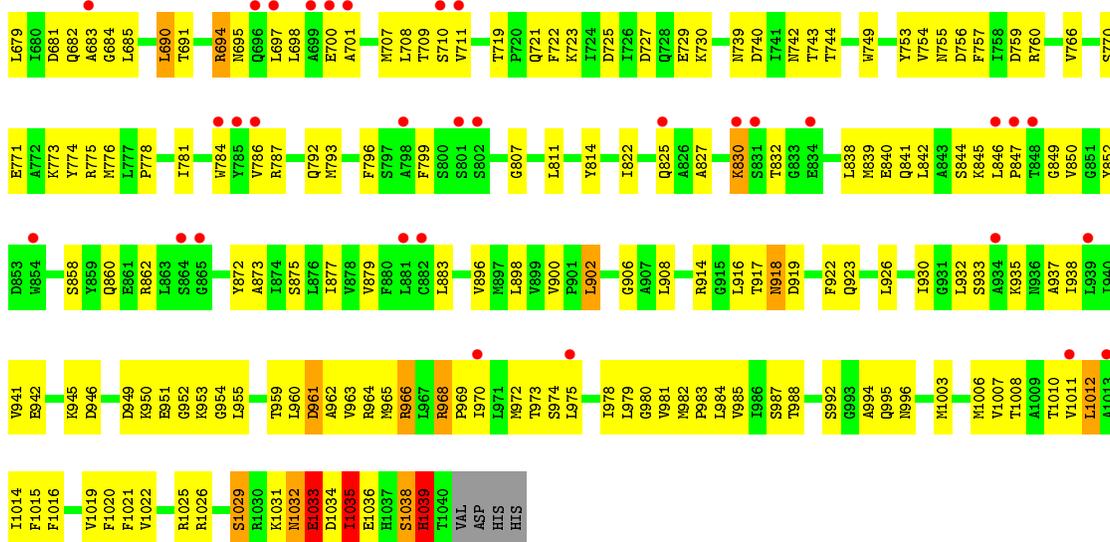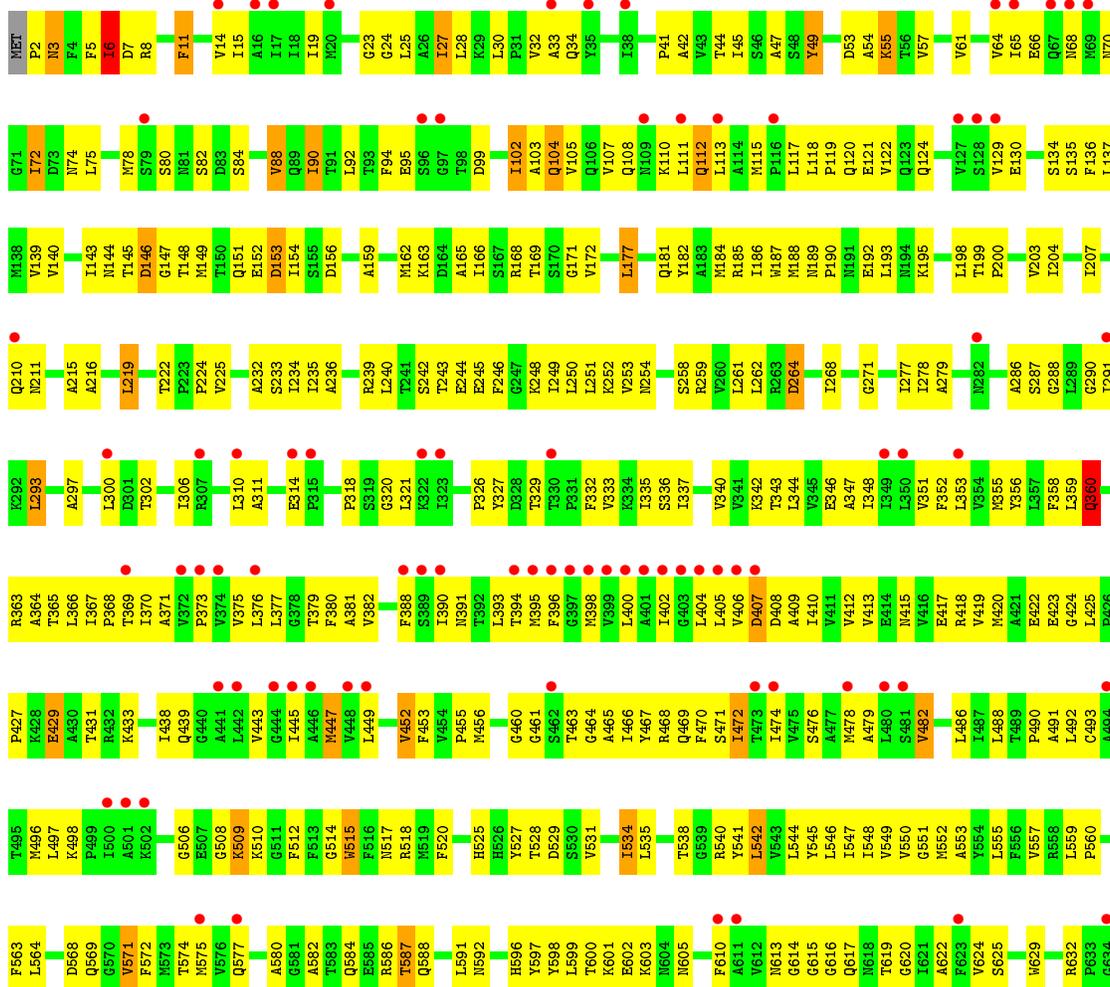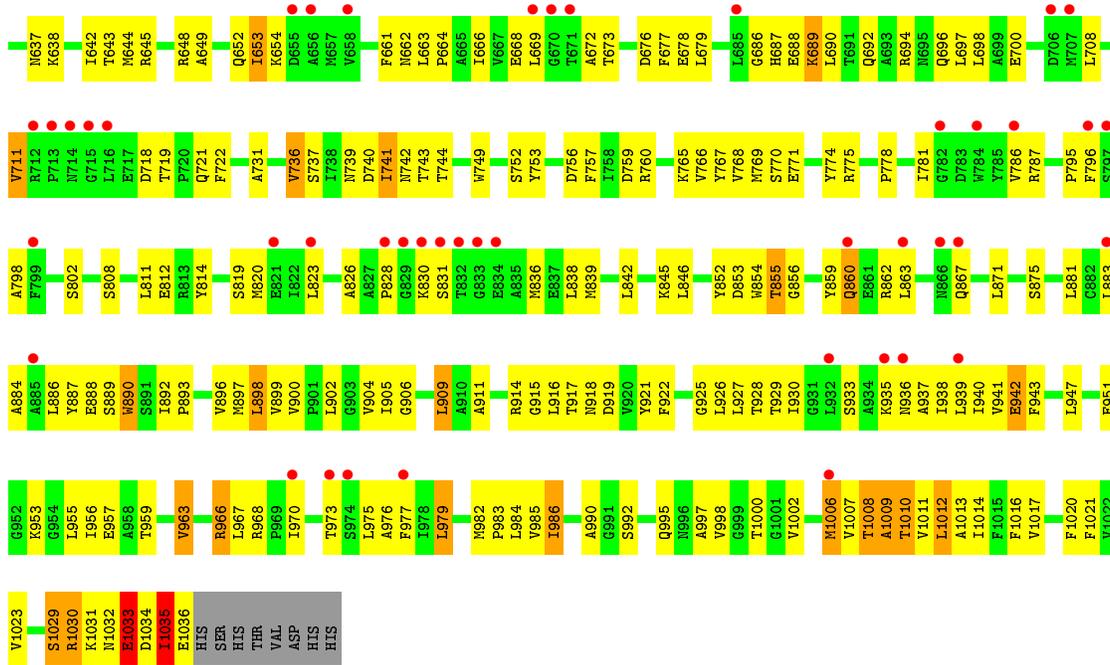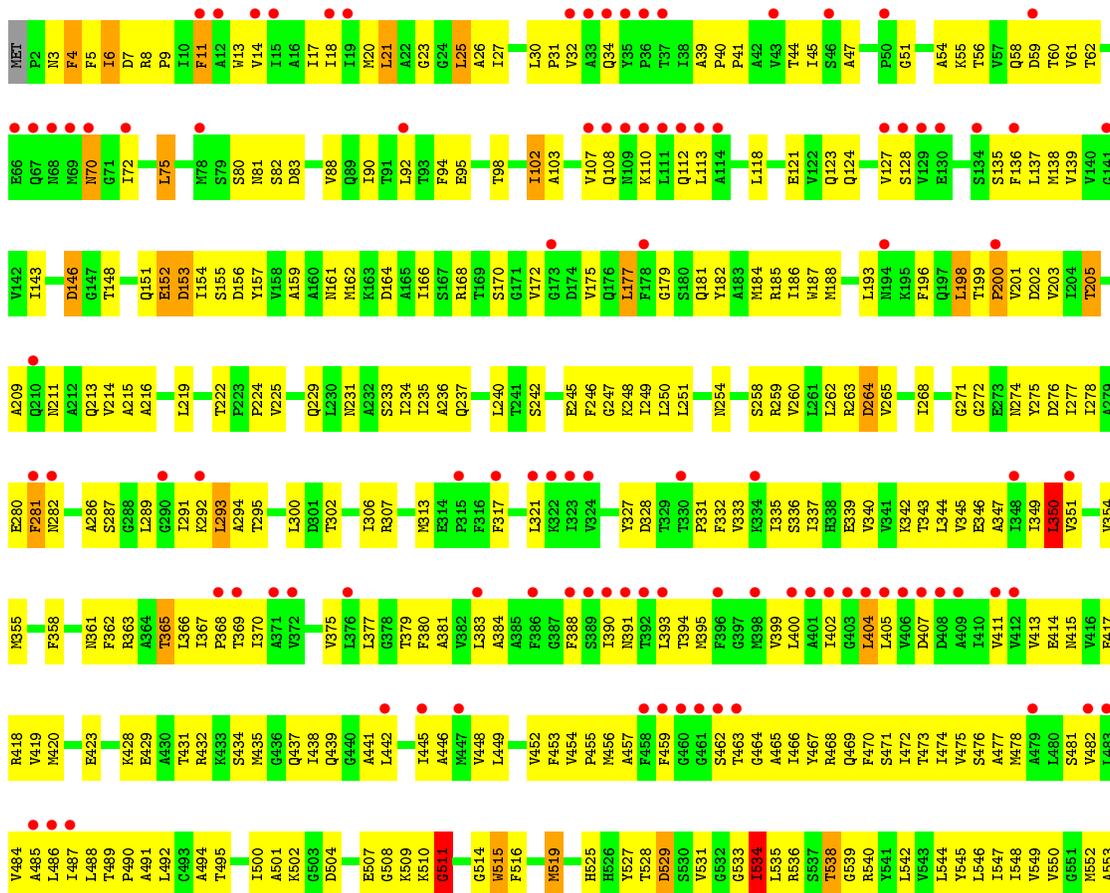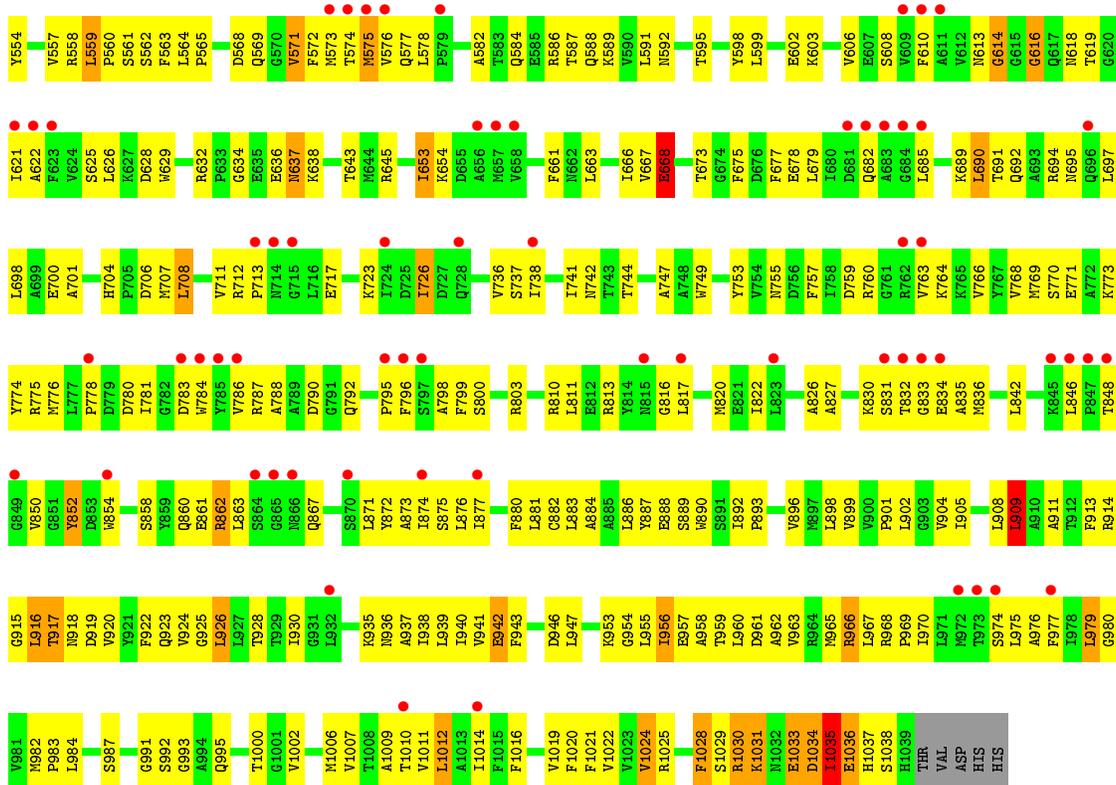
• Molecule 1: Multidrug efflux pump subunit AcrB
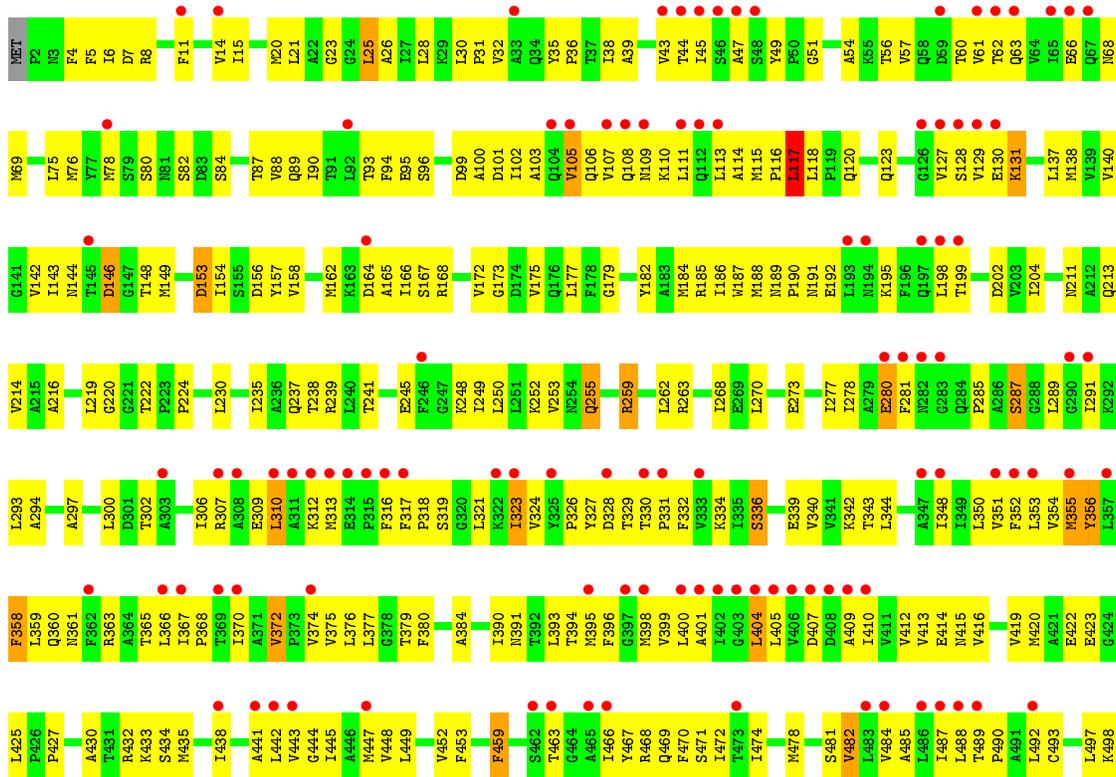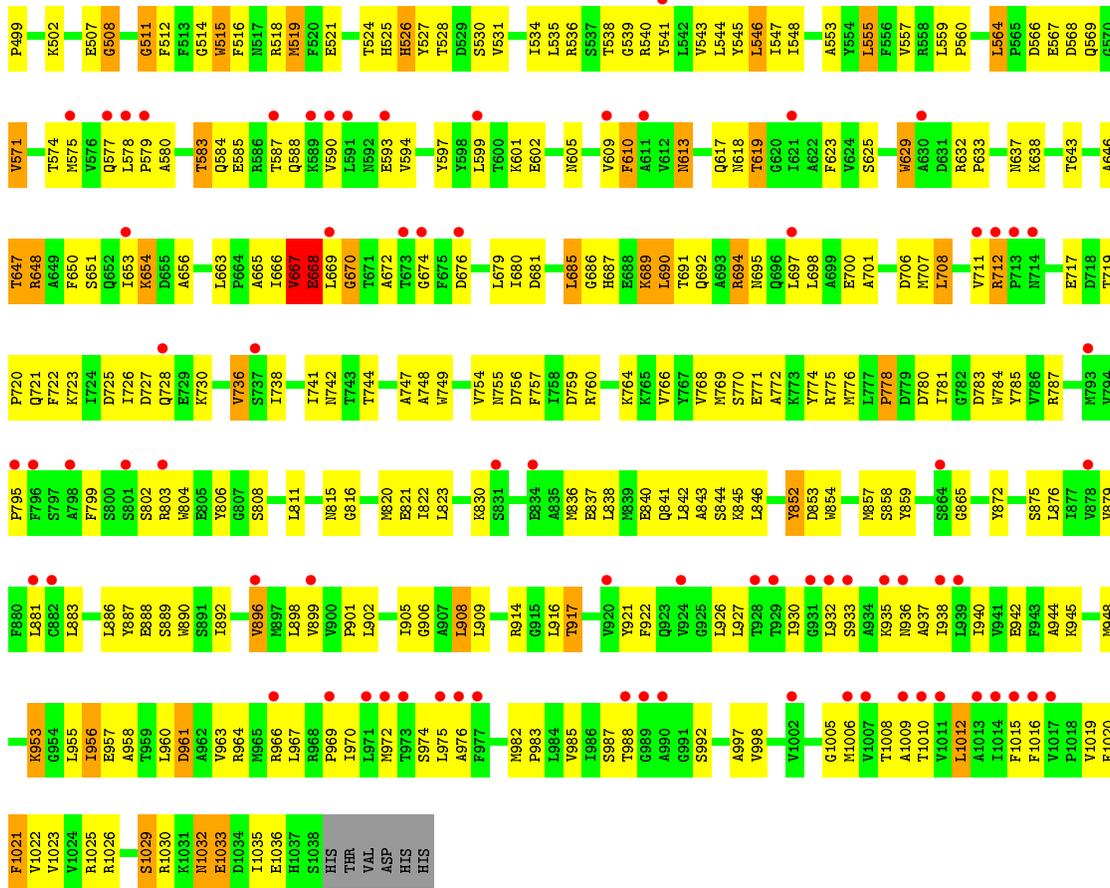
• Molecule 1: Multidrug efflux pump subunit AcrB
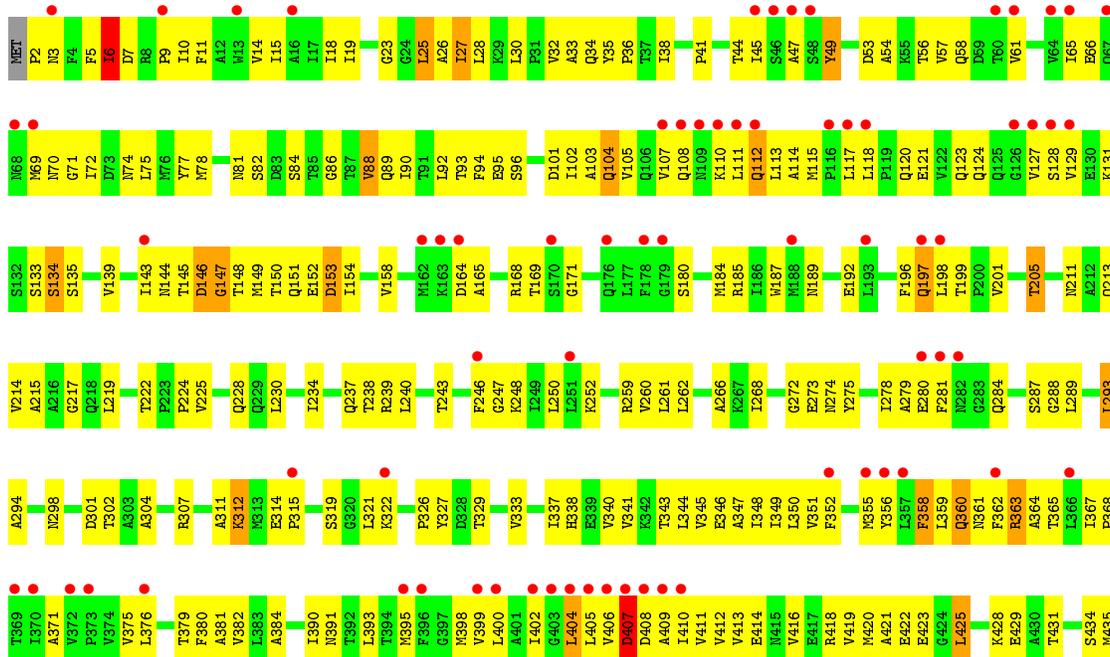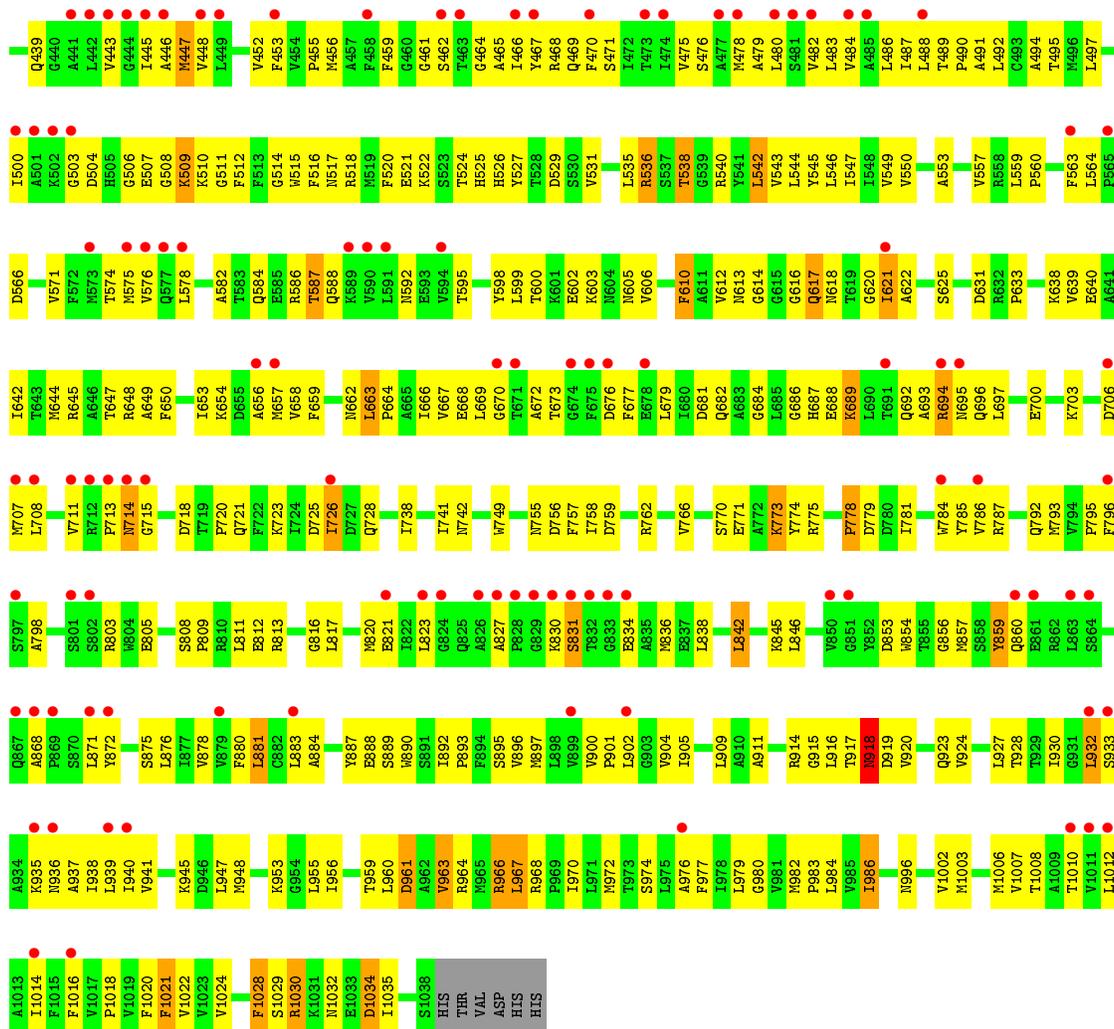
4   Data and refinement statistics (i)

| Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	152.07Å 157.78Å 219.39Å 90.00° 93.14° 90.00°	Depositor
Resolution (Å)	20.00 – 3.40 109.53 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-3.40) 97.9 (109.53-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.275 , 0.349 0.286 , 0.355	Depositor DCC
R_{free} test set	6960 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	98.0	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 74.0	EDS
L-test for twinning[2]	$< |L| > = 0.38, < L^2 > = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.80	EDS
Total number of atoms	47532	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.43 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 9.9288e-05.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, LMT

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.65	1/8043 (0.0%)	0.89	11/10922 (0.1%)
1	B	0.65	1/8050 (0.0%)	0.89	9/10932 (0.1%)
1	C	0.67	1/8015 (0.0%)	0.91	9/10884 (0.1%)
1	D	0.60	1/8043 (0.0%)	0.89	15/10922 (0.1%)
1	E	0.60	1/8032 (0.0%)	0.87	12/10907 (0.1%)
1	F	0.60	0/8032	0.89	7/10907 (0.1%)
All	All	0.63	5/48215 (0.0%)	0.89	63/65474 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	1
1	D	0	1
1	F	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	515	TRP	CB-CG	7.50	1.63	1.50
1	A	515	TRP	CB-CG	6.68	1.62	1.50
1	E	515	TRP	CB-CG	5.77	1.60	1.50
1	B	515	TRP	CB-CG	5.72	1.60	1.50
1	C	515	TRP	CB-CG	5.07	1.59	1.50

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	939	LEU	CA-CB-CG	-8.38	96.02	115.30
1	C	529	ASP	CB-CG-OD1	8.07	125.56	118.30
1	F	529	ASP	CB-CG-OD1	7.98	125.48	118.30
1	A	529	ASP	CB-CG-OD1	7.69	125.22	118.30
1	D	350	LEU	CA-CB-CG	-7.26	98.61	115.30
1	B	480	LEU	CA-CB-CG	-7.17	98.80	115.30
1	D	979	LEU	CA-CB-CG	-6.85	99.55	115.30
1	E	670	GLY	N-CA-C	6.56	129.51	113.10
1	E	908	LEU	CA-CB-CG	6.55	130.37	115.30
1	B	529	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	250	LEU	CA-CB-CG	6.50	130.25	115.30
1	A	939	LEU	CA-CB-CG	-6.47	100.42	115.30
1	C	967	LEU	CA-CB-CG	6.47	130.18	115.30
1	C	72	ILE	CG1-CB-CG2	-6.41	97.31	111.40
1	D	511	GLY	N-CA-C	6.28	128.79	113.10
1	B	690	LEU	CA-CB-CG	6.24	129.65	115.30
1	D	529	ASP	CB-CG-OD1	6.24	123.91	118.30
1	F	425	LEU	CA-CB-CG	6.20	129.56	115.30
1	D	198	LEU	CA-CB-CG	6.20	129.55	115.30
1	E	519	MET	CB-CG-SD	6.13	130.78	112.40
1	F	967	LEU	CA-CB-CG	6.11	129.36	115.30
1	A	946	ASP	CB-CG-OD1	6.10	123.79	118.30
1	D	75	LEU	CA-CB-CG	6.09	129.30	115.30
1	B	293	LEU	CA-CB-CG	6.00	129.09	115.30
1	B	519	MET	CB-CG-SD	5.96	130.28	112.40
1	D	534	ILE	CG1-CB-CG2	-5.96	98.30	111.40
1	A	932	LEU	CA-CB-CG	-5.93	101.67	115.30
1	A	483	LEU	CA-CB-CG	5.92	128.92	115.30
1	D	690	LEU	CA-CB-CG	5.92	128.92	115.30
1	E	117	LEU	CA-CB-CG	5.82	128.69	115.30
1	F	842	LEU	CA-CB-CG	5.80	128.64	115.30
1	D	21	LEU	CA-CB-CG	-5.71	102.17	115.30
1	E	1032	ASN	C-N-CA	5.64	135.79	121.70
1	C	979	LEU	CA-CB-CG	-5.61	102.39	115.30
1	D	967	LEU	CA-CB-CG	5.61	128.19	115.30
1	E	546	LEU	CA-CB-CG	5.59	128.17	115.30
1	D	293	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	118	LEU	CA-CB-CG	5.53	128.02	115.30
1	C	534	ILE	CG1-CB-CG2	-5.42	99.47	111.40
1	E	674	GLY	N-CA-C	5.42	126.65	113.10
1	B	555	LEU	CA-CB-CG	-5.40	102.88	115.30
1	C	542	LEU	CA-CB-CG	-5.38	102.92	115.30
1	C	30	LEU	CA-CB-CG	5.38	127.67	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	287	SER	C-N-CA	-5.33	111.11	122.30
1	A	321	LEU	CA-CB-CG	5.32	127.53	115.30
1	E	449	LEU	CA-CB-CG	-5.32	103.07	115.30
1	F	536	ARG	CG-CD-NE	5.29	122.91	111.80
1	C	1006	MET	CB-CG-SD	5.28	128.24	112.40
1	E	407	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	668	GLU	N-CA-C	5.25	125.17	111.00
1	F	932	LEU	CA-CB-CG	5.22	127.30	115.30
1	A	674	GLY	N-CA-C	5.21	126.13	113.10
1	C	898	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	E	293	LEU	CA-CB-CG	5.13	127.10	115.30
1	A	8	ARG	CB-CG-CD	-5.13	98.27	111.60
1	D	1033	GLU	C-N-CA	5.11	134.47	121.70
1	F	404	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	B	902	LEU	CA-CB-CG	5.09	127.01	115.30
1	B	28	LEU	CB-CG-CD2	5.03	119.56	111.00
1	D	488	LEU	CA-CB-CG	-5.03	103.74	115.30
1	E	865	GLY	N-CA-C	-5.02	100.54	113.10
1	A	966	ARG	CB-CA-C	5.01	120.42	110.40
1	A	357	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1033	GLU	Peptide
1	A	1034	ASP	Peptide
1	A	1036	GLU	Peptide
1	B	1033	GLU	Peptide
1	B	1035	ILE	Peptide
1	C	6	ILE	Peptide
1	D	1035	ILE	Peptide
1	F	6	ILE	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7893	0	8034	457	0
1	B	7900	0	8041	384	0
1	C	7867	0	8015	444	0
1	D	7893	0	8034	515	0
1	E	7883	0	8027	461	0
1	F	7883	0	8027	477	0
2	A	35	0	46	4	0
2	B	35	0	46	3	0
2	C	35	0	46	1	0
2	D	35	0	46	3	0
2	E	35	0	46	8	0
2	F	35	0	46	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
All	All	47532	0	48454	2651	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (2651) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:536:ARG:NE	2:E:1101:LMT:O3B	1.81	1.13
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.38	1.04
1:D:954:GLY:HA2	1:D:1034:ASP:H	1.23	1.03
1:C:686:GLY:HA3	1:C:689:LYS:HD3	1.42	1.01
1:D:533:GLY:HA2	1:D:536:ARG:HD3	1.48	0.95
1:D:113:LEU:HD11	1:F:128:SER:HB3	1.46	0.94
1:A:41:PRO:HG2	1:A:94:PHE:HB2	1.50	0.92
1:E:214:VAL:HG11	1:F:742:ASN:HB3	1.51	0.91
1:F:340:VAL:HG11	1:F:395:MET:HB3	1.53	0.91
1:E:239:ARG:NH1	1:E:756:ASP:O	2.04	0.90
1:E:354:VAL:HG22	1:E:975:LEU:HD23	1.51	0.90
1:C:151:GLN:NE2	1:C:286:ALA:O	2.05	0.89
1:C:151:GLN:NE2	1:C:279:ALA:O	2.04	0.89
1:D:571:VAL:HG22	1:D:625:SER:HA	1.54	0.89
1:D:776:MET:HE1	1:F:225:VAL:H	1.37	0.89
1:E:179:GLY:HA2	1:E:277:ILE:HD11	1.54	0.89
1:E:355:MET:HG2	1:E:365:THR:HA	1.54	0.88
1:B:34:GLN:HG3	1:B:333:VAL:HG22	1.55	0.88
1:A:571:VAL:HG22	1:A:625:SER:HA	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.54	0.88
1:C:61:VAL:HA	1:C:118:LEU:HD22	1.56	0.87
1:E:211:ASN:O	1:E:755:ASN:ND2	2.07	0.87
1:E:680:ILE:HD11	1:E:853:ASP:HB2	1.56	0.87
1:D:446:ALA:HB2	1:D:482:VAL:HG21	1.56	0.87
1:C:156:ASP:OD1	1:C:760:ARG:NH2	2.08	0.87
1:B:350:LEU:HD22	1:B:979:LEU:HB3	1.57	0.86
1:C:939:LEU:HB3	1:C:966:ARG:HD2	1.58	0.86
1:D:70:ASN:O	1:D:110:LYS:NZ	2.09	0.86
1:D:291:ILE:HD13	1:D:306:ILE:HD13	1.57	0.85
1:C:653:ILE:HG13	1:C:654:LYS:HE2	1.58	0.85
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.59	0.85
1:A:723:LYS:NZ	1:C:236:ALA:O	2.09	0.84
1:F:686:GLY:HA3	1:F:689:LYS:HD3	1.58	0.84
1:D:159:ALA:HB2	1:D:177:LEU:HD11	1.57	0.84
1:F:961:ASP:OD1	1:F:964:ARG:NH2	2.11	0.83
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.43	0.83
1:C:264:ASP:OD1	1:C:264:ASP:N	2.12	0.83
1:B:415:ASN:HD22	1:B:434:SER:HB2	1.42	0.83
1:D:457:ALA:O	1:D:468:ARG:NE	2.10	0.83
1:D:156:ASP:OD1	1:D:760:ARG:NH2	2.12	0.83
1:D:187:TRP:HB3	1:D:771:GLU:HA	1.59	0.82
1:D:41:PRO:HG2	1:D:94:PHE:HB2	1.59	0.82
1:B:664:PRO:HB3	1:B:669:LEU:HD12	1.61	0.82
1:D:706:ASP:O	1:D:830:LYS:NZ	2.11	0.82
1:E:307:ARG:NH2	1:E:328:ASP:OD2	2.12	0.82
1:D:400:LEU:HD23	1:D:924:VAL:HG12	1.61	0.81
1:D:60:THR:HG23	1:D:61:VAL:HG23	1.62	0.81
1:D:953:LYS:NZ	1:D:957:GLU:OE1	2.13	0.80
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.63	0.80
1:A:237:GLN:OE1	1:B:742:ASN:ND2	2.14	0.80
1:F:248:LYS:HA	1:F:261:LEU:HD13	1.63	0.80
1:D:453:PHE:O	1:D:471:SER:OG	1.99	0.80
1:A:691:THR:HG23	1:A:694:ARG:HH12	1.47	0.79
1:D:455:PRO:HG2	1:D:875:SER:HB2	1.62	0.79
1:E:1032:ASN:HB3	1:E:1033:GLU:HB3	1.64	0.79
1:A:966:ARG:HE	1:A:970:ILE:HD11	1.46	0.79
1:E:584:GLN:HB2	1:E:617:GLN:HG2	1.64	0.79
1:F:34:GLN:HB2	1:F:333:VAL:HG22	1.64	0.79
1:F:930:ILE:O	1:F:933:SER:OG	2.00	0.79
1:D:139:VAL:HB	1:D:327:TYR:HB3	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:THR:HA	1:D:224:PRO:HD3	1.63	0.79
1:A:153:ASP:OD2	1:A:182:TYR:OH	2.00	0.78
1:C:914:ARG:O	1:C:916:LEU:N	2.16	0.78
1:E:516:PHE:HA	1:E:519:MET:HG3	1.65	0.78
1:C:262:LEU:HG	1:C:268:ILE:HD11	1.65	0.78
1:F:356:TYR:HA	1:F:365:THR:HG21	1.65	0.78
1:A:375:VAL:O	1:A:379:THR:OG1	2.01	0.78
1:A:955:LEU:O	1:A:959:THR:OG1	2.01	0.78
1:A:1034:ASP:HB3	1:A:1035:ILE:HA	1.66	0.78
1:B:427:PRO:HD3	1:B:499:PRO:HB3	1.65	0.78
1:F:45:ILE:HG12	1:F:129:VAL:HG13	1.66	0.78
1:C:360:GLN:OE1	1:C:517:ASN:ND2	2.15	0.78
1:D:414:GLU:OE1	1:D:968:ARG:NH1	2.17	0.78
1:D:344:LEU:HD23	1:D:402:ILE:HD11	1.66	0.78
1:D:211:ASN:O	1:D:755:ASN:ND2	2.18	0.77
1:E:966:ARG:O	1:E:970:ILE:HG12	1.84	0.77
1:C:3:ASN:N	1:C:3:ASN:OD1	2.16	0.77
1:B:327:TYR:HB2	1:B:623:PHE:HE2	1.47	0.77
1:F:82:SER:HB2	1:F:811:LEU:HB2	1.65	0.77
1:D:457:ALA:HA	1:D:468:ARG:HG3	1.67	0.77
1:E:156:ASP:OD1	1:E:760:ARG:NH2	2.18	0.77
1:E:708:LEU:HD21	1:E:838:LEU:HD12	1.67	0.77
1:B:602:GLU:HG3	1:B:605:ASN:HB2	1.66	0.77
1:D:632:ARG:HH12	1:D:638:LYS:HA	1.50	0.77
1:E:507:GLU:HG2	1:E:518:ARG:HA	1.66	0.76
1:F:662:ASN:O	1:F:673:THR:OG1	2.03	0.76
1:A:291:ILE:HD13	1:A:306:ILE:HD13	1.66	0.76
1:C:427:PRO:O	1:C:431:THR:OG1	2.03	0.76
1:A:344:LEU:HD23	1:A:402:ILE:HD11	1.67	0.76
1:C:588:GLN:NE2	1:C:592:ASN:OD1	2.17	0.76
1:C:940:ILE:HG12	1:C:966:ARG:CZ	2.15	0.76
1:D:1036:GLU:HB3	1:D:1037:HIS:HB2	1.68	0.76
1:E:144:ASN:ND2	1:E:319:SER:O	2.15	0.76
1:E:415:ASN:HD22	1:E:434:SER:HB2	1.51	0.76
1:A:214:VAL:HG11	1:B:742:ASN:HB3	1.68	0.76
1:A:34:GLN:HE21	1:A:332:PHE:HE2	1.34	0.76
1:A:491:ALA:O	1:A:495:THR:OG1	2.04	0.76
1:A:605:ASN:HD21	1:A:637:ASN:HA	1.51	0.75
1:E:340:VAL:HG11	1:E:395:MET:HB3	1.68	0.75
1:E:343:THR:HG21	1:E:399:VAL:HG13	1.65	0.75
1:E:241:THR:N	1:E:245:GLU:OE1	2.19	0.75

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:955:LEU:H	1:A:1033:GLU:HA	1.52	0.75
1:C:632:ARG:NH1	1:C:637:ASN:O	2.19	0.75
1:C:460:GLY:O	1:C:867:GLN:NE2	2.20	0.75
1:E:115:MET:O	1:E:123:GLN:NE2	2.18	0.75
1:A:687:HIS:NE2	1:A:718:ASP:OD1	2.19	0.75
1:A:776:MET:HE1	1:C:225:VAL:H	1.50	0.75
1:A:639:VAL:HG11	1:A:662:ASN:HB2	1.67	0.75
1:D:11:PHE:N	1:E:888:GLU:OE1	2.17	0.75
1:C:418:ARG:O	1:C:422:GLU:HB2	1.87	0.75
1:A:415:ASN:HB3	1:A:434:SER:HB2	1.67	0.75
1:E:23:GLY:HA3	1:E:377:LEU:HB3	1.68	0.74
1:C:198:LEU:HD11	1:C:252:LYS:HB2	1.67	0.74
1:C:708:LEU:HD23	1:C:711:VAL:HG21	1.69	0.74
1:D:770:SER:HB3	1:D:775:ARG:HD3	1.68	0.74
1:D:588:GLN:NE2	1:D:592:ASN:OD1	2.18	0.74
1:B:930:ILE:O	1:B:933:SER:OG	2.05	0.74
1:D:966:ARG:HE	1:D:970:ILE:HD11	1.50	0.74
1:F:715:GLY:HA3	1:F:812:GLU:OE1	1.88	0.74
1:A:955:LEU:HD21	1:A:1022:VAL:HG13	1.68	0.74
1:F:598:TYR:HB3	1:F:606:VAL:HG21	1.68	0.74
1:A:38:ILE:HD11	1:A:466:ILE:HD11	1.70	0.74
1:E:39:ALA:HB2	1:E:668:GLU:HG3	1.70	0.74
1:F:936:ASN:HD21	1:F:1010:THR:HG22	1.52	0.74
1:A:175:VAL:HG11	1:A:289:LEU:HD13	1.68	0.74
1:A:531:VAL:O	1:A:534:ILE:HG13	1.87	0.74
1:F:165:ALA:O	1:F:169:THR:OG1	2.03	0.74
1:A:707:MET:HG3	1:A:708:LEU:HD13	1.70	0.73
1:D:448:VAL:HG22	1:D:882:CYS:HB3	1.69	0.73
1:C:418:ARG:NH1	1:C:422:GLU:OE1	2.20	0.73
1:C:420:MET:O	1:C:424:GLY:N	2.20	0.73
1:F:887:TYR:O	1:F:889:SER:N	2.17	0.73
1:A:101:ASP:OD1	1:A:101:ASP:N	2.20	0.73
1:A:414:GLU:HG3	1:A:972:MET:HE1	1.70	0.73
1:A:989:GLY:O	1:A:992:SER:OG	2.06	0.73
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.71	0.73
1:C:49:TYR:HD1	1:C:57:VAL:HG12	1.53	0.73
1:A:186:ILE:HB	1:A:768:VAL:HG22	1.68	0.73
1:D:587:THR:HB	1:D:613:ASN:ND2	2.02	0.73
1:E:945:LYS:HA	1:E:948:MET:HE3	1.70	0.73
1:D:587:THR:HB	1:D:613:ASN:HD21	1.53	0.73
1:E:759:ASP:OD2	1:E:764:LYS:NZ	2.21	0.73

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:ARG:HB3	1:A:966:ARG:HH11	1.53	0.73
1:A:584:GLN:HB2	1:A:617:GLN:HG2	1.71	0.73
1:B:166:ILE:HD11	1:B:310:LEU:HD11	1.69	0.73
1:D:56:THR:OG1	1:F:213:GLN:NE2	2.22	0.72
1:E:445:ILE:HG22	1:E:938:ILE:HD13	1.69	0.72
1:C:574:THR:HG21	1:C:598:TYR:HE2	1.53	0.72
1:D:61:VAL:HA	1:D:118:LEU:HD22	1.70	0.72
1:E:184:MET:HB3	1:E:766:VAL:HG13	1.71	0.72
1:F:65:ILE:HG21	1:F:90:ILE:HD13	1.70	0.72
1:C:49:TYR:CD1	1:C:57:VAL:HG12	2.25	0.72
1:C:453:PHE:HD2	1:C:456:MET:HE1	1.55	0.72
1:D:351:VAL:HG22	1:D:976:ALA:HB1	1.71	0.72
1:E:448:VAL:HG13	1:E:879:VAL:HG13	1.72	0.72
1:C:41:PRO:HG2	1:C:94:PHE:HB2	1.72	0.72
1:C:853:ASP:OD2	1:C:862:ARG:NH2	2.23	0.72
1:B:896:VAL:HG21	1:B:938:ILE:HG13	1.68	0.72
1:D:225:VAL:HG22	1:E:776:MET:HE2	1.72	0.72
1:E:375:VAL:O	1:E:379:THR:OG1	2.07	0.72
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.71	0.72
1:C:580:ALA:HB1	1:C:719:THR:HG22	1.69	0.71
1:A:5:PHE:O	1:A:8:ARG:N	2.15	0.71
1:D:137:LEU:HD23	1:D:291:ILE:HG22	1.69	0.71
1:D:598:TYR:HB3	1:D:606:VAL:HG11	1.71	0.71
1:D:602:GLU:OE2	1:D:645:ARG:NH1	2.23	0.71
1:B:540:ARG:HH22	2:B:2000:LMT:H6'1	1.54	0.71
1:E:351:VAL:HG22	1:E:976:ALA:HB1	1.72	0.71
1:F:61:VAL:HA	1:F:118:LEU:HD22	1.72	0.71
1:A:225:VAL:H	1:B:776:MET:HE1	1.54	0.71
1:D:575:MET:HG2	1:D:661:PHE:HE1	1.54	0.71
1:B:350:LEU:HD13	1:B:980:GLY:HA2	1.70	0.71
1:B:985:VAL:O	1:B:996:ASN:ND2	2.23	0.71
1:F:955:LEU:HD21	1:F:1022:VAL:HA	1.73	0.71
1:C:896:VAL:HG23	1:C:937:ALA:HB3	1.71	0.71
1:B:174:ASP:HB3	1:B:292:LYS:HB2	1.72	0.71
1:B:375:VAL:O	1:B:379:THR:OG1	2.03	0.71
1:D:574:THR:HG23	1:D:622:ALA:HB3	1.71	0.71
1:B:309:GLU:HG3	1:B:313:MET:HE3	1.72	0.71
1:C:2:PRO:O	1:C:6:ILE:HG12	1.90	0.71
1:B:61:VAL:HG21	1:B:122:VAL:HG21	1.72	0.70
1:C:61:VAL:HG13	1:C:118:LEU:HD13	1.71	0.70
1:A:723:LYS:HG2	1:A:803:ARG:NH1	2.06	0.70

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:448:VAL:HG13	1:B:879:VAL:HG13	1.72	0.70
1:D:32:VAL:HG22	1:D:390:ILE:HB	1.73	0.70
1:D:375:VAL:HB	1:D:405:LEU:HD13	1.72	0.70
1:D:880:PHE:CE1	1:D:893:PRO:HB2	2.26	0.70
1:C:186:ILE:HG12	1:C:268:ILE:HG12	1.73	0.70
1:F:45:ILE:HD11	1:F:107:VAL:HG12	1.72	0.70
1:C:940:ILE:HG12	1:C:966:ARG:NH2	2.06	0.70
1:F:544:LEU:HA	1:F:547:ILE:HD12	1.74	0.70
1:F:892:ILE:HG23	1:F:941:VAL:HG11	1.72	0.70
1:A:962:ALA:O	1:A:966:ARG:NH1	2.25	0.70
1:B:974:SER:OG	1:B:1010:THR:HG21	1.92	0.70
1:F:574:THR:HG23	1:F:622:ALA:HB3	1.73	0.70
1:D:941:VAL:HG13	1:D:1021:PHE:CE1	2.26	0.69
1:E:82:SER:HB2	1:E:811:LEU:HB2	1.73	0.69
1:A:424:GLY:O	1:A:502:LYS:NZ	2.25	0.69
1:A:415:ASN:OD1	1:A:418:ARG:NH2	2.25	0.69
1:A:653:ILE:HG13	1:A:654:LYS:HE2	1.75	0.69
1:B:149:MET:HG3	1:B:154:ILE:HG13	1.73	0.69
1:C:248:LYS:HA	1:C:261:LEU:HD13	1.73	0.69
1:D:6:ILE:HG22	1:D:490:PRO:HB2	1.75	0.69
1:D:186:ILE:HG12	1:D:268:ILE:HG12	1.74	0.69
1:F:714:ASN:HB3	1:F:821:GLU:HB3	1.73	0.69
1:A:393:LEU:HD12	1:A:469:GLN:HG3	1.75	0.69
1:A:1034:ASP:CB	1:A:1035:ILE:HA	2.22	0.69
1:B:239:ARG:NH1	1:B:756:ASP:HB2	2.08	0.69
1:F:531:VAL:O	1:F:535:LEU:HG	1.92	0.69
1:B:184:MET:HB2	1:B:757:PHE:CE2	2.28	0.69
1:B:144:ASN:ND2	1:B:319:SER:O	2.23	0.69
1:C:144:ASN:HB3	1:C:148:THR:HG23	1.75	0.69
1:B:422:GLU:OE2	1:B:964:ARG:NH1	2.26	0.68
1:C:587:THR:OG1	1:C:613:ASN:ND2	2.26	0.68
1:C:326:PRO:O	1:C:625:SER:OG	2.11	0.68
1:D:209:ALA:O	1:D:237:GLN:NE2	2.23	0.68
1:D:899:VAL:O	1:D:902:LEU:HB2	1.93	0.68
1:E:185:ARG:NH2	1:E:273:GLU:O	2.24	0.68
1:C:456:MET:HE3	1:C:467:TYR:O	1.92	0.68
1:D:254:ASN:ND2	1:D:258:SER:OG	2.20	0.68
1:B:259:ARG:HD3	1:B:259:ARG:H	1.57	0.68
1:C:45:ILE:HB	1:C:90:ILE:HD12	1.75	0.68
1:D:274:ASN:ND2	1:D:276:ASP:OD2	2.26	0.68
1:E:192:GLU:HA	1:E:195:LYS:HE3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:422:GLU:O	1:E:502:LYS:NZ	2.22	0.68
1:F:368:PRO:HG3	1:F:413:VAL:HG21	1.75	0.68
1:B:383:LEU:HD11	1:B:473:THR:HA	1.74	0.68
1:D:914:ARG:O	1:D:916:LEU:N	2.27	0.68
1:F:149:MET:HG3	1:F:154:ILE:HG13	1.75	0.68
1:F:741:ILE:HG22	1:F:786:VAL:HG21	1.75	0.68
1:B:602:GLU:OE2	1:B:645:ARG:NH1	2.26	0.68
1:C:278:ILE:HG13	1:C:613:ASN:HB3	1.75	0.68
1:A:636:GLU:HB2	1:A:645:ARG:HH22	1.59	0.68
1:D:700:GLU:HB3	1:D:842:LEU:HD22	1.74	0.68
1:A:511:GLY:HA2	1:A:515:TRP:HD1	1.57	0.68
1:B:559:LEU:HD12	1:B:918:ASN:HB2	1.76	0.68
1:E:908:LEU:HD23	1:E:922:PHE:HZ	1.59	0.68
1:A:892:ILE:HG12	1:A:1025:ARG:HD3	1.75	0.67
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.76	0.67
1:C:3:ASN:ND2	1:C:486:LEU:O	2.28	0.67
1:D:250:LEU:HD13	1:D:259:ARG:HB3	1.75	0.67
1:D:707:MET:HG3	1:D:708:LEU:HD13	1.77	0.67
1:E:184:MET:HB2	1:E:757:PHE:CE2	2.29	0.67
1:C:5:PHE:O	1:C:7:ASP:N	2.27	0.67
1:B:219:LEU:HG	1:B:234:ILE:HD11	1.74	0.67
1:C:453:PHE:HD2	1:C:456:MET:CE	2.07	0.67
1:C:112:GLN:HG3	1:C:115:MET:HG3	1.77	0.67
1:C:696:GLN:HE21	1:C:845:LYS:HE3	1.59	0.67
1:D:884:ALA:HA	1:D:889:SER:O	1.94	0.67
1:F:239:ARG:HB2	1:F:758:ILE:HD12	1.75	0.67
1:A:697:LEU:HD12	1:A:846:LEU:HD21	1.75	0.67
1:C:942:GLU:HG3	1:C:943:PHE:N	2.09	0.67
1:D:47:ALA:HB2	1:D:127:VAL:HG13	1.76	0.67
1:E:906:GLY:HA3	1:E:1008:THR:HG21	1.76	0.67
1:E:536:ARG:HE	2:E:1101:LMT:H3O1	1.39	0.67
1:A:1026:ARG:NH1	1:A:1033:GLU:OE1	2.27	0.67
1:A:129:VAL:HG23	1:B:113:LEU:HD11	1.77	0.67
1:D:375:VAL:O	1:D:379:THR:OG1	2.11	0.67
1:F:211:ASN:O	1:F:755:ASN:ND2	2.28	0.67
1:B:156:ASP:OD1	1:B:760:ARG:NH2	2.27	0.67
1:D:954:GLY:HA2	1:D:1034:ASP:N	2.05	0.67
1:E:1021:PHE:HE2	1:E:1025:ARG:HD3	1.58	0.67
1:B:770:SER:HB3	1:B:775:ARG:HD3	1.77	0.67
1:D:400:LEU:HD21	1:D:925:GLY:HA2	1.77	0.67
1:F:418:ARG:O	1:F:422:GLU:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:443:VAL:O	1:F:447:MET:HB3	1.95	0.67
1:B:982:MET:HB3	1:B:983:PRO:HD3	1.77	0.66
1:C:855:THR:HA	1:C:859:TYR:HB2	1.77	0.66
1:D:545:TYR:HD1	1:D:546:LEU:HD23	1.60	0.66
1:D:452:VAL:HA	1:D:875:SER:OG	1.95	0.66
1:F:27:ILE:HG22	1:F:380:PHE:HB3	1.77	0.66
1:A:511:GLY:HA2	1:A:515:TRP:CD1	2.31	0.66
1:A:645:ARG:O	1:A:648:ARG:HB3	1.95	0.66
1:B:24:GLY:O	1:B:27:ILE:HG22	1.95	0.66
1:B:966:ARG:O	1:B:970:ILE:HG12	1.96	0.66
1:D:343:THR:O	1:D:346:GLU:N	2.28	0.66
1:D:367:ILE:HG12	1:D:492:LEU:HB3	1.78	0.66
1:D:80:SER:HB3	1:D:90:ILE:HG23	1.76	0.66
1:F:49:TYR:CD1	1:F:57:VAL:HG12	2.30	0.66
1:C:688:GLU:HB3	1:C:689:LYS:HD2	1.77	0.66
1:C:57:VAL:HG23	1:C:82:SER:HB3	1.76	0.66
1:D:442:LEU:O	1:D:445:ILE:HG13	1.95	0.66
1:C:340:VAL:HG11	1:C:395:MET:HB3	1.76	0.66
1:E:120:GLN:NE2	1:E:123:GLN:OE1	2.29	0.66
1:E:578:LEU:HD21	1:E:590:VAL:HG21	1.77	0.66
1:F:707:MET:O	1:F:827:ALA:N	2.26	0.66
1:A:9:PRO:HG2	1:A:10:ILE:HD12	1.76	0.66
1:D:400:LEU:HD11	1:D:1002:VAL:HG21	1.77	0.66
1:D:697:LEU:HD12	1:D:846:LEU:HD11	1.77	0.66
1:E:204:ILE:HG12	1:E:754:VAL:HG21	1.77	0.66
1:B:683:ALA:O	1:B:685:LEU:N	2.28	0.66
1:E:444:GLY:HA3	1:E:886:LEU:HD22	1.78	0.66
1:E:441:ALA:O	1:E:445:ILE:HG23	1.96	0.66
1:F:755:ASN:O	1:F:766:VAL:HB	1.94	0.66
1:F:41:PRO:HG2	1:F:94:PHE:HB2	1.78	0.66
1:B:453:PHE:O	1:B:471:SER:OG	2.11	0.66
1:A:960:LEU:O	1:A:963:VAL:HG12	1.95	0.66
1:E:559:LEU:HD23	1:E:560:PRO:HD2	1.78	0.66
1:E:774:TYR:O	1:E:784:TRP:NE1	2.25	0.65
1:F:428:LYS:HG2	1:F:494:ALA:HB1	1.78	0.65
1:F:902:LEU:HG	1:F:1012:LEU:HB3	1.78	0.65
1:F:939:LEU:HB3	1:F:966:ARG:HD2	1.78	0.65
1:A:626:LEU:HD11	1:A:639:VAL:HG23	1.76	0.65
1:C:400:LEU:HD23	1:C:474:ILE:HD11	1.78	0.65
1:F:1016:PHE:HB3	1:F:1020:PHE:CE1	2.32	0.65
1:F:880:PHE:HD2	1:F:881:LEU:HD22	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG22	1:A:390:ILE:HB	1.77	0.65
1:D:375:VAL:HG11	1:D:405:LEU:HD22	1.78	0.65
1:D:509:LYS:HG2	1:D:510:LYS:HG3	1.77	0.65
1:E:101:ASP:OD1	1:E:131:LYS:NZ	2.20	0.65
1:F:213:GLN:HA	1:F:237:GLN:O	1.97	0.65
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.79	0.65
1:C:584:GLN:HB2	1:C:617:GLN:HG2	1.79	0.65
1:B:262:LEU:HG	1:B:268:ILE:HD11	1.77	0.65
1:B:567:GLU:OE2	1:B:994:ALA:N	2.29	0.65
1:C:146:ASP:O	1:C:148:THR:N	2.29	0.65
1:F:198:LEU:HD21	1:F:252:LYS:HB2	1.77	0.65
1:F:588:GLN:OE1	1:F:592:ASN:ND2	2.28	0.65
1:A:940:ILE:HG12	1:A:966:ARG:CZ	2.26	0.65
1:C:82:SER:HB2	1:C:811:LEU:HB2	1.79	0.65
1:C:172:VAL:HG13	1:C:291:ILE:HG23	1.79	0.65
1:F:527:TYR:CE1	1:F:1014:ILE:HD12	2.32	0.65
1:C:188:MET:HB3	1:C:193:LEU:HD11	1.78	0.65
1:D:1028:PHE:O	1:D:1030:ARG:N	2.29	0.65
1:E:156:ASP:OD2	1:E:764:LYS:NZ	2.26	0.65
1:F:612:VAL:HB	1:F:621:ILE:HG22	1.78	0.65
1:F:197:GLN:HA	1:F:793:MET:SD	2.36	0.65
1:B:573:MET:HG3	1:B:661:PHE:CE2	2.32	0.65
1:D:511:GLY:HA2	1:D:515:TRP:CD1	2.31	0.65
1:E:5:PHE:HA	1:E:8:ARG:HB2	1.78	0.65
1:F:278:ILE:HG13	1:F:613:ASN:HB3	1.79	0.65
1:F:966:ARG:HH21	1:F:970:ILE:HD11	1.60	0.65
1:A:527:TYR:OH	1:A:1014:ILE:O	2.06	0.65
1:D:694:ARG:NH2	1:D:717:GLU:OE1	2.29	0.65
1:A:143:ILE:O	1:A:321:LEU:HD22	1.96	0.64
1:A:883:LEU:HD22	1:A:887:TYR:CE2	2.32	0.64
1:B:350:LEU:CD2	1:B:979:LEU:HB3	2.27	0.64
1:E:326:PRO:O	1:E:625:SER:OG	2.15	0.64
1:A:1037:HIS:HB3	1:A:1039:HIS:H	1.62	0.64
1:A:538:THR:HG22	1:A:542:LEU:HD22	1.79	0.64
1:B:61:VAL:HG13	1:B:118:LEU:HD22	1.79	0.64
1:A:182:TYR:O	1:A:764:LYS:HD3	1.98	0.64
1:F:664:PRO:HG3	1:F:670:GLY:HA3	1.78	0.64
1:A:184:MET:HB2	1:A:757:PHE:CE2	2.32	0.64
1:B:197:GLN:HA	1:B:793:MET:SD	2.37	0.64
1:F:420:MET:HB3	1:F:500:ILE:HB	1.80	0.64
1:A:368:PRO:HB3	1:A:409:ALA:HB1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:ALA:O	1:E:723:LYS:NZ	2.30	0.64
1:E:330:THR:HG22	1:E:334:LYS:HE2	1.80	0.64
1:B:139:VAL:O	1:B:326:PRO:HD2	1.98	0.64
1:C:249:ILE:HB	1:C:262:LEU:HB2	1.80	0.64
1:C:32:VAL:HG22	1:C:390:ILE:HB	1.80	0.64
1:E:213:GLN:HA	1:E:237:GLN:O	1.97	0.64
1:E:687:HIS:NE2	1:E:808:SER:HB2	2.13	0.64
1:F:582:ALA:HB2	1:F:586:ARG:HH21	1.63	0.64
1:C:388:PHE:CZ	1:C:472:ILE:HG21	2.33	0.64
1:D:200:PRO:HA	1:D:203:VAL:HG23	1.79	0.64
1:E:610:PHE:N	1:E:623:PHE:O	2.26	0.64
1:A:643:THR:HB	1:A:660:ALA:O	1.98	0.64
1:A:827:ALA:HB3	1:A:830:LYS:HB2	1.78	0.64
1:E:605:ASN:OD1	1:E:637:ASN:ND2	2.31	0.64
1:F:164:ASP:HB3	1:F:168:ARG:NH2	2.13	0.64
1:B:572:PHE:HA	1:B:663:LEU:HD21	1.80	0.64
1:F:895:SER:HB3	1:F:1024:VAL:HG11	1.80	0.64
1:F:527:TYR:CE2	1:F:963:VAL:HG13	2.33	0.64
1:A:564:LEU:HB2	1:A:666:ILE:HD11	1.78	0.63
1:A:966:ARG:O	1:A:970:ILE:HG12	1.98	0.63
1:B:222:THR:HA	1:B:224:PRO:HD3	1.81	0.63
1:D:45:ILE:HA	1:D:128:SER:O	1.97	0.63
1:E:579:PRO:HD3	1:E:656:ALA:HB2	1.78	0.63
1:F:240:LEU:HB2	1:F:246:PHE:CE1	2.33	0.63
1:F:75:LEU:HD21	1:F:78:MET:HB2	1.81	0.63
1:A:94:PHE:CE1	1:A:103:ALA:HB1	2.34	0.63
1:E:94:PHE:CE1	1:E:103:ALA:HB1	2.34	0.63
1:F:932:LEU:HD22	1:F:1006:MET:HE1	1.80	0.63
1:F:914:ARG:O	1:F:916:LEU:N	2.28	0.63
1:B:201:VAL:O	1:B:205:THR:OG1	2.11	0.63
1:F:144:ASN:O	1:F:148:THR:OG1	2.11	0.63
1:F:151:GLN:NE2	1:F:279:ALA:O	2.31	0.63
1:F:653:ILE:HD12	1:F:654:LYS:HE2	1.79	0.63
1:B:527:TYR:OH	1:B:1014:ILE:O	2.11	0.63
1:B:190:PRO:HG3	1:B:774:TYR:HB3	1.78	0.63
1:B:455:PRO:HG2	1:B:875:SER:OG	1.97	0.63
1:E:445:ILE:HG21	1:E:935:LYS:HD2	1.80	0.63
1:F:344:LEU:O	1:F:348:ILE:HG13	1.98	0.63
1:F:689:LYS:H	1:F:689:LYS:HD2	1.62	0.63
1:E:778:PRO:O	1:E:781:ILE:HG12	1.98	0.63
1:F:135:SER:HB3	1:F:668:GLU:HB3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:ILE:HB	1:F:90:ILE:HD12	1.79	0.63
1:C:892:ILE:HG23	1:C:941:VAL:HG11	1.80	0.63
1:D:632:ARG:NH1	1:D:637:ASN:O	2.32	0.63
1:D:677:PHE:HD2	1:D:822:ILE:HD12	1.61	0.63
1:E:189:ASN:HB3	1:E:192:GLU:HB2	1.80	0.63
1:E:840:GLU:HG2	1:E:852:TYR:CE1	2.33	0.63
1:F:890:TRP:HA	1:F:890:TRP:CE3	2.33	0.63
1:C:464:GLY:O	1:C:468:ARG:HB2	1.98	0.63
1:D:198:LEU:HD11	1:D:251:LEU:O	1.98	0.63
1:D:394:THR:HG23	1:D:469:GLN:HB3	1.79	0.63
1:D:536:ARG:NH1	2:D:2000:LMT:O3B	2.32	0.63
1:F:54:ALA:HB2	1:F:809:PRO:O	1.99	0.63
1:A:189:ASN:HB3	1:A:192:GLU:HB2	1.80	0.63
1:A:241:THR:N	1:A:245:GLU:OE2	2.29	0.63
1:A:883:LEU:HD22	1:A:887:TYR:HE2	1.63	0.63
1:E:14:VAL:HG22	1:F:881:LEU:HD12	1.79	0.63
1:F:44:THR:HA	1:F:90:ILE:O	1.99	0.63
1:F:66:GLU:OE1	1:F:816:GLY:HA2	1.99	0.63
1:C:99:ASP:HB3	1:C:102:ILE:HB	1.80	0.62
1:E:953:LYS:HB3	1:E:958:ALA:HB2	1.81	0.62
1:F:663:LEU:HD23	1:F:663:LEU:H	1.64	0.62
1:B:978:ILE:HG23	1:B:1003:MET:HG3	1.81	0.62
1:D:361:ASN:O	1:D:365:THR:HG22	1.99	0.62
1:E:100:ALA:HB1	1:E:131:LYS:HE3	1.81	0.62
1:E:165:ALA:HB3	1:E:313:MET:CE	2.29	0.62
1:F:201:VAL:O	1:F:205:THR:OG1	2.14	0.62
1:B:189:ASN:HB3	1:B:192:GLU:HB2	1.79	0.62
1:D:216:ALA:N	1:E:51:GLY:O	2.30	0.62
1:D:871:LEU:HD23	1:D:874:ILE:HD12	1.80	0.62
1:C:577:GLN:HG3	1:C:619:THR:HG22	1.82	0.62
1:E:525:HIS:HA	1:E:528:THR:HG22	1.81	0.62
1:A:137:LEU:HD22	1:A:293:LEU:HD23	1.81	0.62
1:C:757:PHE:CE1	1:C:759:ASP:HB2	2.35	0.62
1:F:146:ASP:O	1:F:148:THR:N	2.30	0.62
1:F:211:ASN:ND2	1:F:246:PHE:HZ	1.97	0.62
1:A:462:SER:O	1:A:466:ILE:HG12	1.99	0.62
1:B:24:GLY:O	1:B:28:LEU:HD23	1.99	0.62
1:C:396:PHE:O	1:C:400:LEU:HB2	2.00	0.62
1:D:445:ILE:O	1:D:449:LEU:HB2	2.00	0.62
1:E:405:LEU:HD22	1:E:481:SER:HB3	1.82	0.62
1:A:966:ARG:HB3	1:A:966:ARG:NH1	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:842:LEU:O	1:B:845:LYS:HB2	2.00	0.62
1:C:453:PHE:HB3	1:C:471:SER:HA	1.82	0.62
1:C:947:LEU:HD23	1:C:951:GLU:HG3	1.81	0.62
1:F:74:ASN:HB3	1:F:95:GLU:HB2	1.81	0.62
1:B:355:MET:HG3	1:B:359:LEU:HD12	1.81	0.62
1:C:545:TYR:CE2	1:C:1020:PHE:HZ	2.17	0.62
1:C:553:ALA:O	1:C:557:VAL:HG23	2.00	0.62
1:D:219:LEU:HG	1:D:234:ILE:HD11	1.81	0.62
1:E:679:LEU:HD22	1:E:822:ILE:HD11	1.81	0.62
1:F:645:ARG:O	1:F:648:ARG:HB3	2.00	0.62
1:A:326:PRO:O	1:A:625:SER:OG	2.17	0.61
1:B:248:LYS:HA	1:B:261:LEU:HD13	1.82	0.61
1:B:435:MET:SD	1:B:490:PRO:HB3	2.40	0.61
1:D:4:PHE:HB2	1:D:5:PHE:CD1	2.35	0.61
1:E:908:LEU:HD23	1:E:922:PHE:CZ	2.34	0.61
1:E:691:THR:HG23	1:E:694:ARG:HH12	1.65	0.61
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.82	0.61
1:A:901:PRO:O	1:A:904:VAL:N	2.33	0.61
1:F:522:LYS:O	1:F:525:HIS:N	2.32	0.61
1:B:941:VAL:HG13	1:B:1021:PHE:HE1	1.64	0.61
1:A:974:SER:OG	1:A:1010:THR:HG21	2.01	0.61
1:B:204:ILE:HG12	1:B:754:VAL:HG21	1.83	0.61
1:D:219:LEU:HD23	1:E:749:TRP:CZ3	2.36	0.61
1:F:902:LEU:HD21	1:F:1016:PHE:HB2	1.82	0.61
1:A:75:LEU:HD13	1:A:92:LEU:HD23	1.81	0.61
1:D:445:ILE:HG21	1:D:935:LYS:HD2	1.81	0.61
1:B:1006:MET:O	1:B:1010:THR:HG23	2.00	0.61
1:B:80:SER:HB3	1:B:90:ILE:HG23	1.82	0.61
1:C:453:PHE:CD2	1:C:456:MET:HE1	2.34	0.61
1:D:344:LEU:CD2	1:D:402:ILE:HD11	2.30	0.61
1:E:280:GLU:HG3	1:E:285:PRO:HA	1.81	0.61
1:E:427:PRO:HD3	1:E:499:PRO:HB3	1.83	0.61
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.83	0.61
1:B:172:VAL:HG13	1:B:291:ILE:HG23	1.83	0.61
1:C:200:PRO:HB2	1:C:744:THR:HG22	1.83	0.61
1:C:348:ILE:HG13	1:C:402:ILE:HD13	1.83	0.61
1:E:531:VAL:O	1:E:534:ILE:HG13	2.01	0.61
1:C:1032:ASN:H	1:C:1033:GLU:HB2	1.65	0.61
1:C:254:ASN:ND2	1:C:258:SER:OG	2.22	0.61
1:E:511:GLY:HA2	1:E:515:TRP:CD1	2.36	0.61
1:F:57:VAL:HG23	1:F:82:SER:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:TYR:HD2	1:B:50:PRO:HD2	1.66	0.61
1:E:694:ARG:HH11	1:E:694:ARG:HB3	1.65	0.61
1:F:34:GLN:O	1:F:391:ASN:HB2	2.01	0.61
1:F:340:VAL:CG1	1:F:395:MET:HB3	2.28	0.61
1:F:121:GLU:O	1:F:124:GLN:HG2	2.00	0.60
1:A:525:HIS:HA	1:A:528:THR:HG22	1.82	0.60
1:B:395:MET:O	1:B:398:MET:HB2	2.00	0.60
1:B:697:LEU:HD22	1:B:846:LEU:HD11	1.83	0.60
1:C:697:LEU:HD12	1:C:846:LEU:HD11	1.82	0.60
1:D:695:ASN:HA	1:D:698:LEU:HD12	1.83	0.60
1:E:76:MET:HE3	1:E:95:GLU:HA	1.83	0.60
1:B:1038:SER:OG	1:B:1039:HIS:N	2.31	0.60
1:C:752:SER:O	1:C:767:TYR:HA	2.00	0.60
1:D:26:ALA:HB1	1:D:384:ALA:HB2	1.84	0.60
1:E:332:PHE:O	1:E:336:SER:OG	2.15	0.60
1:E:544:LEU:O	1:E:548:ILE:HG13	2.01	0.60
1:D:75:LEU:HD11	1:D:92:LEU:HD23	1.82	0.60
1:F:538:THR:HG23	1:F:542:LEU:HD13	1.83	0.60
1:A:448:VAL:HG22	1:A:882:CYS:HB3	1.84	0.60
1:A:723:LYS:HD2	1:C:235:ILE:O	2.01	0.60
1:C:925:GLY:HA2	1:C:1002:VAL:HG22	1.84	0.60
1:E:1006:MET:O	1:E:1010:THR:HG23	2.00	0.60
1:F:896:VAL:HG23	1:F:937:ALA:CB	2.32	0.60
1:A:281:PHE:CE1	1:A:324:VAL:HG21	2.36	0.60
1:A:605:ASN:OD1	1:A:637:ASN:ND2	2.34	0.60
1:C:515:TRP:HD1	1:C:518:ARG:HH12	1.49	0.60
1:C:689:LYS:HA	1:C:692:GLN:OE1	2.01	0.60
1:C:892:ILE:O	1:C:896:VAL:HG12	2.02	0.60
1:E:670:GLY:HA2	1:E:857:MET:SD	2.42	0.60
1:F:576:VAL:HG13	1:F:658:VAL:HG22	1.84	0.60
1:F:638:LYS:HE2	1:F:640:GLU:HG3	1.84	0.60
1:F:935:LYS:HE2	1:F:936:ASN:OD1	2.01	0.60
1:B:213:GLN:HA	1:B:237:GLN:O	2.02	0.60
1:B:7:ASP:OD2	1:B:432:ARG:NH2	2.34	0.60
1:C:676:ASP:HB3	1:C:823:LEU:HD23	1.82	0.60
1:E:57:VAL:HB	1:E:88:VAL:HG23	1.84	0.60
1:A:188:MET:O	1:A:771:GLU:HB2	2.02	0.60
1:B:778:PRO:O	1:B:781:ILE:HG12	2.02	0.60
1:D:3:ASN:O	1:D:6:ILE:N	2.35	0.60
1:E:1008:THR:O	1:E:1012:LEU:HB2	2.01	0.60
1:F:359:LEU:HB2	1:F:365:THR:HG22	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:PHE:HD1	1:A:897:MET:CE	2.15	0.60
1:C:171:GLY:HA3	1:C:302:THR:OG1	2.01	0.60
1:C:582:ALA:HA	1:C:586:ARG:HH21	1.67	0.60
1:C:694:ARG:HD3	1:C:820:MET:SD	2.42	0.60
1:D:30:LEU:HD12	1:D:31:PRO:HD2	1.84	0.60
1:F:379:THR:HG23	1:F:476:SER:OG	2.02	0.60
1:B:757:PHE:HE1	1:B:759:ASP:HB2	1.65	0.59
1:C:1030:ARG:HB2	1:C:1030:ARG:HH21	1.66	0.59
1:C:884:ALA:HB1	1:C:890:TRP:CZ3	2.37	0.59
1:D:13:TRP:CZ2	1:D:492:LEU:HD21	2.36	0.59
1:E:396:PHE:O	1:E:400:LEU:HB2	2.02	0.59
1:F:239:ARG:NH1	1:F:756:ASP:HB2	2.17	0.59
1:A:549:VAL:O	1:A:552:MET:HB3	2.02	0.59
1:C:15:ILE:O	1:C:19:ILE:HG13	2.02	0.59
1:D:95:GLU:HB2	1:D:98:THR:OG1	2.02	0.59
1:F:470:PHE:CD2	1:F:924:VAL:HG11	2.37	0.59
1:F:61:VAL:HG13	1:F:118:LEU:HD13	1.83	0.59
1:F:892:ILE:HD12	1:F:1021:PHE:HE1	1.67	0.59
1:A:216:ALA:HB1	1:A:234:ILE:O	2.02	0.59
1:A:602:GLU:HG3	1:A:605:ASN:HB2	1.84	0.59
1:A:771:GLU:HB3	1:A:774:TYR:HD1	1.68	0.59
1:B:187:TRP:HB3	1:B:771:GLU:HA	1.85	0.59
1:C:291:ILE:HG21	1:C:306:ILE:HD11	1.84	0.59
1:D:941:VAL:HG13	1:D:1021:PHE:HE1	1.68	0.59
1:D:1036:GLU:HB3	1:D:1037:HIS:CB	2.32	0.59
1:D:414:GLU:CD	1:D:969:PRO:HG3	2.22	0.59
1:D:467:TYR:HE1	1:D:920:VAL:HG22	1.66	0.59
1:E:361:ASN:O	1:E:365:THR:HG22	2.01	0.59
1:F:54:ALA:HB2	1:F:809:PRO:C	2.22	0.59
1:A:523:SER:O	1:A:526:HIS:HB2	2.03	0.59
1:A:700:GLU:HB3	1:A:842:LEU:HD22	1.84	0.59
1:B:94:PHE:CE1	1:B:103:ALA:HB1	2.37	0.59
1:B:327:TYR:HB2	1:B:623:PHE:CE2	2.34	0.59
1:B:598:TYR:HB3	1:B:606:VAL:HG21	1.82	0.59
1:F:15:ILE:O	1:F:19:ILE:HG13	2.01	0.59
1:A:721:GLN:HB3	1:C:233:SER:O	2.02	0.59
1:C:249:ILE:O	1:C:262:LEU:N	2.35	0.59
1:C:545:TYR:OH	1:C:898:LEU:O	2.13	0.59
1:E:1032:ASN:CB	1:E:1033:GLU:HB3	2.32	0.59
1:A:610:PHE:O	1:A:622:ALA:HA	2.03	0.59
1:B:143:ILE:HG12	1:B:322:LYS:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:945:LYS:HZ1	1:B:1025:ARG:HH21	1.50	0.59
1:E:545:TYR:OH	1:E:898:LEU:O	2.19	0.59
1:B:677:PHE:HE2	1:B:679:LEU:HB2	1.67	0.59
1:E:853:ASP:OD1	1:E:854:TRP:N	2.35	0.59
1:D:213:GLN:HA	1:D:237:GLN:O	2.02	0.59
1:D:26:ALA:HB1	1:D:384:ALA:CB	2.33	0.59
1:E:140:VAL:HG13	1:E:324:VAL:O	2.02	0.59
1:B:492:LEU:O	1:B:496:MET:HG2	2.03	0.59
1:B:858:SER:O	1:B:862:ARG:HB2	2.02	0.59
1:D:737:SER:O	1:D:741:ILE:HG13	2.03	0.59
1:D:795:PRO:HG2	1:D:798:ALA:HB2	1.84	0.59
1:A:920:VAL:O	1:A:924:VAL:HG23	2.03	0.58
1:C:455:PRO:HG2	1:C:875:SER:HA	1.85	0.58
1:D:694:ARG:NH1	1:D:820:MET:SD	2.76	0.58
1:F:595:THR:O	1:F:599:LEU:HG	2.03	0.58
1:A:593:GLU:OE2	1:A:654:LYS:NZ	2.34	0.58
1:E:955:LEU:HD21	1:E:1022:VAL:HA	1.85	0.58
1:E:599:LEU:HD21	1:E:609:VAL:HG23	1.84	0.58
1:F:133:SER:O	1:F:134:SER:HB2	2.02	0.58
1:F:689:LYS:CD	1:F:689:LYS:H	2.16	0.58
1:A:582:ALA:HB2	1:A:586:ARG:HH21	1.68	0.58
1:A:736:VAL:HG22	1:A:788:ALA:HB2	1.85	0.58
1:D:465:ALA:O	1:D:469:GLN:HG2	2.02	0.58
1:E:7:ASP:CG	1:E:432:ARG:HH21	2.07	0.58
1:C:700:GLU:OE1	1:C:845:LYS:HE2	2.03	0.58
1:D:549:VAL:O	1:D:552:MET:HB3	2.03	0.58
1:D:887:TYR:CD2	1:D:892:ILE:HG22	2.38	0.58
1:E:540:ARG:HH22	2:E:1101:LMT:H6'2	1.68	0.58
1:F:184:MET:HB2	1:F:757:PHE:CE2	2.38	0.58
1:F:452:VAL:O	1:F:455:PRO:HD2	2.03	0.58
1:F:693:ALA:O	1:F:696:GLN:HB3	2.03	0.58
1:A:574:THR:HG21	1:A:598:TYR:CE2	2.32	0.58
1:A:400:LEU:HD12	1:A:928:THR:HG21	1.85	0.58
1:B:908:LEU:HD23	1:B:922:PHE:HZ	1.68	0.58
1:D:181:GLN:HG2	1:D:182:TYR:N	2.18	0.58
1:E:367:ILE:HD11	1:E:497:LEU:HD13	1.84	0.58
1:E:415:ASN:O	1:E:419:VAL:HG23	2.03	0.58
1:E:38:ILE:HD13	1:E:466:ILE:HG12	1.85	0.58
1:E:463:THR:O	1:E:467:TYR:HD1	1.86	0.58
1:D:773:LYS:HB3	1:F:225:VAL:HG11	1.85	0.58
1:F:571:VAL:HG22	1:F:625:SER:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:616:GLY:O	1:F:618:ASN:N	2.37	0.58
1:F:884:ALA:HB2	1:F:893:PRO:HG2	1.85	0.58
1:A:530:SER:HG	2:A:1101:LMT:H2O2	1.49	0.58
1:C:597:TYR:HE1	1:C:601:LYS:HD2	1.68	0.58
1:E:166:ILE:HA	1:E:309:GLU:HG2	1.84	0.58
1:E:526:HIS:O	1:E:530:SER:HB2	2.03	0.58
1:A:770:SER:HB3	1:A:775:ARG:HD3	1.83	0.58
1:B:906:GLY:HA3	1:B:1008:THR:OG1	2.04	0.58
1:A:881:LEU:HB3	1:C:14:VAL:HG13	1.85	0.58
1:D:388:PHE:HE1	1:D:472:ILE:HG21	1.69	0.58
1:A:130:GLU:OE1	1:A:174:ASP:HB2	2.04	0.58
1:B:149:MET:HB2	1:B:153:ASP:HB2	1.86	0.58
1:C:140:VAL:HG11	1:C:310:LEU:HD21	1.86	0.58
1:C:336:SER:O	1:C:340:VAL:HG23	2.04	0.58
1:D:251:LEU:HD11	1:D:262:LEU:HD13	1.84	0.58
1:E:687:HIS:CE1	1:E:808:SER:HB2	2.38	0.58
1:F:563:PHE:CZ	1:F:564:LEU:HD13	2.39	0.58
1:A:1032:ASN:N	1:A:1035:ILE:HD11	2.18	0.58
1:A:728:GLN:HE22	1:A:738:ILE:HG21	1.69	0.58
1:B:545:TYR:CE2	1:B:1020:PHE:HZ	2.21	0.58
1:C:211:ASN:OD1	1:C:240:LEU:HG	2.04	0.58
1:B:602:GLU:OE1	1:B:645:ARG:HD2	2.04	0.58
1:C:222:THR:HA	1:C:224:PRO:HD3	1.85	0.58
1:D:438:ILE:O	1:D:441:ALA:HB3	2.03	0.58
1:F:536:ARG:HD2	2:F:2000:LMT:O4'	2.04	0.58
1:F:185:ARG:NH2	1:F:273:GLU:O	2.28	0.58
1:A:105:VAL:HG13	1:B:109:ASN:HD21	1.68	0.57
1:B:559:LEU:HD22	1:B:560:PRO:HD2	1.85	0.57
1:A:749:TRP:HZ3	1:C:219:LEU:HD23	1.67	0.57
1:E:239:ARG:NH1	1:E:755:ASN:OD1	2.37	0.57
1:E:653:ILE:HG13	1:E:654:LYS:HD2	1.86	0.57
1:E:686:GLY:H	1:E:689:LYS:HB2	1.68	0.57
1:C:216:ALA:HB1	1:C:234:ILE:O	2.05	0.57
1:C:356:TYR:CD1	1:C:365:THR:HG21	2.39	0.57
1:F:164:ASP:CG	1:F:762:ARG:HH22	2.07	0.57
1:F:187:TRP:HB3	1:F:771:GLU:HA	1.85	0.57
1:A:531:VAL:O	1:A:535:LEU:HG	2.05	0.57
1:E:78:MET:N	1:E:815:ASN:OD1	2.33	0.57
1:E:354:VAL:HG21	1:E:976:ALA:HB2	1.86	0.57
1:F:982:MET:HB3	1:F:983:PRO:HD3	1.86	0.57
1:A:1022:VAL:O	1:A:1026:ARG:HG3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1035:ILE:O	1:D:1036:GLU:HG3	2.04	0.57
1:D:264:ASP:N	1:D:264:ASP:OD1	2.37	0.57
1:E:1029:SER:OG	1:E:1030:ARG:N	2.31	0.57
1:E:902:LEU:HG	1:E:1012:LEU:HB3	1.85	0.57
1:A:280:GLU:HG3	1:A:285:PRO:HA	1.85	0.57
1:B:677:PHE:CE2	1:B:822:ILE:HD12	2.39	0.57
1:D:525:HIS:HA	1:D:528:THR:HG22	1.86	0.57
1:A:350:LEU:HD13	1:A:980:GLY:HA2	1.86	0.57
1:B:415:ASN:O	1:B:419:VAL:HG23	2.05	0.57
1:C:756:ASP:OD1	1:C:765:LYS:HA	2.04	0.57
1:E:278:ILE:CG1	1:E:613:ASN:HB3	2.35	0.57
1:E:854:TRP:CE3	1:E:858:SER:HB3	2.40	0.57
1:B:676:ASP:N	1:B:858:SER:OG	2.33	0.57
1:C:597:TYR:CE1	1:C:601:LYS:HD2	2.39	0.57
1:C:739:ASN:O	1:C:743:THR:OG1	2.18	0.57
1:C:75:LEU:HD11	1:C:92:LEU:HD12	1.86	0.57
1:D:527:TYR:O	1:D:531:VAL:HG23	2.05	0.57
1:E:889:SER:HB3	1:E:892:ILE:HG13	1.87	0.57
1:B:531:VAL:HA	1:B:534:ILE:HG12	1.87	0.57
1:A:259:ARG:NH1	1:B:729:GLU:OE2	2.38	0.57
1:C:563:PHE:O	1:C:919:ASP:HB2	2.05	0.57
1:C:884:ALA:HB2	1:C:893:PRO:HG2	1.85	0.57
1:C:939:LEU:C	1:C:966:ARG:HD2	2.24	0.57
1:D:405:LEU:HD21	1:D:477:ALA:HB1	1.87	0.57
1:D:405:LEU:HD22	1:D:481:SER:HB3	1.87	0.57
1:E:577:GLN:NE2	1:E:618:ASN:OD1	2.38	0.57
1:E:643:THR:O	1:E:647:THR:OG1	2.23	0.57
1:B:484:VAL:O	1:B:489:THR:HG23	2.05	0.57
1:D:1030:ARG:HE	1:D:1031:LYS:HB2	1.69	0.57
1:D:453:PHE:CE2	1:D:474:ILE:HG21	2.40	0.57
1:D:677:PHE:CD2	1:D:822:ILE:HD12	2.39	0.57
1:E:540:ARG:HH22	2:E:1101:LMT:C6B	2.18	0.57
1:E:154:ILE:HG22	1:E:287:SER:HB3	1.86	0.57
1:F:393:LEU:HD12	1:F:469:GLN:HG3	1.86	0.57
1:F:435:MET:HE1	1:F:490:PRO:HB3	1.85	0.57
1:F:771:GLU:HB2	1:F:774:TYR:CD1	2.39	0.57
1:A:916:LEU:HD13	1:A:917:THR:HG22	1.87	0.57
1:A:963:VAL:HA	1:A:966:ARG:HH22	1.69	0.57
1:E:697:LEU:HD11	1:E:842:LEU:HB3	1.86	0.57
1:F:23:GLY:HA2	1:F:381:ALA:HB2	1.86	0.57
1:A:133:SER:OG	1:A:134:SER:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ALA:HB2	1:A:471:SER:OG	2.04	0.56
1:D:225:VAL:H	1:E:776:MET:HE1	1.70	0.56
1:E:172:VAL:HG22	1:E:306:ILE:HD11	1.87	0.56
1:A:363:ARG:O	1:A:366:LEU:HB2	2.05	0.56
1:A:448:VAL:O	1:A:451:ALA:HB3	2.05	0.56
1:B:560:PRO:O	1:B:918:ASN:HB3	2.04	0.56
1:C:890:TRP:CE3	1:C:890:TRP:HA	2.41	0.56
1:D:247:GLY:O	1:D:263:ARG:N	2.33	0.56
1:D:393:LEU:HD22	1:D:470:PHE:HE1	1.69	0.56
1:D:516:PHE:HA	1:D:519:MET:HG3	1.86	0.56
1:D:564:LEU:HB2	1:D:666:ILE:HD11	1.87	0.56
1:D:966:ARG:HH11	1:D:966:ARG:HB3	1.70	0.56
1:E:597:TYR:OH	1:E:646:ALA:HA	2.05	0.56
1:A:418:ARG:O	1:A:422:GLU:HB2	2.05	0.56
1:C:352:PHE:HD1	1:C:369:THR:HG21	1.70	0.56
1:D:124:GLN:HA	1:E:117:LEU:HD12	1.87	0.56
1:E:470:PHE:O	1:E:474:ILE:HG13	2.04	0.56
1:E:697:LEU:HD13	1:E:846:LEU:HD21	1.87	0.56
1:F:375:VAL:O	1:F:379:THR:OG1	2.09	0.56
1:C:188:MET:SD	1:C:200:PRO:HG3	2.45	0.56
1:C:449:LEU:O	1:C:452:VAL:HG23	2.06	0.56
1:C:185:ARG:HH12	1:C:769:MET:HB2	1.70	0.56
1:E:842:LEU:O	1:E:845:LYS:HB2	2.05	0.56
1:A:534:ILE:HD12	1:A:535:LEU:HD23	1.87	0.56
1:A:80:SER:HB3	1:A:90:ILE:HG23	1.88	0.56
1:A:399:VAL:HG11	1:A:984:LEU:HD11	1.86	0.56
1:C:154:ILE:HG22	1:C:287:SER:HB3	1.87	0.56
1:C:355:MET:CG	1:C:410:ILE:HD11	2.36	0.56
1:A:978:ILE:HG23	1:A:1003:MET:HG3	1.88	0.56
1:B:525:HIS:NE2	1:B:529:ASP:OD1	2.38	0.56
1:D:393:LEU:HD11	1:D:466:ILE:HD13	1.86	0.56
1:E:1022:VAL:O	1:E:1026:ARG:HG3	2.06	0.56
1:E:35:TYR:HE2	1:E:393:LEU:HD21	1.71	0.56
1:F:514:GLY:HA2	1:F:517:ASN:OD1	2.06	0.56
1:F:945:LYS:HA	1:F:948:MET:HE3	1.88	0.56
1:A:10:ILE:O	1:A:14:VAL:HG23	2.04	0.56
1:A:776:MET:O	1:C:219:LEU:HB3	2.05	0.56
1:D:272:GLY:N	1:D:275:TYR:OH	2.35	0.56
1:E:280:GLU:O	1:E:610:PHE:HA	2.06	0.56
1:F:892:ILE:HD12	1:F:1021:PHE:CE1	2.40	0.56
1:A:795:PRO:HG2	1:A:798:ALA:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:GLU:O	1:D:502:LYS:HB3	2.06	0.56
1:F:347:ALA:HB3	1:F:402:ILE:HD12	1.88	0.56
1:F:414:GLU:HG3	1:F:972:MET:HE1	1.87	0.56
1:C:602:GLU:OE2	1:C:645:ARG:NH1	2.39	0.56
1:E:840:GLU:HG2	1:E:852:TYR:HE1	1.71	0.56
1:B:412:VAL:O	1:B:416:VAL:HG23	2.05	0.56
1:D:455:PRO:HG2	1:D:875:SER:CB	2.35	0.56
1:E:380:PHE:O	1:E:384:ALA:N	2.39	0.56
1:E:442:LEU:O	1:E:445:ILE:HG13	2.06	0.56
1:C:149:MET:HG3	1:C:154:ILE:HG13	1.88	0.56
1:C:921:TYR:HD1	1:C:997:ALA:HB3	1.69	0.56
1:D:423:GLU:C	1:D:502:LYS:HB3	2.26	0.56
1:F:723:LYS:HG2	1:F:803:ARG:NH2	2.20	0.56
1:A:276:ASP:HA	1:C:222:THR:HG21	1.88	0.55
1:A:300:LEU:HD11	1:A:333:VAL:HG11	1.88	0.55
1:A:632:ARG:HB3	1:A:637:ASN:HB3	1.88	0.55
1:F:351:VAL:HG22	1:F:976:ALA:HB1	1.87	0.55
1:A:273:GLU:HG2	1:A:765:LYS:HD2	1.89	0.55
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.40	0.55
1:B:463:THR:HA	1:B:466:ILE:HD12	1.88	0.55
1:B:908:LEU:HD23	1:B:922:PHE:CZ	2.41	0.55
1:C:391:ASN:O	1:C:394:THR:OG1	2.21	0.55
1:D:347:ALA:O	1:D:351:VAL:HG23	2.06	0.55
1:D:701:ALA:HB1	1:D:711:VAL:HG11	1.88	0.55
1:D:185:ARG:HH12	1:D:769:MET:HB2	1.70	0.55
1:E:157:TYR:CZ	1:E:318:PRO:HD3	2.41	0.55
1:F:578:LEU:HD12	1:F:587:THR:HG22	1.88	0.55
1:A:544:LEU:O	1:A:548:ILE:HG13	2.07	0.55
1:D:170:SER:HB2	1:E:75:LEU:H	1.71	0.55
1:D:574:THR:HG21	1:D:598:TYR:HE2	1.71	0.55
1:E:412:VAL:O	1:E:416:VAL:HG23	2.07	0.55
1:F:58:GLN:OE1	1:F:811:LEU:HB3	2.07	0.55
1:F:896:VAL:HG23	1:F:937:ALA:HB1	1.89	0.55
1:A:222:THR:HA	1:A:224:PRO:HD3	1.88	0.55
1:A:572:PHE:HB2	1:A:661:PHE:O	2.05	0.55
1:B:898:LEU:HB3	1:B:1020:PHE:CE2	2.42	0.55
1:C:184:MET:HB3	1:C:766:VAL:HG13	1.88	0.55
1:C:896:VAL:HG23	1:C:937:ALA:CB	2.36	0.55
1:D:59:ASP:OD2	1:F:758:ILE:HD13	2.07	0.55
1:D:888:GLU:OE1	1:F:11:PHE:HB2	2.07	0.55
1:B:1031:LYS:H	1:B:1033:GLU:HG3	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ALA:O	1:C:169:THR:OG1	2.09	0.55
1:C:391:ASN:OD1	1:C:393:LEU:HB2	2.07	0.55
1:D:470:PHE:CD2	1:D:924:VAL:HG21	2.42	0.55
1:E:167:SER:HB3	1:E:175:VAL:HG21	1.88	0.55
1:E:281:PHE:HB2	1:E:610:PHE:CE1	2.41	0.55
1:F:1028:PHE:O	1:F:1030:ARG:N	2.40	0.55
1:F:135:SER:HB2	1:F:667:VAL:HG12	1.89	0.55
1:A:146:ASP:OD2	1:A:146:ASP:N	2.36	0.55
1:C:68:ASN:HB3	1:C:110:LYS:O	2.07	0.55
1:D:448:VAL:HG22	1:D:882:CYS:CB	2.37	0.55
1:D:778:PRO:O	1:D:781:ILE:HG12	2.06	0.55
1:E:613:ASN:C	1:E:613:ASN:HD22	2.10	0.55
1:A:3:ASN:HA	1:A:6:ILE:HG23	1.89	0.55
1:A:514:GLY:C	1:A:516:PHE:H	2.10	0.55
1:B:184:MET:HB2	1:B:757:PHE:CD2	2.42	0.55
1:C:508:GLY:O	1:C:509:LYS:HB2	2.06	0.55
1:C:722:PHE:CE2	1:C:802:SER:HB2	2.42	0.55
1:C:942:GLU:HG3	1:C:943:PHE:HD1	1.71	0.55
1:D:449:LEU:HB3	1:D:478:MET:SD	2.46	0.55
1:D:836:MET:HG2	1:D:854:TRP:CZ2	2.42	0.55
1:E:105:VAL:HG21	1:F:105:VAL:HG13	1.89	0.55
1:F:143:ILE:O	1:F:321:LEU:HD22	2.06	0.55
1:F:298:ASN:HB3	1:F:301:ASP:OD2	2.07	0.55
1:F:412:VAL:O	1:F:416:VAL:HG23	2.06	0.55
1:F:728:GLN:OE1	1:F:738:ILE:HG12	2.07	0.55
1:F:974:SER:HA	1:F:1006:MET:HE3	1.89	0.55
1:D:501:ALA:O	1:D:504:ASP:HB2	2.06	0.55
1:D:723:LYS:HG2	1:D:803:ARG:CZ	2.37	0.55
1:E:569:GLN:NE2	1:E:665:ALA:HA	2.21	0.55
1:A:281:PHE:CD1	1:A:324:VAL:HG11	2.42	0.55
1:A:356:TYR:HD1	1:A:365:THR:HG21	1.72	0.55
1:A:105:VAL:HG13	1:B:109:ASN:ND2	2.22	0.55
1:D:143:ILE:O	1:D:321:LEU:HD22	2.07	0.55
1:E:149:MET:HG3	1:E:154:ILE:HG13	1.89	0.55
1:E:220:GLY:HA3	1:E:230:LEU:O	2.07	0.55
1:A:1002:VAL:O	1:A:1006:MET:HG2	2.07	0.55
1:A:778:PRO:O	1:A:781:ILE:HG12	2.07	0.55
1:B:757:PHE:CE1	1:B:759:ASP:HB2	2.41	0.55
1:C:200:PRO:HA	1:C:203:VAL:CG2	2.37	0.55
1:D:175:VAL:HG11	1:D:289:LEU:HD13	1.88	0.55
1:D:366:LEU:HD23	1:D:369:THR:HB	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:712:ARG:HH21	1:E:823:LEU:HB3	1.71	0.55
1:E:188:MET:O	1:E:771:GLU:HB2	2.06	0.55
1:F:352:PHE:HA	1:F:355:MET:HE2	1.88	0.55
1:F:688:GLU:HB3	1:F:689:LYS:HD2	1.89	0.55
1:A:396:PHE:HZ	1:A:995:GLN:HG2	1.70	0.54
1:B:425:LEU:HD12	1:B:430:ALA:HA	1.89	0.54
1:C:108:GLN:O	1:C:112:GLN:HB2	2.07	0.54
1:C:382:VAL:HG12	1:C:472:ILE:HD11	1.89	0.54
1:C:531:VAL:HA	1:C:534:ILE:HG12	1.89	0.54
1:D:166:ILE:HD12	1:D:306:ILE:HG23	1.88	0.54
1:D:595:THR:O	1:D:599:LEU:HG	2.05	0.54
1:E:352:PHE:HE1	1:E:366:LEU:HD23	1.72	0.54
1:E:435:MET:SD	1:E:490:PRO:HB3	2.46	0.54
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.89	0.54
1:B:404:LEU:HD12	1:B:932:LEU:HD21	1.89	0.54
1:B:631:ASP:C	1:B:633:PRO:HD3	2.28	0.54
1:C:568:ASP:O	1:C:629:TRP:CH2	2.61	0.54
1:C:795:PRO:HG2	1:C:798:ALA:HB2	1.90	0.54
1:D:449:LEU:O	1:D:452:VAL:HG22	2.07	0.54
1:E:355:MET:HB3	1:E:365:THR:OG1	2.06	0.54
1:E:613:ASN:ND2	1:E:619:THR:O	2.40	0.54
1:E:940:ILE:HD11	1:E:970:ILE:HD11	1.90	0.54
1:F:455:PRO:HG3	1:F:878:VAL:HG21	1.89	0.54
1:F:974:SER:OG	1:F:1010:THR:HG21	2.07	0.54
1:A:377:LEU:O	1:A:380:PHE:HB2	2.07	0.54
1:B:586:ARG:O	1:B:589:LYS:HB3	2.07	0.54
1:C:355:MET:HG2	1:C:410:ILE:HD11	1.88	0.54
1:D:188:MET:HB3	1:D:193:LEU:HD11	1.88	0.54
1:E:887:TYR:O	1:E:889:SER:N	2.40	0.54
1:A:158:VAL:HG22	1:A:162:MET:HE3	1.89	0.54
1:A:202:ASP:OD1	1:A:787:ARG:NH2	2.38	0.54
1:A:426:PRO:HD2	1:A:429:GLU:HG3	1.87	0.54
1:B:739:ASN:O	1:B:743:THR:OG1	2.09	0.54
1:C:408:ASP:O	1:C:412:VAL:HG23	2.07	0.54
1:D:955:LEU:N	1:D:1033:GLU:O	2.37	0.54
1:D:108:GLN:O	1:D:112:GLN:HG2	2.08	0.54
1:D:135:SER:O	1:D:292:LYS:HG2	2.07	0.54
1:D:242:SER:O	1:D:246:PHE:HD1	1.91	0.54
1:A:420:MET:HB3	1:A:500:ILE:HB	1.90	0.54
1:B:423:GLU:O	1:B:502:LYS:HD2	2.06	0.54
1:D:54:ALA:HB1	1:D:811:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:631:ASP:C	1:F:633:PRO:HD3	2.27	0.54
1:B:171:GLY:HA3	1:B:302:THR:OG1	2.07	0.54
1:C:883:LEU:HD21	1:C:938:ILE:HD11	1.89	0.54
1:E:36:PRO:HD3	1:E:391:ASN:CG	2.28	0.54
1:A:143:ILE:HG22	1:A:286:ALA:CB	2.38	0.54
1:C:136:PHE:HB2	1:C:327:TYR:HE2	1.72	0.54
1:D:947:LEU:HB2	1:D:958:ALA:HB1	1.90	0.54
1:F:681:ASP:O	1:F:817:LEU:HD13	2.07	0.54
1:F:936:ASN:ND2	1:F:1010:THR:HG22	2.22	0.54
1:A:565:PRO:HG2	1:A:567:GLU:OE2	2.08	0.54
1:B:172:VAL:HG22	1:B:306:ILE:HD11	1.89	0.54
1:C:1006:MET:O	1:C:1010:THR:OG1	2.25	0.54
1:C:24:GLY:HA2	1:C:27:ILE:HG23	1.89	0.54
1:C:642:ILE:O	1:C:645:ARG:HG2	2.08	0.54
1:D:538:THR:HG23	1:D:542:LEU:HD13	1.90	0.54
1:D:904:VAL:HG22	1:D:926:LEU:HD21	1.89	0.54
1:D:962:ALA:O	1:D:965:MET:HG2	2.07	0.54
1:E:444:GLY:O	1:E:448:VAL:HG23	2.08	0.54
1:E:44:THR:HA	1:E:90:ILE:O	2.07	0.54
1:E:545:TYR:CE2	1:E:1020:PHE:HZ	2.25	0.54
1:E:663:LEU:HD23	1:E:663:LEU:H	1.72	0.54
1:F:677:PHE:HB2	1:F:854:TRP:CZ3	2.43	0.54
1:A:936:ASN:O	1:A:940:ILE:HG13	2.08	0.54
1:B:941:VAL:HG13	1:B:1021:PHE:CE1	2.42	0.54
1:B:412:VAL:HG22	1:B:438:ILE:HD11	1.89	0.54
1:B:771:GLU:HB3	1:B:774:TYR:CD1	2.43	0.54
1:C:395:MET:O	1:C:398:MET:HB2	2.07	0.54
1:D:1033:GLU:HB3	1:D:1034:ASP:HB2	1.90	0.54
1:D:692:GLN:HA	1:D:695:ASN:HB2	1.89	0.54
1:E:536:ARG:CZ	2:E:1101:LMT:O3B	2.55	0.54
1:E:770:SER:HB3	1:E:775:ARG:HD3	1.89	0.54
1:F:164:ASP:OD1	1:F:762:ARG:NH2	2.40	0.54
1:A:34:GLN:HE22	1:A:569:GLN:NE2	2.06	0.54
1:B:198:LEU:HD21	1:B:252:LYS:HB2	1.90	0.54
1:B:272:GLY:N	1:B:275:TYR:OH	2.21	0.54
1:C:520:PHE:CE2	1:C:968:ARG:HD2	2.43	0.54
1:D:559:LEU:HD23	1:D:560:PRO:HD2	1.90	0.54
1:E:138:MET:HG3	1:E:327:TYR:O	2.08	0.54
1:E:593:GLU:OE1	1:E:654:LYS:NZ	2.34	0.54
1:F:114:ALA:O	1:F:118:LEU:HG	2.08	0.54
1:F:435:MET:O	1:F:439:GLN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:488:LEU:O	1:F:491:ALA:HB3	2.07	0.54
1:A:220:GLY:HA3	1:A:230:LEU:O	2.08	0.53
1:A:166:ILE:HD11	1:A:306:ILE:HG23	1.90	0.53
1:A:545:TYR:O	1:A:549:VAL:HG23	2.08	0.53
1:A:577:GLN:OE1	1:A:619:THR:HG23	2.08	0.53
1:A:769:MET:HG2	1:A:770:SER:H	1.72	0.53
1:B:468:ARG:HG2	1:B:472:ILE:HD13	1.89	0.53
1:D:694:ARG:HD2	1:D:713:PRO:HB3	1.90	0.53
1:E:1019:VAL:O	1:E:1023:VAL:HG23	2.08	0.53
1:F:38:ILE:HD13	1:F:466:ILE:HD13	1.90	0.53
1:A:340:VAL:HG11	1:A:395:MET:HB3	1.90	0.53
1:A:896:VAL:HG21	1:A:938:ILE:HG13	1.90	0.53
1:B:1034:ASP:N	1:B:1035:ILE:HG22	2.24	0.53
1:B:945:LYS:NZ	1:B:1025:ARG:HH21	2.07	0.53
1:D:186:ILE:HB	1:D:768:VAL:HG22	1.91	0.53
1:D:21:LEU:O	1:D:25:LEU:HB2	2.08	0.53
1:D:185:ARG:HB2	1:D:271:GLY:HA3	1.89	0.53
1:D:908:LEU:HD23	1:D:922:PHE:CZ	2.43	0.53
1:A:492:LEU:O	1:A:496:MET:HG2	2.08	0.53
1:A:728:GLN:NE2	1:A:738:ILE:HG21	2.23	0.53
1:A:451:ALA:HB1	1:A:878:VAL:HG12	1.91	0.53
1:A:940:ILE:HG12	1:A:966:ARG:NE	2.23	0.53
1:C:893:PRO:HA	1:C:896:VAL:HG12	1.89	0.53
1:C:935:LYS:NZ	1:C:973:THR:HG21	2.24	0.53
1:D:17:ILE:HA	1:D:20:MET:HE2	1.89	0.53
1:D:491:ALA:O	1:D:495:THR:OG1	2.24	0.53
1:D:776:MET:HE1	1:F:225:VAL:HG22	1.89	0.53
1:A:281:PHE:HB2	1:A:610:PHE:CE1	2.43	0.53
1:A:143:ILE:HG22	1:A:286:ALA:HB1	1.91	0.53
1:A:157:TYR:CZ	1:A:318:PRO:HD3	2.44	0.53
1:B:902:LEU:HD11	1:B:1016:PHE:HD2	1.73	0.53
1:C:23:GLY:HA2	1:C:381:ALA:HB2	1.91	0.53
1:C:366:LEU:O	1:C:370:ILE:HG13	2.08	0.53
1:C:525:HIS:HA	1:C:528:THR:HG22	1.91	0.53
1:C:935:LYS:HE2	1:C:936:ASN:OD1	2.09	0.53
1:D:873:ALA:O	1:D:877:ILE:HG12	2.08	0.53
1:E:553:ALA:O	1:E:557:VAL:HG23	2.08	0.53
1:F:446:ALA:HB3	1:F:482:VAL:HG22	1.89	0.53
1:F:184:MET:HB2	1:F:757:PHE:CD2	2.42	0.53
1:B:108:GLN:HA	1:B:129:VAL:HG21	1.90	0.53
1:C:574:THR:HG21	1:C:598:TYR:CE2	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:LYS:O	1:D:431:THR:N	2.42	0.53
1:D:578:LEU:HB2	1:D:618:ASN:O	2.09	0.53
1:D:559:LEU:HD12	1:D:908:LEU:HD22	1.90	0.53
1:E:482:VAL:O	1:E:485:ALA:HB3	2.09	0.53
1:E:926:LEU:O	1:E:930:ILE:HG13	2.09	0.53
1:E:942:GLU:O	1:E:945:LYS:N	2.42	0.53
1:F:197:GLN:HG3	1:F:793:MET:SD	2.49	0.53
1:A:954:GLY:HA2	1:A:1034:ASP:H	1.74	0.53
1:B:952:GLY:O	1:B:1036:GLU:HA	2.08	0.53
1:C:367:ILE:HB	1:C:368:PRO:HD3	1.90	0.53
1:C:184:MET:HB3	1:C:766:VAL:HG22	1.91	0.53
1:D:723:LYS:HG2	1:D:803:ARG:NH1	2.23	0.53
1:E:974:SER:OG	1:E:1010:THR:HG21	2.09	0.53
1:E:26:ALA:O	1:E:30:LEU:HB2	2.09	0.53
1:D:219:LEU:HD23	1:E:749:TRP:HZ3	1.73	0.53
1:E:80:SER:HB3	1:E:90:ILE:HG23	1.90	0.53
1:A:953:LYS:O	1:A:1035:ILE:HB	2.09	0.53
1:C:479:ALA:O	1:C:482:VAL:HG23	2.09	0.53
1:D:233:SER:HB2	1:E:721:GLN:HB3	1.91	0.53
1:D:428:LYS:HG2	1:D:494:ALA:HB1	1.91	0.53
1:E:140:VAL:HA	1:E:326:PRO:HD2	1.91	0.53
1:E:20:MET:HG3	1:E:374:VAL:HG22	1.91	0.53
1:E:468:ARG:HG2	1:E:472:ILE:CD1	2.39	0.53
1:E:670:GLY:C	1:E:672:ALA:H	2.12	0.53
1:B:902:LEU:HD21	1:B:1016:PHE:HB2	1.90	0.53
1:A:888:GLU:OE1	1:C:11:PHE:HB2	2.09	0.53
1:C:544:LEU:O	1:C:547:ILE:HB	2.08	0.53
1:C:770:SER:HB3	1:C:775:ARG:HD3	1.91	0.53
1:D:335:ILE:O	1:D:339:GLU:HG2	2.09	0.53
1:E:1005:GLY:O	1:E:1009:ALA:HB2	2.08	0.53
1:F:700:GLU:HA	1:F:703:LYS:NZ	2.24	0.53
1:A:21:LEU:O	1:A:25:LEU:HB2	2.09	0.53
1:A:44:THR:HA	1:A:90:ILE:O	2.09	0.53
1:A:13:TRP:HE1	1:A:492:LEU:HD21	1.73	0.53
1:A:626:LEU:HD11	1:A:639:VAL:CG2	2.39	0.53
1:B:154:ILE:O	1:B:158:VAL:HG23	2.09	0.53
1:B:82:SER:HA	1:B:88:VAL:HG22	1.89	0.53
1:C:65:ILE:HG23	1:C:111:LEU:HD23	1.90	0.53
1:C:571:VAL:HG22	1:C:625:SER:HA	1.91	0.53
1:C:899:VAL:O	1:C:902:LEU:HB2	2.09	0.53
1:A:234:ILE:HD11	1:B:749:TRP:CE3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:VAL:O	1:A:478:MET:HB3	2.08	0.52
1:A:763:VAL:HG12	1:B:63:GLN:HE21	1.73	0.52
1:C:415:ASN:O	1:C:419:VAL:HG23	2.10	0.52
1:E:701:ALA:HB1	1:E:711:VAL:HG11	1.90	0.52
1:F:3:ASN:ND2	1:F:435:MET:SD	2.77	0.52
1:F:45:ILE:HD13	1:F:111:LEU:HG	1.89	0.52
1:F:676:ASP:HB3	1:F:823:LEU:HD23	1.91	0.52
1:F:75:LEU:HD11	1:F:92:LEU:HD12	1.91	0.52
1:F:966:ARG:NE	1:F:966:ARG:O	2.40	0.52
1:A:527:TYR:CE1	1:A:1014:ILE:HD12	2.44	0.52
1:A:536:ARG:NH1	2:A:1101:LMT:O4'	2.41	0.52
1:A:910:ALA:HB2	1:A:1004:GLY:HA3	1.90	0.52
1:B:377:LEU:O	1:B:380:PHE:HB2	2.09	0.52
1:B:841:GLN:O	1:B:844:SER:OG	2.26	0.52
1:C:151:GLN:HE22	1:C:286:ALA:H	1.56	0.52
1:C:663:LEU:HA	1:C:672:ALA:HA	1.91	0.52
1:C:917:THR:O	1:C:919:ASP:N	2.43	0.52
1:C:977:PHE:HE2	1:C:1002:VAL:HG12	1.75	0.52
1:D:211:ASN:OD1	1:D:240:LEU:HG	2.09	0.52
1:D:137:LEU:HD13	1:D:293:LEU:HB2	1.91	0.52
1:D:991:GLY:O	1:D:993:GLY:N	2.42	0.52
1:E:355:MET:SD	1:E:368:PRO:HG2	2.48	0.52
1:E:15:ILE:HD12	1:E:487:ILE:HG21	1.91	0.52
1:E:854:TRP:HE3	1:E:858:SER:HB3	1.72	0.52
1:F:452:VAL:C	1:F:455:PRO:HD2	2.30	0.52
1:A:940:ILE:HD12	1:A:1017:VAL:HG11	1.90	0.52
1:A:8:ARG:O	1:A:11:PHE:N	2.42	0.52
1:B:677:PHE:CD2	1:B:822:ILE:HD12	2.45	0.52
1:C:371:ALA:O	1:C:375:VAL:HG23	2.10	0.52
1:D:366:LEU:HA	1:D:369:THR:HB	1.90	0.52
1:D:896:VAL:HG21	1:D:938:ILE:HG13	1.90	0.52
1:E:445:ILE:HG22	1:E:938:ILE:CD1	2.38	0.52
1:E:961:ASP:O	1:E:964:ARG:HB3	2.09	0.52
1:F:154:ILE:HG22	1:F:287:SER:HB3	1.90	0.52
1:F:446:ALA:CB	1:F:482:VAL:HG22	2.40	0.52
1:F:47:ALA:HB2	1:F:127:VAL:HG13	1.92	0.52
1:A:272:GLY:N	1:A:275:TYR:OH	2.34	0.52
1:C:244:GLU:HG2	1:C:248:LYS:HE3	1.90	0.52
1:C:600:THR:O	1:C:603:LYS:HG3	2.09	0.52
1:D:278:ILE:CG1	1:D:613:ASN:HB3	2.40	0.52
1:D:434:SER:O	1:D:438:ILE:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:VAL:HA	1:A:875:SER:OG	2.09	0.52
1:B:36:PRO:HD3	1:B:391:ASN:CG	2.30	0.52
1:C:190:PRO:HG3	1:C:774:TYR:CG	2.44	0.52
1:C:940:ILE:HA	1:C:966:ARG:NH1	2.25	0.52
1:D:121:GLU:O	1:D:124:GLN:HG2	2.10	0.52
1:D:546:LEU:O	1:D:550:VAL:HG23	2.10	0.52
1:D:673:THR:HA	1:D:832:THR:OG1	2.10	0.52
1:E:982:MET:HB3	1:E:983:PRO:HD3	1.91	0.52
1:F:329:THR:O	1:F:333:VAL:HG23	2.09	0.52
1:F:456:MET:HA	1:F:459:PHE:CD1	2.45	0.52
1:B:953:LYS:O	1:B:1035:ILE:HG12	2.09	0.52
1:B:796:PHE:HA	1:B:799:PHE:CZ	2.45	0.52
1:C:11:PHE:O	1:C:15:ILE:HG13	2.10	0.52
1:C:355:MET:SD	1:C:368:PRO:HB2	2.50	0.52
1:D:153:ASP:OD2	1:D:153:ASP:N	2.42	0.52
1:F:184:MET:HB3	1:F:766:VAL:HG22	1.91	0.52
1:A:4:PHE:HB3	1:A:8:ARG:CZ	2.39	0.52
1:A:966:ARG:C	1:A:969:PRO:HD2	2.30	0.52
1:B:510:LYS:HB3	1:B:513:PHE:HB3	1.92	0.52
1:C:189:ASN:HB3	1:C:192:GLU:HB2	1.91	0.52
1:C:662:ASN:O	1:C:673:THR:N	2.37	0.52
1:D:278:ILE:HD13	1:D:584:GLN:OE1	2.09	0.52
1:E:199:THR:HG21	1:E:787:ARG:H	1.73	0.52
1:E:524:THR:O	1:E:527:TYR:HB3	2.09	0.52
1:F:408:ASP:O	1:F:412:VAL:HG23	2.09	0.52
1:A:708:LEU:HD21	1:A:838:LEU:HD12	1.90	0.52
1:C:251:LEU:HD11	1:C:262:LEU:HD13	1.92	0.52
1:C:549:VAL:O	1:C:552:MET:HB3	2.10	0.52
1:D:478:MET:O	1:D:482:VAL:HG23	2.09	0.52
1:D:653:ILE:HG13	1:D:654:LYS:HE2	1.92	0.52
1:D:771:GLU:HB3	1:D:774:TYR:HD1	1.75	0.52
1:D:940:ILE:HG12	1:D:966:ARG:CZ	2.39	0.52
1:E:47:ALA:O	1:E:87:THR:HA	2.10	0.52
1:F:94:PHE:CE1	1:F:103:ALA:HB1	2.45	0.52
1:F:314:GLU:HB2	1:F:315:PRO:HD3	1.92	0.52
1:F:559:LEU:HD11	1:F:911:ALA:HB1	1.92	0.52
1:A:968:ARG:HG2	1:A:972:MET:CE	2.40	0.52
1:C:545:TYR:CE2	1:C:1020:PHE:CZ	2.98	0.52
1:C:884:ALA:HB1	1:C:890:TRP:HZ3	1.74	0.52
1:D:17:ILE:HA	1:D:20:MET:CE	2.40	0.52
1:D:542:LEU:O	1:D:546:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:858:SER:HA	1:D:861:GLU:CD	2.31	0.52
1:F:757:PHE:HE1	1:F:759:ASP:HB2	1.74	0.52
1:A:902:LEU:HD21	1:A:1016:PHE:CD1	2.44	0.52
1:A:415:ASN:HD22	1:A:434:SER:HB2	1.74	0.52
1:B:340:VAL:HG11	1:B:395:MET:HB3	1.91	0.52
1:B:58:GLN:O	1:B:63:GLN:HG3	2.09	0.52
1:D:137:LEU:HB3	1:D:291:ILE:O	2.10	0.52
1:D:23:GLY:HA2	1:D:381:ALA:HB2	1.90	0.52
1:D:361:ASN:HD21	1:D:363:ARG:HG2	1.74	0.52
1:D:27:ILE:HG23	1:D:390:ILE:HD11	1.91	0.52
1:D:276:ASP:O	1:D:614:GLY:HA2	2.10	0.52
1:D:936:ASN:ND2	1:D:970:ILE:HG23	2.25	0.52
1:E:695:ASN:O	1:E:698:LEU:HB2	2.10	0.52
1:F:453:PHE:HB2	1:F:475:VAL:HG23	1.90	0.52
1:F:778:PRO:O	1:F:781:ILE:HG12	2.10	0.52
1:F:986:ILE:HG23	1:F:986:ILE:O	2.10	0.52
1:A:442:LEU:O	1:A:445:ILE:HG13	2.10	0.51
1:A:553:ALA:O	1:A:557:VAL:HG23	2.10	0.51
1:B:30:LEU:HD12	1:B:31:PRO:HD2	1.92	0.51
1:B:413:VAL:O	1:B:417:GLU:HG2	2.11	0.51
1:C:493:CYS:O	1:C:497:LEU:HB2	2.11	0.51
1:E:757:PHE:HD2	1:E:766:VAL:HG22	1.75	0.51
1:D:225:VAL:H	1:E:776:MET:CE	2.22	0.51
1:F:872:TYR:O	1:F:876:LEU:HD12	2.09	0.51
1:F:905:ILE:O	1:F:909:LEU:HB2	2.10	0.51
1:A:694:ARG:NH2	1:A:717:GLU:OE1	2.43	0.51
1:B:549:VAL:O	1:B:552:MET:HB3	2.10	0.51
1:B:578:LEU:HB2	1:B:618:ASN:O	2.10	0.51
1:D:201:VAL:O	1:D:205:THR:OG1	2.26	0.51
1:D:974:SER:OG	1:D:1010:THR:HG21	2.10	0.51
1:E:32:VAL:HG21	1:E:300:LEU:HD13	1.90	0.51
1:E:514:GLY:C	1:E:516:PHE:N	2.63	0.51
1:E:76:MET:HB2	1:E:93:THR:O	2.09	0.51
1:A:13:TRP:O	1:A:17:ILE:HG13	2.09	0.51
1:C:219:LEU:HD12	1:C:232:ALA:HB3	1.92	0.51
1:C:906:GLY:HA3	1:C:1008:THR:OG1	2.10	0.51
1:D:636:GLU:HB2	1:D:645:ARG:NH2	2.25	0.51
1:D:881:LEU:HD13	1:F:18:ILE:HG13	1.92	0.51
1:D:966:ARG:C	1:D:969:PRO:HD2	2.30	0.51
1:E:534:ILE:HG21	2:E:1101:LMT:H12	1.92	0.51
1:F:382:VAL:HG21	1:F:476:SER:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HG21	1:A:281:PHE:CD2	2.45	0.51
1:A:58:GLN:HA	1:A:62:THR:HB	1.92	0.51
1:B:52:ALA:HB1	1:B:56:THR:HB	1.93	0.51
1:B:700:GLU:HB3	1:B:842:LEU:HD22	1.92	0.51
1:B:950:LYS:O	1:B:951:GLU:HG2	2.10	0.51
1:C:985:VAL:HG13	1:C:1000:THR:OG1	2.10	0.51
1:C:110:LYS:O	1:C:113:LEU:HB2	2.10	0.51
1:C:781:ILE:O	1:C:796:PHE:HB2	2.11	0.51
1:D:56:THR:O	1:D:60:THR:HG22	2.10	0.51
1:D:575:MET:HG2	1:D:661:PHE:CE1	2.42	0.51
1:D:757:PHE:CE1	1:D:759:ASP:HB2	2.45	0.51
1:E:484:VAL:HG12	1:E:489:THR:HG23	1.92	0.51
1:A:417:GLU:HG2	1:A:497:LEU:HD21	1.92	0.51
1:A:632:ARG:NH1	1:A:637:ASN:O	2.44	0.51
1:A:841:GLN:O	1:A:844:SER:OG	2.25	0.51
1:B:515:TRP:O	1:B:519:MET:HG3	2.11	0.51
1:B:560:PRO:HG2	1:B:917:THR:HA	1.93	0.51
1:B:673:THR:HA	1:B:832:THR:OG1	2.11	0.51
1:C:568:ASP:CG	1:C:632:ARG:HH22	2.13	0.51
1:C:445:ILE:HG12	1:C:935:LYS:HG3	1.91	0.51
1:D:113:LEU:HD11	1:F:128:SER:CB	2.30	0.51
1:D:340:VAL:HG11	1:D:395:MET:HB3	1.92	0.51
1:D:363:ARG:O	1:D:366:LEU:HB2	2.10	0.51
1:F:110:LYS:O	1:F:113:LEU:HB2	2.10	0.51
1:F:395:MET:O	1:F:398:MET:HB2	2.11	0.51
1:F:422:GLU:HB3	1:F:423:GLU:HG3	1.93	0.51
1:F:667:VAL:HB	1:F:668:GLU:OE2	2.10	0.51
1:F:666:ILE:HD12	1:F:857:MET:SD	2.51	0.51
1:B:375:VAL:HG11	1:B:405:LEU:HD22	1.92	0.51
1:B:44:THR:HA	1:B:90:ILE:O	2.10	0.51
1:C:538:THR:CG2	1:C:542:LEU:HD13	2.41	0.51
1:C:568:ASP:O	1:C:629:TRP:HH2	1.94	0.51
1:C:80:SER:HB3	1:C:90:ILE:HG23	1.92	0.51
1:C:982:MET:O	1:C:985:VAL:N	2.44	0.51
1:D:457:ALA:CA	1:D:468:ARG:HG3	2.37	0.51
1:D:899:VAL:HA	1:D:902:LEU:HD22	1.92	0.51
1:E:1016:PHE:O	1:E:1019:VAL:HB	2.10	0.51
1:E:162:MET:HA	1:E:313:MET:HE1	1.91	0.51
1:D:225:VAL:HG12	1:E:772:ALA:HB1	1.93	0.51
1:F:639:VAL:HA	1:F:642:ILE:HD12	1.92	0.51
1:F:892:ILE:CG2	1:F:941:VAL:HG11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LEU:HD11	1:A:925:GLY:HA2	1.92	0.51
1:B:393:LEU:HD22	1:B:470:PHE:HE1	1.76	0.51
1:B:544:LEU:HA	1:B:547:ILE:HD12	1.92	0.51
1:C:778:PRO:O	1:C:781:ILE:HG12	2.10	0.51
1:E:438:ILE:O	1:E:441:ALA:HB3	2.11	0.51
1:E:511:GLY:HA2	1:E:515:TRP:HD1	1.76	0.51
1:F:144:ASN:O	1:F:284:GLN:NE2	2.42	0.51
1:F:375:VAL:HA	1:F:480:LEU:HD13	1.91	0.51
1:F:455:PRO:HG2	1:F:875:SER:HA	1.91	0.51
1:F:770:SER:HB2	1:F:784:TRP:CZ2	2.46	0.51
1:A:166:ILE:HG22	1:A:175:VAL:HG21	1.93	0.51
1:D:573:MET:HG3	1:D:661:PHE:CE2	2.45	0.51
1:E:68:ASN:HB3	1:E:114:ALA:HB2	1.92	0.51
1:A:209:ALA:O	1:A:237:GLN:NE2	2.43	0.51
1:A:219:LEU:HD13	1:A:230:LEU:HD21	1.93	0.51
1:B:143:ILE:O	1:B:321:LEU:HG	2.11	0.51
1:B:415:ASN:OD1	1:B:418:ARG:NH1	2.44	0.51
1:B:678:GLU:HG2	1:B:814:TYR:CG	2.46	0.51
1:C:329:THR:O	1:C:332:PHE:HB3	2.11	0.51
1:C:616:GLY:N	1:C:619:THR:OG1	2.43	0.51
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.93	0.51
1:C:966:ARG:O	1:C:970:ILE:HG13	2.11	0.51
1:C:982:MET:HB3	1:C:983:PRO:HD3	1.93	0.51
1:D:562:SER:N	1:D:917:THR:OG1	2.39	0.51
1:E:109:ASN:OD1	1:E:110:LYS:N	2.44	0.51
1:E:7:ASP:OD1	1:E:432:ARG:NH2	2.44	0.51
1:F:409:ALA:O	1:F:413:VAL:HG23	2.11	0.51
1:F:542:LEU:O	1:F:546:LEU:HG	2.11	0.51
1:F:687:HIS:NE2	1:F:718:ASP:OD1	2.43	0.51
1:E:237:GLN:OE1	1:F:742:ASN:ND2	2.44	0.51
1:A:571:VAL:CG2	1:A:625:SER:HA	2.35	0.51
1:B:372:VAL:O	1:B:376:LEU:HG	2.10	0.51
1:B:501:ALA:O	1:B:504:ASP:HB2	2.10	0.51
1:C:287:SER:OG	1:C:288:GLY:N	2.42	0.51
1:D:216:ALA:HB1	1:D:234:ILE:O	2.10	0.51
1:D:577:GLN:OE1	1:D:619:THR:HG22	2.11	0.51
1:D:678:GLU:HA	1:D:678:GLU:OE1	2.11	0.51
1:D:168:ARG:NH2	1:E:816:GLY:HA3	2.26	0.51
1:F:406:VAL:O	1:F:407:ASP:C	2.49	0.51
1:F:465:ALA:HA	1:F:468:ARG:NH1	2.25	0.51
1:A:228:GLN:NE2	1:A:230:LEU:H	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:GLU:OE1	1:A:627:LYS:HA	2.12	0.50
1:B:181:GLN:HG2	1:B:182:TYR:N	2.25	0.50
1:B:574:THR:HA	1:B:660:ALA:HA	1.92	0.50
1:E:281:PHE:CZ	1:E:324:VAL:HG21	2.46	0.50
1:E:423:GLU:O	1:E:502:LYS:HB2	2.11	0.50
1:E:953:LYS:HG3	1:E:957:GLU:CD	2.31	0.50
1:F:445:ILE:HG12	1:F:935:LYS:HG3	1.93	0.50
1:F:830:LYS:HG3	1:F:831:SER:N	2.26	0.50
1:A:605:ASN:ND2	1:A:637:ASN:HA	2.24	0.50
1:B:307:ARG:NH2	1:B:328:ASP:OD2	2.44	0.50
1:B:375:VAL:HG11	1:B:481:SER:HB3	1.92	0.50
1:C:393:LEU:HD11	1:C:466:ILE:HD13	1.92	0.50
1:D:368:PRO:HD3	1:D:413:VAL:HG21	1.94	0.50
1:F:836:MET:HG2	1:F:854:TRP:CH2	2.46	0.50
1:A:511:GLY:CA	1:A:515:TRP:CD1	2.94	0.50
1:A:908:LEU:O	1:A:911:ALA:HB3	2.10	0.50
1:B:493:CYS:O	1:B:497:LEU:HB2	2.11	0.50
1:C:129:VAL:O	1:C:130:GLU:HG3	2.10	0.50
1:C:377:LEU:O	1:C:380:PHE:HB2	2.12	0.50
1:C:666:ILE:HD13	1:C:669:LEU:HD12	1.94	0.50
1:C:939:LEU:HB3	1:C:966:ARG:CD	2.37	0.50
1:D:200:PRO:HA	1:D:203:VAL:CG2	2.41	0.50
1:D:899:VAL:HG21	1:D:937:ALA:HB2	1.93	0.50
1:E:583:THR:HG23	1:E:585:GLU:H	1.77	0.50
1:F:262:LEU:HG	1:F:268:ILE:HD11	1.93	0.50
1:F:508:GLY:O	1:F:509:LYS:HB2	2.09	0.50
1:F:49:TYR:N	1:F:86:GLY:O	2.40	0.50
1:F:947:LEU:HD22	1:F:953:LYS:CE	2.42	0.50
1:A:372:VAL:HG13	1:A:405:LEU:HD12	1.94	0.50
1:A:567:GLU:HG2	1:A:665:ALA:HB2	1.92	0.50
1:B:917:THR:O	1:B:919:ASP:N	2.45	0.50
1:C:737:SER:O	1:C:741:ILE:HG22	2.10	0.50
1:C:927:LEU:O	1:C:930:ILE:HB	2.11	0.50
1:D:691:THR:HG23	1:D:694:ARG:NH2	2.26	0.50
1:D:83:ASP:OD2	1:D:810:ARG:NH1	2.44	0.50
1:E:115:MET:SD	1:E:123:GLN:HG2	2.52	0.50
1:F:338:HIS:O	1:F:341:VAL:HB	2.12	0.50
1:F:3:ASN:OD1	1:F:486:LEU:HB3	2.11	0.50
1:F:918:ASN:ND2	1:F:918:ASN:O	2.39	0.50
1:A:894:PHE:HA	1:A:897:MET:HE3	1.93	0.50
1:C:11:PHE:HD2	1:C:11:PHE:O	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:860:GLN:O	1:C:863:LEU:HB3	2.11	0.50
1:C:456:MET:HB3	1:C:871:LEU:HD21	1.94	0.50
1:C:887:TYR:O	1:C:889:SER:N	2.42	0.50
1:C:927:LEU:O	1:C:928:THR:C	2.50	0.50
1:C:953:LYS:HG2	1:C:957:GLU:OE2	2.11	0.50
1:D:616:GLY:N	1:D:619:THR:OG1	2.44	0.50
1:E:355:MET:HB3	1:E:365:THR:CB	2.41	0.50
1:E:45:ILE:O	1:E:89:GLN:HA	2.12	0.50
1:E:700:GLU:HB3	1:E:842:LEU:HD22	1.93	0.50
1:A:375:VAL:HG13	1:A:480:LEU:CB	2.42	0.50
1:A:649:ALA:O	1:A:653:ILE:HG12	2.12	0.50
1:A:989:GLY:N	1:A:992:SER:OG	2.44	0.50
1:B:573:MET:HG3	1:B:661:PHE:HE2	1.77	0.50
1:B:80:SER:HB3	1:B:90:ILE:HG12	1.94	0.50
1:C:68:ASN:O	1:C:110:LYS:HB3	2.11	0.50
1:C:963:VAL:HA	1:C:966:ARG:HH22	1.77	0.50
1:D:172:VAL:HG22	1:D:302:THR:HG23	1.93	0.50
1:D:917:THR:O	1:D:919:ASP:N	2.45	0.50
1:F:406:VAL:O	1:F:408:ASP:N	2.45	0.50
1:F:773:LYS:HG3	1:F:774:TYR:CZ	2.47	0.50
1:A:394:THR:HG22	1:A:473:THR:OG1	2.12	0.50
1:B:27:ILE:HD13	1:B:380:PHE:CG	2.47	0.50
1:C:311:ALA:O	1:C:314:GLU:HB2	2.12	0.50
1:D:242:SER:OG	1:D:245:GLU:HG2	2.11	0.50
1:D:545:TYR:HB2	1:D:1016:PHE:HE2	1.76	0.50
1:D:747:ALA:O	1:D:769:MET:HA	2.12	0.50
1:E:697:LEU:HD12	1:E:700:GLU:HB2	1.94	0.50
1:F:355:MET:SD	1:F:368:PRO:HB2	2.52	0.50
1:F:893:PRO:O	1:F:897:MET:HG2	2.11	0.50
2:B:2000:LMT:H6E	2:B:2000:LMT:O5B	2.11	0.50
1:B:595:THR:O	1:B:599:LEU:HG	2.12	0.50
1:C:162:MET:O	1:C:166:ILE:N	2.41	0.50
1:D:188:MET:HB3	1:D:193:LEU:CD1	2.42	0.50
1:D:222:THR:HA	1:D:224:PRO:CD	2.38	0.50
1:D:249:ILE:O	1:D:262:LEU:N	2.45	0.50
1:D:525:HIS:NE2	1:D:529:ASP:OD1	2.45	0.50
1:D:854:TRP:CE3	1:D:858:SER:HB2	2.46	0.50
1:E:468:ARG:HG2	1:E:472:ILE:HD13	1.94	0.50
1:E:632:ARG:NH1	1:E:637:ASN:O	2.45	0.50
1:F:1016:PHE:HB3	1:F:1020:PHE:CZ	2.46	0.50
1:B:771:GLU:HB3	1:B:774:TYR:HD1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:LYS:HG2	1:D:263:ARG:HH21	1.76	0.50
1:D:168:ARG:HB3	1:E:75:LEU:HD22	1.93	0.50
1:E:76:MET:SD	1:E:859:TYR:HE2	2.35	0.50
1:F:112:GLN:HG3	1:F:115:MET:HG3	1.93	0.50
1:F:219:LEU:HD12	1:F:219:LEU:H	1.76	0.50
1:F:966:ARG:NH2	1:F:970:ILE:HD11	2.25	0.50
1:A:408:ASP:O	1:A:412:VAL:HG23	2.12	0.49
1:A:431:THR:HG21	1:A:490:PRO:O	2.12	0.49
1:B:709:THR:HB	1:B:827:ALA:HA	1.94	0.49
1:B:962:ALA:O	1:B:965:MET:HG2	2.12	0.49
1:C:602:GLU:OE1	1:C:645:ARG:HD2	2.12	0.49
1:C:740:ASP:O	1:C:744:THR:OG1	2.22	0.49
1:D:337:ILE:HA	1:D:340:VAL:HG23	1.94	0.49
1:D:51:GLY:O	1:F:217:GLY:N	2.44	0.49
1:D:632:ARG:NH1	1:D:638:LYS:HA	2.23	0.49
1:D:889:SER:HB3	1:D:892:ILE:HB	1.92	0.49
1:D:920:VAL:HA	1:D:923:GLN:OE1	2.11	0.49
1:E:452:VAL:HA	1:E:875:SER:OG	2.12	0.49
1:F:484:VAL:O	1:F:487:ILE:N	2.38	0.49
1:F:5:PHE:O	1:F:7:ASP:N	2.42	0.49
1:C:687:HIS:NE2	1:C:718:ASP:OD2	2.35	0.49
1:D:154:ILE:HG22	1:D:287:SER:HB3	1.94	0.49
1:E:281:PHE:HB2	1:E:610:PHE:HE1	1.77	0.49
1:A:753:TYR:HB2	1:A:767:TYR:CE1	2.47	0.49
1:B:412:VAL:HG22	1:B:438:ILE:CD1	2.41	0.49
1:C:465:ALA:O	1:C:469:GLN:HG2	2.12	0.49
1:D:1006:MET:O	1:D:1009:ALA:HB3	2.11	0.49
1:E:172:VAL:HG13	1:E:291:ILE:HG23	1.95	0.49
1:E:356:TYR:HD1	1:E:365:THR:HG21	1.76	0.49
1:E:478:MET:O	1:E:482:VAL:HG12	2.12	0.49
1:E:748:ALA:O	1:E:770:SER:HB3	2.12	0.49
1:E:769:MET:HG2	1:E:770:SER:H	1.77	0.49
1:F:479:ALA:O	1:F:483:LEU:HG	2.12	0.49
1:F:893:PRO:HA	1:F:896:VAL:HG12	1.93	0.49
1:A:212:ALA:HA	1:A:239:ARG:HE	1.78	0.49
1:A:475:VAL:HA	1:A:478:MET:HE1	1.95	0.49
1:B:57:VAL:HG11	1:B:86:GLY:O	2.11	0.49
1:C:425:LEU:HB3	1:C:429:GLU:CG	2.42	0.49
1:C:569:GLN:OE1	1:C:663:LEU:HD11	2.12	0.49
1:D:695:ASN:O	1:D:698:LEU:HB2	2.12	0.49
1:E:146:ASP:OD2	1:E:146:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ILE:HG13	1:E:881:LEU:HD23	1.93	0.49
1:E:987:SER:O	1:E:992:SER:HB2	2.12	0.49
1:A:177:LEU:HD13	1:A:179:GLY:O	2.11	0.49
1:A:475:VAL:HA	1:A:478:MET:CE	2.43	0.49
1:B:770:SER:HG	1:B:775:ARG:HG2	1.76	0.49
1:D:249:ILE:HB	1:D:262:LEU:HB2	1.94	0.49
1:D:415:ASN:O	1:D:419:VAL:HG23	2.13	0.49
1:D:393:LEU:HD12	1:D:469:GLN:HG3	1.94	0.49
1:D:691:THR:HG23	1:D:694:ARG:HH22	1.77	0.49
1:D:826:ALA:HB2	1:D:835:ALA:HB2	1.93	0.49
1:E:484:VAL:HG13	1:E:488:LEU:HB3	1.95	0.49
1:F:272:GLY:N	1:F:275:TYR:OH	2.22	0.49
1:A:695:ASN:HA	1:A:698:LEU:HD12	1.94	0.49
1:B:906:GLY:HA3	1:B:1008:THR:HG21	1.95	0.49
1:B:428:LYS:HG2	1:B:494:ALA:HB1	1.95	0.49
1:B:574:THR:HG23	1:B:622:ALA:HB3	1.92	0.49
1:B:961:ASP:O	1:B:964:ARG:HB3	2.11	0.49
1:E:434:SER:O	1:E:438:ILE:HG12	2.13	0.49
1:E:514:GLY:C	1:E:516:PHE:H	2.15	0.49
1:E:747:ALA:O	1:E:769:MET:HA	2.13	0.49
1:A:952:GLY:HA2	1:A:1035:ILE:HG22	1.93	0.49
1:B:174:ASP:HB3	1:B:292:LYS:HD2	1.94	0.49
1:B:280:GLU:HG2	1:B:283:GLY:C	2.32	0.49
1:B:362:PHE:HA	1:B:365:THR:CG2	2.42	0.49
1:B:56:THR:O	1:B:60:THR:OG1	2.19	0.49
1:E:527:TYR:O	1:E:531:VAL:HG23	2.13	0.49
1:F:365:THR:O	1:F:368:PRO:HD2	2.13	0.49
1:A:156:ASP:OD2	1:A:182:TYR:HB2	2.12	0.49
1:B:896:VAL:HG23	1:B:937:ALA:HB3	1.93	0.49
1:D:475:VAL:HA	1:D:478:MET:HE1	1.94	0.49
1:D:278:ILE:HG13	1:D:613:ASN:HB3	1.93	0.49
1:E:43:VAL:HG13	1:E:130:GLU:C	2.33	0.49
1:E:356:TYR:C	1:E:358:PHE:H	2.16	0.49
1:E:375:VAL:HG11	1:E:481:SER:HB3	1.95	0.49
1:F:213:GLN:OE1	1:F:238:THR:HA	2.13	0.49
1:F:406:VAL:O	1:F:409:ALA:N	2.45	0.49
1:F:81:ASN:HB2	1:F:89:GLN:HB2	1.95	0.49
1:A:636:GLU:HA	1:A:641:ALA:CB	2.42	0.49
1:A:199:THR:HG21	1:A:786:VAL:HA	1.95	0.49
1:B:988:THR:HA	1:B:992:SER:OG	2.13	0.49
1:C:599:LEU:O	1:C:603:LYS:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:GLN:HG3	1:D:152:GLU:N	2.28	0.49
1:F:144:ASN:ND2	1:F:319:SER:O	2.40	0.49
1:F:75:LEU:CD1	1:F:92:LEU:HD12	2.43	0.49
1:A:1016:PHE:HB3	1:A:1020:PHE:CE1	2.48	0.49
1:A:330:THR:HB	1:A:331:PRO:HD3	1.95	0.49
1:A:453:PHE:O	1:A:471:SER:OG	2.23	0.49
1:A:574:THR:HG23	1:A:622:ALA:HB3	1.94	0.49
1:C:492:LEU:O	1:C:496:MET:HG2	2.12	0.49
1:C:678:GLU:HG2	1:C:814:TYR:CG	2.48	0.49
1:C:708:LEU:HD21	1:C:839:MET:HG2	1.95	0.49
1:D:281:PHE:CZ	1:D:608:SER:HB2	2.47	0.49
1:D:375:VAL:HG22	1:D:484:VAL:HG21	1.95	0.49
1:F:133:SER:OG	1:F:293:LEU:O	2.14	0.49
1:F:375:VAL:HB	1:F:405:LEU:HD22	1.95	0.49
1:A:225:VAL:HG11	1:B:773:LYS:HA	1.95	0.48
1:A:645:ARG:HA	1:A:648:ARG:HB3	1.95	0.48
1:D:462:SER:O	1:D:466:ILE:HG12	2.13	0.48
1:D:527:TYR:CE1	1:D:1014:ILE:HD12	2.47	0.48
1:D:860:GLN:O	1:D:863:LEU:HB2	2.13	0.48
1:F:311:ALA:HA	1:F:314:GLU:HG3	1.95	0.48
1:F:900:VAL:O	1:F:904:VAL:HG23	2.12	0.48
1:A:697:LEU:HD21	1:A:839:MET:HE1	1.95	0.48
1:B:508:GLY:O	1:B:510:LYS:N	2.42	0.48
1:C:686:GLY:O	1:C:690:LEU:N	2.37	0.48
1:D:155:SER:OG	1:D:179:GLY:HA3	2.13	0.48
1:D:413:VAL:O	1:D:417:GLU:HG2	2.13	0.48
1:D:749:TRP:HZ3	1:F:219:LEU:HG	1.78	0.48
1:E:101:ASP:HA	1:E:131:LYS:HZ2	1.78	0.48
1:A:378:GLY:O	1:A:381:ALA:HB3	2.14	0.48
1:A:401:ALA:O	1:A:405:LEU:HG	2.13	0.48
1:A:948:MET:O	1:A:1035:ILE:HG21	2.13	0.48
1:B:441:ALA:HB2	1:B:942:GLU:OE1	2.13	0.48
1:C:538:THR:HG23	1:C:542:LEU:HD13	1.94	0.48
1:C:520:PHE:HE2	1:C:968:ARG:HD2	1.76	0.48
1:D:184:MET:HB3	1:D:766:VAL:HG22	1.95	0.48
1:D:966:ARG:HB3	1:D:966:ARG:NH1	2.28	0.48
1:E:359:LEU:C	1:E:360:GLN:HG2	2.32	0.48
1:E:187:TRP:CZ3	1:E:769:MET:HB3	2.48	0.48
1:F:2:PRO:O	1:F:5:PHE:HB3	2.13	0.48
1:A:573:MET:HG3	1:A:661:PHE:CE2	2.48	0.48
1:A:795:PRO:O	1:A:798:ALA:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ALA:HB3	1:A:88:VAL:HG13	1.94	0.48
1:C:356:TYR:HD1	1:C:365:THR:HG21	1.77	0.48
1:C:645:ARG:O	1:C:648:ARG:HB3	2.13	0.48
1:B:175:VAL:HG23	1:C:70:ASN:HD22	1.78	0.48
1:C:72:ILE:HD13	1:C:107:VAL:HG22	1.95	0.48
1:D:375:VAL:HG11	1:D:481:SER:HB3	1.96	0.48
1:D:391:ASN:O	1:D:395:MET:HG2	2.13	0.48
1:D:568:ASP:OD1	1:D:632:ARG:NH2	2.43	0.48
1:D:7:ASP:OD2	1:D:432:ARG:NH2	2.41	0.48
1:D:354:VAL:HG22	1:D:975:LEU:HD23	1.96	0.48
1:E:137:LEU:HD12	1:E:329:THR:HG22	1.94	0.48
1:F:189:ASN:HB3	1:F:192:GLU:HB2	1.95	0.48
1:F:36:PRO:HD3	1:F:391:ASN:ND2	2.29	0.48
1:A:225:VAL:HG22	1:B:776:MET:HE2	1.95	0.48
1:A:577:GLN:O	1:A:656:ALA:HB1	2.14	0.48
1:B:277:ILE:HG13	1:B:277:ILE:H	1.44	0.48
1:C:185:ARG:HB2	1:C:271:GLY:HA3	1.95	0.48
1:D:32:VAL:HB	1:D:300:LEU:HD22	1.94	0.48
1:E:372:VAL:O	1:E:376:LEU:HG	2.12	0.48
1:E:43:VAL:HG22	1:E:131:LYS:HG3	1.94	0.48
1:E:757:PHE:CD2	1:E:766:VAL:HG22	2.49	0.48
1:F:361:ASN:ND2	1:F:364:ALA:HB2	2.28	0.48
1:F:9:PRO:HB3	1:F:495:THR:HG21	1.96	0.48
1:B:344:LEU:HD23	1:B:402:ILE:HG12	1.96	0.48
1:B:559:LEU:HA	1:B:560:PRO:HD2	1.45	0.48
1:C:54:ALA:HB3	1:C:808:SER:O	2.14	0.48
1:C:6:ILE:H	1:C:6:ILE:HG12	1.43	0.48
1:C:925:GLY:O	1:C:929:THR:OG1	2.24	0.48
1:D:830:LYS:HG2	1:D:834:GLU:OE2	2.13	0.48
1:D:836:MET:HE1	1:D:862:ARG:HD2	1.94	0.48
1:D:896:VAL:HG23	1:D:937:ALA:HB3	1.95	0.48
1:D:936:ASN:O	1:D:940:ILE:HG13	2.14	0.48
1:E:239:ARG:HH12	1:E:756:ASP:H	1.60	0.48
1:F:400:LEU:O	1:F:404:LEU:HD22	2.14	0.48
1:F:587:THR:HG21	1:F:617:GLN:O	2.13	0.48
1:F:940:ILE:HA	1:F:966:ARG:NH1	2.28	0.48
1:A:607:GLU:HB2	1:A:627:LYS:N	2.28	0.48
1:B:349:ILE:O	1:B:352:PHE:HB3	2.13	0.48
1:B:872:TYR:HA	1:B:875:SER:HB2	1.95	0.48
1:B:954:GLY:HA2	1:B:1035:ILE:HG23	1.96	0.48
1:C:318:PRO:HG2	1:C:321:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:LEU:HB3	1:D:470:PHE:CE1	2.49	0.48
1:D:514:GLY:C	1:D:516:PHE:H	2.16	0.48
1:D:571:VAL:CG2	1:D:625:SER:HA	2.35	0.48
1:E:317:PHE:CZ	1:E:323:ILE:HG12	2.49	0.48
1:E:422:GLU:O	1:E:502:LYS:HG3	2.13	0.48
1:D:75:LEU:HD23	1:F:168:ARG:HB3	1.96	0.48
1:F:362:PHE:H	1:F:363:ARG:NH2	2.12	0.48
1:F:414:GLU:OE1	1:F:968:ARG:NH1	2.43	0.48
1:F:900:VAL:HG22	1:F:930:ILE:HG23	1.95	0.48
1:B:535:LEU:HD21	1:B:1019:VAL:HA	1.96	0.48
1:C:902:LEU:HG	1:C:1012:LEU:HB3	1.95	0.48
1:C:1031:LYS:HD2	1:C:1033:GLU:HB2	1.95	0.48
1:F:152:GLU:HG2	1:F:275:TYR:HE2	1.79	0.48
1:F:58:GLN:OE1	1:F:813:ARG:HD2	2.14	0.48
1:F:853:ASP:OD2	1:F:854:TRP:N	2.46	0.48
1:A:70:ASN:OD1	1:A:110:LYS:HD2	2.14	0.48
1:A:361:ASN:O	1:A:365:THR:HG22	2.14	0.48
1:A:532:GLY:O	1:A:536:ARG:HG2	2.14	0.48
1:A:723:LYS:HB2	1:A:805:GLU:OE2	2.14	0.48
1:B:952:GLY:HA2	1:B:1035:ILE:HD11	1.95	0.48
1:C:278:ILE:HD13	1:C:584:GLN:OE1	2.14	0.48
1:C:654:LYS:HD3	1:C:654:LYS:HA	1.51	0.48
1:C:893:PRO:O	1:C:897:MET:HG2	2.14	0.48
1:D:956:ILE:HD12	1:D:957:GLU:H	1.79	0.48
1:E:143:ILE:O	1:E:321:LEU:HG	2.13	0.48
1:E:78:MET:O	1:E:815:ASN:N	2.35	0.48
1:E:887:TYR:HB3	1:E:892:ILE:HD12	1.95	0.48
1:E:906:GLY:HA3	1:E:1008:THR:CG2	2.41	0.48
1:F:459:PHE:CE1	1:F:871:LEU:HG	2.48	0.48
1:A:893:PRO:HB2	1:A:897:MET:HE2	1.94	0.48
1:B:535:LEU:HD13	1:B:1022:VAL:HG21	1.96	0.48
1:C:110:LYS:HD3	1:C:110:LYS:HA	1.68	0.48
1:D:61:VAL:HG13	1:D:118:LEU:HD13	1.95	0.48
1:E:401:ALA:HB2	1:E:474:ILE:HG23	1.96	0.48
1:E:414:GLU:HG3	1:E:969:PRO:HB3	1.96	0.48
1:F:901:PRO:O	1:F:904:VAL:N	2.47	0.48
1:F:956:ILE:H	1:F:956:ILE:HD12	1.79	0.48
1:A:157:TYR:OH	1:A:316:PHE:O	2.32	0.47
1:B:277:ILE:HD12	1:B:277:ILE:O	2.14	0.47
1:B:708:LEU:HG	1:B:838:LEU:HD12	1.95	0.47
1:B:753:TYR:OH	1:B:756:ASP:OD1	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1032:ASN:OD1	1:C:1033:GLU:HA	2.14	0.47
1:C:211:ASN:CG	1:C:240:LEU:HG	2.35	0.47
1:D:164:ASP:HB3	1:D:168:ARG:NH2	2.28	0.47
1:D:890:TRP:NE1	1:F:10:ILE:HG12	2.29	0.47
1:D:908:LEU:HD23	1:D:922:PHE:HZ	1.79	0.47
1:E:906:GLY:CA	1:E:1008:THR:HG21	2.44	0.47
1:E:339:GLU:HA	1:E:342:LYS:HB2	1.95	0.47
1:F:103:ALA:O	1:F:107:VAL:HG23	2.14	0.47
1:F:120:GLN:HG3	1:F:123:GLN:OE1	2.14	0.47
1:F:398:MET:HE3	1:F:398:MET:HB3	1.77	0.47
1:F:54:ALA:HB3	1:F:808:SER:O	2.13	0.47
1:F:692:GLN:HA	1:F:695:ASN:HB2	1.96	0.47
1:F:770:SER:HB3	1:F:775:ARG:HD3	1.95	0.47
1:F:983:PRO:HA	1:F:986:ILE:HG22	1.94	0.47
1:A:278:ILE:CG1	1:A:613:ASN:HB3	2.44	0.47
1:B:352:PHE:HZ	1:B:362:PHE:CE1	2.32	0.47
1:B:422:GLU:O	1:B:502:LYS:NZ	2.47	0.47
1:C:409:ALA:O	1:C:413:VAL:HG23	2.13	0.47
1:C:551:GLY:O	1:C:555:LEU:HB2	2.14	0.47
1:E:99:ASP:HB3	1:E:102:ILE:HB	1.96	0.47
1:D:233:SER:O	1:E:721:GLN:HB2	2.14	0.47
1:E:57:VAL:HG23	1:E:82:SER:HB3	1.96	0.47
1:E:887:TYR:C	1:E:889:SER:H	2.17	0.47
1:F:917:THR:O	1:F:919:ASP:N	2.47	0.47
1:A:165:ALA:HB3	1:A:313:MET:CE	2.44	0.47
1:A:241:THR:HG23	1:A:758:ILE:O	2.14	0.47
1:A:669:LEU:HA	1:A:669:LEU:HD23	1.61	0.47
1:B:45:ILE:HA	1:B:128:SER:O	2.14	0.47
1:D:137:LEU:HD22	1:D:293:LEU:HB2	1.96	0.47
1:E:20:MET:CG	1:E:374:VAL:HG22	2.44	0.47
1:E:638:LYS:NZ	1:E:988:THR:HG23	2.29	0.47
1:F:914:ARG:C	1:F:916:LEU:H	2.16	0.47
1:F:959:THR:O	1:F:963:VAL:HB	2.14	0.47
1:A:143:ILE:HG12	1:A:322:LYS:O	2.15	0.47
1:A:317:PHE:CD2	1:A:321:LEU:HD12	2.49	0.47
1:A:2:PRO:HB2	1:A:3:ASN:H	1.45	0.47
1:A:127:VAL:O	1:B:113:LEU:HD13	2.15	0.47
1:B:625:SER:O	1:B:626:LEU:HD23	2.14	0.47
1:B:773:LYS:HG3	1:B:774:TYR:CZ	2.49	0.47
1:C:242:SER:HB2	1:C:245:GLU:H	1.78	0.47
1:C:826:ALA:HB3	1:C:830:LYS:HG3	1.96	0.47

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:574:THR:HG21	1:D:598:TYR:CE2	2.49	0.47
1:D:872:TYR:O	1:D:876:LEU:HB2	2.14	0.47
1:A:169:THR:HB	1:A:172:VAL:CG2	2.45	0.47
1:C:544:LEU:HD12	1:C:547:ILE:HD12	1.97	0.47
1:D:400:LEU:HA	1:D:400:LEU:HD12	1.52	0.47
1:E:165:ALA:HB3	1:E:313:MET:HE2	1.97	0.47
1:E:148:THR:HG21	1:E:319:SER:HB2	1.96	0.47
1:E:356:TYR:O	1:E:358:PHE:N	2.47	0.47
1:E:35:TYR:CE2	1:E:393:LEU:HD21	2.49	0.47
1:E:543:VAL:HA	1:E:546:LEU:HG	1.95	0.47
1:A:864:SER:OG	1:A:865:GLY:N	2.47	0.47
1:A:880:PHE:HD1	1:A:897:MET:HE2	1.79	0.47
1:B:167:SER:HB3	1:B:175:VAL:HG21	1.97	0.47
1:B:364:ALA:O	1:B:368:PRO:HD3	2.14	0.47
1:C:119:PRO:O	1:C:122:VAL:HB	2.15	0.47
1:C:203:VAL:O	1:C:207:ILE:HG13	2.14	0.47
1:C:395:MET:HA	1:C:398:MET:HG3	1.97	0.47
1:C:966:ARG:HE	1:C:970:ILE:HD11	1.79	0.47
1:D:531:VAL:HG13	1:D:534:ILE:HD11	1.96	0.47
1:D:282:ASN:HD21	1:D:608:SER:HA	1.78	0.47
1:D:675:PHE:HB2	1:D:854:TRP:CZ3	2.49	0.47
1:E:518:ARG:O	1:E:521:GLU:N	2.47	0.47
1:D:235:ILE:O	1:E:723:LYS:HD2	2.14	0.47
1:E:749:TRP:CZ2	1:E:781:ILE:HD13	2.50	0.47
1:F:144:ASN:HB3	1:F:148:THR:HG23	1.95	0.47
1:F:248:LYS:O	1:F:261:LEU:HD22	2.14	0.47
1:A:587:THR:HB	1:A:613:ASN:ND2	2.30	0.47
1:A:602:GLU:OE1	1:A:645:ARG:HD2	2.14	0.47
1:B:418:ARG:O	1:B:422:GLU:HB2	2.15	0.47
1:B:49:TYR:HB3	1:B:57:VAL:HG12	1.97	0.47
1:B:513:PHE:O	1:B:515:TRP:N	2.48	0.47
1:B:653:ILE:O	1:B:654:LYS:HD2	2.15	0.47
1:D:1030:ARG:HE	1:D:1031:LYS:N	2.13	0.47
1:D:456:MET:HE2	1:D:471:SER:HA	1.97	0.47
1:D:736:VAL:HG21	1:D:799:PHE:CE1	2.50	0.47
1:D:776:MET:CE	1:F:225:VAL:HG22	2.45	0.47
1:D:905:ILE:O	1:D:909:LEU:HB2	2.15	0.47
1:E:351:VAL:O	1:E:354:VAL:HB	2.13	0.47
1:E:355:MET:CE	1:E:410:ILE:HG12	2.44	0.47
1:E:571:VAL:HG13	1:E:623:PHE:HE1	1.80	0.47
1:E:780:ASP:O	1:E:783:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:836:MET:O	1:E:840:GLU:HG3	2.13	0.47
1:F:1008:THR:O	1:F:1012:LEU:HB2	2.15	0.47
1:A:157:TYR:HE2	1:A:317:PHE:CD1	2.33	0.47
1:A:770:SER:HG	1:A:775:ARG:HG2	1.80	0.47
1:B:1035:ILE:H	1:B:1036:GLU:HG3	1.79	0.47
1:B:770:SER:HB2	1:B:784:TRP:CZ2	2.50	0.47
1:C:203:VAL:HG12	1:C:207:ILE:HD11	1.97	0.47
1:C:351:VAL:HG11	1:C:406:VAL:HG21	1.97	0.47
1:D:188:MET:SD	1:D:200:PRO:HG3	2.55	0.47
1:D:582:ALA:HA	1:D:586:ARG:HH21	1.79	0.47
1:E:182:TYR:O	1:E:764:LYS:HD3	2.15	0.47
1:E:508:GLY:HA2	1:E:514:GLY:O	2.14	0.47
1:E:578:LEU:O	1:E:618:ASN:ND2	2.38	0.47
1:F:228:GLN:NE2	1:F:230:LEU:O	2.45	0.47
1:F:480:LEU:O	1:F:484:VAL:HG23	2.15	0.47
1:F:689:LYS:N	1:F:689:LYS:HD2	2.29	0.47
1:B:1007:VAL:O	1:B:1011:VAL:HG23	2.14	0.47
1:B:960:LEU:O	1:B:963:VAL:HG12	2.15	0.47
1:C:204:ILE:O	1:C:207:ILE:HB	2.15	0.47
1:C:402:ILE:O	1:C:406:VAL:HG22	2.15	0.47
1:D:103:ALA:O	1:D:107:VAL:HG23	2.15	0.47
1:D:199:THR:O	1:D:202:ASP:N	2.47	0.47
1:D:770:SER:HB2	1:D:784:TRP:CZ2	2.49	0.47
1:E:944:ALA:HB3	1:E:1021:PHE:HE1	1.78	0.47
1:F:1006:MET:O	1:F:1010:THR:HG23	2.15	0.47
1:F:356:TYR:C	1:F:358:PHE:H	2.16	0.47
1:F:407:ASP:O	1:F:411:VAL:HG23	2.15	0.47
1:F:516:PHE:O	1:F:520:PHE:N	2.43	0.47
1:A:300:LEU:O	1:A:303:ALA:HB3	2.15	0.47
1:A:23:GLY:HA3	1:A:377:LEU:O	2.14	0.47
1:A:41:PRO:HD3	1:A:97:GLY:H	1.79	0.47
1:A:826:ALA:HB2	1:A:835:ALA:HB2	1.97	0.47
1:B:740:ASP:O	1:B:744:THR:OG1	2.23	0.47
1:E:410:ILE:HD13	1:E:972:MET:HB3	1.97	0.47
1:E:466:ILE:HD13	1:E:564:LEU:HD11	1.97	0.47
1:F:154:ILE:O	1:F:158:VAL:HG23	2.15	0.47
1:F:222:THR:HA	1:F:224:PRO:HD3	1.97	0.47
1:A:1032:ASN:O	1:A:1033:GLU:HB2	2.13	0.47
1:A:68:ASN:O	1:A:110:LYS:HB3	2.16	0.47
1:A:190:PRO:HG3	1:A:784:TRP:CH2	2.50	0.47
1:A:559:LEU:HD13	1:A:918:ASN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:THR:O	1:B:1012:LEU:HB2	2.15	0.47
1:C:413:VAL:O	1:C:417:GLU:HG2	2.15	0.47
1:C:422:GLU:HB3	1:C:423:GLU:HG3	1.96	0.47
1:C:669:LEU:HA	1:C:669:LEU:HD23	1.61	0.47
1:D:404:LEU:HD21	1:D:449:LEU:HD13	1.96	0.47
1:E:61:VAL:HG22	1:E:118:LEU:HD22	1.97	0.47
1:E:594:VAL:HG22	1:E:650:PHE:CE2	2.50	0.47
1:E:932:LEU:HA	1:E:932:LEU:HD23	1.72	0.47
1:F:371:ALA:O	1:F:375:VAL:HG23	2.15	0.47
1:F:471:SER:O	1:F:475:VAL:HB	2.14	0.47
1:F:506:GLY:C	1:F:508:GLY:H	2.18	0.47
1:F:53:ASP:OD1	1:F:56:THR:OG1	2.28	0.47
1:F:559:LEU:HA	1:F:560:PRO:HD2	1.49	0.47
1:F:69:MET:SD	1:F:72:ILE:HD11	2.55	0.47
1:B:480:LEU:HA	1:B:480:LEU:HD23	1.68	0.46
1:B:583:THR:HG23	1:B:585:GLU:H	1.80	0.46
1:B:959:THR:HG21	1:B:1022:VAL:HG23	1.97	0.46
1:C:104:GLN:HG3	1:C:105:VAL:N	2.29	0.46
1:C:340:VAL:CG1	1:C:395:MET:HB3	2.43	0.46
1:E:318:PRO:HG2	1:E:321:LEU:HB2	1.97	0.46
1:E:356:TYR:CD1	1:E:365:THR:HG21	2.50	0.46
1:E:728:GLN:NE2	1:E:738:ILE:HG21	2.30	0.46
1:E:785:TYR:CZ	1:E:795:PRO:HB3	2.50	0.46
1:D:742:ASN:ND2	1:F:214:VAL:HG21	2.30	0.46
1:F:510:LYS:O	1:F:512:PHE:N	2.40	0.46
1:F:697:LEU:HD12	1:F:846:LEU:HD11	1.97	0.46
1:F:723:LYS:HG2	1:F:803:ARG:CZ	2.45	0.46
1:A:166:ILE:HD13	1:A:166:ILE:HA	1.59	0.46
1:A:340:VAL:O	1:A:343:THR:HB	2.15	0.46
1:B:344:LEU:HD11	1:B:398:MET:HE2	1.98	0.46
1:B:393:LEU:HD22	1:B:470:PHE:CE1	2.50	0.46
1:B:709:THR:O	1:B:710:SER:OG	2.31	0.46
1:C:527:TYR:HE2	1:C:963:VAL:HG13	1.80	0.46
1:D:880:PHE:HA	1:D:883:LEU:HD12	1.97	0.46
1:F:486:LEU:O	1:F:490:PRO:HG2	2.15	0.46
1:F:563:PHE:CE2	1:F:564:LEU:HD13	2.50	0.46
1:A:190:PRO:HG2	1:A:774:TYR:CG	2.51	0.46
1:A:281:PHE:HB2	1:A:610:PHE:HE1	1.80	0.46
1:A:200:PRO:HB2	1:A:744:THR:HG22	1.98	0.46
1:A:932:LEU:HD23	1:A:932:LEU:HA	1.51	0.46
1:B:366:LEU:O	1:B:369:THR:HB	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:772:ALA:HB1	1:C:225:VAL:HG12	1.97	0.46
1:C:572:PHE:CE1	1:C:643:THR:HG22	2.51	0.46
1:C:587:THR:HG21	1:C:617:GLN:O	2.15	0.46
1:C:899:VAL:CG2	1:C:1017:VAL:HG22	2.45	0.46
1:D:23:GLY:O	1:D:27:ILE:HG13	2.15	0.46
1:D:544:LEU:O	1:D:548:ILE:HG13	2.16	0.46
1:E:101:ASP:HA	1:E:131:LYS:NZ	2.30	0.46
1:F:351:VAL:O	1:F:355:MET:HE2	2.15	0.46
1:F:419:VAL:HG21	1:F:434:SER:HB3	1.96	0.46
1:F:859:TYR:HD2	1:F:859:TYR:O	1.98	0.46
1:A:172:VAL:HG13	1:A:291:ILE:HG23	1.96	0.46
1:A:412:VAL:HG22	1:A:438:ILE:HD11	1.96	0.46
1:A:574:THR:HG22	1:A:624:VAL:CG2	2.45	0.46
1:A:836:MET:HG2	1:A:854:TRP:CH2	2.49	0.46
1:B:293:LEU:HD22	1:B:297:ALA:HB3	1.97	0.46
1:B:507:GLU:O	1:B:509:LYS:HG3	2.16	0.46
1:C:1007:VAL:O	1:C:1011:VAL:HG23	2.16	0.46
1:C:293:LEU:HD22	1:C:297:ALA:HB3	1.96	0.46
1:C:45:ILE:HG21	1:C:111:LEU:HG	1.96	0.46
1:D:55:LYS:HE2	1:D:55:LYS:HB3	1.71	0.46
1:E:394:THR:HG23	1:E:469:GLN:HB3	1.98	0.46
1:E:653:ILE:C	1:E:654:LYS:HD2	2.36	0.46
1:E:841:GLN:O	1:E:844:SER:OG	2.33	0.46
1:D:749:TRP:CZ3	1:F:219:LEU:HG	2.51	0.46
1:F:288:GLY:O	1:F:289:LEU:HD23	2.16	0.46
1:F:36:PRO:HD3	1:F:391:ASN:CG	2.35	0.46
1:F:795:PRO:HG2	1:F:798:ALA:HB2	1.97	0.46
1:A:379:THR:HG21	1:A:477:ALA:HB2	1.96	0.46
1:B:462:SER:O	1:B:466:ILE:HG13	2.15	0.46
1:B:527:TYR:CE1	1:B:1014:ILE:HD12	2.51	0.46
1:B:525:HIS:HA	1:B:528:THR:HG22	1.97	0.46
1:B:932:LEU:HD23	1:B:932:LEU:HA	1.78	0.46
1:C:153:ASP:N	1:C:153:ASP:OD2	2.47	0.46
1:D:621:ILE:HD12	1:D:622:ALA:H	1.79	0.46
1:D:698:LEU:HD21	1:D:713:PRO:HD3	1.96	0.46
1:D:796:PHE:O	1:D:800:SER:OG	2.30	0.46
1:E:453:PHE:O	1:E:471:SER:OG	2.32	0.46
1:E:484:VAL:O	1:E:489:THR:HG23	2.15	0.46
1:E:720:PRO:HA	1:E:806:TYR:HA	1.96	0.46
1:F:139:VAL:O	1:F:326:PRO:HD2	2.15	0.46
1:F:293:LEU:HD13	1:F:294:ALA:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:96:SER:HB3	1:F:461:GLY:HA2	1.98	0.46
1:F:6:ILE:H	1:F:6:ILE:HG12	1.40	0.46
1:A:211:ASN:O	1:A:755:ASN:ND2	2.46	0.46
1:A:21:LEU:HA	1:A:21:LEU:HD13	1.74	0.46
1:A:359:LEU:C	1:A:360:GLN:HG2	2.34	0.46
1:A:375:VAL:HG13	1:A:480:LEU:HB2	1.97	0.46
1:B:394:THR:HG23	1:B:469:GLN:OE1	2.15	0.46
1:B:840:GLU:HG2	1:B:852:TYR:CE1	2.51	0.46
1:B:76:MET:HB2	1:B:93:THR:O	2.16	0.46
1:A:749:TRP:CZ3	1:C:219:LEU:HD23	2.49	0.46
1:C:242:SER:O	1:C:246:PHE:HD1	1.99	0.46
1:C:855:THR:HG23	1:C:856:GLY:N	2.31	0.46
1:C:47:ALA:HB3	1:C:88:VAL:HG13	1.98	0.46
1:D:21:LEU:HA	1:D:21:LEU:HD13	1.57	0.46
1:D:30:LEU:CD1	1:D:384:ALA:HA	2.46	0.46
1:D:420:MET:HB3	1:D:500:ILE:HB	1.98	0.46
1:D:749:TRP:CE3	1:F:234:ILE:HD11	2.51	0.46
1:E:222:THR:HA	1:E:224:PRO:HD3	1.98	0.46
1:E:896:VAL:HG23	1:E:937:ALA:HB3	1.98	0.46
1:F:664:PRO:HD3	1:F:672:ALA:C	2.36	0.46
1:F:967:LEU:HA	1:F:970:ILE:HD12	1.98	0.46
1:A:1006:MET:O	1:A:1010:THR:HG23	2.16	0.46
1:B:352:PHE:C	1:B:352:PHE:CD2	2.88	0.46
1:C:210:GLN:OE1	1:C:249:ILE:HG23	2.15	0.46
1:C:135:SER:HB3	1:C:668:GLU:HA	1.98	0.46
1:C:900:VAL:O	1:C:904:VAL:HG23	2.16	0.46
1:D:277:ILE:HG12	1:D:614:GLY:HA3	1.98	0.46
1:D:136:PHE:CE2	1:D:292:LYS:HE3	2.50	0.46
1:D:787:ARG:HA	1:D:792:GLN:O	2.15	0.46
1:A:100:ALA:HB1	1:A:131:LYS:HD2	1.98	0.46
1:A:212:ALA:HA	1:A:239:ARG:NE	2.30	0.46
1:A:249:ILE:HB	1:A:262:LEU:HB2	1.97	0.46
1:A:255:GLN:H	1:A:255:GLN:HG3	1.57	0.46
1:A:375:VAL:HG21	1:A:481:SER:HA	1.97	0.46
1:A:636:GLU:HA	1:A:641:ALA:HB3	1.98	0.46
1:B:727:ASP:OD1	1:B:730:LYS:HG3	2.16	0.46
1:B:906:GLY:HA3	1:B:1008:THR:CG2	2.46	0.46
1:C:250:LEU:CD1	1:C:259:ARG:HB3	2.45	0.46
1:C:144:ASN:HA	1:C:320:GLY:O	2.16	0.46
1:C:534:ILE:HD13	1:C:534:ILE:HG21	1.67	0.46
1:C:277:ILE:HA	1:C:614:GLY:HA2	1.98	0.46

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:757:PHE:HE1	1:D:759:ASP:HB2	1.81	0.46
1:E:648:ARG:O	1:E:651:SER:OG	2.34	0.46
1:F:105:VAL:HA	1:F:108:GLN:HE21	1.80	0.46
1:F:10:ILE:O	1:F:14:VAL:HG23	2.16	0.46
1:F:421:ALA:O	1:F:503:GLY:N	2.30	0.46
1:F:757:PHE:CE1	1:F:759:ASP:HB2	2.50	0.46
1:A:325:TYR:HA	1:A:326:PRO:HD2	1.86	0.46
1:A:438:ILE:O	1:A:442:LEU:HG	2.16	0.46
1:B:667:VAL:HB	1:B:668:GLU:CD	2.36	0.46
1:B:677:PHE:HB3	1:B:822:ILE:O	2.16	0.46
1:B:900:VAL:HG22	1:B:930:ILE:HG23	1.98	0.46
1:C:902:LEU:HD23	1:C:1013:ALA:HA	1.97	0.46
1:C:731:ALA:HA	1:C:736:VAL:HG23	1.97	0.46
1:D:30:LEU:HD13	1:D:384:ALA:HA	1.98	0.46
1:F:425:LEU:HB3	1:F:429:GLU:HG2	1.98	0.46
1:F:738:ILE:O	1:F:741:ILE:HG13	2.16	0.46
1:A:72:ILE:HD13	1:A:107:VAL:HG22	1.98	0.46
1:B:68:ASN:CB	1:B:114:ALA:HB2	2.46	0.46
1:B:457:ALA:HB2	1:B:471:SER:OG	2.16	0.46
1:B:544:LEU:O	1:B:547:ILE:HB	2.16	0.46
1:B:787:ARG:HA	1:B:792:GLN:O	2.15	0.46
1:C:2:PRO:HB2	1:C:3:ASN:OD1	2.15	0.46
1:C:836:MET:HA	1:C:854:TRP:CH2	2.51	0.46
1:E:190:PRO:HB3	1:E:784:TRP:CE2	2.51	0.46
1:E:4:PHE:O	1:E:8:ARG:HD2	2.15	0.46
1:E:691:THR:HA	1:E:694:ARG:NH1	2.31	0.46
1:E:748:ALA:O	1:E:769:MET:HG2	2.16	0.46
1:F:30:LEU:HD23	1:F:390:ILE:HD11	1.98	0.46
1:F:352:PHE:HA	1:F:355:MET:CE	2.46	0.46
1:F:26:ALA:HB1	1:F:384:ALA:CB	2.45	0.46
1:F:566:ASP:CG	1:F:673:THR:HG23	2.36	0.46
1:F:945:LYS:O	1:F:948:MET:N	2.49	0.46
1:A:488:LEU:O	1:A:491:ALA:HB3	2.15	0.45
1:A:514:GLY:C	1:A:516:PHE:N	2.69	0.45
1:A:516:PHE:HA	1:A:519:MET:HG3	1.98	0.45
1:B:110:LYS:HA	1:B:110:LYS:HD3	1.51	0.45
1:B:427:PRO:O	1:B:430:ALA:HB3	2.17	0.45
1:B:455:PRO:HG2	1:B:875:SER:HG	1.81	0.45
1:C:423:GLU:HB2	1:C:425:LEU:HG	1.98	0.45
1:C:986:ILE:O	1:C:986:ILE:HD13	2.16	0.45
1:D:136:PHE:HD2	1:D:292:LYS:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:LEU:CD1	1:D:259:ARG:HB3	2.44	0.45
1:D:332:PHE:CD1	1:D:569:GLN:HG2	2.50	0.45
1:D:559:LEU:HD13	1:D:918:ASN:HB2	1.96	0.45
1:E:748:ALA:HB3	1:E:749:TRP:HD1	1.81	0.45
1:F:110:LYS:HA	1:F:110:LYS:HD3	1.61	0.45
1:F:344:LEU:HD13	1:F:402:ILE:HD11	1.98	0.45
1:F:654:LYS:HB3	1:F:656:ALA:H	1.81	0.45
1:A:681:ASP:OD1	1:A:684:GLY:N	2.47	0.45
1:B:470:PHE:O	1:B:474:ILE:HG13	2.15	0.45
1:C:200:PRO:HA	1:C:203:VAL:HG23	1.98	0.45
1:C:343:THR:HG23	1:C:983:PRO:HB2	1.98	0.45
1:C:33:ALA:O	1:C:391:ASN:HA	2.16	0.45
1:C:542:LEU:O	1:C:546:LEU:HG	2.16	0.45
1:C:890:TRP:HA	1:C:890:TRP:HE3	1.81	0.45
1:D:3:ASN:O	1:D:5:PHE:N	2.49	0.45
1:D:184:MET:HB3	1:D:766:VAL:HG13	1.97	0.45
1:E:955:LEU:HD13	1:E:1025:ARG:HG2	1.98	0.45
1:E:106:GLN:HA	1:E:109:ASN:ND2	2.31	0.45
1:E:172:VAL:CG2	1:E:306:ILE:HD11	2.46	0.45
1:E:445:ILE:HG21	1:E:935:LYS:CD	2.46	0.45
1:F:101:ASP:OD1	1:F:131:LYS:NZ	2.46	0.45
1:F:171:GLY:HA3	1:F:302:THR:OG1	2.15	0.45
1:A:363:ARG:O	1:A:366:LEU:N	2.49	0.45
1:A:278:ILE:HG13	1:A:613:ASN:HB3	1.97	0.45
1:B:119:PRO:HG2	1:B:122:VAL:CG2	2.46	0.45
1:B:363:ARG:HD2	1:B:498:LYS:HD2	1.97	0.45
1:B:23:GLY:HA3	1:B:377:LEU:HB3	1.99	0.45
1:B:469:GLN:O	1:B:473:THR:OG1	2.14	0.45
1:B:510:LYS:HB2	1:B:514:GLY:H	1.82	0.45
1:C:1006:MET:HA	1:C:1009:ALA:HB3	1.97	0.45
1:C:514:GLY:O	1:C:518:ARG:HD3	2.16	0.45
1:D:470:PHE:CE2	1:D:924:VAL:HG21	2.51	0.45
1:D:72:ILE:HD13	1:D:107:VAL:HG22	1.99	0.45
1:D:974:SER:CB	1:D:1010:THR:HG21	2.47	0.45
1:E:186:ILE:O	1:E:768:VAL:HA	2.16	0.45
1:F:1003:MET:O	1:F:1007:VAL:HG23	2.16	0.45
1:F:941:VAL:HG13	1:F:1021:PHE:CZ	2.52	0.45
1:F:77:TYR:CE1	1:F:93:THR:HG21	2.52	0.45
1:F:676:ASP:HB3	1:F:823:LEU:CD2	2.46	0.45
1:F:65:ILE:HD13	1:F:90:ILE:HD11	1.97	0.45
1:A:349:ILE:O	1:A:352:PHE:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:LYS:HA	1:A:654:LYS:HD3	1.62	0.45
1:B:347:ALA:O	1:B:351:VAL:HG23	2.16	0.45
1:B:418:ARG:HD2	1:B:965:MET:HB2	1.98	0.45
1:C:407:ASP:OD1	1:C:407:ASP:N	2.48	0.45
1:C:662:ASN:OD1	1:C:663:LEU:HD23	2.16	0.45
1:E:166:ILE:HG23	1:E:306:ILE:HG12	1.99	0.45
1:E:54:ALA:N	1:E:84:SER:HA	2.31	0.45
1:E:876:LEU:HD23	1:E:876:LEU:HA	1.82	0.45
1:E:982:MET:O	1:E:985:VAL:HG23	2.16	0.45
1:F:459:PHE:CZ	1:F:871:LEU:HG	2.52	0.45
1:A:377:LEU:HA	1:A:377:LEU:HD23	1.78	0.45
1:A:981:VAL:O	1:A:984:LEU:N	2.46	0.45
1:C:527:TYR:OH	1:C:1014:ILE:O	2.24	0.45
1:C:527:TYR:CE2	1:C:963:VAL:HG13	2.52	0.45
1:C:812:GLU:HB2	1:C:819:SER:O	2.16	0.45
1:C:892:ILE:HD12	1:C:1021:PHE:HE1	1.81	0.45
1:D:293:LEU:HD13	1:D:294:ALA:O	2.16	0.45
1:D:414:GLU:OE2	1:D:969:PRO:HG3	2.16	0.45
1:D:3:ASN:O	1:D:4:PHE:C	2.55	0.45
1:D:572:PHE:CE1	1:D:643:THR:HG22	2.50	0.45
1:E:331:PRO:HA	1:E:334:LYS:HD2	1.98	0.45
1:E:697:LEU:HD12	1:E:697:LEU:HA	1.75	0.45
1:F:694:ARG:HD3	1:F:820:MET:SD	2.57	0.45
1:A:30:LEU:HD11	1:A:384:ALA:HA	1.98	0.45
1:A:708:LEU:HA	1:A:825:GLN:O	2.16	0.45
1:A:900:VAL:O	1:A:904:VAL:HG23	2.17	0.45
1:A:948:MET:HG3	1:A:954:GLY:O	2.17	0.45
1:B:373:PRO:O	1:B:376:LEU:HB2	2.17	0.45
1:B:442:LEU:O	1:B:445:ILE:HG13	2.16	0.45
1:B:961:ASP:OD2	1:B:964:ARG:NH2	2.50	0.45
1:C:121:GLU:O	1:C:124:GLN:HG2	2.15	0.45
1:C:786:VAL:HG23	1:C:796:PHE:CE2	2.51	0.45
1:D:251:LEU:HD12	1:D:265:VAL:HG21	1.99	0.45
1:E:377:LEU:O	1:E:380:PHE:HB2	2.17	0.45
1:E:415:ASN:HD22	1:E:434:SER:CB	2.27	0.45
1:F:250:LEU:HD13	1:F:259:ARG:HB3	1.98	0.45
1:F:642:ILE:O	1:F:645:ARG:HG2	2.17	0.45
1:F:980:GLY:O	1:F:983:PRO:HD2	2.17	0.45
1:A:941:VAL:HG22	1:A:1021:PHE:CD1	2.52	0.45
1:B:647:THR:CG2	1:B:660:ALA:H	2.29	0.45
1:B:580:ALA:HB1	1:B:719:THR:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:THR:O	1:C:398:MET:HG2	2.17	0.45
1:D:977:PHE:HD2	1:D:1006:MET:HG3	1.82	0.45
1:D:1016:PHE:O	1:D:1019:VAL:HB	2.17	0.45
1:D:383:LEU:HD22	1:D:388:PHE:CD1	2.52	0.45
1:D:383:LEU:HD22	1:D:388:PHE:HD1	1.81	0.45
1:D:618:ASN:N	1:D:618:ASN:OD1	2.50	0.45
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.98	0.45
1:E:708:LEU:HG	1:E:708:LEU:H	1.42	0.45
1:E:354:VAL:CG1	1:E:972:MET:HG2	2.46	0.45
1:F:361:ASN:HD22	1:F:364:ALA:HB2	1.80	0.45
1:F:5:PHE:HD2	1:F:6:ILE:HG12	1.82	0.45
1:F:932:LEU:O	1:F:935:LYS:HB3	2.17	0.45
1:A:597:TYR:CD2	1:A:650:PHE:CZ	3.05	0.45
1:A:184:MET:HB3	1:A:766:VAL:HG13	1.98	0.45
1:A:873:ALA:O	1:A:877:ILE:HG12	2.16	0.45
1:A:956:ILE:HG13	1:A:956:ILE:H	1.38	0.45
1:B:139:VAL:HA	1:B:289:LEU:O	2.16	0.45
1:B:293:LEU:HD11	1:B:297:ALA:O	2.17	0.45
1:B:428:LYS:O	1:B:431:THR:N	2.49	0.45
1:C:376:LEU:HD22	1:C:398:MET:CE	2.47	0.45
1:C:379:THR:HG23	1:C:476:SER:OG	2.17	0.45
1:D:240:LEU:HD22	1:D:245:GLU:OE1	2.16	0.45
1:D:763:VAL:HG12	1:E:63:GLN:OE1	2.17	0.45
1:D:7:ASP:O	1:D:8:ARG:HG3	2.16	0.45
1:D:880:PHE:O	1:D:883:LEU:HB2	2.17	0.45
1:D:979:LEU:HA	1:D:979:LEU:HD23	1.34	0.45
1:E:425:LEU:HD12	1:E:430:ALA:HA	1.99	0.45
1:E:564:LEU:CD1	1:E:666:ILE:HD12	2.47	0.45
1:E:564:LEU:HD13	1:E:666:ILE:HD12	1.98	0.45
1:F:521:GLU:O	1:F:524:THR:HB	2.16	0.45
1:F:700:GLU:HA	1:F:703:LYS:HZ2	1.82	0.45
1:F:787:ARG:HA	1:F:792:GLN:O	2.17	0.45
1:A:158:VAL:HA	1:A:162:MET:HE2	1.99	0.45
1:A:882:CYS:O	1:A:885:ALA:HB3	2.16	0.45
1:B:445:ILE:HG21	1:B:935:LYS:HD2	1.98	0.45
1:C:181:GLN:HG2	1:C:182:TYR:N	2.31	0.45
1:D:441:ALA:HB2	1:D:942:GLU:OE2	2.17	0.45
1:A:444:GLY:O	1:A:448:VAL:HG23	2.17	0.45
1:A:720:PRO:HA	1:A:805:GLU:O	2.16	0.45
1:A:75:LEU:CD1	1:A:92:LEU:HD23	2.47	0.45
1:B:383:LEU:HD22	1:B:472:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:PHE:HB3	1:B:658:VAL:HB	1.99	0.45
1:B:354:VAL:HG22	1:B:975:LEU:HD23	1.99	0.45
1:C:461:GLY:HA3	1:C:863:LEU:HD21	1.99	0.45
1:D:343:THR:O	1:D:344:LEU:C	2.55	0.45
1:D:685:LEU:O	1:D:689:LYS:HD2	2.16	0.45
1:E:108:GLN:CD	1:F:112:GLN:HG2	2.37	0.45
1:E:367:ILE:CD1	1:E:497:LEU:HD13	2.47	0.45
1:E:427:PRO:O	1:E:430:ALA:HB3	2.16	0.45
1:F:363:ARG:CZ	1:F:363:ARG:H	2.29	0.45
1:F:887:TYR:C	1:F:889:SER:N	2.70	0.45
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.52	0.44
1:A:35:TYR:CE2	1:A:564:LEU:HD21	2.52	0.44
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.83	0.44
1:B:525:HIS:O	1:B:528:THR:HG22	2.17	0.44
1:B:674:GLY:HA2	1:B:825:GLN:HA	1.98	0.44
1:B:723:LYS:HE3	1:B:725:ASP:OD2	2.17	0.44
1:B:873:ALA:O	1:B:877:ILE:HG13	2.17	0.44
1:C:163:LYS:HE3	1:C:177:LEU:HB2	1.99	0.44
1:C:694:ARG:HG2	1:C:698:LEU:HD12	1.98	0.44
1:C:845:LYS:HD2	1:C:845:LYS:O	2.17	0.44
1:D:214:VAL:HG21	1:E:742:ASN:ND2	2.32	0.44
1:D:262:LEU:HG	1:D:268:ILE:HD11	1.99	0.44
1:D:831:SER:OG	1:D:832:THR:N	2.49	0.44
1:D:685:LEU:HD21	1:D:848:THR:O	2.18	0.44
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.98	0.44
1:E:108:GLN:HA	1:E:129:VAL:HG21	1.98	0.44
1:E:571:VAL:HG22	1:E:625:SER:HA	1.98	0.44
1:F:187:TRP:O	1:F:266:ALA:HB1	2.17	0.44
1:F:614:GLY:O	1:F:616:GLY:HA3	2.16	0.44
1:A:388:PHE:CE2	1:A:472:ILE:HD13	2.53	0.44
1:A:470:PHE:CD2	1:A:924:VAL:HG11	2.52	0.44
1:A:722:PHE:CD1	1:A:804:TRP:CE2	3.05	0.44
1:A:904:VAL:HA	1:A:926:LEU:HD21	1.99	0.44
1:B:329:THR:O	1:B:333:VAL:HG23	2.16	0.44
1:B:576:VAL:HG22	1:B:658:VAL:HG22	1.99	0.44
1:D:307:ARG:HA	1:D:307:ARG:HD3	1.88	0.44
1:D:336:SER:O	1:D:340:VAL:HG23	2.17	0.44
1:D:723:LYS:HB3	1:D:803:ARG:HG2	2.00	0.44
1:E:102:ILE:O	1:E:106:GLN:HG3	2.17	0.44
1:E:255:GLN:HG3	1:E:255:GLN:H	1.38	0.44
1:E:329:THR:O	1:E:332:PHE:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:409:ALA:O	1:E:413:VAL:HG23	2.17	0.44
1:E:568:ASP:O	1:E:629:TRP:CZ3	2.70	0.44
1:D:214:VAL:HG11	1:E:742:ASN:CG	2.38	0.44
1:E:770:SER:OG	1:E:775:ARG:HG2	2.18	0.44
1:F:65:ILE:O	1:F:69:MET:HG2	2.17	0.44
1:F:940:ILE:HG12	1:F:966:ARG:NH2	2.32	0.44
1:A:213:GLN:HA	1:A:237:GLN:O	2.17	0.44
1:A:663:LEU:HD12	1:A:667:VAL:HG13	1.98	0.44
1:A:871:LEU:O	1:A:874:ILE:HB	2.17	0.44
1:B:330:THR:HB	1:B:331:PRO:HD3	1.98	0.44
1:B:65:ILE:O	1:B:69:MET:HG2	2.17	0.44
1:B:984:LEU:HB3	1:B:995:GLN:O	2.17	0.44
1:C:615:GLY:HA2	1:C:616:GLY:HA3	1.69	0.44
1:B:235:ILE:HD11	1:C:721:GLN:OE1	2.17	0.44
1:D:463:THR:HG22	1:D:467:TYR:CE2	2.51	0.44
1:D:827:ALA:O	1:D:830:LYS:N	2.39	0.44
1:D:123:GLN:HB3	1:E:116:PRO:HB3	1.99	0.44
1:A:34:GLN:O	1:A:392:THR:OG1	2.16	0.44
1:A:376:LEU:HD22	1:A:398:MET:SD	2.57	0.44
1:A:344:LEU:CD2	1:A:402:ILE:HD11	2.45	0.44
1:A:650:PHE:HD1	1:A:653:ILE:HD11	1.83	0.44
1:D:531:VAL:O	1:D:535:LEU:HG	2.17	0.44
1:D:833:GLY:O	1:D:836:MET:HB2	2.17	0.44
1:D:871:LEU:HA	1:D:871:LEU:HD23	1.66	0.44
1:D:911:ALA:HB2	1:D:922:PHE:CE1	2.53	0.44
1:E:344:LEU:O	1:E:348:ILE:HG13	2.18	0.44
1:E:632:ARG:HB3	1:E:637:ASN:HB3	1.99	0.44
1:E:837:GLU:O	1:E:840:GLU:HB2	2.18	0.44
1:F:247:GLY:O	1:F:261:LEU:HB3	2.18	0.44
1:F:312:LYS:HD3	1:F:312:LYS:O	2.17	0.44
1:A:892:ILE:HG12	1:A:1025:ARG:CD	2.46	0.44
1:C:103:ALA:O	1:C:107:VAL:HG23	2.18	0.44
1:C:343:THR:HA	1:C:346:GLU:OE1	2.17	0.44
1:C:53:ASP:HA	1:C:84:SER:HB2	1.99	0.44
1:D:328:ASP:O	1:D:331:PRO:HD2	2.18	0.44
1:D:366:LEU:HD22	1:D:370:ILE:HG13	2.00	0.44
1:D:982:MET:HB3	1:D:983:PRO:HD3	2.00	0.44
1:E:568:ASP:O	1:E:629:TRP:HZ3	2.00	0.44
1:E:685:LEU:HD11	1:E:690:LEU:HG	1.99	0.44
1:F:400:LEU:HD11	1:F:1002:VAL:HG21	1.99	0.44
1:F:728:GLN:HE22	1:F:738:ILE:HG21	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:VAL:HA	1:A:493:CYS:SG	2.57	0.44
1:A:691:THR:HG23	1:A:694:ARG:NH1	2.25	0.44
1:A:769:MET:HG2	1:A:770:SER:N	2.33	0.44
1:A:959:THR:HG21	1:A:1022:VAL:HG23	1.99	0.44
1:B:399:VAL:HA	1:B:402:ILE:HG13	2.00	0.44
1:B:61:VAL:HG22	1:B:119:PRO:HD2	1.99	0.44
1:B:707:MET:SD	1:B:830:LYS:HG2	2.58	0.44
1:C:538:THR:HG21	1:C:1023:VAL:CG2	2.48	0.44
1:C:6:ILE:HG22	1:C:8:ARG:O	2.17	0.44
1:D:345:VAL:O	1:D:349:ILE:HD12	2.18	0.44
1:D:400:LEU:HG	1:D:928:THR:OG1	2.18	0.44
1:D:682:GLN:HG3	1:D:817:LEU:HD13	2.00	0.44
1:E:198:LEU:HD21	1:E:252:LYS:HB2	1.99	0.44
1:E:309:GLU:OE2	1:E:313:MET:HE3	2.17	0.44
1:E:420:MET:SD	1:E:499:PRO:HA	2.58	0.44
1:E:610:PHE:HB2	1:E:623:PHE:HB3	2.00	0.44
1:E:728:GLN:HE22	1:E:738:ILE:HG21	1.82	0.44
1:F:1018:PRO:O	1:F:1022:VAL:HG23	2.18	0.44
1:F:484:VAL:C	1:F:486:LEU:N	2.71	0.44
1:F:647:THR:HG23	1:F:659:PHE:CE1	2.53	0.44
1:F:927:LEU:O	1:F:928:THR:C	2.55	0.44
1:A:415:ASN:O	1:A:419:VAL:HG23	2.17	0.44
1:A:424:GLY:C	1:A:502:LYS:HZ2	2.20	0.44
1:B:478:MET:O	1:B:482:VAL:HG12	2.17	0.44
1:C:65:ILE:HD11	1:C:118:LEU:HD11	1.99	0.44
1:C:574:THR:HG23	1:C:622:ALA:HB3	1.98	0.44
1:C:955:LEU:O	1:C:959:THR:HG23	2.17	0.44
1:C:975:LEU:O	1:C:976:ALA:C	2.55	0.44
1:D:346:GLU:O	1:D:350:LEU:HD12	2.17	0.44
1:D:395:MET:O	1:D:399:VAL:HG23	2.17	0.44
1:D:514:GLY:C	1:D:516:PHE:N	2.71	0.44
1:D:975:LEU:HA	1:D:975:LEU:HD12	1.82	0.44
1:E:21:LEU:O	1:E:25:LEU:HB2	2.18	0.44
1:E:694:ARG:NH2	1:E:717:GLU:OE1	2.50	0.44
1:F:101:ASP:O	1:F:105:VAL:HG23	2.17	0.44
1:F:345:VAL:O	1:F:349:ILE:HD12	2.18	0.44
1:F:468:ARG:HA	1:F:471:SER:OG	2.18	0.44
1:B:72:ILE:HG12	1:B:106:GLN:HB3	1.99	0.44
1:B:13:TRP:O	1:B:17:ILE:HG13	2.17	0.44
1:D:164:ASP:HB3	1:D:168:ARG:HH21	1.82	0.44
1:D:956:ILE:H	1:D:956:ILE:HG13	1.16	0.44

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:602:GLU:HB3	1:F:606:VAL:HG23	1.99	0.44
1:F:916:LEU:HD23	1:F:916:LEU:HA	1.76	0.44
1:A:130:GLU:HB3	1:A:132:SER:HB2	2.00	0.44
1:A:324:VAL:HG22	1:A:325:TYR:H	1.82	0.44
1:A:483:LEU:HD13	1:A:487:ILE:HD12	1.99	0.44
1:A:636:GLU:HB2	1:A:645:ARG:NH2	2.30	0.44
1:A:895:SER:HB2	1:A:1021:PHE:HA	1.99	0.44
1:B:399:VAL:O	1:B:402:ILE:HG13	2.18	0.44
1:B:445:ILE:HD12	1:B:449:LEU:HD12	2.00	0.44
1:B:721:GLN:CD	1:B:807:GLY:HA3	2.38	0.44
1:B:975:LEU:O	1:B:979:LEU:HB2	2.18	0.44
1:C:429:GLU:O	1:C:433:LYS:HB2	2.18	0.44
1:C:663:LEU:H	1:C:663:LEU:HD23	1.83	0.44
2:D:2000:LMT:H6E	2:D:2000:LMT:O5B	2.18	0.44
1:D:563:PHE:O	1:D:564:LEU:HD12	2.18	0.44
1:E:172:VAL:HG22	1:E:302:THR:HG23	2.00	0.44
1:E:515:TRP:O	1:E:519:MET:HG3	2.18	0.44
1:E:905:ILE:HG23	1:E:906:GLY:N	2.33	0.44
1:F:669:LEU:HD22	1:F:856:GLY:HA2	1.98	0.44
1:A:270:LEU:HA	1:A:270:LEU:HD12	1.85	0.43
1:A:451:ALA:CB	1:A:878:VAL:HG12	2.48	0.43
1:B:959:THR:HG21	1:B:1022:VAL:CG2	2.48	0.43
1:B:214:VAL:HG21	1:C:742:ASN:ND2	2.32	0.43
1:B:194:ASN:HA	1:B:793:MET:HE2	2.00	0.43
1:B:902:LEU:HD11	1:B:1016:PHE:CD2	2.53	0.43
1:C:370:ILE:C	1:C:373:PRO:HD2	2.39	0.43
1:C:722:PHE:CZ	1:C:802:SER:HB2	2.53	0.43
1:D:196:PHE:CG	1:D:260:VAL:HG11	2.53	0.43
1:D:377:LEU:O	1:D:380:PHE:HB2	2.17	0.43
1:D:712:ARG:O	1:D:822:ILE:HG23	2.17	0.43
1:E:110:LYS:HD3	1:E:110:LYS:HA	1.60	0.43
1:E:149:MET:HB2	1:E:153:ASP:CB	2.43	0.43
1:F:146:ASP:OD2	1:F:147:GLY:N	2.49	0.43
1:F:281:PHE:HB2	1:F:610:PHE:CE1	2.53	0.43
1:F:343:THR:O	1:F:346:GLU:N	2.51	0.43
1:F:35:TYR:HB3	1:F:38:ILE:HD12	2.00	0.43
1:F:425:LEU:HB3	1:F:429:GLU:HB3	2.00	0.43
1:F:49:TYR:CD1	1:F:57:VAL:HA	2.52	0.43
1:F:770:SER:OG	1:F:775:ARG:HG2	2.18	0.43
1:A:1035:ILE:O	1:A:1036:GLU:HB2	2.18	0.43
1:A:788:ALA:HB3	1:A:790:ASP:OD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:GLY:HA3	1:B:502:LYS:HB2	2.00	0.43
1:B:526:HIS:O	1:B:529:ASP:HB2	2.18	0.43
1:B:691:THR:HG23	1:B:694:ARG:NH1	2.33	0.43
1:B:755:ASN:O	1:B:766:VAL:HB	2.18	0.43
1:D:1020:PHE:O	1:D:1024:VAL:HB	2.18	0.43
1:D:34:GLN:HB2	1:D:333:VAL:HG22	2.00	0.43
1:D:960:LEU:HD23	1:D:960:LEU:HA	1.75	0.43
1:E:187:TRP:HZ3	1:E:769:MET:HB3	1.82	0.43
1:E:370:ILE:HD12	1:E:492:LEU:HD13	2.00	0.43
1:E:676:ASP:HA	1:E:823:LEU:HD23	1.99	0.43
1:E:821:GLU:HG2	1:E:822:ILE:N	2.33	0.43
1:F:343:THR:HA	1:F:346:GLU:OE1	2.18	0.43
1:F:610:PHE:O	1:F:622:ALA:HA	2.18	0.43
1:A:158:VAL:HA	1:A:162:MET:CE	2.48	0.43
1:A:480:LEU:HA	1:A:480:LEU:HD23	1.78	0.43
1:A:527:TYR:O	1:A:530:SER:HB3	2.18	0.43
1:A:667:VAL:HG12	1:A:668:GLU:OE1	2.19	0.43
1:A:770:SER:OG	1:A:775:ARG:HG2	2.18	0.43
1:A:962:ALA:O	1:A:965:MET:HG2	2.18	0.43
1:B:544:LEU:O	1:B:548:ILE:HG13	2.18	0.43
1:C:405:LEU:HD12	1:C:406:VAL:N	2.34	0.43
1:C:679:LEU:O	1:C:819:SER:HB2	2.18	0.43
1:C:905:ILE:HG13	1:C:909:LEU:HD23	2.00	0.43
1:C:911:ALA:HB2	1:C:922:PHE:CE1	2.52	0.43
1:D:246:PHE:O	1:D:262:LEU:HD23	2.18	0.43
1:D:343:THR:HG21	1:D:984:LEU:HD21	2.00	0.43
1:D:559:LEU:HA	1:D:560:PRO:HD2	1.68	0.43
1:D:588:GLN:NE2	1:D:588:GLN:O	2.51	0.43
1:D:691:THR:HA	1:D:694:ARG:NH1	2.33	0.43
1:D:415:ASN:ND2	1:D:943:PHE:HZ	2.15	0.43
1:E:238:THR:HG22	1:E:239:ARG:O	2.17	0.43
1:E:559:LEU:CD2	1:E:560:PRO:HD2	2.46	0.43
1:F:143:ILE:HG12	1:F:322:LYS:O	2.19	0.43
1:F:348:ILE:HG12	1:F:402:ILE:HD13	2.00	0.43
1:F:650:PHE:HB2	1:F:658:VAL:O	2.18	0.43
1:F:707:MET:HB2	1:F:708:LEU:HD12	2.00	0.43
1:A:154:ILE:HG22	1:A:287:SER:HB3	2.01	0.43
1:A:615:GLY:HA2	1:A:617:GLN:H	1.82	0.43
1:A:695:ASN:O	1:A:698:LEU:HB2	2.18	0.43
1:A:722:PHE:HD1	1:A:804:TRP:CE2	2.37	0.43
1:A:932:LEU:O	1:A:935:LYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1031:LYS:HA	1:B:1032:ASN:HA	1.68	0.43
1:B:452:VAL:HG23	1:B:453:PHE:CD2	2.53	0.43
1:B:574:THR:HG21	1:B:598:TYR:HE2	1.83	0.43
1:B:594:VAL:HG22	1:B:650:PHE:CZ	2.53	0.43
1:C:1031:LYS:HD2	1:C:1033:GLU:CB	2.49	0.43
1:C:143:ILE:HG22	1:C:286:ALA:CB	2.48	0.43
1:C:146:ASP:O	1:C:148:THR:OG1	2.36	0.43
1:C:363:ARG:NH2	1:C:498:LYS:HD2	2.33	0.43
1:D:1007:VAL:O	1:D:1011:VAL:HG23	2.18	0.43
1:D:454:VAL:O	1:D:457:ALA:HB3	2.19	0.43
1:D:124:GLN:NE2	1:D:753:TYR:HD2	2.16	0.43
1:D:771:GLU:HB3	1:D:774:TYR:CD1	2.53	0.43
1:D:786:VAL:HG23	1:D:796:PHE:CE2	2.53	0.43
1:D:81:ASN:O	1:D:88:VAL:HG23	2.19	0.43
1:F:144:ASN:OD1	1:F:148:THR:HA	2.18	0.43
1:E:173:GLY:O	1:F:71:GLY:HA3	2.18	0.43
1:F:54:ALA:HB1	1:F:811:LEU:HG	2.00	0.43
1:F:84:SER:HB3	1:F:809:PRO:O	2.17	0.43
1:A:137:LEU:HD13	1:A:293:LEU:HG	1.99	0.43
1:A:189:ASN:HA	1:A:190:PRO:HD3	1.74	0.43
1:B:681:ASP:HA	1:B:849:GLY:O	2.18	0.43
1:C:546:LEU:O	1:C:550:VAL:HG23	2.18	0.43
1:D:199:THR:HG21	1:D:787:ARG:H	1.82	0.43
1:D:959:THR:HG21	1:D:1022:VAL:CG2	2.49	0.43
1:E:30:LEU:HA	1:E:30:LEU:HD12	1.78	0.43
1:E:597:TYR:O	1:E:601:LYS:HB2	2.18	0.43
1:F:196:PHE:CD2	1:F:260:VAL:HG21	2.54	0.43
1:F:544:LEU:O	1:F:547:ILE:HB	2.18	0.43
1:F:771:GLU:HB2	1:F:774:TYR:HD1	1.82	0.43
1:A:3:ASN:O	1:A:4:PHE:C	2.57	0.43
1:A:530:SER:O	1:A:533:GLY:N	2.51	0.43
1:A:639:VAL:CG1	1:A:662:ASN:HB2	2.42	0.43
1:A:79:SER:HA	1:A:813:ARG:O	2.19	0.43
1:A:814:TYR:OH	1:A:854:TRP:O	2.29	0.43
1:B:1033:GLU:OE2	1:B:1034:ASP:HB2	2.18	0.43
1:B:281:PHE:HB2	1:B:610:PHE:CE1	2.53	0.43
1:B:407:ASP:OD1	1:B:973:THR:HG21	2.19	0.43
1:B:949:ASP:O	1:B:951:GLU:N	2.52	0.43
1:B:981:VAL:O	1:B:982:MET:C	2.57	0.43
1:C:531:VAL:O	1:C:535:LEU:HG	2.19	0.43
1:C:836:MET:HG2	1:C:854:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:927:LEU:O	1:C:930:ILE:N	2.51	0.43
1:C:963:VAL:HA	1:C:966:ARG:HH12	1.82	0.43
1:D:852:TYR:CD2	1:D:852:TYR:N	2.86	0.43
1:D:966:ARG:O	1:D:970:ILE:HG12	2.18	0.43
1:E:250:LEU:HD21	1:E:253:VAL:HG22	2.00	0.43
1:F:38:ILE:HD13	1:F:466:ILE:CD1	2.49	0.43
1:F:462:SER:O	1:F:466:ILE:HG12	2.19	0.43
1:F:602:GLU:HG3	1:F:605:ASN:HB2	2.01	0.43
1:A:1013:ALA:C	1:A:1015:PHE:H	2.21	0.43
1:A:540:ARG:HH22	2:A:1101:LMT:H6'2	1.84	0.43
1:A:142:VAL:O	1:A:286:ALA:HB1	2.18	0.43
1:A:497:LEU:HD12	1:A:497:LEU:HA	1.79	0.43
1:A:728:GLN:OE1	1:A:738:ILE:HG12	2.19	0.43
1:A:946:ASP:OD1	1:A:946:ASP:C	2.56	0.43
1:B:535:LEU:CD2	1:B:1019:VAL:HA	2.49	0.43
1:B:26:ALA:HB1	1:B:384:ALA:CB	2.49	0.43
1:C:188:MET:HB3	1:C:193:LEU:CD1	2.46	0.43
1:C:677:PHE:CE1	1:C:852:TYR:HB2	2.53	0.43
1:C:966:ARG:HG2	1:C:966:ARG:O	2.19	0.43
1:E:324:VAL:O	1:E:326:PRO:HD3	2.19	0.43
1:E:602:GLU:O	1:E:602:GLU:HG3	2.19	0.43
1:D:102:ILE:HD12	1:F:101:ASP:HB3	2.01	0.43
1:F:344:LEU:CD2	1:F:402:ILE:HD11	2.48	0.43
1:F:376:LEU:HD22	1:F:398:MET:CE	2.49	0.43
1:F:49:TYR:CE1	1:F:57:VAL:HA	2.53	0.43
1:F:49:TYR:CG	1:F:57:VAL:HG12	2.54	0.43
1:F:706:ASP:OD1	1:F:706:ASP:N	2.49	0.43
1:A:242:SER:OG	1:A:245:GLU:HG2	2.19	0.43
1:A:722:PHE:HB2	1:A:804:TRP:CZ3	2.52	0.43
1:A:893:PRO:O	1:A:896:VAL:HG13	2.18	0.43
1:C:166:ILE:HG23	1:C:172:VAL:HG11	2.01	0.43
1:C:211:ASN:OD1	1:C:239:ARG:HA	2.18	0.43
1:C:139:VAL:HG22	1:C:290:GLY:HA2	1.99	0.43
1:C:66:GLU:HG2	1:C:78:MET:SD	2.59	0.43
1:C:979:LEU:HA	1:C:979:LEU:HD23	1.51	0.43
1:D:339:GLU:HA	1:D:342:LYS:HB2	2.00	0.43
1:D:464:GLY:O	1:D:468:ARG:HB2	2.18	0.43
1:D:470:PHE:HD2	1:D:924:VAL:HG11	1.84	0.43
1:D:507:GLU:O	1:D:509:LYS:N	2.52	0.43
1:D:531:VAL:HA	1:D:534:ILE:CG1	2.49	0.43
1:D:553:ALA:O	1:D:557:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:663:LEU:H	1:D:663:LEU:HD23	1.83	0.43
1:E:45:ILE:HA	1:E:128:SER:O	2.19	0.43
1:E:248:LYS:HG2	1:E:263:ARG:NH2	2.33	0.43
1:E:350:LEU:O	1:E:353:LEU:HB2	2.19	0.43
1:D:14:VAL:HG13	1:E:881:LEU:HB3	2.01	0.43
1:F:180:SER:CB	1:F:274:ASN:H	2.31	0.43
1:F:681:ASP:CG	1:F:682:GLN:N	2.71	0.43
1:A:545:TYR:HA	1:A:548:ILE:HD12	1.99	0.43
1:A:748:ALA:HB3	1:A:749:TRP:HD1	1.83	0.43
1:A:966:ARG:NE	1:A:970:ILE:HD11	2.25	0.43
1:B:352:PHE:HD2	1:B:353:LEU:HD23	1.84	0.43
1:C:393:LEU:HD13	1:C:466:ILE:HA	2.00	0.43
1:C:548:ILE:CD1	1:C:1016:PHE:HE1	2.32	0.43
1:C:992:SER:HA	1:C:995:GLN:HG3	2.00	0.43
1:D:1035:ILE:HG22	1:D:1036:GLU:O	2.19	0.43
1:D:293:LEU:HD22	1:D:294:ALA:H	1.83	0.43
1:D:485:ALA:O	1:D:490:PRO:HD3	2.18	0.43
1:D:83:ASP:OD1	1:D:810:ARG:HD3	2.18	0.43
1:D:867:GLN:HB3	1:D:871:LEU:HD12	2.00	0.43
1:E:32:VAL:HA	1:E:390:ILE:O	2.19	0.43
1:E:899:VAL:CG1	1:E:933:SER:HB2	2.48	0.43
1:F:344:LEU:CD1	1:F:402:ILE:HD11	2.48	0.43
1:F:871:LEU:HD22	1:F:927:LEU:HD21	2.01	0.43
1:A:763:VAL:HG12	1:B:63:GLN:NE2	2.33	0.43
1:A:969:PRO:HA	1:A:972:MET:CE	2.49	0.43
1:C:291:ILE:HD13	1:C:306:ILE:HD13	2.01	0.43
1:C:544:LEU:O	1:C:548:ILE:HG13	2.19	0.43
1:C:559:LEU:HA	1:C:560:PRO:HD2	1.77	0.43
1:D:402:ILE:HD13	1:D:402:ILE:HG21	1.81	0.43
1:D:5:PHE:CD2	1:D:487:ILE:HG23	2.53	0.43
1:D:992:SER:HA	1:D:995:GLN:HG3	2.00	0.43
1:E:219:LEU:HD23	1:F:749:TRP:CZ3	2.53	0.43
1:E:685:LEU:HD12	1:E:686:GLY:O	2.18	0.43
1:E:580:ALA:HB1	1:E:719:THR:HG21	2.00	0.43
1:E:723:LYS:HE3	1:E:725:ASP:HB2	2.01	0.43
1:F:355:MET:CG	1:F:410:ILE:HD11	2.49	0.43
1:F:53:ASP:O	1:F:57:VAL:HG13	2.19	0.43
1:A:26:ALA:O	1:A:30:LEU:HB2	2.19	0.42
1:A:726:ILE:H	1:A:726:ILE:HG12	1.13	0.42
1:B:612:VAL:HB	1:B:621:ILE:HG23	2.01	0.42
1:B:695:ASN:O	1:B:698:LEU:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:969:PRO:HA	1:B:972:MET:HE3	2.00	0.42
1:B:982:MET:HB3	1:B:983:PRO:CD	2.48	0.42
1:C:1034:ASP:O	1:C:1035:ILE:HG12	2.19	0.42
1:C:356:TYR:HA	1:C:365:THR:HG21	2.01	0.42
1:C:415:ASN:ND2	1:C:438:ILE:HG21	2.34	0.42
1:C:447:MET:SD	1:C:886:LEU:HD22	2.59	0.42
1:D:157:TYR:O	1:D:161:ASN:ND2	2.46	0.42
1:D:25:LEU:HD12	1:D:25:LEU:HA	1.64	0.42
1:D:82:SER:HB2	1:D:811:LEU:HB2	2.00	0.42
1:E:164:ASP:O	1:E:168:ARG:HG3	2.19	0.42
1:E:191:ASN:O	1:E:195:LYS:HB2	2.19	0.42
1:E:597:TYR:HH	1:E:646:ALA:HA	1.84	0.42
1:E:190:PRO:HG3	1:E:774:TYR:CG	2.54	0.42
1:F:114:ALA:HA	1:F:117:LEU:HD12	2.00	0.42
1:F:356:TYR:C	1:F:358:PHE:N	2.73	0.42
1:F:344:LEU:HD11	1:F:376:LEU:HD11	2.01	0.42
1:A:1008:THR:O	1:A:1012:LEU:HB2	2.20	0.42
1:B:9:PRO:O	1:B:12:ALA:HB3	2.18	0.42
1:C:184:MET:HE3	1:C:185:ARG:N	2.34	0.42
1:C:649:ALA:O	1:C:653:ILE:HG12	2.19	0.42
1:D:564:LEU:HA	1:D:565:PRO:HD2	1.84	0.42
1:D:959:THR:HG21	1:D:1022:VAL:HG22	2.01	0.42
1:E:459:PHE:HE1	1:E:872:TYR:HH	1.65	0.42
1:F:686:GLY:CA	1:F:689:LYS:HD3	2.40	0.42
1:F:920:VAL:HA	1:F:923:GLN:OE1	2.19	0.42
1:A:776:MET:HE2	1:C:225:VAL:HG22	2.02	0.42
1:B:5:PHE:CE1	1:B:487:ILE:HG12	2.53	0.42
1:B:984:LEU:HA	1:B:984:LEU:HD23	1.77	0.42
1:C:352:PHE:CD2	1:C:352:PHE:C	2.93	0.42
1:B:219:LEU:HD23	1:C:749:TRP:HZ3	1.84	0.42
1:D:1012:LEU:O	1:D:1016:PHE:HB2	2.19	0.42
1:D:13:TRP:HB3	1:E:890:TRP:HZ2	1.84	0.42
1:D:576:VAL:HG21	1:D:591:LEU:HD21	2.00	0.42
1:E:430:ALA:O	1:E:433:LYS:HB3	2.19	0.42
1:F:464:GLY:HA2	1:F:467:TYR:CD1	2.53	0.42
1:F:483:LEU:O	1:F:486:LEU:HB2	2.19	0.42
1:A:34:GLN:HB2	1:A:333:VAL:HG22	2.00	0.42
1:A:80:SER:HA	1:A:89:GLN:O	2.18	0.42
1:B:2:PRO:HB2	1:B:439:GLN:OE1	2.19	0.42
1:B:667:VAL:HB	1:B:668:GLU:OE2	2.20	0.42
1:B:847:PRO:O	1:B:850:VAL:HB	2.20	0.42

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:GLU:O	1:C:195:LYS:HB3	2.19	0.42
1:C:347:ALA:HB3	1:C:402:ILE:HD12	2.01	0.42
1:C:836:MET:HG2	1:C:854:TRP:CH2	2.54	0.42
1:C:42:ALA:HA	1:C:92:LEU:O	2.19	0.42
1:D:39:ALA:HA	1:D:40:PRO:HD2	1.76	0.42
1:D:626:LEU:HB3	1:D:632:ARG:HD3	2.01	0.42
1:D:883:LEU:CB	1:D:893:PRO:HB3	2.49	0.42
1:D:976:ALA:O	1:D:980:GLY:N	2.52	0.42
1:E:310:LEU:CD2	1:E:323:ILE:HG21	2.49	0.42
1:E:356:TYR:C	1:E:358:PHE:N	2.71	0.42
1:E:404:LEU:HD12	1:E:404:LEU:HA	1.84	0.42
1:E:588:GLN:NE2	1:E:588:GLN:O	2.52	0.42
1:E:898:LEU:O	1:E:901:PRO:HD2	2.19	0.42
1:F:32:VAL:HG22	1:F:390:ILE:HB	2.01	0.42
1:F:603:LYS:HB3	1:F:603:LYS:HE2	1.65	0.42
1:A:1030:ARG:O	1:A:1031:LYS:HG2	2.20	0.42
1:A:219:LEU:HD11	1:B:722:PHE:HB2	2.01	0.42
1:A:368:PRO:HB3	1:A:409:ALA:CB	2.47	0.42
1:A:677:PHE:CZ	1:A:852:TYR:HB2	2.54	0.42
1:A:916:LEU:HB3	1:A:917:THR:H	1.66	0.42
1:B:525:HIS:O	1:B:526:HIS:C	2.58	0.42
1:B:574:THR:HG21	1:B:598:TYR:CE2	2.55	0.42
1:C:1008:THR:C	1:C:1010:THR:H	2.23	0.42
1:C:249:ILE:HB	1:C:262:LEU:CB	2.49	0.42
1:C:423:GLU:OE1	1:C:425:LEU:HD11	2.19	0.42
1:D:1021:PHE:O	1:D:1025:ARG:HG2	2.19	0.42
1:D:182:TYR:O	1:D:764:LYS:HD3	2.20	0.42
1:D:30:LEU:HD12	1:D:31:PRO:CD	2.48	0.42
1:D:586:ARG:O	1:D:589:LYS:HB3	2.19	0.42
1:D:813:ARG:NH2	1:D:816:GLY:O	2.53	0.42
1:E:695:ASN:HA	1:E:698:LEU:HD12	2.01	0.42
1:E:692:GLN:O	1:E:695:ASN:HB2	2.20	0.42
1:E:69:MET:HE1	1:E:107:VAL:HG13	2.01	0.42
1:F:307:ARG:NH2	1:F:311:ALA:HB2	2.35	0.42
1:F:638:LYS:HE2	1:F:640:GLU:CG	2.48	0.42
1:F:723:LYS:HG3	1:F:725:ASP:OD1	2.20	0.42
1:A:142:VAL:O	1:A:287:SER:N	2.51	0.42
1:A:679:LEU:HD12	1:A:679:LEU:HA	1.76	0.42
1:A:895:SER:HB3	1:A:1024:VAL:HB	2.02	0.42
1:B:5:PHE:C	1:B:8:ARG:H	2.22	0.42
1:B:281:PHE:CE1	1:B:608:SER:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:300:LEU:HD11	1:C:333:VAL:HG11	2.02	0.42
1:C:353:LEU:HA	1:C:353:LEU:HD23	1.79	0.42
1:C:360:GLN:HE21	1:C:360:GLN:HB3	1.66	0.42
1:C:425:LEU:HB3	1:C:429:GLU:HG3	1.99	0.42
1:C:506:GLY:O	1:C:508:GLY:N	2.48	0.42
1:C:541:TYR:OH	2:C:1101:LMT:O6'	2.34	0.42
1:D:251:LEU:CD1	1:D:265:VAL:HG21	2.50	0.42
1:D:538:THR:HG22	1:D:539:GLY:N	2.34	0.42
1:D:562:SER:H	1:D:917:THR:HG1	1.61	0.42
1:E:534:ILE:CG2	2:E:1101:LMT:H12	2.49	0.42
1:E:443:VAL:O	1:E:447:MET:HG2	2.20	0.42
1:E:633:PRO:HD2	1:E:637:ASN:OD1	2.19	0.42
1:E:690:LEU:HB3	1:E:820:MET:SD	2.59	0.42
1:E:883:LEU:HA	1:E:883:LEU:HD23	1.85	0.42
1:E:944:ALA:HB3	1:E:1021:PHE:CE1	2.54	0.42
1:F:1010:THR:O	1:F:1014:ILE:HG23	2.20	0.42
1:F:152:GLU:HG2	1:F:275:TYR:CE2	2.55	0.42
1:F:831:SER:HB3	1:F:834:GLU:HG3	2.01	0.42
1:A:409:ALA:O	1:A:413:VAL:HG23	2.20	0.42
1:A:81:ASN:O	1:A:88:VAL:HA	2.20	0.42
1:A:855:THR:OG1	1:A:856:GLY:N	2.52	0.42
1:A:982:MET:HB3	1:A:983:PRO:HD3	2.01	0.42
1:B:1022:VAL:O	1:B:1026:ARG:HG3	2.19	0.42
1:B:345:VAL:O	1:B:348:ILE:HB	2.20	0.42
1:B:375:VAL:HG22	1:B:484:VAL:HG21	2.01	0.42
1:B:553:ALA:O	1:B:557:VAL:HG23	2.20	0.42
1:C:102:ILE:HD13	1:C:102:ILE:HA	1.78	0.42
1:C:488:LEU:O	1:C:491:ALA:HB3	2.20	0.42
1:C:571:VAL:HG22	1:C:624:VAL:O	2.19	0.42
1:C:186:ILE:O	1:C:768:VAL:HG23	2.19	0.42
1:D:914:ARG:HD2	1:D:1000:THR:HG21	2.02	0.42
1:D:146:ASP:OD2	1:D:146:ASP:N	2.52	0.42
1:D:200:PRO:HB2	1:D:744:THR:HG22	2.02	0.42
1:D:435:MET:O	1:D:439:GLN:HB2	2.20	0.42
1:D:578:LEU:HD11	1:D:587:THR:N	2.35	0.42
1:E:463:THR:O	1:E:467:TYR:CD1	2.69	0.42
1:F:211:ASN:OD1	1:F:240:LEU:HG	2.19	0.42
1:F:304:ALA:O	1:F:307:ARG:HB3	2.19	0.42
1:F:932:LEU:HD11	1:F:977:PHE:CE2	2.55	0.42
1:A:166:ILE:HG23	1:A:166:ILE:HD12	1.74	0.42
1:A:13:TRP:NE1	1:A:492:LEU:HD21	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:MET:SD	1:A:955:LEU:HA	2.58	0.42
1:B:26:ALA:O	1:B:30:LEU:HB2	2.20	0.42
1:B:409:ALA:O	1:B:413:VAL:HG23	2.20	0.42
1:B:607:GLU:OE1	1:B:627:LYS:HG2	2.20	0.42
1:B:701:ALA:HB3	1:B:711:VAL:HG11	2.01	0.42
1:D:475:VAL:O	1:D:478:MET:HB3	2.20	0.42
1:D:886:LEU:HA	1:D:886:LEU:HD12	1.76	0.42
1:F:399:VAL:HG11	1:F:984:LEU:HD21	2.02	0.42
1:F:509:LYS:HA	1:F:509:LYS:HD2	1.83	0.42
1:A:199:THR:HG21	1:A:787:ARG:H	1.85	0.42
1:B:3:ASN:O	1:B:6:ILE:HB	2.20	0.42
1:B:671:THR:O	1:B:671:THR:OG1	2.35	0.42
1:B:898:LEU:HB3	1:B:1020:PHE:CZ	2.54	0.42
1:C:343:THR:HG21	1:C:984:LEU:HD23	2.02	0.42
1:C:55:LYS:HE2	1:C:55:LYS:HB3	1.72	0.42
1:C:926:LEU:HA	1:C:926:LEU:HD23	1.82	0.42
1:D:852:TYR:HD2	1:D:852:TYR:N	2.18	0.42
1:E:113:LEU:HA	1:E:113:LEU:HD23	1.80	0.42
1:E:294:ALA:HB3	1:E:297:ALA:HB2	2.01	0.42
1:E:30:LEU:HA	1:E:31:PRO:HD3	1.82	0.42
1:E:544:LEU:O	1:E:547:ILE:HB	2.19	0.42
1:E:843:ALA:O	1:E:846:LEU:HG	2.20	0.42
1:E:921:TYR:HB3	1:E:998:VAL:HG23	2.02	0.42
1:F:25:LEU:HD12	1:F:25:LEU:HA	1.62	0.42
1:F:41:PRO:O	1:F:94:PHE:HB2	2.20	0.42
1:E:235:ILE:HD11	1:F:721:GLN:OE1	2.20	0.42
1:F:883:LEU:HD11	1:F:938:ILE:HD11	2.00	0.42
1:F:974:SER:HA	1:F:1006:MET:CE	2.49	0.42
1:A:282:ASN:HD21	1:A:608:SER:CB	2.33	0.42
1:A:442:LEU:HA	1:A:442:LEU:HD23	1.84	0.42
1:A:563:PHE:O	1:A:564:LEU:HD12	2.20	0.42
1:A:694:ARG:HH11	1:A:694:ARG:HB3	1.85	0.42
1:B:955:LEU:O	1:B:959:THR:HG23	2.20	0.42
1:C:159:ALA:HB2	1:C:177:LEU:HD11	2.02	0.42
1:C:335:ILE:HG12	1:C:990:ALA:HB2	2.02	0.42
1:C:753:TYR:HD1	1:C:767:TYR:HE2	1.66	0.42
1:D:193:LEU:CD2	1:D:265:VAL:HB	2.50	0.42
1:D:836:MET:CE	1:D:862:ARG:HD2	2.49	0.42
1:D:941:VAL:HG22	1:D:1021:PHE:CD1	2.55	0.42
1:E:1029:SER:HG	1:E:1030:ARG:H	1.61	0.42
1:E:43:VAL:HG13	1:E:130:GLU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:722:PHE:CZ	1:E:802:SER:HB2	2.55	0.42
1:E:722:PHE:CD1	1:E:804:TRP:CE2	3.08	0.42
1:E:960:LEU:O	1:E:963:VAL:HG12	2.20	0.42
1:F:364:ALA:O	1:F:368:PRO:HD3	2.19	0.42
1:F:786:VAL:HG23	1:F:796:PHE:CE2	2.55	0.42
1:F:960:LEU:HD23	1:F:960:LEU:HA	1.89	0.42
1:A:585:GLU:O	1:A:588:GLN:HB3	2.20	0.41
1:B:15:ILE:HD13	1:B:15:ILE:HG21	1.86	0.41
1:C:148:THR:HG22	1:C:149:MET:O	2.20	0.41
1:C:24:GLY:CA	1:C:27:ILE:HG23	2.50	0.41
1:C:453:PHE:CD2	1:C:456:MET:CE	2.95	0.41
1:C:278:ILE:CG1	1:C:613:ASN:HB3	2.48	0.41
1:C:855:THR:CA	1:C:859:TYR:HB2	2.47	0.41
1:C:899:VAL:HG12	1:C:933:SER:HB2	2.02	0.41
1:C:977:PHE:HE2	1:C:1002:VAL:CG1	2.32	0.41
1:D:152:GLU:CD	1:D:152:GLU:H	2.24	0.41
1:D:235:ILE:HG23	1:D:235:ILE:HD12	1.74	0.41
1:D:393:LEU:HD13	1:D:466:ILE:HA	2.02	0.41
1:D:470:PHE:CD2	1:D:924:VAL:HG11	2.54	0.41
1:E:579:PRO:HD3	1:E:656:ALA:CB	2.48	0.41
1:E:727:ASP:OD1	1:E:730:LYS:HG3	2.20	0.41
1:E:741:ILE:O	1:E:744:THR:OG1	2.34	0.41
1:F:355:MET:HG2	1:F:410:ILE:HD11	2.01	0.41
1:F:3:ASN:HD21	1:F:486:LEU:HA	1.85	0.41
1:F:587:THR:HG21	1:F:618:ASN:HA	2.02	0.41
1:A:149:MET:HG3	1:A:154:ILE:HG13	2.02	0.41
1:A:427:PRO:O	1:A:430:ALA:HB3	2.19	0.41
1:A:55:LYS:HB3	1:A:55:LYS:HE2	1.76	0.41
1:A:901:PRO:HA	1:A:904:VAL:HB	2.02	0.41
1:B:1015:PHE:CZ	2:B:2000:LMT:H52	2.55	0.41
1:B:248:LYS:O	1:B:261:LEU:HD22	2.20	0.41
1:B:368:PRO:HG3	1:B:413:VAL:HG21	2.02	0.41
1:B:486:LEU:HA	1:B:486:LEU:HD23	1.77	0.41
1:B:4:PHE:CZ	1:B:8:ARG:HD3	2.55	0.41
1:B:914:ARG:NH1	1:B:985:VAL:HG12	2.35	0.41
1:C:443:VAL:O	1:C:447:MET:HB3	2.20	0.41
1:C:584:GLN:N	1:C:617:GLN:HB3	2.34	0.41
1:C:187:TRP:HB3	1:C:771:GLU:HA	2.02	0.41
1:E:493:CYS:O	1:E:497:LEU:HB2	2.19	0.41
1:E:363:ARG:CZ	1:E:498:LYS:HE3	2.49	0.41
1:F:344:LEU:HD22	1:F:402:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:504:ASP:C	1:F:506:GLY:N	2.72	0.41
1:A:169:THR:HB	1:A:172:VAL:HG23	2.02	0.41
1:B:363:ARG:NH1	1:B:498:LYS:HG3	2.35	0.41
1:B:463:THR:O	1:B:466:ILE:HB	2.20	0.41
1:B:480:LEU:O	1:B:484:VAL:HG23	2.20	0.41
1:B:482:VAL:O	1:B:485:ALA:HB3	2.20	0.41
1:B:527:TYR:O	1:B:531:VAL:HG23	2.20	0.41
1:B:701:ALA:CB	1:B:711:VAL:HG11	2.50	0.41
1:C:443:VAL:HG12	1:C:886:LEU:HD21	2.01	0.41
1:C:753:TYR:HD1	1:C:767:TYR:CE2	2.38	0.41
1:C:966:ARG:HH21	1:C:970:ILE:HD11	1.85	0.41
1:D:459:PHE:O	1:D:468:ARG:NH2	2.54	0.41
1:D:482:VAL:O	1:D:486:LEU:HG	2.20	0.41
1:E:202:ASP:OD2	1:E:787:ARG:NH2	2.46	0.41
1:E:158:VAL:HG11	1:E:289:LEU:HG	2.01	0.41
1:E:306:ILE:O	1:E:309:GLU:HB3	2.20	0.41
1:E:62:THR:O	1:E:66:GLU:HG3	2.21	0.41
1:E:927:LEU:HA	1:E:930:ILE:HD12	2.02	0.41
1:F:356:TYR:HD1	1:F:365:THR:HG21	1.84	0.41
1:F:578:LEU:HA	1:F:656:ALA:HB1	2.02	0.41
1:A:1017:VAL:HB	1:A:1018:PRO:HD3	2.02	0.41
1:A:54:ALA:HB2	1:A:809:PRO:O	2.20	0.41
1:A:273:GLU:CG	1:A:765:LYS:HD2	2.50	0.41
1:B:27:ILE:HD12	1:B:27:ILE:HA	1.86	0.41
1:B:576:VAL:HG13	1:B:658:VAL:HG22	2.01	0.41
1:B:676:ASP:H	1:B:858:SER:HG	1.62	0.41
1:B:968:ARG:O	1:B:972:MET:HE2	2.20	0.41
1:C:614:GLY:O	1:C:616:GLY:HA3	2.20	0.41
1:C:664:PRO:HG2	1:C:666:ILE:O	2.20	0.41
1:D:432:ARG:HH11	1:D:432:ARG:HD2	1.68	0.41
1:D:531:VAL:O	1:D:534:ILE:HG13	2.20	0.41
1:D:544:LEU:O	1:D:547:ILE:HB	2.20	0.41
1:D:5:PHE:CE1	1:D:487:ILE:HG12	2.55	0.41
1:D:679:LEU:HD11	1:D:850:VAL:HG12	2.02	0.41
1:D:726:ILE:H	1:D:726:ILE:HG12	1.24	0.41
1:D:898:LEU:O	1:D:901:PRO:HD2	2.20	0.41
1:D:941:VAL:HG13	1:D:1021:PHE:CD1	2.56	0.41
1:E:1015:PHE:O	1:E:1019:VAL:HG23	2.21	0.41
1:E:448:VAL:HG13	1:E:879:VAL:CG1	2.47	0.41
1:D:234:ILE:HA	1:E:722:PHE:O	2.20	0.41
1:E:7:ASP:O	1:E:8:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:578:LEU:CD1	1:F:587:THR:HG22	2.50	0.41
1:A:165:ALA:HA	1:A:168:ARG:NH1	2.35	0.41
1:A:446:ALA:CB	1:A:482:VAL:HG21	2.51	0.41
1:B:572:PHE:CE1	1:B:643:THR:HG22	2.56	0.41
1:D:473:THR:O	1:D:476:SER:OG	2.38	0.41
1:D:531:VAL:HA	1:D:534:ILE:HD11	2.01	0.41
1:D:634:GLY:O	1:D:638:LYS:HG3	2.20	0.41
1:D:9:PRO:O	1:D:13:TRP:CD1	2.74	0.41
1:E:697:LEU:HA	1:E:700:GLU:HB2	2.02	0.41
1:F:149:MET:HB2	1:F:153:ASP:HB3	2.03	0.41
1:F:620:GLY:O	1:F:621:ILE:HD12	2.20	0.41
1:F:666:ILE:HD13	1:F:669:LEU:HD12	2.03	0.41
1:F:694:ARG:HE	1:F:713:PRO:HB3	1.85	0.41
1:F:720:PRO:HA	1:F:805:GLU:O	2.20	0.41
1:F:199:THR:HG22	1:F:785:TYR:O	2.20	0.41
1:A:118:LEU:HA	1:A:119:PRO:HD3	1.77	0.41
1:A:578:LEU:HB2	1:A:618:ASN:HA	2.02	0.41
1:A:650:PHE:HB3	1:A:658:VAL:HB	2.02	0.41
1:A:204:ILE:HG12	1:A:754:VAL:HG21	2.02	0.41
1:B:121:GLU:O	1:B:125:GLN:HB2	2.21	0.41
1:B:149:MET:H	1:B:149:MET:HG2	1.75	0.41
1:B:167:SER:HB2	1:C:70:ASN:HB3	2.02	0.41
1:C:376:LEU:HD22	1:C:398:MET:HE3	2.02	0.41
1:C:836:MET:O	1:C:854:TRP:HZ2	2.03	0.41
1:D:138:MET:CG	1:D:291:ILE:HB	2.51	0.41
1:D:355:MET:HE2	1:D:368:PRO:HG2	2.03	0.41
1:D:418:ARG:HH21	1:D:943:PHE:HE2	1.69	0.41
1:D:44:THR:HA	1:D:90:ILE:O	2.20	0.41
1:D:58:GLN:HA	1:D:62:THR:HB	2.03	0.41
1:E:189:ASN:O	1:E:192:GLU:HB2	2.21	0.41
1:E:262:LEU:HG	1:E:268:ILE:HD11	2.02	0.41
1:E:175:VAL:HG11	1:E:289:LEU:HD13	2.02	0.41
1:E:559:LEU:HA	1:E:560:PRO:HD2	1.55	0.41
1:E:585:GLU:O	1:E:588:GLN:HB3	2.20	0.41
1:E:914:ARG:NH1	1:E:985:VAL:HG12	2.36	0.41
1:E:927:LEU:O	1:E:930:ILE:HB	2.21	0.41
1:F:540:ARG:O	1:F:543:VAL:HB	2.20	0.41
1:F:679:LEU:HD23	1:F:820:MET:HB2	2.03	0.41
1:F:970:ILE:H	1:F:970:ILE:HG13	1.64	0.41
1:A:367:ILE:HD13	1:A:367:ILE:HG21	1.84	0.41
1:A:66:GLU:OE1	1:A:816:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ASN:HA	1:B:321:LEU:HA	2.02	0.41
1:C:1012:LEU:HD12	1:C:1012:LEU:HA	1.85	0.41
1:C:370:ILE:O	1:C:373:PRO:HD2	2.20	0.41
1:C:591:LEU:HD11	1:C:620:GLY:HA3	2.01	0.41
1:C:689:LYS:CD	1:C:689:LYS:H	2.33	0.41
1:D:366:LEU:HD23	1:D:366:LEU:HA	1.74	0.41
1:D:572:PHE:CD1	1:D:643:THR:HG22	2.56	0.41
1:D:667:VAL:HG12	1:D:668:GLU:OE1	2.20	0.41
1:D:788:ALA:HB3	1:D:790:ASP:OD2	2.20	0.41
1:E:250:LEU:HD13	1:E:259:ARG:HB2	2.02	0.41
1:F:510:LYS:HA	1:F:518:ARG:HH12	1.86	0.41
1:F:914:ARG:NH1	1:F:996:ASN:HB3	2.36	0.41
2:A:1101:LMT:H51	2:A:1101:LMT:H81	1.51	0.41
1:A:11:PHE:CE1	1:A:15:ILE:HD11	2.56	0.41
1:A:355:MET:HE1	1:A:368:PRO:HG2	2.02	0.41
1:A:574:THR:OG1	1:A:659:PHE:O	2.22	0.41
1:A:694:ARG:HD2	1:A:713:PRO:HB3	2.03	0.41
1:A:82:SER:HB2	1:A:811:LEU:HB2	2.02	0.41
1:A:57:VAL:CG1	1:A:88:VAL:HB	2.50	0.41
1:A:979:LEU:HD23	1:A:979:LEU:HA	1.80	0.41
1:A:343:THR:HG21	1:A:984:LEU:HD21	2.02	0.41
1:B:82:SER:HB2	1:B:811:LEU:HB2	2.03	0.41
1:B:883:LEU:HA	1:B:883:LEU:HD23	1.88	0.41
1:B:923:GLN:O	1:B:926:LEU:HB2	2.21	0.41
1:C:153:ASP:HA	1:C:182:TYR:OH	2.20	0.41
1:E:224:PRO:HD2	1:F:584:GLN:NE2	2.35	0.41
1:E:186:ILE:HG12	1:E:268:ILE:HG12	2.02	0.41
1:E:555:LEU:HB3	1:E:908:LEU:HD13	2.03	0.41
1:E:916:LEU:HD11	1:E:997:ALA:HA	2.03	0.41
1:F:120:GLN:O	1:F:123:GLN:HB2	2.21	0.41
1:F:345:VAL:HA	1:F:348:ILE:HD12	2.03	0.41
1:F:356:TYR:O	1:F:358:PHE:N	2.53	0.41
1:F:407:ASP:HB3	1:F:445:ILE:HD13	2.03	0.41
1:F:600:THR:C	1:F:602:GLU:H	2.22	0.41
1:F:61:VAL:O	1:F:65:ILE:HG13	2.19	0.41
1:F:649:ALA:O	1:F:653:ILE:HG12	2.20	0.41
1:F:741:ILE:HG22	1:F:786:VAL:HG11	2.03	0.41
1:E:219:LEU:HD23	1:F:749:TRP:HZ3	1.85	0.41
1:F:803:ARG:NH1	1:F:805:GLU:OE2	2.54	0.41
1:A:189:ASN:O	1:A:192:GLU:HB2	2.20	0.41
1:A:223:PRO:HD2	1:B:775:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:LEU:O	1:A:265:VAL:HG22	2.21	0.41
1:A:492:LEU:HD22	1:A:496:MET:SD	2.61	0.41
1:A:645:ARG:C	1:A:648:ARG:HB3	2.41	0.41
1:B:40:PRO:HA	1:B:41:PRO:HD3	1.82	0.41
1:C:1029:SER:OG	1:C:1030:ARG:N	2.48	0.41
1:B:105:VAL:HG21	1:C:105:VAL:HG13	2.03	0.41
1:C:64:VAL:HG11	1:C:117:LEU:HB2	2.01	0.41
1:D:293:LEU:HD22	1:D:294:ALA:N	2.36	0.41
1:D:770:SER:OG	1:D:775:ARG:HG2	2.20	0.41
1:D:963:VAL:HA	1:D:966:ARG:HH12	1.85	0.41
1:E:535:LEU:HD13	1:E:1022:VAL:HG21	2.02	0.41
1:E:685:LEU:HD13	1:E:689:LYS:HB3	2.02	0.41
1:D:11:PHE:HB2	1:E:888:GLU:OE2	2.21	0.41
1:E:527:TYR:CE2	1:E:967:LEU:HG	2.56	0.41
1:F:33:ALA:HB2	1:F:298:ASN:OD1	2.21	0.41
1:F:510:LYS:HA	1:F:518:ARG:NH1	2.35	0.41
1:F:545:TYR:O	1:F:549:VAL:HG23	2.21	0.41
1:F:932:LEU:HD11	1:F:977:PHE:HE2	1.85	0.41
1:A:75:LEU:HD23	1:C:168:ARG:HB3	2.03	0.41
1:B:361:ASN:O	1:B:365:THR:HG22	2.21	0.41
1:B:80:SER:CB	1:B:90:ILE:HG12	2.51	0.41
1:C:605:ASN:HD21	1:C:637:ASN:HA	1.85	0.41
1:C:930:ILE:HG21	1:C:930:ILE:HD13	1.87	0.41
1:D:166:ILE:HA	1:D:166:ILE:HD13	1.91	0.41
1:E:103:ALA:O	1:E:107:VAL:HG23	2.21	0.41
1:E:313:MET:HA	1:E:316:PHE:HD2	1.86	0.41
1:E:559:LEU:HD22	1:E:917:THR:HA	2.03	0.41
1:F:379:THR:N	1:F:480:LEU:HD11	2.35	0.41
1:F:553:ALA:O	1:F:557:VAL:HG23	2.20	0.41
1:A:757:PHE:CE1	1:A:759:ASP:HB2	2.55	0.41
1:A:903:GLY:HA2	1:A:1009:ALA:HB2	2.03	0.41
1:B:407:ASP:O	1:B:411:VAL:HG23	2.21	0.41
1:B:914:ARG:HH12	1:B:985:VAL:HG12	1.86	0.41
1:B:926:LEU:HD23	1:B:926:LEU:HA	1.69	0.41
1:B:914:ARG:NH2	1:B:996:ASN:HB3	2.36	0.41
1:C:404:LEU:HB3	1:C:478:MET:SD	2.61	0.41
1:C:509:LYS:HA	1:C:509:LYS:HD2	1.83	0.41
1:C:199:THR:HG21	1:C:787:ARG:H	1.86	0.41
1:C:65:ILE:HG21	1:C:90:ILE:HD13	2.03	0.41
1:D:317:PHE:CD1	1:D:321:LEU:HD12	2.56	0.41
1:D:339:GLU:OE1	1:D:342:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:780:ASP:O	1:D:783:ASP:HB2	2.20	0.41
1:E:142:VAL:O	1:E:154:ILE:HD13	2.21	0.41
1:E:235:ILE:HB	1:F:723:LYS:HA	2.01	0.41
1:E:567:GLU:O	1:E:569:GLN:HG3	2.21	0.41
1:E:838:LEU:HD22	1:E:841:GLN:HB2	2.02	0.41
1:F:726:ILE:H	1:F:726:ILE:HG13	1.65	0.41
1:F:979:LEU:HD23	1:F:979:LEU:HA	1.75	0.41
1:A:678:GLU:HG2	1:A:814:TYR:CG	2.56	0.40
1:B:138:MET:HE2	1:B:138:MET:HB2	1.94	0.40
1:B:773:LYS:HG3	1:B:774:TYR:CE2	2.56	0.40
1:C:1010:THR:O	1:C:1014:ILE:HG23	2.21	0.40
1:C:497:LEU:HA	1:C:497:LEU:HD12	1.82	0.40
1:C:632:ARG:HH12	1:C:638:LYS:HA	1.86	0.40
1:D:143:ILE:HG22	1:D:286:ALA:HB2	2.02	0.40
1:D:442:LEU:HA	1:D:442:LEU:HD23	1.70	0.40
1:D:591:LEU:HD23	1:D:591:LEU:HA	1.71	0.40
1:D:654:LYS:HD3	1:D:654:LYS:HA	1.77	0.40
1:D:940:ILE:HG12	1:D:966:ARG:NH2	2.36	0.40
1:E:343:THR:HG21	1:E:399:VAL:CG1	2.43	0.40
1:E:56:THR:O	1:E:60:THR:OG1	2.25	0.40
1:E:723:LYS:HG2	1:E:803:ARG:NH1	2.36	0.40
1:E:736:VAL:HB	1:E:741:ILE:HD11	2.03	0.40
1:F:104:GLN:OE1	1:F:108:GLN:NE2	2.54	0.40
1:F:217:GLY:O	1:F:234:ILE:HB	2.22	0.40
1:C:527:TYR:O	1:C:531:VAL:HG23	2.21	0.40
1:C:963:VAL:HA	1:C:966:ARG:NH2	2.37	0.40
1:C:984:LEU:HB3	1:C:995:GLN:O	2.21	0.40
1:D:540:ARG:NH2	2:D:2000:LMT:H6'2	2.36	0.40
1:D:162:MET:HA	1:D:313:MET:SD	2.62	0.40
1:D:404:LEU:HD21	1:D:449:LEU:HD22	2.02	0.40
1:D:564:LEU:CD2	1:D:666:ILE:HG12	2.51	0.40
1:D:564:LEU:HD22	1:D:666:ILE:HG12	2.04	0.40
1:E:541:TYR:HH	2:E:1101:LMT:H6'	1.54	0.40
1:E:330:THR:HB	1:E:331:PRO:HD3	2.03	0.40
1:E:516:PHE:HA	1:E:519:MET:CG	2.45	0.40
1:E:956:ILE:HG13	1:E:956:ILE:H	1.27	0.40
1:F:941:VAL:HG13	1:F:1021:PHE:CE1	2.56	0.40
1:F:489:THR:HA	1:F:492:LEU:HB2	2.03	0.40
1:F:868:ALA:HB2	1:F:923:GLN:NE2	2.36	0.40
1:A:676:ASP:HB2	1:A:857:MET:HE3	2.04	0.40
1:A:697:LEU:HA	1:A:700:GLU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:PHE:HB2	1:A:804:TRP:CH2	2.56	0.40
1:A:969:PRO:HA	1:A:972:MET:HE2	2.03	0.40
1:B:233:SER:HB2	1:C:721:GLN:HG2	2.03	0.40
1:B:786:VAL:HG23	1:B:796:PHE:CE2	2.55	0.40
1:B:983:PRO:O	1:B:987:SER:HB2	2.22	0.40
1:C:152:GLU:H	1:C:152:GLU:CD	2.24	0.40
1:C:364:ALA:O	1:C:368:PRO:HD3	2.21	0.40
1:C:584:GLN:N	1:C:617:GLN:OE1	2.31	0.40
1:D:231:ASN:ND2	1:E:617:GLN:HE22	2.20	0.40
1:D:511:GLY:CA	1:D:515:TRP:CD1	3.01	0.40
1:E:667:VAL:H	1:E:667:VAL:HG23	1.58	0.40
1:A:19:ILE:HD13	1:A:19:ILE:HG21	1.83	0.40
1:A:351:VAL:O	1:A:355:MET:HG2	2.22	0.40
1:A:340:VAL:HB	1:A:395:MET:HE2	2.02	0.40
1:A:467:TYR:CE2	1:A:920:VAL:HG22	2.55	0.40
1:C:137:LEU:HB2	1:C:293:LEU:HB2	2.03	0.40
1:C:188:MET:O	1:C:771:GLU:HG3	2.20	0.40
1:C:252:LYS:HE2	1:C:253:VAL:O	2.21	0.40
1:C:431:THR:HG21	1:C:490:PRO:O	2.22	0.40
1:C:55:LYS:HA	1:C:811:LEU:HD11	2.03	0.40
1:D:188:MET:HE3	1:D:188:MET:HB2	1.78	0.40
1:D:281:PHE:C	1:D:281:PHE:CD2	2.95	0.40
1:E:587:THR:HB	1:E:613:ASN:OD1	2.21	0.40
1:E:681:ASP:HB2	1:E:690:LEU:HG	2.04	0.40
1:E:722:PHE:HD1	1:E:804:TRP:CE2	2.40	0.40
1:F:180:SER:HB3	1:F:273:GLU:CB	2.51	0.40
1:F:525:HIS:O	1:F:526:HIS:C	2.60	0.40
1:F:546:LEU:O	1:F:550:VAL:HG23	2.21	0.40
1:A:142:VAL:N	1:A:287:SER:O	2.44	0.40
1:A:615:GLY:HA2	1:A:616:GLY:HA2	1.75	0.40
1:A:778:PRO:HG3	1:A:804:TRP:HZ2	1.87	0.40
1:B:534:ILE:HD13	1:B:534:ILE:HG21	1.91	0.40
1:B:58:GLN:OE1	1:B:811:LEU:HB3	2.21	0.40
1:C:1031:LYS:HD3	1:C:1031:LYS:HA	1.86	0.40
1:C:359:LEU:HB2	1:C:365:THR:HG22	2.03	0.40
1:C:44:THR:HA	1:C:90:ILE:O	2.21	0.40
1:D:407:ASP:O	1:D:411:VAL:HG23	2.22	0.40
1:D:554:TYR:CE2	1:D:558:ARG:HG3	2.56	0.40
1:D:704:HIS:CE1	1:D:842:LEU:HD21	2.56	0.40
1:D:916:LEU:HB3	1:D:917:THR:H	1.68	0.40
1:D:984:LEU:HB3	1:D:995:GLN:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:936:ASN:ND2	1:E:970:ILE:HG23	2.36	0.40
1:F:337:ILE:HD11	1:F:391:ASN:HA	2.04	0.40
1:F:348:ILE:HG13	1:F:348:ILE:H	1.68	0.40
1:F:478:MET:O	1:F:482:VAL:HG23	2.21	0.40
1:F:497:LEU:HD12	1:F:497:LEU:HA	1.75	0.40
1:F:527:TYR:O	1:F:531:VAL:HG23	2.21	0.40
1:F:887:TYR:C	1:F:889:SER:H	2.13	0.40
1:F:343:THR:HG21	1:F:984:LEU:HD23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1036/1044 (99%)	942 (91%)	79 (8%)	15 (1%)	14	55
1	B	1037/1044 (99%)	942 (91%)	85 (8%)	10 (1%)	19	63
1	C	1033/1044 (99%)	931 (90%)	84 (8%)	18 (2%)	11	51
1	D	1036/1044 (99%)	934 (90%)	83 (8%)	19 (2%)	11	50
1	E	1035/1044 (99%)	937 (90%)	87 (8%)	11 (1%)	17	61
1	F	1035/1044 (99%)	926 (90%)	84 (8%)	25 (2%)	7	44
All	All	6212/6264 (99%)	5612 (90%)	502 (8%)	98 (2%)	12	53

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	672	ALA
1	A	986	ILE
1	A	1029	SER
1	A	1033	GLU

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Mol	Chain	Res	Type
1	B	617	GLN
1	B	1029	SER
1	B	1038	SER
1	C	509	LYS
1	C	915	GLY
1	C	1009	ALA
1	C	1029	SER
1	C	1035	ILE
1	D	508	GLY
1	D	511	GLY
1	D	668	GLU
1	D	915	GLY
1	D	1029	SER
1	D	1034	ASP
1	D	1035	ILE
1	D	1036	GLU
1	D	1038	SER
1	E	667	VAL
1	E	1029	SER
1	E	1033	GLU
1	E	1036	GLU
1	F	134	SER
1	F	145	THR
1	F	509	LYS
1	F	617	GLN
1	F	888	GLU
1	F	1029	SER
1	F	1032	ASN
1	F	1035	ILE
1	A	915	GLY
1	A	987	SER
1	A	1032	ASN
1	B	514	GLY
1	B	684	GLY
1	B	1035	ILE
1	C	147	GLY
1	C	831	SER
1	D	4	PHE
1	D	987	SER
1	D	1028	PHE
1	D	1031	LYS
1	E	668	GLU

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Mol	Chain	Res	Type
1	F	6	ILE
1	F	146	ASP
1	F	147	GLY
1	F	511	GLY
1	F	684	GLY
1	F	918	ASN
1	F	1028	PHE
1	A	615	GLY
1	A	1031	LYS
1	B	918	ASN
1	C	134	SER
1	C	146	ASP
1	C	360	GLN
1	C	888	GLU
1	F	407	ASP
1	F	507	GLU
1	F	831	SER
1	F	1034	ASP
1	A	215	ALA
1	B	215	ALA
1	C	6	ILE
1	C	1033	GLU
1	D	614	GLY
1	D	653	ILE
1	D	909	LEU
1	F	360	GLN
1	A	918	ASN
1	A	1036	GLU
1	B	1039	HIS
1	C	215	ALA
1	C	918	ASN
1	D	215	ALA
1	E	216	ALA
1	F	150	THR
1	F	215	ALA
1	A	509	LYS
1	E	778	PRO
1	F	773	LYS
1	F	915	GLY
1	A	666	ILE
1	A	778	PRO
1	C	998	VAL

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Mol	Chain	Res	Type
1	E	511	GLY
1	E	1035	ILE
1	D	616	GLY
1	C	828	PRO
1	E	508	GLY
1	E	539	GLY
1	F	778	PRO
1	B	318	PRO
1	C	653	ILE
1	D	200	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	846/852 (99%)	781 (92%)	65 (8%)	16	53
1	B	847/852 (99%)	789 (93%)	58 (7%)	20	60
1	C	843/852 (99%)	774 (92%)	69 (8%)	14	50
1	D	846/852 (99%)	789 (93%)	57 (7%)	20	60
1	E	845/852 (99%)	775 (92%)	70 (8%)	14	49
1	F	845/852 (99%)	789 (93%)	56 (7%)	21	61
All	All	5072/5112 (99%)	4697 (93%)	375 (7%)	17	55

All (375) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	25	LEU
1	A	44	THR
1	A	49	TYR
1	A	70	ASN
1	A	101	ASP
1	A	146	ASP
1	A	148	THR

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Mol	Chain	Res	Type
1	A	152	GLU
1	A	166	ILE
1	A	177	LEU
1	A	243	THR
1	A	255	GLN
1	A	281	PHE
1	A	293	LEU
1	A	295	THR
1	A	337	ILE
1	A	342	LYS
1	A	349	ILE
1	A	350	LEU
1	A	360	GLN
1	A	362	PHE
1	A	400	LEU
1	A	429	GLU
1	A	434	SER
1	A	437	GLN
1	A	463	THR
1	A	483	LEU
1	A	489	THR
1	A	502	LYS
1	A	512	PHE
1	A	519	MET
1	A	524	THR
1	A	536	ARG
1	A	538	THR
1	A	542	LEU
1	A	558	ARG
1	A	566	ASP
1	A	575	MET
1	A	603	LYS
1	A	610	PHE
1	A	669	LEU
1	A	682	GLN
1	A	690	LEU
1	A	694	ARG
1	A	708	LEU
1	A	711	VAL
1	A	726	ILE
1	A	736	VAL
1	A	830	LYS

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Mol	Chain	Res	Type
1	A	896	VAL
1	A	916	LEU
1	A	917	THR
1	A	926	LEU
1	A	942	GLU
1	A	946	ASP
1	A	956	ILE
1	A	959	THR
1	A	966	ARG
1	A	977	PHE
1	A	985	VAL
1	A	1012	LEU
1	A	1014	ILE
1	A	1024	VAL
1	A	1035	ILE
1	B	6	ILE
1	B	10	ILE
1	B	11	PHE
1	B	29	LYS
1	B	34	GLN
1	B	49	TYR
1	B	96	SER
1	B	117	LEU
1	B	131	LYS
1	B	177	LEU
1	B	185	ARG
1	B	229	GLN
1	B	243	THR
1	B	255	GLN
1	B	259	ARG
1	B	293	LEU
1	B	295	THR
1	B	323	ILE
1	B	350	LEU
1	B	355	MET
1	B	358	PHE
1	B	360	GLN
1	B	365	THR
1	B	372	VAL
1	B	389	SER
1	B	400	LEU
1	B	422	GLU

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Mol	Chain	Res	Type
1	B	482	VAL
1	B	489	THR
1	B	538	THR
1	B	542	LEU
1	B	559	LEU
1	B	563	PHE
1	B	571	VAL
1	B	575	MET
1	B	578	LEU
1	B	583	THR
1	B	610	PHE
1	B	663	LEU
1	B	668	GLU
1	B	673	THR
1	B	682	GLN
1	B	690	LEU
1	B	694	ARG
1	B	830	LYS
1	B	839	MET
1	B	860	GLN
1	B	916	LEU
1	B	946	ASP
1	B	961	ASP
1	B	966	ARG
1	B	968	ARG
1	B	1012	LEU
1	B	1029	SER
1	B	1032	ASN
1	B	1033	GLU
1	B	1035	ILE
1	B	1039	HIS
1	C	3	ASN
1	C	6	ILE
1	C	11	PHE
1	C	25	LEU
1	C	27	ILE
1	C	28	LEU
1	C	49	TYR
1	C	55	LYS
1	C	88	VAL
1	C	90	ILE
1	C	102	ILE

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Mol	Chain	Res	Type
1	C	104	GLN
1	C	112	GLN
1	C	120	GLN
1	C	145	THR
1	C	153	ASP
1	C	177	LEU
1	C	219	LEU
1	C	243	THR
1	C	264	ASP
1	C	293	LEU
1	C	337	ILE
1	C	342	LYS
1	C	358	PHE
1	C	360	GLN
1	C	407	ASP
1	C	429	GLU
1	C	439	GLN
1	C	447	MET
1	C	452	VAL
1	C	463	THR
1	C	470	PHE
1	C	472	ILE
1	C	482	VAL
1	C	510	LYS
1	C	512	PHE
1	C	540	ARG
1	C	564	LEU
1	C	571	VAL
1	C	575	MET
1	C	587	THR
1	C	596	HIS
1	C	610	PHE
1	C	644	MET
1	C	652	GLN
1	C	661	PHE
1	C	689	LYS
1	C	711	VAL
1	C	736	VAL
1	C	741	ILE
1	C	838	LEU
1	C	842	LEU
1	C	855	THR

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Mol	Chain	Res	Type
1	C	860	GLN
1	C	881	LEU
1	C	890	TRP
1	C	909	LEU
1	C	942	GLU
1	C	956	ILE
1	C	963	VAL
1	C	966	ARG
1	C	986	ILE
1	C	1008	THR
1	C	1010	THR
1	C	1012	LEU
1	C	1030	ARG
1	C	1033	GLU
1	C	1035	ILE
1	C	1036	GLU
1	D	6	ILE
1	D	11	PHE
1	D	25	LEU
1	D	70	ASN
1	D	102	ILE
1	D	146	ASP
1	D	148	THR
1	D	152	GLU
1	D	153	ASP
1	D	177	LEU
1	D	205	THR
1	D	229	GLN
1	D	264	ASP
1	D	280	GLU
1	D	281	PHE
1	D	295	THR
1	D	350	LEU
1	D	358	PHE
1	D	362	PHE
1	D	365	THR
1	D	404	LEU
1	D	429	GLU
1	D	437	GLN
1	D	489	THR
1	D	519	MET
1	D	534	ILE

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Mol	Chain	Res	Type
1	D	538	THR
1	D	559	LEU
1	D	561	SER
1	D	571	VAL
1	D	575	MET
1	D	603	LYS
1	D	610	PHE
1	D	628	ASP
1	D	629	TRP
1	D	637	ASN
1	D	690	LEU
1	D	708	LEU
1	D	726	ILE
1	D	738	ILE
1	D	852	TYR
1	D	862	ARG
1	D	909	LEU
1	D	913	PHE
1	D	916	LEU
1	D	917	THR
1	D	926	LEU
1	D	930	ILE
1	D	942	GLU
1	D	946	ASP
1	D	956	ILE
1	D	961	ASP
1	D	966	ARG
1	D	1012	LEU
1	D	1024	VAL
1	D	1030	ARG
1	D	1035	ILE
1	E	6	ILE
1	E	11	PHE
1	E	25	LEU
1	E	28	LEU
1	E	49	TYR
1	E	96	SER
1	E	105	VAL
1	E	117	LEU
1	E	131	LYS
1	E	146	ASP
1	E	153	ASP

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Mol	Chain	Res	Type
1	E	177	LEU
1	E	249	ILE
1	E	255	GLN
1	E	259	ARG
1	E	270	LEU
1	E	280	GLU
1	E	310	LEU
1	E	312	LYS
1	E	323	ILE
1	E	336	SER
1	E	355	MET
1	E	356	TYR
1	E	358	PHE
1	E	372	VAL
1	E	398	MET
1	E	404	LEU
1	E	459	PHE
1	E	482	VAL
1	E	512	PHE
1	E	526	HIS
1	E	538	THR
1	E	555	LEU
1	E	564	LEU
1	E	566	ASP
1	E	571	VAL
1	E	574	THR
1	E	575	MET
1	E	583	THR
1	E	610	PHE
1	E	613	ASN
1	E	619	THR
1	E	629	TRP
1	E	647	THR
1	E	648	ARG
1	E	654	LYS
1	E	667	VAL
1	E	668	GLU
1	E	669	LEU
1	E	685	LEU
1	E	689	LYS
1	E	690	LEU
1	E	694	ARG

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Mol	Chain	Res	Type
1	E	706	ASP
1	E	707	MET
1	E	708	LEU
1	E	712	ARG
1	E	726	ILE
1	E	736	VAL
1	E	799	PHE
1	E	830	LYS
1	E	852	TYR
1	E	896	VAL
1	E	909	LEU
1	E	917	THR
1	E	953	LYS
1	E	956	ILE
1	E	961	ASP
1	E	1012	LEU
1	E	1021	PHE
1	F	6	ILE
1	F	25	LEU
1	F	27	ILE
1	F	28	LEU
1	F	49	TYR
1	F	70	ASN
1	F	88	VAL
1	F	102	ILE
1	F	104	GLN
1	F	112	GLN
1	F	153	ASP
1	F	197	GLN
1	F	205	THR
1	F	243	THR
1	F	280	GLU
1	F	293	LEU
1	F	312	LYS
1	F	327	TYR
1	F	350	LEU
1	F	358	PHE
1	F	360	GLN
1	F	363	ARG
1	F	407	ASP
1	F	431	THR
1	F	447	MET

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Mol	Chain	Res	Type
1	F	448	VAL
1	F	515	TRP
1	F	538	THR
1	F	542	LEU
1	F	575	MET
1	F	587	THR
1	F	610	PHE
1	F	621	ILE
1	F	644	MET
1	F	657	MET
1	F	663	LEU
1	F	689	LYS
1	F	694	ARG
1	F	711	VAL
1	F	714	ASN
1	F	726	ILE
1	F	779	ASP
1	F	838	LEU
1	F	842	LEU
1	F	845	LYS
1	F	859	TYR
1	F	860	GLN
1	F	881	LEU
1	F	918	ASN
1	F	961	ASP
1	F	963	VAL
1	F	966	ARG
1	F	986	ILE
1	F	1021	PHE
1	F	1030	ARG
1	F	1034	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	237	GLN
1	A	569	GLN
1	B	63	GLN
1	B	109	ASN
1	B	742	ASN
1	C	151	GLN

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Mol	Chain	Res	Type
1	C	613	ASN
1	C	755	ASN
1	D	109	ASN
1	D	231	ASN
1	D	437	GLN
1	D	742	ASN
1	E	34	GLN
1	E	67	GLN
1	E	231	ASN
1	E	569	GLN
1	E	605	ASN
1	E	613	ASN
1	E	637	ASN
1	E	732	GLN
1	F	108	GLN
1	F	584	GLN
1	F	613	ASN
1	F	682	GLN
1	F	704	HIS
1	F	732	GLN
1	F	755	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link

column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	LMT	A	1101	-	36,36,36	1.76	11 (30%)	47,47,47	1.40	6 (12%)
2	LMT	B	2000	-	36,36,36	1.78	11 (30%)	47,47,47	1.55	9 (19%)
2	LMT	C	1101	-	36,36,36	1.81	9 (25%)	47,47,47	1.55	7 (14%)
2	LMT	D	2000	-	36,36,36	1.83	9 (25%)	47,47,47	1.82	8 (17%)
2	LMT	E	1101	-	36,36,36	1.80	10 (27%)	47,47,47	2.01	10 (21%)
2	LMT	F	2000	-	36,36,36	1.81	8 (22%)	47,47,47	1.13	5 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LMT	A	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	B	2000	-	-	0/21/61/61	0/2/2/2
2	LMT	C	1101	-	-	0/21/61/61	0/2/2/2
2	LMT	D	2000	-	1/1/10/10	0/21/61/61	0/2/2/2
2	LMT	E	1101	-	1/1/10/10	0/21/61/61	0/2/2/2
2	LMT	F	2000	-	-	0/21/61/61	0/2/2/2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	LMT	C6'-C5'	-3.30	1.40	1.51
2	F	2000	LMT	C6'-C5'	-3.26	1.40	1.51
2	E	1101	LMT	C6'-C5'	-3.19	1.40	1.51
2	B	2000	LMT	C6'-C5'	-3.10	1.40	1.51
2	A	1101	LMT	C6'-C5'	-3.05	1.41	1.51
2	D	2000	LMT	C3'-C2'	-3.04	1.44	1.52
2	D	2000	LMT	C6'-C5'	-2.92	1.41	1.51
2	B	2000	LMT	C3'-C2'	-2.84	1.44	1.52
2	B	2000	LMT	C3B-C2B	-2.78	1.45	1.52
2	E	1101	LMT	C3'-C2'	-2.74	1.45	1.52
2	E	1101	LMT	O1B-C1B	-2.73	1.34	1.41
2	F	2000	LMT	C3'-C2'	-2.71	1.45	1.52
2	D	2000	LMT	C3B-C2B	-2.58	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	LMT	C3'-C2'	-2.55	1.45	1.52
2	C	1101	LMT	C3'-C2'	-2.26	1.46	1.52
2	E	1101	LMT	O1B-C4'	-2.25	1.38	1.43
2	A	1101	LMT	C1'-C2'	-2.24	1.45	1.52
2	A	1101	LMT	C3B-C2B	-2.16	1.46	1.52
2	A	1101	LMT	O1B-C1B	-2.08	1.36	1.41
2	F	2000	LMT	C5-C4	2.03	1.63	1.51
2	B	2000	LMT	O3'-C3'	2.04	1.47	1.43
2	B	2000	LMT	O2'-C2'	2.06	1.47	1.43
2	B	2000	LMT	C5-C4	2.07	1.63	1.51
2	C	1101	LMT	O3'-C3'	2.07	1.47	1.43
2	E	1101	LMT	O3'-C3'	2.07	1.47	1.43
2	B	2000	LMT	O3B-C3B	2.24	1.48	1.43
2	A	1101	LMT	O3B-C3B	2.27	1.48	1.43
2	C	1101	LMT	O2'-C2'	2.33	1.48	1.43
2	A	1101	LMT	O2'-C2'	2.35	1.48	1.43
2	F	2000	LMT	O3B-C3B	2.39	1.48	1.43
2	D	2000	LMT	O2'-C2'	2.52	1.48	1.43
2	A	1101	LMT	O5'-C1'	2.64	1.48	1.41
2	E	1101	LMT	O3B-C3B	2.69	1.49	1.43
2	D	2000	LMT	O5'-C1'	2.85	1.49	1.41
2	D	2000	LMT	O3B-C3B	2.87	1.49	1.43
2	B	2000	LMT	O1'-C1'	2.90	1.45	1.40
2	B	2000	LMT	O5'-C1'	2.95	1.49	1.41
2	C	1101	LMT	O3B-C3B	3.06	1.50	1.43
2	E	1101	LMT	O5B-C1B	3.11	1.49	1.41
2	A	1101	LMT	O1'-C1'	3.16	1.45	1.40
2	B	2000	LMT	O5B-C1B	3.18	1.50	1.41
2	C	1101	LMT	O5B-C1B	3.19	1.50	1.41
2	C	1101	LMT	O5'-C1'	3.32	1.50	1.41
2	A	1101	LMT	O5B-C1B	3.35	1.50	1.41
2	F	2000	LMT	O5B-C1B	3.38	1.50	1.41
2	C	1101	LMT	O1'-C1'	3.45	1.46	1.40
2	E	1101	LMT	O5'-C1'	3.46	1.50	1.41
2	E	1101	LMT	O5'-C5'	3.48	1.53	1.44
2	D	2000	LMT	O5B-C1B	3.50	1.50	1.41
2	D	2000	LMT	O1'-C1'	3.72	1.46	1.40
2	D	2000	LMT	O5'-C5'	3.72	1.53	1.44
2	F	2000	LMT	O1'-C1'	3.73	1.46	1.40
2	A	1101	LMT	O5'-C5'	3.78	1.53	1.44
2	F	2000	LMT	O5'-C5'	3.84	1.54	1.44
2	B	2000	LMT	O5'-C5'	3.84	1.54	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1101	LMT	O1'-C1'	3.97	1.47	1.40
2	C	1101	LMT	O5'-C5'	3.97	1.54	1.44
2	F	2000	LMT	O5'-C1'	4.05	1.52	1.41

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1101	LMT	O1B-C4'-C5'	-5.32	95.18	109.33
2	E	1101	LMT	O4'-C4B-C3B	-3.77	101.86	110.36
2	B	2000	LMT	C1'-C2'-C3'	-3.74	102.57	109.98
2	B	2000	LMT	C1B-O1B-C4'	-3.62	108.39	118.00
2	D	2000	LMT	C1B-O1B-C4'	-3.11	109.73	118.00
2	B	2000	LMT	O3B-C3B-C2B	-3.11	103.34	110.36
2	D	2000	LMT	C1'-C2'-C3'	-2.96	104.11	109.98
2	F	2000	LMT	C1B-O5B-C5B	-2.84	108.17	113.74
2	E	1101	LMT	O1B-C1B-C2B	-2.82	101.11	108.12
2	C	1101	LMT	C1'-C2'-C3'	-2.81	104.40	109.98
2	C	1101	LMT	C3'-C4'-C5'	-2.53	105.07	110.85
2	A	1101	LMT	O3B-C3B-C4B	-2.35	105.06	110.36
2	B	2000	LMT	C1'-O5'-C5'	-2.31	109.21	113.74
2	C	1101	LMT	C1B-O1B-C4'	-2.28	111.94	118.00
2	E	1101	LMT	O2'-C2'-C3'	-2.04	105.76	110.36
2	C	1101	LMT	O1B-C4'-C3'	2.01	112.42	107.18
2	B	2000	LMT	O3'-C3'-C4'	2.02	114.66	109.89
2	F	2000	LMT	O5'-C1'-C2'	2.02	114.47	110.28
2	F	2000	LMT	O5B-C5B-C6B	2.10	111.82	106.38
2	A	1101	LMT	O1'-C1'-C2'	2.16	110.65	108.00
2	D	2000	LMT	C4B-C3B-C2B	2.19	114.81	110.79
2	A	1101	LMT	O5B-C1B-C2B	2.21	114.86	110.28
2	C	1101	LMT	C1B-C2B-C3B	2.26	114.46	109.98
2	F	2000	LMT	O5B-C5B-C4B	2.27	114.00	109.67
2	F	2000	LMT	C1'-O5'-C5'	2.29	118.23	113.74
2	B	2000	LMT	C1B-O5B-C5B	2.43	118.51	113.74
2	E	1101	LMT	O2'-C2'-C1'	2.45	115.44	110.01
2	A	1101	LMT	C1B-C2B-C3B	2.51	114.96	109.98
2	B	2000	LMT	O1B-C1B-C2B	2.55	114.46	108.12
2	E	1101	LMT	O5B-C5B-C4B	2.64	114.70	109.67
2	D	2000	LMT	O3'-C3'-C4'	2.74	116.37	109.89
2	C	1101	LMT	O3'-C3'-C4'	2.81	116.54	109.89
2	D	2000	LMT	C1'-O5'-C5'	2.93	119.49	113.74
2	E	1101	LMT	O5'-C5'-C6'	2.95	114.03	106.38
2	B	2000	LMT	O5B-C5B-C4B	3.55	116.44	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2000	LMT	O1'-C1'-C2'	3.56	112.38	108.00
2	A	1101	LMT	O5B-C5B-C4B	3.84	116.99	109.67
2	D	2000	LMT	O2'-C2'-C1'	3.98	118.84	110.01
2	D	2000	LMT	C1-O1'-C1'	4.37	121.63	114.00
2	A	1101	LMT	C1B-O5B-C5B	4.40	122.37	113.74
2	E	1101	LMT	C4B-C3B-C2B	4.59	119.23	110.79
2	E	1101	LMT	C3B-C4B-C5B	4.71	118.63	110.23
2	E	1101	LMT	O1'-C1'-C2'	5.51	114.78	108.00
2	C	1101	LMT	O1'-C1'-C2'	6.43	115.91	108.00
2	D	2000	LMT	O1'-C1'-C2'	6.73	116.28	108.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2000	LMT	C3B
2	E	1101	LMT	C2B

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	LMT	4	0
2	B	2000	LMT	3	0
2	C	1101	LMT	1	0
2	D	2000	LMT	3	0
2	E	1101	LMT	8	0
2	F	2000	LMT	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	1038/1044 (99%)	0.42	127 (12%)	5	5	27, 75, 109, 132	0
1	B	1039/1044 (99%)	0.38	102 (9%)	10	10	18, 68, 104, 130	0
1	C	1035/1044 (99%)	0.50	125 (12%)	6	6	17, 69, 104, 126	0
1	D	1038/1044 (99%)	0.59	162 (15%)	3	3	16, 90, 130, 173	0
1	E	1037/1044 (99%)	0.69	181 (17%)	2	2	40, 91, 115, 134	0
1	F	1037/1044 (99%)	0.73	177 (17%)	2	2	24, 84, 118, 142	0
All	All	6224/6264 (99%)	0.55	874 (14%)	4	4	16, 80, 115, 173	0

All (874) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	128	SER	16.7
1	E	314	GLU	14.0
1	E	315	PRO	12.2
1	F	714	ASN	11.8
1	F	442	LEU	11.3
1	F	128	SER	11.2
1	F	481	SER	10.4
1	E	311	ALA	10.4
1	F	832	THR	10.3
1	F	830	LYS	10.1
1	F	831	SER	10.0
1	C	403	GLY	9.3
1	C	402	ILE	9.2
1	E	406	VAL	9.1
1	C	714	ASN	8.7
1	E	405	LEU	8.5
1	C	715	GLY	8.5
1	B	315	PRO	8.5
1	D	459	PHE	8.4

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Mol	Chain	Res	Type	RSRZ
1	E	129	VAL	8.4
1	F	936	ASN	8.0
1	A	371	ALA	7.9
1	F	127	VAL	7.8
1	D	685	LEU	7.7
1	B	314	GLU	7.6
1	C	831	SER	7.5
1	F	823	LEU	7.5
1	E	973	THR	7.3
1	D	461	GLY	7.2
1	D	322	LYS	7.2
1	D	683	ALA	7.1
1	D	864	SER	7.1
1	F	410	ILE	7.1
1	F	715	GLY	6.9
1	E	409	ALA	6.9
1	C	832	THR	6.8
1	E	407	ASP	6.8
1	A	369	THR	6.7
1	F	406	VAL	6.7
1	E	488	LEU	6.7
1	F	695	ASN	6.7
1	F	448	VAL	6.6
1	D	407	ASP	6.5
1	D	389	SER	6.5
1	F	407	ASP	6.5
1	D	462	SER	6.5
1	F	694	ARG	6.5
1	E	928	THR	6.4
1	B	164	ASP	6.4
1	E	976	ALA	6.4
1	D	35	TYR	6.4
1	C	670	GLY	6.3
1	B	128	SER	6.3
1	E	864	SER	6.3
1	F	405	LEU	6.2
1	F	46	SER	6.1
1	E	127	VAL	6.1
1	D	282	ASN	6.1
1	A	396	PHE	6.1
1	C	671	THR	6.1
1	F	107	VAL	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	372	VAL	6.0
1	E	487	ILE	6.0
1	E	307	ARG	6.0
1	D	67	GLN	5.9
1	A	656	ALA	5.9
1	E	408	ASP	5.9
1	A	404	LEU	5.9
1	F	441	ALA	5.9
1	A	400	LEU	5.9
1	F	315	PRO	5.9
1	D	108	GLN	5.9
1	F	111	LEU	5.9
1	F	109	ASN	5.8
1	A	445	ILE	5.8
1	F	500	ILE	5.8
1	F	671	THR	5.7
1	E	972	MET	5.7
1	A	35	TYR	5.7
1	F	449	LEU	5.7
1	D	70	ASN	5.7
1	C	716	LEU	5.7
1	E	310	LEU	5.7
1	E	932	LEU	5.6
1	C	406	VAL	5.6
1	F	193	LEU	5.6
1	F	178	PHE	5.6
1	D	486	LEU	5.6
1	D	460	GLY	5.6
1	F	47	ALA	5.6
1	F	821	GLU	5.5
1	C	401	ALA	5.5
1	D	834	GLU	5.5
1	B	111	LEU	5.5
1	D	111	LEU	5.4
1	E	578	LEU	5.4
1	E	410	ILE	5.4
1	D	658	VAL	5.4
1	A	48	SER	5.4
1	E	312	LYS	5.4
1	B	129	VAL	5.4
1	F	372	VAL	5.4
1	A	894	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	D	847	PRO	5.3
1	B	487	ILE	5.3
1	C	830	LYS	5.3
1	C	821	GLU	5.3
1	A	16	ALA	5.3
1	F	482	VAL	5.3
1	E	67	GLN	5.3
1	C	404	LEU	5.3
1	F	872	TYR	5.2
1	C	405	LEU	5.2
1	D	404	LEU	5.2
1	B	109	ASN	5.2
1	E	1014	ILE	5.2
1	C	398	MET	5.2
1	E	351	VAL	5.2
1	E	355	MET	5.2
1	D	846	LEU	5.2
1	F	501	ALA	5.2
1	B	831	SER	5.2
1	E	352	PHE	5.2
1	E	834	GLU	5.2
1	E	442	LEU	5.2
1	A	482	VAL	5.2
1	F	474	ILE	5.1
1	A	635	GLU	5.1
1	C	445	ILE	5.0
1	F	463	THR	5.0
1	E	466	ILE	5.0
1	E	330	THR	5.0
1	E	403	GLY	5.0
1	C	707	MET	4.9
1	C	481	SER	4.9
1	F	833	GLY	4.9
1	F	502	LYS	4.9
1	F	60	THR	4.9
1	D	32	VAL	4.9
1	E	362	PHE	4.9
1	B	697	LEU	4.9
1	D	141	GLY	4.9
1	E	590	VAL	4.8
1	F	129	VAL	4.8
1	E	366	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	E	939	LEU	4.8
1	F	443	VAL	4.8
1	D	330	THR	4.8
1	D	112	GLN	4.8
1	D	68	ASN	4.8
1	F	473	THR	4.8
1	B	830	LYS	4.7
1	E	198	LEU	4.7
1	C	833	GLY	4.7
1	D	411	VAL	4.7
1	B	108	GLN	4.7
1	F	879	VAL	4.7
1	D	487	ILE	4.7
1	E	484	VAL	4.7
1	C	79	SER	4.6
1	E	483	LEU	4.6
1	A	407	ASP	4.6
1	E	291	ILE	4.6
1	C	713	PRO	4.6
1	C	936	ASN	4.6
1	F	467	TYR	4.6
1	A	1008	THR	4.6
1	D	323	ILE	4.6
1	F	408	ASP	4.6
1	B	656	ALA	4.6
1	C	706	ASP	4.6
1	F	362	PHE	4.5
1	C	473	THR	4.5
1	F	883	LEU	4.5
1	F	670	GLY	4.5
1	E	107	VAL	4.5
1	E	1010	THR	4.5
1	E	369	THR	4.5
1	A	368	PRO	4.5
1	A	974	SER	4.4
1	A	578	LEU	4.4
1	D	684	GLY	4.4
1	A	401	ALA	4.4
1	A	128	SER	4.4
1	B	700	GLU	4.4
1	F	713	PRO	4.4
1	D	714	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	863	LEU	4.4
1	A	376	LEU	4.4
1	E	443	VAL	4.4
1	F	116	PRO	4.4
1	B	864	SER	4.4
1	F	706	ASP	4.3
1	D	849	GLY	4.3
1	F	48	SER	4.3
1	B	282	ASN	4.3
1	F	485	ALA	4.3
1	E	313	MET	4.3
1	B	696	GLN	4.3
1	A	486	LEU	4.3
1	A	127	VAL	4.3
1	C	323	ILE	4.3
1	E	348	ILE	4.3
1	C	314	GLU	4.2
1	F	824	GLY	4.2
1	E	669	LEU	4.2
1	D	575	MET	4.2
1	D	874	ILE	4.2
1	C	127	VAL	4.2
1	F	282	ASN	4.2
1	D	610	PHE	4.2
1	C	444	GLY	4.2
1	E	1006	MET	4.1
1	E	621	ILE	4.1
1	B	710	SER	4.1
1	A	15	ILE	4.1
1	F	402	ILE	4.1
1	A	397	GLY	4.1
1	D	682	GLN	4.1
1	F	868	ALA	4.1
1	E	46	SER	4.1
1	E	402	ILE	4.1
1	E	404	LEU	4.1
1	C	64	VAL	4.1
1	C	442	LEU	4.1
1	F	829	GLY	4.1
1	D	848	THR	4.1
1	F	357	LEU	4.1
1	D	784	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	864	SER	4.1
1	E	924	VAL	4.1
1	D	110	LYS	4.1
1	C	16	ALA	4.1
1	E	463	THR	4.0
1	E	282	ASN	4.0
1	D	178	PHE	4.0
1	E	1013	ALA	4.0
1	D	681	ASP	4.0
1	B	447	MET	4.0
1	A	405	LEU	4.0
1	E	990	ALA	4.0
1	C	474	ILE	4.0
1	B	67	GLN	4.0
1	F	589	LYS	4.0
1	D	408	ASP	4.0
1	D	870	SER	4.0
1	C	68	ASN	3.9
1	D	371	ALA	3.9
1	D	400	LEU	3.9
1	E	353	LEU	3.9
1	A	339	GLU	3.9
1	A	410	ILE	3.9
1	E	308	ALA	3.9
1	E	400	LEU	3.9
1	F	68	ASN	3.9
1	F	369	THR	3.9
1	C	784	TRP	3.9
1	F	503	GLY	3.9
1	B	701	ALA	3.9
1	D	656	ALA	3.9
1	B	848	THR	3.8
1	E	975	LEU	3.8
1	C	65	ILE	3.8
1	F	112	GLN	3.8
1	E	1009	ALA	3.8
1	D	621	ILE	3.8
1	F	445	ILE	3.8
1	C	866	ASN	3.8
1	E	462	SER	3.8
1	F	396	PHE	3.8
1	B	113	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	136	PHE	3.8
1	D	18	ILE	3.8
1	F	712	ARG	3.7
1	E	370	ILE	3.7
1	C	394	THR	3.7
1	A	463	THR	3.7
1	E	65	ILE	3.7
1	F	707	MET	3.7
1	D	128	SER	3.7
1	A	403	GLY	3.7
1	C	502	LYS	3.7
1	F	446	ALA	3.7
1	F	826	ALA	3.7
1	B	400	LEU	3.7
1	F	65	ILE	3.7
1	B	406	VAL	3.7
1	D	113	LEU	3.6
1	F	356	TYR	3.6
1	E	111	LEU	3.6
1	E	333	VAL	3.6
1	E	1011	VAL	3.6
1	F	373	PRO	3.6
1	C	939	LEU	3.6
1	E	935	LYS	3.6
1	B	107	VAL	3.6
1	F	118	LEU	3.6
1	B	575	MET	3.6
1	F	850	VAL	3.6
1	C	829	GLY	3.6
1	F	45	ILE	3.6
1	C	400	LEU	3.6
1	C	67	GLN	3.6
1	A	327	TYR	3.6
1	D	406	VAL	3.5
1	E	920	VAL	3.5
1	E	936	ASN	3.5
1	E	989	GLY	3.5
1	E	105	VAL	3.5
1	D	458	PHE	3.5
1	C	390	ILE	3.5
1	B	316	PHE	3.5
1	E	929	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	1012	LEU	3.5
1	B	311	ALA	3.5
1	C	935	LYS	3.5
1	E	322	LYS	3.5
1	C	823	LEU	3.5
1	C	129	VAL	3.5
1	E	317	PHE	3.5
1	A	593	GLU	3.5
1	B	145	THR	3.5
1	C	69	MET	3.5
1	D	78	MET	3.5
1	B	410	ILE	3.5
1	F	871	LEU	3.5
1	E	283	GLY	3.5
1	E	194	ASN	3.4
1	E	108	GLN	3.4
1	E	882	CYS	3.4
1	C	867	GLN	3.4
1	F	834	GLU	3.4
1	B	683	ALA	3.4
1	D	401	ALA	3.4
1	C	388	PHE	3.4
1	E	712	ARG	3.4
1	A	574	THR	3.4
1	C	860	GLN	3.4
1	E	398	MET	3.4
1	C	656	ALA	3.4
1	E	357	LEU	3.4
1	C	480	LEU	3.4
1	D	92	LEU	3.4
1	D	576	VAL	3.4
1	E	977	PHE	3.4
1	A	933	SER	3.4
1	D	15	ILE	3.3
1	F	198	LEU	3.3
1	E	673	THR	3.3
1	C	116	PRO	3.3
1	F	179	GLY	3.3
1	F	197	GLN	3.3
1	F	867	GLN	3.3
1	C	374	VAL	3.3
1	F	444	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	939	LEU	3.3
1	A	467	TYR	3.3
1	D	390	ILE	3.3
1	F	575	MET	3.3
1	C	322	LYS	3.3
1	D	405	LEU	3.3
1	A	406	VAL	3.3
1	D	479	ALA	3.3
1	D	623	PHE	3.3
1	B	322	LYS	3.3
1	F	708	LEU	3.3
1	D	210	GLN	3.3
1	F	176	GLN	3.3
1	C	38	ILE	3.3
1	B	881	LEU	3.3
1	E	48	SER	3.2
1	A	365	THR	3.2
1	D	369	THR	3.2
1	C	448	VAL	3.2
1	C	395	MET	3.2
1	A	411	VAL	3.2
1	D	317	PHE	3.2
1	D	482	VAL	3.2
1	A	1012	LEU	3.2
1	C	407	ASP	3.2
1	F	466	ILE	3.2
1	F	462	SER	3.2
1	B	44	THR	3.2
1	E	931	GLY	3.2
1	F	478	MET	3.2
1	A	13	TRP	3.2
1	A	398	MET	3.2
1	A	390	ILE	3.2
1	D	783	ASP	3.2
1	D	609	VAL	3.2
1	A	353	LEU	3.2
1	B	488	LEU	3.2
1	C	449	LEU	3.2
1	D	972	MET	3.2
1	E	109	ASN	3.2
1	E	33	ALA	3.2
1	D	483	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	404	LEU	3.1
1	D	281	PHE	3.1
1	F	281	PHE	3.1
1	F	484	VAL	3.1
1	B	408	ASP	3.1
1	C	330	THR	3.1
1	A	69	MET	3.1
1	D	657	MET	3.1
1	C	834	GLU	3.1
1	D	66	GLU	3.1
1	D	36	PRO	3.1
1	D	866	ASN	3.1
1	E	126	GLY	3.1
1	B	443	VAL	3.1
1	C	307	ARG	3.1
1	F	869	PRO	3.1
1	B	198	LEU	3.1
1	D	109	ASN	3.1
1	F	453	PHE	3.1
1	E	78	MET	3.1
1	E	465	ALA	3.1
1	F	801	SER	3.1
1	B	65	ILE	3.1
1	D	130	GLU	3.1
1	A	573	MET	3.1
1	E	969	PRO	3.1
1	A	408	ASP	3.1
1	E	112	GLN	3.1
1	E	896	VAL	3.1
1	A	902	LEU	3.1
1	D	321	LEU	3.1
1	E	316	PHE	3.0
1	E	593	GLU	3.0
1	E	674	GLY	3.0
1	B	46	SER	3.0
1	E	59	ASP	3.0
1	B	308	ALA	3.0
1	C	109	ASN	3.0
1	E	899	VAL	3.0
1	D	114	ALA	3.0
1	A	355	MET	3.0
1	F	355	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	323	ILE	3.0
1	B	127	VAL	3.0
1	F	64	VAL	3.0
1	A	481	SER	3.0
1	E	104	GLN	3.0
1	D	865	GLY	3.0
1	F	400	LEU	3.0
1	B	11	PHE	3.0
1	B	112	GLN	3.0
1	D	403	GLY	3.0
1	B	45	ILE	3.0
1	D	12	ALA	3.0
1	A	579	PRO	3.0
1	F	656	ALA	2.9
1	B	834	GLU	2.9
1	D	715	GLY	2.9
1	C	885	ALA	2.9
1	F	117	LEU	2.9
1	D	59	ASP	2.9
1	C	712	ARG	2.9
1	F	110	LYS	2.9
1	C	883	LEU	2.9
1	D	463	THR	2.9
1	E	44	THR	2.9
1	E	579	PRO	2.9
1	B	177	LEU	2.9
1	F	594	VAL	2.9
1	E	473	THR	2.9
1	A	354	VAL	2.9
1	A	661	PHE	2.9
1	C	96	SER	2.9
1	C	310	LEU	2.9
1	F	1011	VAL	2.9
1	C	494	ALA	2.9
1	F	470	PHE	2.9
1	C	397	GLY	2.9
1	E	938	ILE	2.9
1	F	784	TRP	2.9
1	C	399	VAL	2.9
1	F	9	PRO	2.9
1	C	1006	MET	2.9
1	D	393	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	797	SER	2.9
1	D	796	PHE	2.9
1	F	1016	PHE	2.9
1	B	1013	ALA	2.9
1	D	292	LYS	2.9
1	B	251	LEU	2.9
1	C	113	LEU	2.9
1	A	1007	VAL	2.8
1	F	13	TRP	2.8
1	A	145	THR	2.8
1	D	33	ALA	2.8
1	F	399	VAL	2.8
1	E	541	TYR	2.8
1	E	798	ALA	2.8
1	F	935	LYS	2.8
1	F	932	LEU	2.8
1	D	372	VAL	2.8
1	E	14	VAL	2.8
1	B	801	SER	2.8
1	A	195	LYS	2.8
1	E	325	TYR	2.8
1	C	799	PHE	2.8
1	E	1016	PHE	2.8
1	B	573	MET	2.8
1	D	854	TRP	2.8
1	D	351	VAL	2.8
1	F	861	GLU	2.8
1	C	373	PRO	2.8
1	C	111	LEU	2.8
1	F	409	ALA	2.8
1	F	827	ALA	2.8
1	F	67	GLN	2.8
1	E	676	ASP	2.8
1	F	591	LEU	2.8
1	A	977	PHE	2.8
1	C	786	VAL	2.8
1	C	462	SER	2.8
1	C	478	MET	2.8
1	C	300	LEU	2.8
1	E	803	ARG	2.8
1	A	383	LEU	2.8
1	B	394	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	1015	PHE	2.8
1	E	395	MET	2.7
1	C	372	VAL	2.7
1	D	200	PRO	2.7
1	D	324	VAL	2.7
1	F	246	PHE	2.7
1	F	828	PRO	2.7
1	A	386	PHE	2.7
1	D	622	ALA	2.7
1	A	971	LEU	2.7
1	A	577	GLN	2.7
1	F	108	GLN	2.7
1	E	145	THR	2.7
1	E	591	LEU	2.7
1	A	658	VAL	2.7
1	D	396	PHE	2.7
1	C	376	LEU	2.7
1	D	14	VAL	2.7
1	A	487	ILE	2.7
1	A	874	ILE	2.7
1	F	726	ILE	2.7
1	D	11	PHE	2.7
1	F	863	LEU	2.7
1	F	675	PHE	2.7
1	B	854	TRP	2.7
1	A	281	PHE	2.7
1	A	1011	VAL	2.7
1	F	576	VAL	2.7
1	A	970	ILE	2.7
1	B	369	THR	2.7
1	B	934	ALA	2.7
1	E	45	ILE	2.7
1	A	322	LYS	2.7
1	B	110	LYS	2.7
1	E	1007	VAL	2.7
1	B	798	ALA	2.7
1	C	17	ILE	2.7
1	E	401	ALA	2.7
1	B	407	ASP	2.7
1	A	630	ALA	2.7
1	B	92	LEU	2.6
1	B	711	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	188	MET	2.6
1	D	391	ASN	2.6
1	D	973	THR	2.6
1	E	280	GLU	2.6
1	F	786	VAL	2.6
1	B	699	ALA	2.6
1	C	446	ALA	2.6
1	A	336	SER	2.6
1	F	590	VAL	2.6
1	F	657	MET	2.6
1	A	785	TYR	2.6
1	B	785	TYR	2.6
1	E	47	ALA	2.6
1	D	831	SER	2.6
1	A	107	VAL	2.6
1	D	368	PRO	2.6
1	A	590	VAL	2.6
1	A	70	ASN	2.6
1	A	666	ILE	2.6
1	A	714	ASN	2.6
1	C	210	GLN	2.6
1	D	579	PRO	2.6
1	E	66	GLU	2.6
1	E	447	MET	2.6
1	A	357	LEU	2.6
1	F	976	ALA	2.6
1	C	932	LEU	2.6
1	E	577	GLN	2.6
1	E	164	ASP	2.6
1	E	246	PHE	2.6
1	A	374	VAL	2.6
1	D	173	GLY	2.6
1	F	851	GLY	2.6
1	A	876	LEU	2.6
1	D	445	ILE	2.6
1	E	697	LEU	2.6
1	A	315	PRO	2.6
1	D	786	VAL	2.6
1	E	290	GLY	2.6
1	F	1010	THR	2.6
1	A	449	LEU	2.6
1	D	69	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	113	LEU	2.6
1	C	828	PRO	2.6
1	D	713	PRO	2.6
1	E	599	LEU	2.6
1	C	97	GLY	2.6
1	A	834	GLU	2.5
1	C	369	THR	2.5
1	F	403	GLY	2.5
1	F	352	PHE	2.5
1	D	43	VAL	2.5
1	F	674	GLY	2.5
1	F	370	ILE	2.5
1	B	91	THR	2.5
1	B	786	VAL	2.5
1	E	587	THR	2.5
1	B	12	ALA	2.5
1	A	33	ALA	2.5
1	D	37	THR	2.5
1	E	130	GLU	2.5
1	E	793	MET	2.5
1	B	882	CYS	2.5
1	A	12	ALA	2.5
1	A	129	VAL	2.5
1	D	290	GLY	2.5
1	A	877	ILE	2.5
1	B	188	MET	2.5
1	C	575	MET	2.5
1	A	485	ALA	2.5
1	F	488	LEU	2.5
1	B	666	ILE	2.5
1	D	46	SER	2.5
1	D	447	MET	2.5
1	D	412	VAL	2.5
1	F	899	VAL	2.5
1	E	331	PRO	2.5
1	F	164	ASP	2.5
1	F	376	LEU	2.4
1	E	988	THR	2.4
1	D	50	PRO	2.4
1	D	877	ILE	2.4
1	A	198	LEU	2.4
1	E	711	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	409	ALA	2.4
1	C	441	ALA	2.4
1	D	815	ASN	2.4
1	D	778	PRO	2.4
1	E	63	GLN	2.4
1	B	290	GLY	2.4
1	D	376	LEU	2.4
1	F	162	MET	2.4
1	E	197	GLN	2.4
1	A	321	LEU	2.4
1	F	676	ASP	2.4
1	D	409	ALA	2.4
1	D	34	GLN	2.4
1	E	489	THR	2.4
1	F	711	VAL	2.4
1	A	196	PHE	2.4
1	B	355	MET	2.4
1	E	367	ILE	2.4
1	E	881	LEU	2.4
1	A	334	LYS	2.4
1	D	845	LYS	2.4
1	A	67	GLN	2.4
1	A	761	GLY	2.4
1	E	43	VAL	2.4
1	F	860	GLN	2.4
1	F	3	ASN	2.4
1	D	611	ALA	2.4
1	B	411	VAL	2.4
1	D	763	VAL	2.4
1	F	395	MET	2.4
1	F	16	ALA	2.4
1	B	591	LEU	2.4
1	B	450	SER	2.4
1	F	69	MET	2.4
1	A	19	ILE	2.4
1	B	43	VAL	2.3
1	C	14	VAL	2.3
1	D	392	THR	2.3
1	C	782	GLY	2.3
1	E	1017	VAL	2.3
1	E	281	PHE	2.3
1	B	371	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	966	ARG	2.3
1	A	164	ASP	2.3
1	A	348	ILE	2.3
1	B	802	SER	2.3
1	C	797	SER	2.3
1	D	19	ILE	2.3
1	D	72	ILE	2.3
1	F	563	PHE	2.3
1	E	328	ASP	2.3
1	B	975	LEU	2.3
1	C	350	LEU	2.3
1	D	383	LEU	2.3
1	D	977	PHE	2.3
1	E	796	PHE	2.3
1	B	542	LEU	2.3
1	C	973	THR	2.3
1	E	92	LEU	2.3
1	E	303	ALA	2.3
1	F	458	PHE	2.3
1	E	713	PRO	2.3
1	E	795	PRO	2.3
1	D	932	LEU	2.3
1	F	61	VAL	2.3
1	D	129	VAL	2.3
1	E	737	SER	2.3
1	F	170	SER	2.3
1	A	14	VAL	2.3
1	A	399	VAL	2.3
1	E	878	VAL	2.3
1	D	573	MET	2.3
1	C	970	ILE	2.3
1	D	107	VAL	2.3
1	F	477	ALA	2.3
1	D	833	GLY	2.3
1	D	832	THR	2.3
1	E	486	LEU	2.3
1	C	128	SER	2.3
1	E	801	SER	2.3
1	B	404	LEU	2.2
1	B	486	LEU	2.2
1	E	714	ASN	2.2
1	A	36	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	370	ILE	2.2
1	B	865	GLY	2.2
1	C	685	LEU	2.2
1	D	398	MET	2.2
1	F	251	LEU	2.2
1	A	470	PHE	2.2
1	D	1014	ILE	2.2
1	D	696	GLN	2.2
1	A	591	LEU	2.2
1	A	657	MET	2.2
1	A	351	VAL	2.2
1	E	630	ALA	2.2
1	E	728	GLN	2.2
1	F	577	GLN	2.2
1	C	389	SER	2.2
1	F	480	LEU	2.2
1	C	611	ALA	2.2
1	D	315	PRO	2.2
1	F	280	GLU	2.2
1	A	975	LEU	2.2
1	B	405	LEU	2.2
1	F	902	LEU	2.2
1	A	797	SER	2.2
1	A	762	ARG	2.2
1	D	334	LYS	2.2
1	F	797	SER	2.2
1	F	802	SER	2.2
1	A	898	LEU	2.2
1	D	817	LEU	2.2
1	C	610	PHE	2.2
1	B	72	ILE	2.2
1	D	134	SER	2.2
1	E	397	GLY	2.2
1	B	847	PRO	2.2
1	E	971	LEU	2.2
1	F	366	LEU	2.2
1	A	483	LEU	2.2
1	B	18	ILE	2.2
1	B	970	ILE	2.2
1	D	574	THR	2.2
1	B	784	TRP	2.2
1	C	33	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	823	LEU	2.2
1	E	611	ALA	2.2
1	A	382	VAL	2.2
1	B	392	THR	2.2
1	D	127	VAL	2.2
1	B	846	LEU	2.2
1	B	939	LEU	2.2
1	E	438	ILE	2.2
1	E	589	LYS	2.2
1	F	163	LYS	2.2
1	D	485	ALA	2.1
1	C	623	PHE	2.1
1	C	977	PHE	2.1
1	F	933	SER	2.1
1	C	349	ILE	2.1
1	E	609	VAL	2.1
1	A	194	ASN	2.1
1	D	442	LEU	2.1
1	E	193	LEU	2.1
1	E	347	ALA	2.1
1	A	43	VAL	2.1
1	B	79	SER	2.1
1	B	658	VAL	2.1
1	C	669	LEU	2.1
1	D	388	PHE	2.1
1	D	762	ARG	2.1
1	D	738	ILE	2.1
1	C	315	PRO	2.1
1	E	831	SER	2.1
1	F	565	PRO	2.1
1	A	934	ALA	2.1
1	C	501	ALA	2.1
1	C	796	PHE	2.1
1	C	658	VAL	2.1
1	D	348	ILE	2.1
1	C	974	SER	2.1
1	D	795	PRO	2.1
1	B	246	PHE	2.1
1	A	32	VAL	2.1
1	A	472	ILE	2.1
1	E	492	LEU	2.1
1	A	623	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	785	TYR	2.1
1	F	940	ILE	2.1
1	F	322	LYS	2.1
1	F	678	GLU	2.1
1	A	45	ILE	2.1
1	C	291	ILE	2.1
1	B	657	MET	2.1
1	C	577	GLN	2.1
1	C	634	GLY	2.1
1	D	194	ASN	2.1
1	A	611	ALA	2.1
1	A	622	ALA	2.1
1	C	35	TYR	2.1
1	D	724	ILE	2.1
1	E	374	VAL	2.1
1	E	653	ILE	2.1
1	F	621	ILE	2.1
1	E	575	MET	2.1
1	E	11	PHE	2.1
1	F	796	PHE	2.1
1	E	933	SER	2.1
1	A	792	GLN	2.1
1	D	1010	THR	2.1
1	B	578	LEU	2.1
1	D	402	ILE	2.1
1	B	825	GLN	2.0
1	A	489	THR	2.0
1	B	71	GLY	2.0
1	C	353	LEU	2.0
1	A	831	SER	2.0
1	B	281	PHE	2.0
1	C	20	MET	2.0
1	C	396	PHE	2.0
1	F	1014	ILE	2.0
1	D	386	PHE	2.0
1	D	728	GLN	2.0
1	F	573	MET	2.0
1	C	655	ASP	2.0
1	A	711	VAL	2.0
1	E	61	VAL	2.0
1	C	500	ILE	2.0
1	F	143	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	136	PHE	2.0
1	C	282	ASN	2.0
1	E	62	THR	2.0
1	A	108	GLN	2.0
1	B	197	GLN	2.0
1	A	881	LEU	2.0
1	E	441	ALA	2.0
1	F	126	GLY	2.0
1	F	691	THR	2.0
1	D	974	SER	2.0
1	F	578	LEU	2.0
1	A	461	GLY	2.0
1	E	199	THR	2.0
1	B	1011	VAL	2.0
1	E	1002	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	LMT	B	2000	35/35	0.73	0.43	1.69	31,50,60,69	0
2	LMT	D	2000	35/35	0.82	0.34	0.78	21,41,56,63	0
2	LMT	C	1101	35/35	0.82	0.33	0.75	12,41,56,72	0
2	LMT	F	2000	35/35	0.82	0.40	0.65	40,64,89,94	0
2	LMT	A	1101	35/35	0.86	0.32	0.53	31,41,90,99	0
2	LMT	E	1101	35/35	0.78	0.42	0.12	41,74,104,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NI	E	1102	1/1	0.96	0.15	-	170,170,170,170	0
3	NI	C	1102	1/1	0.98	0.09	-	41,41,41,41	0
3	NI	A	1102	1/1	0.97	0.19	-	154,154,154,154	0

6.5 Other polymers (i)

There are no such residues in this entry.