Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:18 PM GMT

PDB ID	:	4XAM
Title	:	Complement component C4b
Authors	:	Mortensen, S.; Kidmose, R.T.; Petersen, S.V.; Szilagyi, A.; Andersen, G.R.
Deposited on	:	2014-12-15
Resolution	:	4.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

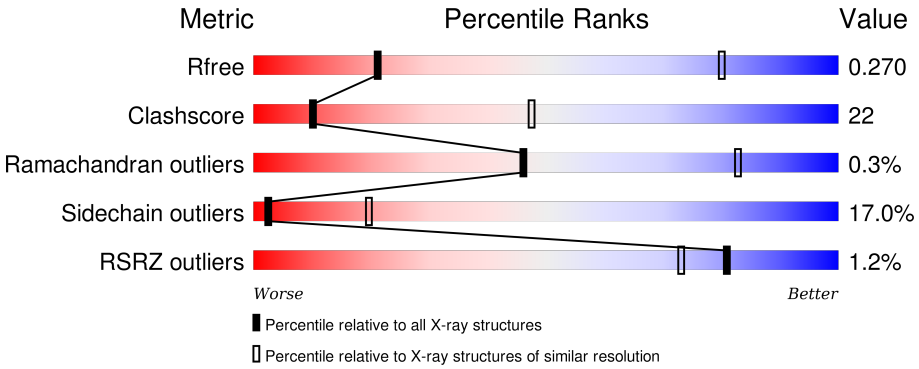
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 4.20 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	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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	656	52% 41% 7%
1	B	656	49% 42% 8%
2	C	690	2% 46% 38% 7% 8%
2	E	690	2% 46% 37% 7% 8%
3	D	291	% 47% 39% 10%

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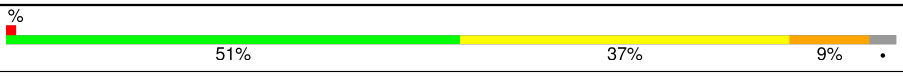
Mol	Chain	Length	Quality of chain
3	F	291	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 24258 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 Complement C4-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5012	3185	872	939	16			
1	B	651	Total	C	N	O	S	0	0	0
			5012	3185	872	939	16			

- Molecule 2 is a protein called Complement C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	632	Total	C	N	O	S	0	0	0
			4876	3085	844	932	15			
2	E	632	Total	C	N	O	S	0	0	0
			4876	3085	844	932	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1201	SER	THR	conflict	UNP P0C0L4
E	1201	SER	THR	conflict	UNP P0C0L4

- Molecule 3 is a protein called Complement C4-A.

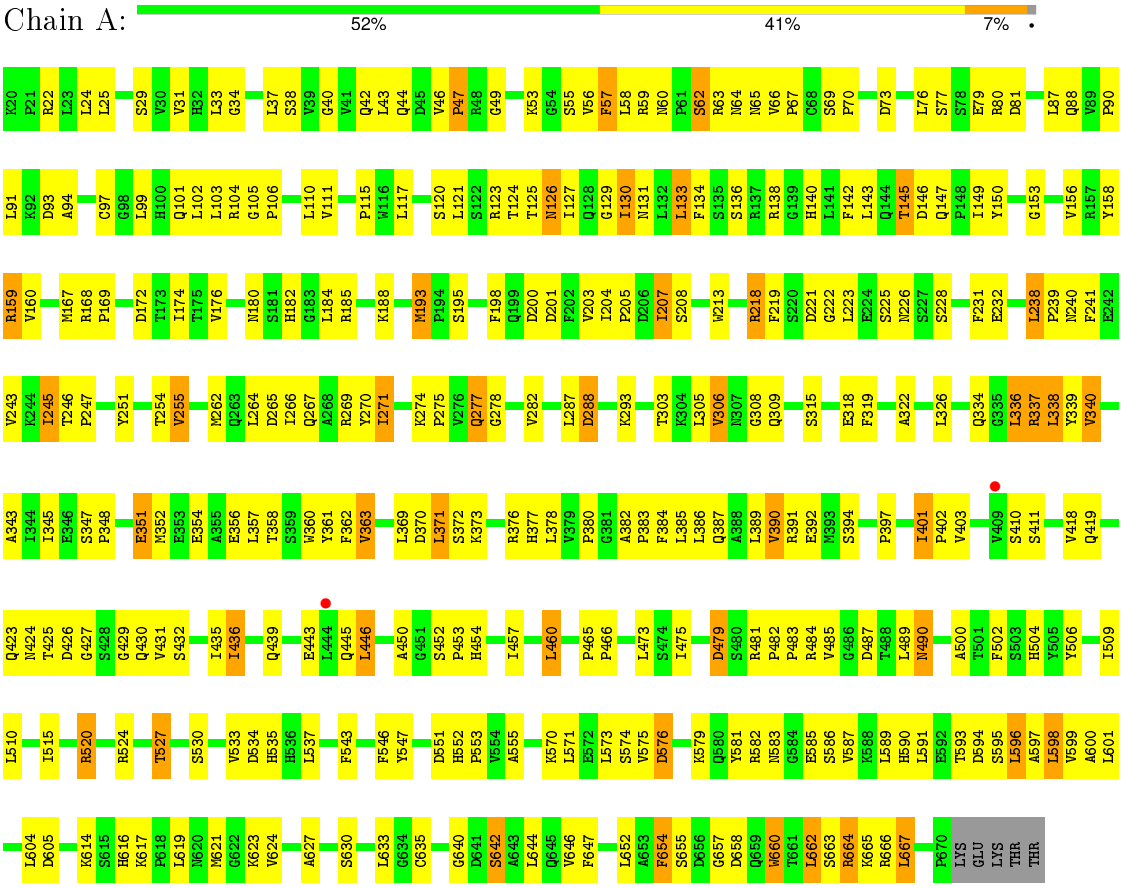
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	281	Total	C	N	O	S	0	0	0
			2241	1407	400	417	17			
3	F	281	Total	C	N	O	S	0	0	0
			2241	1407	400	417	17			

3 Residue-property plots (i)

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.

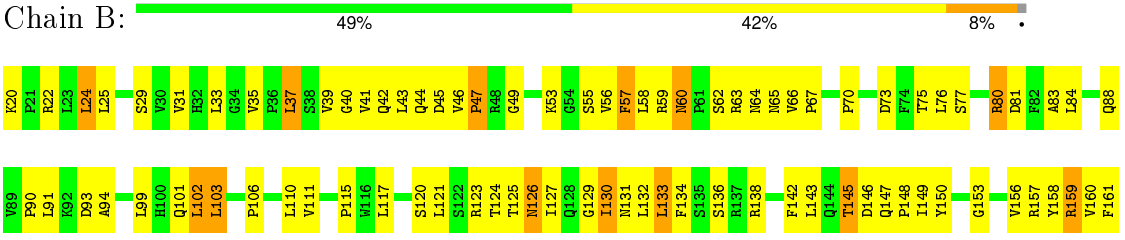
- Molecule 1: Complement C4-B

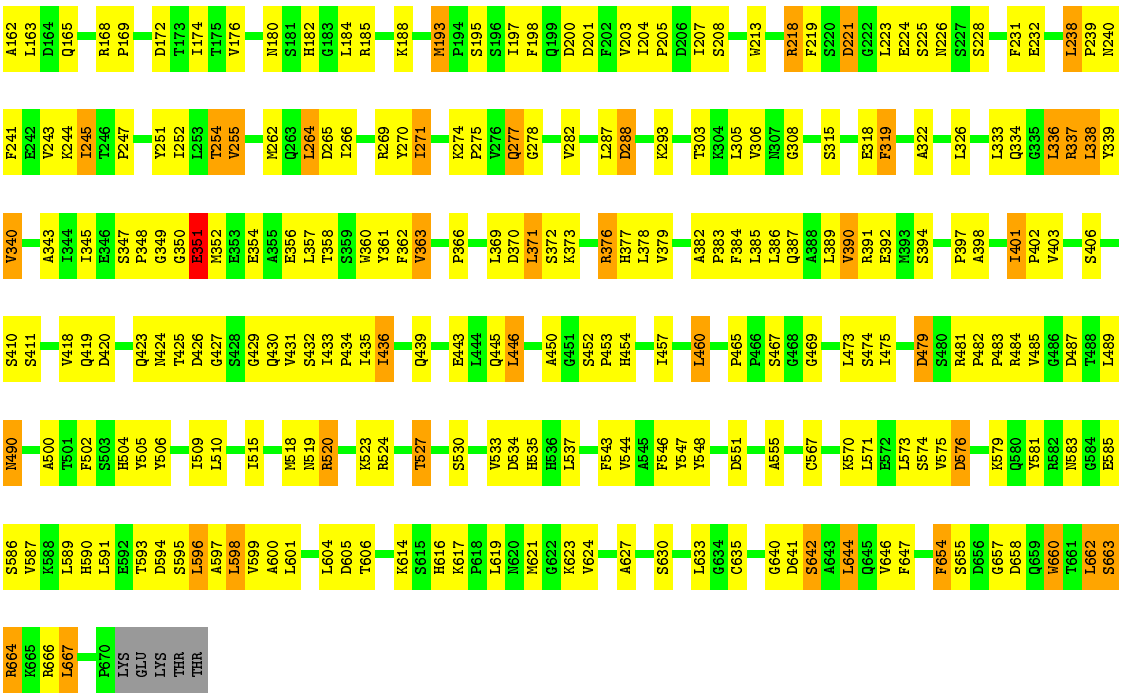
Chain A:



- Molecule 1: Complement C4-B

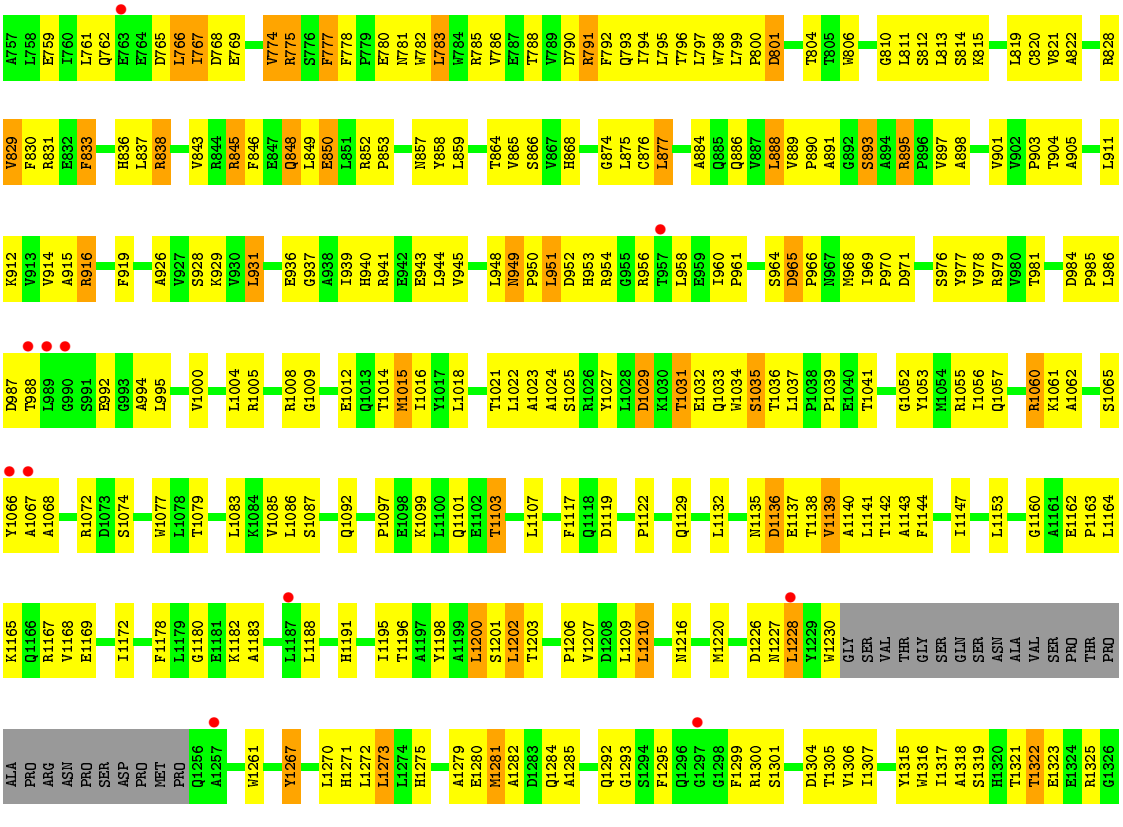
Chain B:

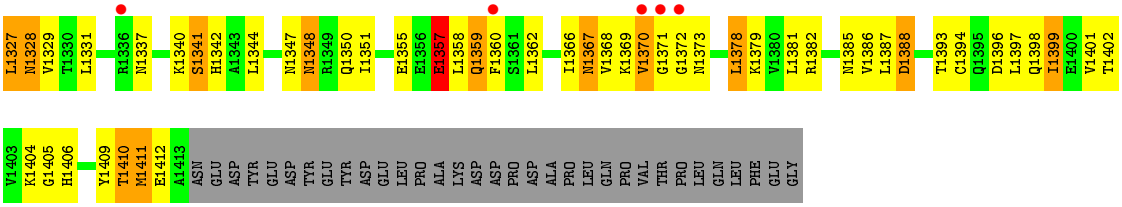




• Molecule 2: Complement C4-A

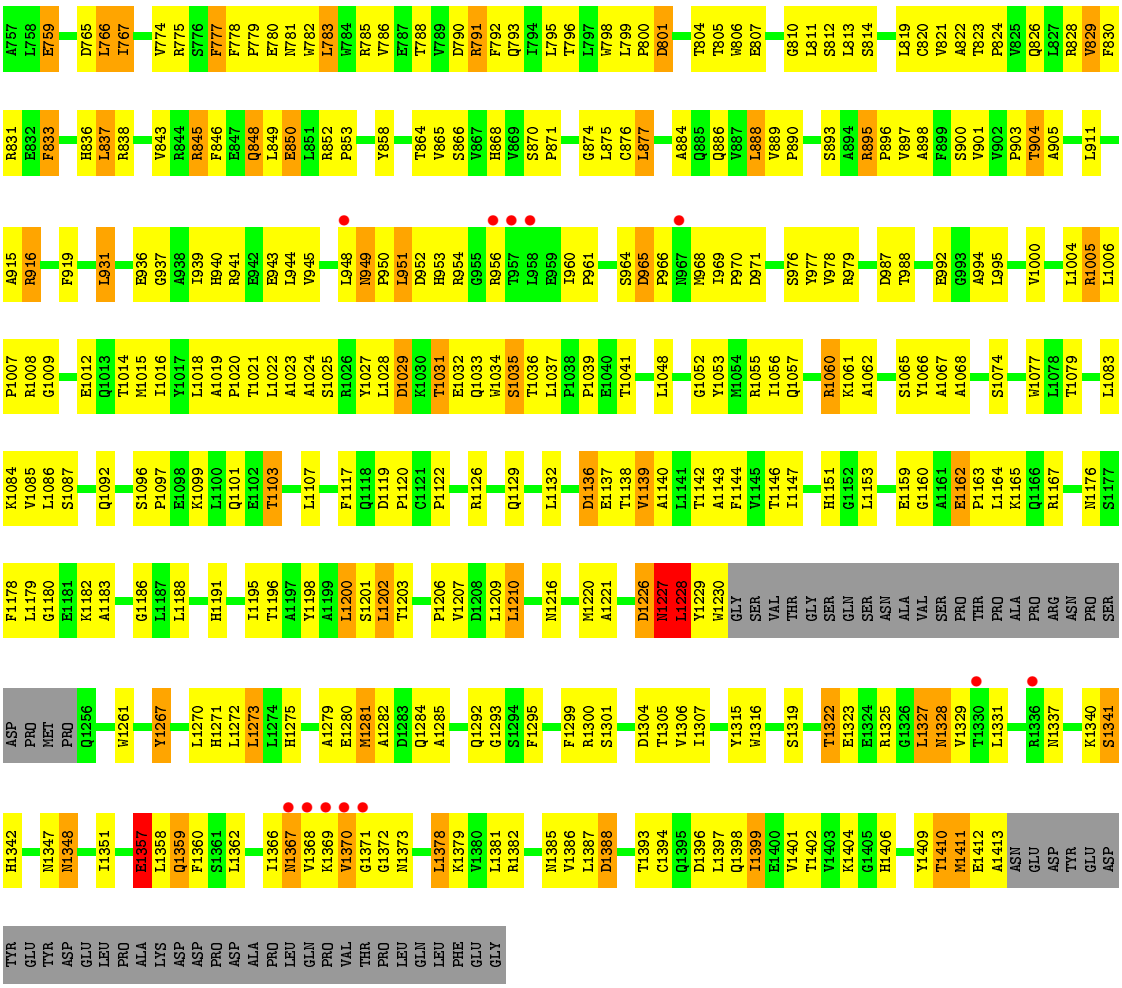
Chain C:





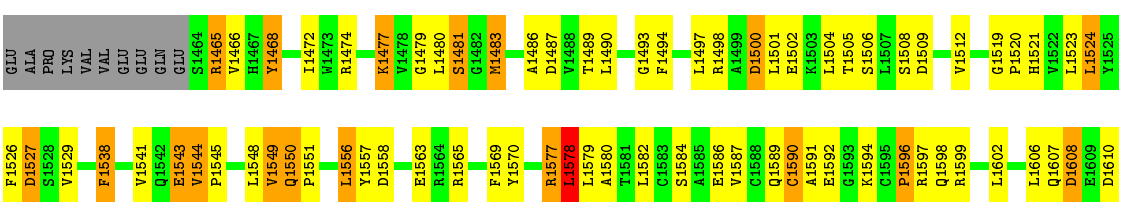
• Molecule 2: Complement C4-A

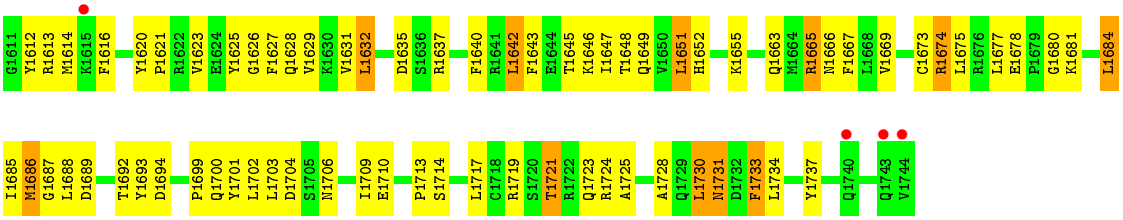
Chain E:



• Molecule 3: Complement C4-A

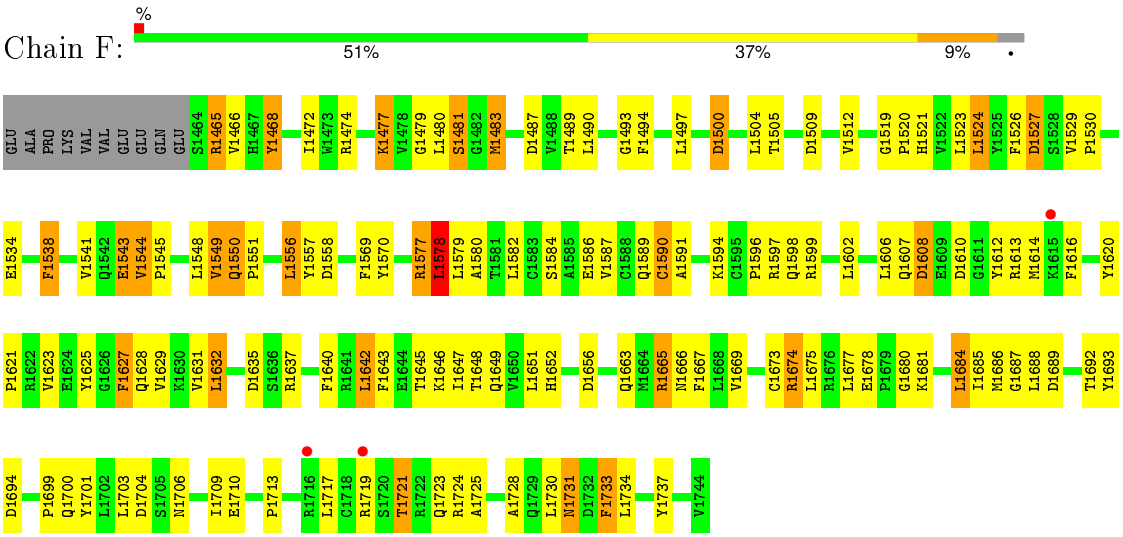
Chain D:





- Molecule 3: Complement C4-A

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.50Å 161.08Å 131.60Å 90.00° 107.26° 90.00°	Depositor
Resolution (Å)	49.54 – 4.20 49.54 – 4.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.54-4.20) 98.5 (49.54-4.20)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 4.14Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, R_{free}	0.217 , 0.273 0.211 , 0.270	Depositor DCC
R_{free} test set	1167 reflections (3.35%)	DCC
Wilson B-factor (Å^2)	103.4	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 134.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 34863 reflections	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	24258	wwPDB-VP
Average B, all atoms (Å^2)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.52	0/5128	0.72	1/6961 (0.0%)
1	B	0.57	0/5128	0.74	3/6961 (0.0%)
2	C	0.45	2/4975 (0.0%)	0.63	0/6765
2	E	0.46	2/4975 (0.0%)	0.64	1/6765 (0.0%)
3	D	0.49	0/2288	0.71	1/3090 (0.0%)
3	F	0.46	0/2288	0.70	2/3090 (0.1%)
All	All	0.50	4/24782 (0.0%)	0.69	8/33632 (0.0%)

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	3
2	C	0	8
2	E	0	8
3	D	0	2
3	F	0	1
All	All	0	25

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1092	GLN	CD-NE2	-6.23	1.17	1.32
2	C	1092	GLN	CD-NE2	-6.07	1.17	1.32
2	C	1092	GLN	CD-OE1	-5.59	1.11	1.24
2	E	1092	GLN	CD-OE1	-5.19	1.12	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	24	LEU	CB-CG-CD1	-6.30	100.28	111.00
1	A	338	LEU	CA-CB-CG	6.26	129.69	115.30
1	B	338	LEU	CA-CB-CG	6.02	129.16	115.30
3	D	1578	LEU	CA-CB-CG	5.72	128.46	115.30
3	F	1578	LEU	CA-CB-CG	5.69	128.39	115.30
3	F	1556	LEU	CA-CB-CG	5.50	127.94	115.30
2	E	1227	ASN	C-N-CA	5.10	134.44	121.70
1	B	60	ASN	C-N-CD	5.04	138.98	128.40

There are no chirality outliers.

All (25) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	GLU	Peptide
1	A	47	PRO	Peptide
1	A	596	LEU	Peptide
1	B	351	GLU	Peptide
1	B	47	PRO	Peptide
1	B	596	LEU	Peptide
2	C	1062	ALA	Peptide
2	C	1322	THR	Peptide
2	C	1357	GLU	Peptide
2	C	1359	GLN	Peptide
2	C	1388	ASP	Peptide
2	C	1409	TYR	Peptide
2	C	1410	THR	Peptide
2	C	969	ILE	Peptide
3	D	1578	LEU	Peptide
3	D	1596	PRO	Peptide
2	E	1062	ALA	Peptide
2	E	1322	THR	Peptide
2	E	1357	GLU	Peptide
2	E	1359	GLN	Peptide
2	E	1388	ASP	Peptide
2	E	1409	TYR	Peptide
2	E	1410	THR	Peptide
2	E	969	ILE	Peptide
3	F	1578	LEU	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	5012	0	5026	233	0
1	B	5012	0	5026	260	1
2	C	4876	0	4846	222	1
2	E	4876	0	4846	221	0
3	D	2241	0	2184	112	0
3	F	2241	0	2184	104	0
All	All	24258	0	24112	1056	1

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 22.

All (1056) 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:B:241:PHE:HE2	1:B:352:MET:HB3	1.26	1.00
1:A:241:PHE:HE2	1:A:352:MET:HB3	1.27	0.96
1:B:370:ASP:HB2	1:B:391:ARG:HD2	1.54	0.90
1:A:370:ASP:HB2	1:A:391:ARG:HD2	1.54	0.88
2:C:1411:MET:N	2:C:1411:MET:SD	2.45	0.88
1:A:619:LEU:HG	1:A:623:LYS:HD2	1.58	0.85
1:B:90:PRO:HG2	1:B:93:ASP:HB2	1.60	0.83
1:B:77:SER:HB3	1:B:80:ARG:H	1.41	0.83
1:B:619:LEU:HG	1:B:623:LYS:HD2	1.60	0.83
2:C:889:VAL:HG22	2:C:895:ARG:HB2	1.58	0.82
3:F:1594:LYS:HD3	3:F:1674:ARG:HH22	1.45	0.81
2:E:1411:MET:SD	2:E:1411:MET:N	2.53	0.81
1:A:90:PRO:HG2	1:A:93:ASP:HB2	1.63	0.81
3:F:1597:ARG:HH21	3:F:1599:ARG:HD2	1.46	0.81
1:A:129:GLY:HA3	2:C:1039:PRO:HG2	1.62	0.80
1:B:251:TYR:HB2	1:B:363:VAL:HG21	1.63	0.80
2:E:804:THR:H	2:E:829:VAL:HG23	1.46	0.80
1:A:77:SER:HB3	1:A:80:ARG:H	1.45	0.80
3:F:1570:TYR:HA	3:F:1577:ARG:HH21	1.46	0.80
2:C:1328:ASN:HB2	2:C:1370:VAL:HG13	1.64	0.79
2:E:889:VAL:HG22	2:E:895:ARG:HB2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:HD3	1:A:188:LYS:HB2	1.62	0.79
2:E:1328:ASN:HB2	2:E:1370:VAL:HG13	1.64	0.79
1:A:585:GLU:H	2:C:799:LEU:HB2	1.45	0.79
3:D:1524:LEU:HB2	3:D:1526:PHE:HE1	1.48	0.79
3:D:1594:LYS:HD3	3:D:1674:ARG:HH22	1.46	0.79
2:C:936:GLU:HG2	2:C:1385:ASN:HB3	1.65	0.78
1:A:278:GLY:H	1:A:305:LEU:HB2	1.47	0.78
2:E:936:GLU:HG2	2:E:1385:ASN:HB3	1.64	0.78
2:E:1299:PHE:O	2:E:1300:ARG:NE	2.12	0.78
1:B:278:GLY:H	1:B:305:LEU:HB2	1.46	0.78
1:B:159:ARG:HH21	1:B:600:ALA:HB1	1.48	0.78
3:F:1703:LEU:HD22	3:F:1709:ILE:HD11	1.65	0.78
3:D:1570:TYR:HA	3:D:1577:ARG:HH21	1.47	0.78
1:B:136:SER:N	1:B:224:GLU:OE1	2.16	0.77
3:D:1703:LEU:HD22	3:D:1709:ILE:HD11	1.65	0.77
2:C:1299:PHE:O	2:C:1300:ARG:NE	2.14	0.77
1:B:193:MET:HG2	1:B:198:PHE:HB2	1.66	0.77
2:C:804:THR:H	2:C:829:VAL:HG23	1.48	0.77
1:B:185:ARG:HD3	1:B:188:LYS:HB2	1.64	0.77
3:D:1597:ARG:HH21	3:D:1599:ARG:HD2	1.49	0.77
1:B:121:LEU:HD12	1:B:123:ARG:HE	1.50	0.77
2:C:1272:LEU:HD11	2:C:1281:MET:HB2	1.67	0.76
1:A:193:MET:HG2	1:A:198:PHE:HB2	1.67	0.76
1:B:138:ARG:NH2	1:B:221:ASP:OD2	2.15	0.76
1:A:159:ARG:HH21	1:A:600:ALA:HB1	1.49	0.76
1:B:43:LEU:HD22	1:B:46:VAL:HG21	1.68	0.75
1:B:389:LEU:HB3	1:B:391:ARG:HG3	1.68	0.74
1:A:597:ALA:HB2	2:C:814:SER:HB3	1.69	0.74
1:B:585:GLU:H	2:E:799:LEU:HB2	1.49	0.74
1:B:129:GLY:HA3	2:E:1039:PRO:HG2	1.66	0.74
1:B:110:LEU:HB3	1:B:130:ILE:HG13	1.69	0.74
3:F:1637:ARG:HG3	3:F:1642:LEU:HD12	1.69	0.74
1:B:241:PHE:CE2	1:B:352:MET:HB3	2.18	0.74
1:A:389:LEU:HB3	1:A:391:ARG:HG3	1.70	0.74
1:B:597:ALA:HB2	2:E:814:SER:HB3	1.70	0.73
2:E:1301:SER:O	2:E:1305:THR:OG1	2.05	0.73
2:E:1272:LEU:HD11	2:E:1281:MET:HB2	1.70	0.73
1:A:174:ILE:HG22	1:A:219:PHE:HA	1.70	0.73
2:C:1301:SER:O	2:C:1305:THR:OG1	2.05	0.73
3:F:1628:GLN:HG3	3:F:1648:THR:HB	1.71	0.73
1:B:633:LEU:HB3	1:B:664:ARG:HH22	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:ILE:HG22	1:B:219:PHE:HA	1.71	0.73
1:A:110:LEU:HB3	1:A:130:ILE:HG13	1.71	0.73
1:A:43:LEU:HD22	1:A:46:VAL:HG21	1.71	0.72
1:B:238:LEU:HD22	1:B:239:PRO:HD2	1.70	0.72
1:B:348:PRO:HA	3:F:1521:HIS:ND1	2.03	0.72
1:A:121:LEU:HD12	1:A:123:ARG:HE	1.53	0.72
2:C:794:ILE:H	1:B:75:THR:HG21	1.54	0.72
1:A:241:PHE:CE2	1:A:352:MET:HB3	2.18	0.72
2:E:1413:ALA:C	3:F:1594:LYS:HG2	2.11	0.71
1:A:287:LEU:HB3	1:A:338:LEU:HG	1.71	0.71
1:B:245:ILE:HD12	1:B:358:THR:HG23	1.72	0.71
2:C:1057:GLN:O	2:C:1060:ARG:HB3	1.91	0.71
1:B:401:ILE:HG12	1:B:402:PRO:HD2	1.72	0.71
2:E:819:LEU:HD22	2:E:820:CYS:H	1.55	0.71
2:E:1057:GLN:O	2:E:1060:ARG:HB3	1.90	0.71
1:B:255:VAL:HA	1:B:334:GLN:OE1	1.91	0.70
2:E:948:LEU:HD11	2:E:1378:LEU:HD23	1.72	0.70
3:D:1637:ARG:HG3	3:D:1642:LEU:HD12	1.73	0.70
2:E:799:LEU:HD23	2:E:800:PRO:HD2	1.73	0.70
1:A:585:GLU:N	2:C:799:LEU:HB2	2.07	0.70
1:B:600:ALA:HB3	2:E:811:LEU:HB2	1.74	0.70
3:D:1692:THR:OG1	3:D:1700:GLN:O	2.10	0.69
3:F:1524:LEU:HB2	3:F:1526:PHE:HE1	1.55	0.69
2:E:1008:ARG:O	2:E:1014:THR:OG1	2.10	0.69
1:B:22:ARG:HH12	1:B:658:ASP:HB2	1.58	0.69
2:C:790:ASP:OD1	2:C:791:ARG:NH2	2.24	0.69
1:A:31:VAL:HG11	1:A:58:LEU:HD21	1.74	0.69
2:E:1136:ASP:O	2:E:1140:ALA:N	2.26	0.69
1:A:633:LEU:HB3	1:A:664:ARG:HH22	1.56	0.69
1:A:315:SER:HB3	1:A:318:GLU:HB2	1.74	0.68
2:E:1085:VAL:HG12	2:E:1086:LEU:HD23	1.74	0.68
1:A:238:LEU:HD22	1:A:239:PRO:HD2	1.74	0.68
1:A:245:ILE:HD12	1:A:358:THR:HG23	1.74	0.68
2:C:948:LEU:HD11	2:C:1378:LEU:HD23	1.75	0.68
3:D:1597:ARG:HB3	3:D:1709:ILE:HB	1.75	0.68
2:E:790:ASP:OD1	2:E:791:ARG:NH2	2.26	0.68
1:B:24:LEU:HB2	1:B:42:GLN:HB3	1.75	0.67
1:A:104:ARG:HH22	2:C:1033:GLN:HG2	1.59	0.67
2:C:1008:ARG:O	2:C:1014:THR:OG1	2.12	0.67
1:B:31:VAL:HG11	1:B:58:LEU:HD21	1.76	0.67
3:F:1663:GLN:OE1	3:F:1665:ARG:NH2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLY:HA2	1:A:348:PRO:HD3	1.76	0.67
3:D:1678:GLU:HB2	3:D:1681:LYS:HB2	1.76	0.67
1:A:111:VAL:HG13	1:A:127:ILE:HG23	1.77	0.67
1:B:373:LYS:HG3	1:B:389:LEU:HD13	1.76	0.67
3:F:1721:THR:HA	3:F:1724:ARG:HB3	1.76	0.67
3:F:1597:ARG:HB3	3:F:1709:ILE:HB	1.77	0.67
2:C:874:GLY:HA2	2:C:904:THR:HB	1.76	0.67
1:B:315:SER:HB3	1:B:318:GLU:HB2	1.75	0.67
2:E:845:ARG:HA	2:E:903:PRO:HG2	1.75	0.66
3:D:1628:GLN:HG3	3:D:1648:THR:HB	1.76	0.66
1:A:600:ALA:HB3	2:C:811:LEU:HB2	1.77	0.66
3:F:1678:GLU:HB2	3:F:1681:LYS:HB2	1.77	0.66
1:B:287:LEU:HB3	1:B:338:LEU:HG	1.75	0.66
2:E:1009:GLY:HA2	2:E:1055:ARG:HH21	1.59	0.66
2:E:874:GLY:HA2	2:E:904:THR:HB	1.75	0.66
2:E:874:GLY:O	2:E:904:THR:N	2.29	0.66
1:B:110:LEU:HD23	1:B:130:ILE:HD11	1.78	0.66
1:A:401:ILE:HG12	1:A:402:PRO:HD2	1.76	0.66
2:C:819:LEU:HD22	2:C:820:CYS:H	1.58	0.66
2:C:845:ARG:HA	2:C:903:PRO:HG2	1.77	0.66
1:B:336:LEU:O	1:B:337:ARG:NE	2.28	0.66
1:A:24:LEU:HB2	1:A:42:GLN:HB3	1.78	0.66
2:E:830:PHE:HZ	2:E:858:TYR:HD1	1.44	0.66
1:A:571:LEU:HG	2:C:822:ALA:HB2	1.77	0.66
2:C:1183:ALA:HA	2:C:1188:LEU:HD11	1.78	0.65
2:E:1183:ALA:HA	2:E:1188:LEU:HD11	1.78	0.65
3:D:1663:GLN:OE1	3:D:1665:ARG:NH2	2.29	0.65
1:B:29:SER:HB3	1:B:664:ARG:HH21	1.61	0.65
1:A:29:SER:HB3	1:A:664:ARG:HH21	1.62	0.65
1:B:403:VAL:HG21	1:B:431:VAL:HG21	1.78	0.65
1:A:485:VAL:HA	1:A:533:VAL:HG12	1.79	0.65
1:B:504:HIS:CD2	1:B:520:ARG:HE	2.15	0.65
1:B:24:LEU:HD22	1:B:654:PHE:HE1	1.61	0.65
1:A:425:THR:HG23	1:A:431:VAL:HG23	1.79	0.65
2:C:1018:LEU:HD13	2:C:1052:GLY:HA3	1.79	0.64
1:B:614:LYS:HD3	1:B:616:HIS:HB2	1.78	0.64
2:C:1009:GLY:HA2	2:C:1055:ARG:HH21	1.61	0.64
2:C:799:LEU:HD23	2:C:800:PRO:HD2	1.79	0.64
1:B:585:GLU:N	2:E:799:LEU:HB2	2.12	0.64
3:D:1631:VAL:O	3:D:1680:GLY:N	2.30	0.64
1:A:33:LEU:HD21	1:A:134:PHE:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:TYR:HB2	1:A:363:VAL:HG21	1.79	0.64
1:B:510:LEU:HD22	1:B:515:ILE:HG12	1.79	0.64
3:D:1721:THR:HA	3:D:1724:ARG:HB3	1.78	0.64
1:B:600:ALA:HA	2:E:786:VAL:HG22	1.80	0.64
1:A:664:ARG:NH1	1:A:666:ARG:O	2.31	0.64
2:C:1085:VAL:HG12	2:C:1086:LEU:HD23	1.78	0.64
3:D:1519:GLY:O	3:D:1521:HIS:N	2.28	0.64
2:C:830:PHE:HZ	2:C:858:TYR:HD1	1.46	0.64
2:C:1136:ASP:O	2:C:1140:ALA:N	2.31	0.64
1:A:31:VAL:HB	1:A:134:PHE:HB3	1.80	0.63
1:B:106:PRO:O	1:B:133:LEU:HA	1.98	0.63
1:B:126:ASN:OD1	1:B:126:ASN:N	2.30	0.63
3:D:1719:ARG:O	3:D:1724:ARG:NE	2.30	0.63
1:A:218:ARG:HA	1:A:225:SER:HB2	1.79	0.63
3:D:1589:GLN:HG2	3:D:1590:CYS:N	2.14	0.63
3:F:1719:ARG:O	3:F:1724:ARG:NE	2.31	0.63
1:A:106:PRO:O	1:A:133:LEU:HA	1.98	0.63
3:F:1692:THR:OG1	3:F:1700:GLN:O	2.13	0.63
1:B:278:GLY:HA2	1:B:348:PRO:HD3	1.79	0.63
3:F:1521:HIS:CE1	3:F:1523:LEU:HD21	2.34	0.63
1:A:104:ARG:NH2	2:C:1033:GLN:HG2	2.13	0.63
3:F:1631:VAL:O	3:F:1680:GLY:N	2.32	0.63
2:C:1201:SER:HB3	2:C:1210:LEU:HD21	1.80	0.63
1:B:485:VAL:HA	1:B:533:VAL:HG12	1.81	0.63
1:A:336:LEU:O	1:A:337:ARG:NE	2.31	0.63
3:F:1616:PHE:O	3:F:1621:PRO:HD2	1.98	0.62
1:B:218:ARG:HA	1:B:225:SER:HB2	1.80	0.62
1:A:110:LEU:HD23	1:A:130:ILE:HD11	1.81	0.62
2:E:1207:VAL:HA	2:E:1210:LEU:HB3	1.81	0.62
3:D:1717:LEU:O	3:D:1723:GLN:NE2	2.32	0.62
3:F:1487:ASP:OD1	3:F:1521:HIS:NE2	2.26	0.62
1:B:24:LEU:HD11	1:B:44:GLN:NE2	2.14	0.62
1:A:403:VAL:HG21	1:A:431:VAL:HG21	1.80	0.62
2:C:852:ARG:NH2	3:D:1489:THR:OG1	2.33	0.62
2:C:979:ARG:NH2	2:C:1357:GLU:OE1	2.32	0.62
1:A:287:LEU:HD12	1:A:338:LEU:HD23	1.81	0.62
1:B:425:THR:HG23	1:B:431:VAL:HG23	1.81	0.62
1:A:614:LYS:HD3	1:A:616:HIS:HB2	1.80	0.62
2:E:848:GLN:N	2:E:848:GLN:OE1	2.32	0.62
1:A:533:VAL:HA	1:A:537:LEU:HD22	1.82	0.62
1:B:103:LEU:HD22	2:E:1316:TRP:CZ3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD11	1:A:44:GLN:NE2	2.15	0.62
1:B:271:ILE:HB	2:E:805:THR:HG22	1.80	0.62
3:D:1616:PHE:O	3:D:1621:PRO:HD2	1.99	0.62
1:A:373:LYS:HG3	1:A:389:LEU:HD13	1.80	0.62
3:D:1487:ASP:OD1	3:D:1521:HIS:NE2	2.29	0.62
1:B:571:LEU:HG	2:E:822:ALA:HB2	1.81	0.62
1:A:168:ARG:HD2	2:C:815:LYS:O	2.00	0.62
2:E:976:SER:HB2	2:E:1360:PHE:CD1	2.35	0.61
1:B:111:VAL:HG13	1:B:127:ILE:HG23	1.82	0.61
2:E:1164:LEU:HA	2:E:1167:ARG:HG2	1.82	0.61
2:C:1340:LYS:HZ2	2:C:1359:GLN:HA	1.65	0.61
1:B:243:VAL:HG21	1:B:345:ILE:HD13	1.81	0.61
2:E:1201:SER:HB3	2:E:1210:LEU:HD21	1.81	0.61
1:A:504:HIS:CD2	1:A:520:ARG:HE	2.18	0.61
3:D:1550:GLN:HG2	3:D:1551:PRO:HD2	1.82	0.61
2:C:1207:VAL:HA	2:C:1210:LEU:HB3	1.83	0.61
2:C:848:GLN:N	2:C:848:GLN:OE1	2.34	0.61
3:D:1692:THR:HB	3:D:1700:GLN:HB3	1.83	0.61
3:D:1643:PHE:CG	3:D:1677:LEU:HD22	2.34	0.61
3:F:1596:PRO:HB2	3:F:1598:GLN:HB2	1.83	0.61
2:E:1412:GLU:HG3	3:F:1549:VAL:HG11	1.83	0.61
1:A:598:LEU:HD12	2:C:813:LEU:O	2.01	0.60
1:A:243:VAL:HG21	1:A:345:ILE:HD13	1.82	0.60
1:B:533:VAL:HA	1:B:537:LEU:HD22	1.83	0.60
1:A:510:LEU:HD22	1:A:515:ILE:HG12	1.82	0.60
2:E:1018:LEU:HD13	2:E:1052:GLY:HA3	1.82	0.60
1:B:160:VAL:HG22	1:B:198:PHE:HB3	1.83	0.60
1:B:500:ALA:HB1	1:B:502:PHE:CE2	2.37	0.60
2:E:1340:LYS:NZ	2:E:1359:GLN:HA	2.16	0.60
1:A:131:ASN:OD1	2:C:1035:SER:HA	2.01	0.60
1:A:500:ALA:HB1	1:A:502:PHE:CE2	2.37	0.60
1:B:621:MET:SD	2:E:821:VAL:HG12	2.41	0.60
2:C:769:GLU:HG3	2:C:914:VAL:HG11	1.84	0.60
3:F:1519:GLY:O	3:F:1521:HIS:N	2.33	0.60
3:F:1551:PRO:HG3	3:F:1578:LEU:HB2	1.83	0.60
2:C:943:GLU:HB3	2:C:1381:LEU:HD13	1.84	0.60
2:C:960:ILE:HG22	2:C:1366:ILE:HD12	1.83	0.60
2:C:853:PRO:HD2	2:C:897:VAL:O	2.02	0.60
2:E:940:HIS:HB2	2:E:1386:VAL:HB	1.83	0.60
3:F:1550:GLN:HG2	3:F:1551:PRO:HD2	1.83	0.59
1:B:278:GLY:HA2	1:B:348:PRO:CD	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:960:ILE:HG22	2:E:1366:ILE:HD12	1.83	0.59
1:A:277:GLN:O	1:A:277:GLN:NE2	2.35	0.59
3:F:1717:LEU:O	3:F:1723:GLN:NE2	2.35	0.59
3:F:1692:THR:HB	3:F:1700:GLN:HB3	1.84	0.59
2:E:1340:LYS:HZ2	2:E:1359:GLN:HA	1.67	0.59
2:E:1226:ASP:OD1	2:E:1226:ASP:N	2.36	0.59
3:D:1521:HIS:CE1	3:D:1523:LEU:HD21	2.38	0.59
2:C:1412:GLU:HG3	3:D:1549:VAL:HG11	1.84	0.59
2:C:1160:GLY:O	2:C:1163:PRO:HD2	2.03	0.59
2:E:830:PHE:CZ	2:E:858:TYR:HD1	2.20	0.58
2:C:865:VAL:HG11	2:C:915:ALA:HB1	1.85	0.58
2:E:1399:ILE:HB	3:F:1472:ILE:HG22	1.85	0.58
1:A:278:GLY:HA2	1:A:348:PRO:CD	2.33	0.58
2:C:1340:LYS:NZ	2:C:1359:GLN:HA	2.18	0.58
2:E:1027:TYR:O	2:E:1031:THR:OG1	2.14	0.58
1:B:465:PRO:HB3	1:B:641:ASP:HA	1.86	0.58
1:B:251:TYR:HB2	1:B:363:VAL:CG2	2.33	0.58
1:B:599:VAL:HA	2:E:811:LEU:O	2.03	0.58
2:E:1053:TYR:CD1	2:E:1086:LEU:HD22	2.38	0.58
1:B:640:GLY:HA3	1:B:646:VAL:HG22	1.85	0.58
1:B:664:ARG:NH1	1:B:666:ARG:O	2.36	0.58
1:B:31:VAL:HB	1:B:134:PHE:HB3	1.86	0.58
1:B:33:LEU:HD21	1:B:134:PHE:HB2	1.84	0.58
2:E:865:VAL:HG11	2:E:915:ALA:HB1	1.85	0.58
2:E:1160:GLY:O	2:E:1163:PRO:HD2	2.02	0.58
2:C:1117:PHE:HD2	2:C:1142:THR:HG23	1.69	0.58
3:F:1699:PRO:HB2	3:F:1701:TYR:HE1	1.69	0.58
1:A:160:VAL:HG22	1:A:198:PHE:HB3	1.85	0.58
1:A:126:ASN:N	1:A:126:ASN:OD1	2.36	0.58
1:A:600:ALA:HA	2:C:786:VAL:HG22	1.86	0.58
1:A:153:GLY:H	1:A:204:ILE:HB	1.68	0.58
1:B:145:THR:HG1	1:B:150:TYR:HH	1.52	0.58
2:E:943:GLU:HB3	2:E:1381:LEU:HD13	1.86	0.58
2:E:1066:TYR:HD1	2:E:1079:THR:HG23	1.68	0.58
1:B:158:TYR:CE1	1:B:200:ASP:HB3	2.39	0.57
1:A:22:ARG:HH12	1:A:658:ASP:HB2	1.69	0.57
2:C:1404:LYS:O	3:D:1466:VAL:HG13	2.04	0.57
3:D:1474:ARG:HE	3:D:1477:LYS:HG3	1.69	0.57
1:B:45:ASP:HB2	1:B:548:TYR:HE2	1.69	0.57
3:D:1699:PRO:HB2	3:D:1701:TYR:HE1	1.68	0.57
3:F:1684:LEU:HD23	3:F:1710:GLU:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:LEU:HD11	1:B:44:GLN:HE21	1.69	0.57
1:B:287:LEU:HD12	1:B:338:LEU:HD23	1.86	0.57
1:A:120:SER:OG	1:A:121:LEU:N	2.37	0.57
3:F:1483:MET:HB2	3:F:1526:PHE:O	2.05	0.57
1:A:509:ILE:HG21	1:A:537:LEU:HD11	1.87	0.57
3:D:1483:MET:HB2	3:D:1526:PHE:O	2.04	0.57
1:B:293:LYS:NZ	1:B:340:VAL:HG21	2.19	0.57
2:C:874:GLY:O	2:C:904:THR:N	2.35	0.57
1:B:333:LEU:HD13	1:B:362:PHE:CE2	2.39	0.57
1:B:158:TYR:CZ	1:B:200:ASP:HB3	2.40	0.57
1:B:282:VAL:HG13	1:B:343:ALA:HB2	1.85	0.57
2:E:1153:LEU:HD11	2:E:1165:LYS:HG3	1.87	0.57
2:C:911:LEU:HD23	2:C:931:LEU:HB2	1.86	0.57
1:A:599:VAL:HA	2:C:811:LEU:O	2.05	0.56
2:C:1053:TYR:CD1	2:C:1086:LEU:HD22	2.39	0.56
2:C:761:LEU:HD11	3:D:1545:PRO:HG2	1.86	0.56
2:C:1317:ILE:O	2:C:1321:THR:OG1	2.14	0.56
2:C:1399:ILE:HB	3:D:1472:ILE:HG22	1.87	0.56
2:C:1153:LEU:HD11	2:C:1165:LYS:HG3	1.87	0.56
2:C:1272:LEU:HD21	2:C:1279:ALA:HB3	1.87	0.56
1:B:338:LEU:HD12	1:B:339:TYR:H	1.70	0.56
2:C:976:SER:HB2	2:C:1360:PHE:CD1	2.39	0.56
1:B:275:PRO:HB3	1:B:308:GLY:HA3	1.87	0.56
2:C:965:ASP:HB2	2:C:1362:LEU:HA	1.88	0.56
1:A:293:LYS:NZ	1:A:340:VAL:HG21	2.21	0.56
1:B:426:ASP:HB2	1:B:430:GLN:HB2	1.86	0.56
1:B:277:GLN:O	1:B:277:GLN:NE2	2.38	0.56
2:C:868:HIS:HB3	2:C:884:ALA:HA	1.88	0.56
2:C:940:HIS:HB2	2:C:1386:VAL:HB	1.86	0.56
3:D:1596:PRO:HB2	3:D:1598:GLN:HB2	1.88	0.56
2:E:979:ARG:NH2	2:E:1357:GLU:OE1	2.38	0.56
2:C:845:ARG:HD2	2:C:846:PHE:CE2	2.40	0.56
1:B:621:MET:HA	1:B:624:VAL:HG23	1.88	0.56
2:C:1031:THR:HB	2:C:1033:GLN:HG3	1.86	0.56
1:B:509:ILE:HG21	1:B:537:LEU:HD11	1.87	0.56
3:F:1589:GLN:HG2	3:F:1590:CYS:N	2.18	0.56
3:D:1684:LEU:HD23	3:D:1710:GLU:HB3	1.87	0.56
3:F:1643:PHE:CG	3:F:1677:LEU:HD22	2.41	0.55
1:B:391:ARG:NH1	1:B:392:GLU:OE2	2.33	0.55
1:B:278:GLY:N	1:B:305:LEU:HB2	2.18	0.55
2:E:845:ARG:HD2	2:E:846:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:VAL:HG12	1:A:425:THR:HG21	1.88	0.55
2:C:830:PHE:CZ	2:C:858:TYR:HD1	2.25	0.55
1:B:274:LYS:HG2	2:E:858:TYR:CZ	2.41	0.55
1:A:251:TYR:HB2	1:A:363:VAL:CG2	2.36	0.55
2:C:945:VAL:HG12	2:C:1379:LYS:HG2	1.89	0.55
1:A:621:MET:HA	1:A:624:VAL:HG23	1.88	0.55
1:B:627:ALA:O	1:B:630:SER:OG	2.20	0.55
2:C:1164:LEU:HA	2:C:1167:ARG:HG2	1.88	0.55
2:E:812:SER:HB3	2:E:820:CYS:HB3	1.89	0.55
2:C:762:GLN:N	2:C:886:GLN:OE1	2.37	0.55
3:D:1551:PRO:HB3	3:D:1577:ARG:O	2.07	0.55
2:E:830:PHE:HZ	2:E:858:TYR:CD1	2.23	0.55
2:E:853:PRO:HD2	2:E:897:VAL:O	2.06	0.55
2:C:877:LEU:HB3	2:C:901:VAL:HG22	1.89	0.55
3:D:1524:LEU:HB2	3:D:1526:PHE:CE1	2.36	0.55
2:E:988:THR:OG1	2:E:1323:GLU:OE1	2.25	0.55
2:E:951:LEU:HD23	2:E:1373:ASN:HD21	1.72	0.55
1:B:426:ASP:HB3	1:B:430:GLN:H	1.72	0.54
1:B:33:LEU:HD21	1:B:134:PHE:CD1	2.42	0.54
1:A:274:LYS:HG2	2:C:858:TYR:CZ	2.42	0.54
1:B:153:GLY:H	1:B:204:ILE:HB	1.72	0.54
1:B:53:LYS:O	1:B:115:PRO:HD2	2.08	0.54
1:A:426:ASP:HB2	1:A:430:GLN:HB2	1.89	0.54
2:E:895:ARG:HG2	3:F:1520:PRO:HD2	1.89	0.54
3:F:1635:ASP:HB2	3:F:1642:LEU:HB3	1.89	0.54
1:A:338:LEU:HD12	1:A:339:TYR:H	1.73	0.54
1:A:33:LEU:HD21	1:A:134:PHE:CD1	2.42	0.54
2:E:1315:TYR:O	2:E:1319:SER:N	2.35	0.54
3:F:1614:MET:HB2	3:F:1733:PHE:HD1	1.71	0.54
1:A:278:GLY:N	1:A:305:LEU:HB2	2.21	0.54
1:B:120:SER:OG	1:B:121:LEU:N	2.41	0.54
2:E:1272:LEU:HD21	2:E:1279:ALA:HB3	1.89	0.54
2:C:904:THR:HG22	2:C:905:ALA:H	1.73	0.54
2:E:911:LEU:HD23	2:E:931:LEU:HB2	1.88	0.54
2:E:877:LEU:HB3	2:E:901:VAL:HG22	1.88	0.54
1:B:205:PRO:O	1:B:208:SER:OG	2.18	0.54
1:A:125:THR:HB	1:A:127:ILE:H	1.72	0.54
1:B:606:THR:HB	2:E:805:THR:HG23	1.89	0.54
3:F:1642:LEU:HD21	3:F:1666:ASN:HB3	1.90	0.54
2:C:895:ARG:HG2	3:D:1520:PRO:HD2	1.89	0.54
3:F:1472:ILE:HD13	3:F:1529:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:PRO:HB3	1:A:308:GLY:HA3	1.89	0.54
1:A:158:TYR:CE1	1:A:200:ASP:HB3	2.43	0.54
3:D:1551:PRO:HG3	3:D:1578:LEU:HB2	1.88	0.54
2:E:978:VAL:HG22	2:E:1382:ARG:HA	1.89	0.54
2:C:1273:LEU:HD11	2:C:1315:TYR:HA	1.89	0.54
2:C:1138:THR:HG23	2:C:1178:PHE:HZ	1.73	0.54
1:A:53:LYS:O	1:A:115:PRO:HD2	2.08	0.54
1:B:81:ASP:OD2	1:B:81:ASP:N	2.28	0.54
2:C:978:VAL:HG22	2:C:1382:ARG:HA	1.90	0.54
2:E:777:PHE:HB3	2:E:801:ASP:H	1.73	0.54
3:F:1474:ARG:HE	3:F:1477:LYS:HG3	1.73	0.54
3:F:1466:VAL:HB	3:F:1494:PHE:HE2	1.73	0.54
3:D:1614:MET:HB2	3:D:1733:PHE:HD1	1.72	0.54
1:A:585:GLU:HG2	1:A:586:SER:H	1.73	0.53
1:B:642:SER:O	1:B:646:VAL:HG23	2.08	0.53
1:B:350:GLY:N	2:E:896:PRO:HD3	2.22	0.53
3:D:1493:GLY:O	3:D:1543:GLU:N	2.38	0.53
2:E:936:GLU:HG3	2:E:937:GLY:N	2.23	0.53
1:A:153:GLY:HA2	1:A:204:ILE:O	2.08	0.53
1:B:379:VAL:HG11	1:B:474:SER:HB2	1.90	0.53
2:E:1117:PHE:HD2	2:E:1142:THR:HG23	1.72	0.53
2:C:951:LEU:HD23	2:C:1373:ASN:HD21	1.74	0.53
1:A:33:LEU:CD2	1:A:134:PHE:HB2	2.38	0.53
1:A:142:PHE:CZ	1:A:624:VAL:HG13	2.43	0.53
2:C:766:LEU:HD22	2:C:866:SER:HB3	1.90	0.53
3:F:1493:GLY:O	3:F:1543:GLU:N	2.37	0.53
1:B:655:SER:OG	1:B:660:TRP:HB3	2.08	0.53
3:D:1642:LEU:HD21	3:D:1666:ASN:HB3	1.91	0.53
2:E:1273:LEU:HD11	2:E:1315:TYR:HA	1.90	0.53
1:A:604:LEU:O	2:C:806:TRP:HE3	1.91	0.53
1:B:148:PRO:HB3	1:B:616:HIS:HB3	1.91	0.53
3:F:1594:LYS:HD3	3:F:1674:ARG:NH2	2.21	0.53
2:C:1327:LEU:HD12	2:C:1329:VAL:HG23	1.90	0.53
2:E:1139:VAL:HG11	2:E:1188:LEU:HD13	1.91	0.53
1:A:207:ILE:HD12	2:C:941:ARG:NH1	2.23	0.53
1:A:655:SER:OG	1:A:660:TRP:HB3	2.08	0.53
1:A:136:SER:OG	1:A:222:GLY:HA2	2.09	0.53
2:E:1031:THR:HB	2:E:1033:GLN:HG3	1.91	0.53
3:F:1597:ARG:NH2	3:F:1599:ARG:HD2	2.22	0.52
2:E:900:SER:HB3	3:F:1578:LEU:HD12	1.90	0.52
1:B:125:THR:HB	1:B:127:ILE:H	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:GLU:OE1	1:B:445:GLN:NE2	2.42	0.52
2:E:1138:THR:HG23	2:E:1178:PHE:HZ	1.74	0.52
2:C:936:GLU:HG3	2:C:937:GLY:N	2.24	0.52
1:B:369:LEU:HD21	1:B:450:ALA:HB3	1.90	0.52
1:B:581:TYR:CD1	1:B:587:VAL:HG22	2.44	0.52
1:A:322:ALA:O	1:A:326:LEU:HG	2.09	0.52
1:B:377:HIS:ND1	1:B:640:GLY:HA2	2.24	0.52
2:C:1066:TYR:HD1	2:C:1079:THR:HG23	1.71	0.52
1:B:159:ARG:NH2	1:B:600:ALA:HB1	2.21	0.52
1:A:392:GLU:HB3	1:A:394:SER:H	1.73	0.52
1:A:593:THR:O	2:C:791:ARG:HA	2.09	0.52
2:E:1413:ALA:O	3:F:1594:LYS:NZ	2.39	0.52
1:B:146:ASP:OD1	1:B:147:GLN:HG3	2.09	0.52
3:F:1580:ALA:HB1	3:F:1591:ALA:O	2.10	0.52
2:E:970:PRO:O	2:E:1386:VAL:HA	2.09	0.52
2:C:777:PHE:HB3	2:C:801:ASP:H	1.75	0.52
1:A:81:ASP:N	1:A:81:ASP:OD2	2.30	0.52
1:B:660:TRP:N	1:B:660:TRP:CE3	2.78	0.52
2:E:868:HIS:HB3	2:E:884:ALA:HA	1.92	0.52
2:E:965:ASP:HB2	2:E:1362:LEU:HA	1.92	0.52
3:F:1527:ASP:OD1	3:F:1527:ASP:N	2.42	0.52
2:E:1413:ALA:O	3:F:1594:LYS:HG2	2.08	0.52
1:B:338:LEU:HD13	1:B:361:TYR:CZ	2.45	0.52
2:C:1139:VAL:HG11	2:C:1188:LEU:HD13	1.90	0.52
3:F:1582:LEU:HD22	3:F:1692:THR:HG22	1.92	0.52
1:A:158:TYR:CZ	1:A:200:ASP:HB3	2.44	0.52
3:F:1551:PRO:HB3	3:F:1577:ARG:O	2.10	0.52
1:A:348:PRO:HA	3:D:1521:HIS:ND1	2.24	0.52
3:D:1597:ARG:NH2	3:D:1599:ARG:HD2	2.23	0.52
1:B:598:LEU:HD12	2:E:813:LEU:O	2.09	0.52
2:E:979:ARG:HB3	2:E:1357:GLU:HB2	1.92	0.52
1:A:423:GLN:HG2	1:A:424:ASN:H	1.74	0.52
1:A:205:PRO:O	1:A:208:SER:OG	2.21	0.52
1:B:662:LEU:HD12	1:B:663:SER:H	1.74	0.52
2:C:1027:TYR:O	2:C:1031:THR:OG1	2.17	0.51
3:D:1632:LEU:HD21	3:D:1646:LYS:HB2	1.93	0.51
1:A:391:ARG:NH1	1:A:392:GLU:OE2	2.36	0.51
2:E:1279:ALA:HB3	2:E:1282:ALA:H	1.75	0.51
3:D:1472:ILE:HD13	3:D:1529:VAL:HG22	1.93	0.51
1:A:660:TRP:CE3	1:A:660:TRP:N	2.78	0.51
1:B:390:VAL:HG12	1:B:425:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASN:OD1	1:A:65:ASN:ND2	2.43	0.51
1:A:147:GLN:OE1	2:C:780:GLU:HB3	2.10	0.51
2:C:966:PRO:HB2	2:C:968:MET:O	2.10	0.51
1:B:423:GLN:HG2	1:B:424:ASN:H	1.74	0.51
2:E:852:ARG:NH2	3:F:1489:THR:OG1	2.43	0.51
1:A:570:LYS:HB3	1:A:594:ASP:H	1.75	0.51
2:C:1394:CYS:HB3	2:C:1398:GLN:HG2	1.93	0.51
1:A:443:GLU:OE1	1:A:445:GLN:NE2	2.43	0.51
2:E:945:VAL:HG12	2:E:1379:LYS:HG2	1.91	0.51
1:A:277:GLN:O	1:A:348:PRO:HD2	2.11	0.51
3:D:1635:ASP:HB2	3:D:1642:LEU:HB3	1.92	0.51
2:E:1061:LYS:HA	2:E:1065:SER:O	2.11	0.51
1:A:426:ASP:HB3	1:A:430:GLN:H	1.76	0.51
1:A:339:TYR:HB2	1:A:362:PHE:CE1	2.45	0.51
1:B:33:LEU:HD21	1:B:134:PHE:HD1	1.76	0.51
1:B:47:PRO:O	1:B:49:GLY:N	2.43	0.51
1:A:598:LEU:HD13	2:C:813:LEU:HB3	1.91	0.51
1:B:585:GLU:HG2	1:B:586:SER:H	1.75	0.51
1:B:245:ILE:HG23	1:B:266:ILE:HG12	1.93	0.51
1:B:33:LEU:CD2	1:B:134:PHE:HB2	2.41	0.51
3:D:1613:ARG:NH1	3:D:1730:LEU:HD21	2.26	0.51
2:C:1097:PRO:O	2:C:1101:GLN:HG3	2.11	0.51
1:B:348:PRO:HB3	3:F:1523:LEU:HD11	1.92	0.51
2:C:970:PRO:O	2:C:1386:VAL:HA	2.11	0.51
2:E:1327:LEU:HD12	2:E:1329:VAL:HG23	1.93	0.51
2:C:891:ALA:O	2:C:893:SER:OG	2.28	0.50
1:B:99:LEU:HD22	1:B:134:PHE:CZ	2.46	0.50
2:E:950:PRO:HG3	2:E:1368:VAL:HG12	1.92	0.50
1:B:333:LEU:HD22	1:B:362:PHE:CD1	2.46	0.50
2:C:950:PRO:HG3	2:C:1368:VAL:HG12	1.92	0.50
1:B:473:LEU:HB2	1:B:547:TYR:HE2	1.76	0.50
3:D:1731:ASN:O	3:D:1734:LEU:HB3	2.11	0.50
1:B:81:ASP:OD1	1:B:506:TYR:OH	2.16	0.50
2:C:1119:ASP:HB3	2:C:1122:PRO:HD3	1.92	0.50
1:B:150:TYR:CZ	1:B:156:VAL:HG13	2.46	0.50
2:E:904:THR:HG22	2:E:905:ALA:H	1.76	0.50
2:C:1143:ALA:O	2:C:1147:ILE:HG13	2.11	0.50
1:B:392:GLU:HB3	1:B:394:SER:H	1.77	0.50
1:B:598:LEU:HD12	1:B:598:LEU:H	1.77	0.50
1:B:22:ARG:NH1	1:B:658:ASP:HB2	2.26	0.50
2:E:966:PRO:HB2	2:E:968:MET:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1083:LEU:O	2:C:1087:SER:OG	2.19	0.50
1:B:382:ALA:HB1	1:B:383:PRO:HD2	1.93	0.50
3:D:1597:ARG:HG3	3:D:1599:ARG:HB3	1.94	0.50
1:B:66:VAL:HG13	1:B:67:PRO:HD2	1.92	0.50
2:E:1119:ASP:HB3	2:E:1122:PRO:HD3	1.92	0.50
2:C:1077:TRP:CZ2	2:C:1129:GLN:HA	2.47	0.50
1:A:282:VAL:HG13	1:A:343:ALA:HB2	1.93	0.49
2:E:1394:CYS:HB3	2:E:1398:GLN:HG2	1.93	0.49
2:C:1198:TYR:CE1	2:C:1270:LEU:HB3	2.47	0.49
3:F:1647:ILE:HD11	3:F:1665:ARG:HG2	1.94	0.49
3:D:1647:ILE:HD11	3:D:1665:ARG:HG2	1.93	0.49
1:B:506:TYR:CD2	1:B:520:ARG:HB3	2.46	0.49
3:F:1616:PHE:CE2	3:F:1621:PRO:HG3	2.48	0.49
2:C:761:LEU:HD21	3:D:1544:VAL:HG23	1.93	0.49
1:A:642:SER:O	1:A:646:VAL:HG23	2.12	0.49
1:A:475:ILE:HD13	1:A:543:PHE:HE1	1.77	0.49
1:A:385:LEU:HG	1:A:387:GLN:HG2	1.93	0.49
3:F:1632:LEU:HD21	3:F:1646:LYS:HB2	1.93	0.49
2:E:1180:GLY:HA3	2:E:1209:LEU:HD23	1.94	0.49
3:D:1647:ILE:HD12	3:D:1663:GLN:HB2	1.94	0.49
1:A:524:ARG:H	1:A:527:THR:HB	1.78	0.49
1:A:581:TYR:CD1	1:A:587:VAL:HG22	2.48	0.49
1:A:348:PRO:HB3	3:D:1523:LEU:HD11	1.95	0.49
1:B:546:PHE:HB3	1:B:555:ALA:HB2	1.94	0.49
2:E:1097:PRO:O	2:E:1101:GLN:HG3	2.13	0.49
1:A:185:ARG:HH21	2:C:1351:ILE:HG21	1.78	0.49
3:D:1631:VAL:HA	3:D:1645:THR:HG22	1.94	0.49
1:B:57:PHE:CE1	1:B:59:ARG:HD2	2.47	0.49
1:B:59:ARG:HG2	1:B:67:PRO:HA	1.94	0.49
3:D:1465:ARG:H	3:D:1465:ARG:HD2	1.78	0.49
1:A:337:ARG:HB3	1:A:362:PHE:CD1	2.47	0.49
1:A:621:MET:SD	2:C:821:VAL:HG12	2.53	0.49
1:A:484:ARG:O	1:A:487:ASP:HB2	2.12	0.49
3:F:1616:PHE:CE1	3:F:1621:PRO:HD3	2.48	0.48
3:D:1616:PHE:CE1	3:D:1621:PRO:HD3	2.48	0.48
2:C:1280:GLU:O	2:C:1284:GLN:HG3	2.13	0.48
2:E:1000:VAL:HG12	2:E:1024:ALA:HB1	1.95	0.48
2:E:1012:GLU:HG3	2:E:1068:ALA:HB2	1.95	0.48
2:C:988:THR:OG1	2:C:1323:GLU:OE1	2.24	0.48
1:B:524:ARG:H	1:B:527:THR:HB	1.77	0.48
1:B:371:LEU:HA	1:B:371:LEU:HD13	1.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1468:TYR:CE1	3:D:1490:LEU:HD22	2.48	0.48
2:C:875:LEU:HD23	2:C:903:PRO:HA	1.95	0.48
3:D:1556:LEU:HD13	3:D:1556:LEU:O	2.13	0.48
2:C:888:LEU:HD12	2:C:888:LEU:H	1.78	0.48
3:F:1613:ARG:NH1	3:F:1730:LEU:HD21	2.28	0.48
1:A:619:LEU:HA	1:A:623:LYS:HD2	1.96	0.48
2:E:1077:TRP:CZ2	2:E:1129:GLN:HA	2.49	0.48
2:E:1142:THR:O	2:E:1146:THR:OG1	2.24	0.48
1:B:427:GLY:N	1:B:429:GLY:H	2.11	0.48
2:E:759:GLU:HB3	3:F:1545:PRO:HD3	1.94	0.48
1:A:401:ILE:H	1:A:425:THR:HB	1.79	0.48
1:B:205:PRO:HB2	1:B:208:SER:HB3	1.95	0.48
1:B:277:GLN:O	1:B:348:PRO:HD2	2.14	0.48
1:A:97:CYS:SG	1:A:99:LEU:HG	2.54	0.48
2:E:976:SER:HB2	2:E:1360:PHE:CG	2.49	0.48
3:F:1625:TYR:CG	3:F:1701:TYR:HE2	2.32	0.48
1:A:640:GLY:HA3	1:A:646:VAL:HG22	1.96	0.48
1:B:322:ALA:O	1:B:326:LEU:HG	2.13	0.48
1:A:255:VAL:HA	1:A:334:GLN:OE1	2.14	0.48
1:B:35:VAL:HG21	1:B:165:GLN:HE21	1.78	0.48
1:A:371:LEU:HA	1:A:371:LEU:HD13	1.62	0.48
1:A:338:LEU:HD13	1:A:361:TYR:CZ	2.48	0.48
3:D:1582:LEU:HD22	3:D:1692:THR:HG22	1.96	0.48
2:E:1337:ASN:HB2	2:E:1340:LYS:HZ1	1.79	0.48
3:F:1652:HIS:HB2	3:F:1737:TYR:CE2	2.49	0.48
1:A:662:LEU:HD12	1:A:663:SER:H	1.76	0.48
1:A:390:VAL:CG1	1:A:425:THR:HG21	2.43	0.48
3:D:1616:PHE:CE2	3:D:1621:PRO:HG3	2.48	0.48
1:B:60:ASN:ND2	1:B:111:VAL:HG21	2.29	0.48
1:A:446:LEU:HB2	1:A:460:LEU:O	2.14	0.48
2:C:912:LYS:HG3	2:C:928:SER:HB2	1.96	0.48
3:F:1578:LEU:HG	3:F:1579:LEU:HB2	1.95	0.48
3:D:1667:PHE:HE2	3:D:1685:ILE:HG21	1.79	0.48
2:C:1315:TYR:O	2:C:1319:SER:N	2.37	0.48
2:E:1280:GLU:O	2:E:1284:GLN:HG3	2.13	0.48
1:A:386:LEU:O	1:A:432:SER:HA	2.14	0.48
3:F:1731:ASN:O	3:F:1734:LEU:HB3	2.13	0.48
2:C:1000:VAL:HG12	2:C:1024:ALA:HB1	1.93	0.48
2:E:1143:ALA:O	2:E:1147:ILE:HG13	2.14	0.48
3:F:1465:ARG:H	3:F:1465:ARG:HD2	1.79	0.48
2:C:1279:ALA:HB3	2:C:1282:ALA:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1647:ILE:HD12	3:F:1663:GLN:HB2	1.96	0.48
2:E:1370:VAL:HG12	2:E:1371:GLY:H	1.79	0.47
1:A:277:GLN:H	1:A:277:GLN:CD	2.18	0.47
1:A:598:LEU:HD12	1:A:598:LEU:H	1.79	0.47
2:C:1230:TRP:HB2	2:C:1261:TRP:CG	2.49	0.47
3:D:1652:HIS:HB2	3:D:1737:TYR:CE2	2.48	0.47
1:A:269:ARG:HG2	1:A:270:TYR:O	2.15	0.47
1:B:484:ARG:O	1:B:487:ASP:HB2	2.15	0.47
2:E:1397:LEU:HD11	3:F:1558:ASP:HB2	1.95	0.47
2:C:1322:THR:OG1	2:C:1322:THR:O	2.27	0.47
2:C:1012:GLU:HG3	2:C:1068:ALA:HB2	1.94	0.47
1:B:385:LEU:HG	1:B:387:GLN:HG2	1.97	0.47
1:A:33:LEU:HD21	1:A:134:PHE:HD1	1.79	0.47
2:C:1067:ALA:HB2	2:C:1074:SER:HA	1.96	0.47
2:E:795:LEU:HA	2:E:795:LEU:HD23	1.78	0.47
1:B:604:LEU:O	2:E:806:TRP:HE3	1.98	0.47
2:C:1397:LEU:HD11	3:D:1558:ASP:HB2	1.96	0.47
2:C:792:PHE:HZ	1:B:77:SER:HB2	1.78	0.47
1:A:205:PRO:HB2	1:A:208:SER:HB3	1.96	0.47
2:E:956:ARG:HH21	2:E:1369:LYS:NZ	2.13	0.47
1:B:475:ILE:HD13	1:B:543:PHE:HE1	1.79	0.47
2:E:1230:TRP:HB2	2:E:1261:TRP:CG	2.48	0.47
2:C:979:ARG:HB3	2:C:1357:GLU:HB2	1.96	0.47
1:A:180:ASN:HA	1:A:213:TRP:CD2	2.49	0.47
2:C:1061:LYS:HA	2:C:1065:SER:O	2.14	0.47
1:A:389:LEU:HD11	1:A:430:GLN:OE1	2.14	0.47
1:B:153:GLY:HA2	1:B:204:ILE:O	2.13	0.47
1:B:123:ARG:HH22	1:B:657:GLY:HA3	1.78	0.47
1:B:570:LYS:HB3	1:B:594:ASP:H	1.78	0.47
2:E:811:LEU:HA	2:E:811:LEU:HD23	1.64	0.47
1:B:401:ILE:H	1:B:425:THR:HB	1.80	0.47
1:B:64:ASN:HB3	1:B:66:VAL:HG23	1.97	0.47
1:A:482:PRO:HA	1:A:483:PRO:HD2	1.74	0.47
2:C:1344:LEU:HA	2:C:1344:LEU:HD23	1.78	0.47
1:A:392:GLU:HA	1:A:397:PRO:HA	1.97	0.47
1:B:373:LYS:HB3	1:B:387:GLN:HB3	1.97	0.47
1:A:99:LEU:HD22	1:A:134:PHE:CZ	2.50	0.47
2:C:1337:ASN:HB2	2:C:1340:LYS:HZ1	1.80	0.47
2:C:1029:ASP:HA	2:C:1034:TRP:HE1	1.80	0.47
1:A:64:ASN:HB3	1:A:66:VAL:HG23	1.97	0.47
1:B:142:PHE:CZ	1:B:624:VAL:HG13	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:965:ASP:HB2	2:C:1362:LEU:CA	2.46	0.46
1:B:251:TYR:CZ	1:B:366:PRO:HB3	2.51	0.46
3:F:1551:PRO:HB2	3:F:1569:PHE:HD2	1.80	0.46
2:C:1327:LEU:HA	2:C:1370:VAL:HG21	1.97	0.46
1:B:149:ILE:HA	1:B:232:GLU:O	2.16	0.46
2:E:1292:GLN:O	2:E:1295:PHE:HB2	2.15	0.46
1:B:386:LEU:O	1:B:432:SER:HA	2.15	0.46
1:A:369:LEU:HD21	1:A:450:ALA:HB3	1.97	0.46
2:E:1023:ALA:HB2	2:E:1306:VAL:HG13	1.96	0.46
2:E:783:LEU:HD22	2:E:783:LEU:HA	1.66	0.46
1:B:180:ASN:HA	1:B:213:TRP:CD2	2.50	0.46
3:F:1597:ARG:HG3	3:F:1599:ARG:HB3	1.96	0.46
1:B:142:PHE:C	1:B:143:LEU:HD23	2.36	0.46
1:A:60:ASN:ND2	1:A:111:VAL:HG21	2.30	0.46
2:C:778:PHE:CZ	2:C:929:LYS:HE2	2.51	0.46
1:B:389:LEU:HD11	1:B:430:GLN:OE1	2.16	0.46
2:C:1370:VAL:HB	2:C:1372:GLY:H	1.80	0.46
1:A:287:LEU:HD13	1:A:288:ASP:N	2.31	0.46
2:E:954:ARG:HB3	2:E:960:ILE:HG12	1.97	0.46
2:C:1061:LYS:HB3	2:C:1065:SER:H	1.80	0.46
1:B:99:LEU:HA	1:B:99:LEU:HD23	1.65	0.46
3:F:1631:VAL:HA	3:F:1645:THR:HG22	1.98	0.46
1:B:269:ARG:HG2	1:B:270:TYR:O	2.15	0.46
3:D:1688:LEU:HD13	3:D:1706:ASN:HB3	1.98	0.46
1:A:575:VAL:HG12	1:A:579:LYS:HG2	1.98	0.46
1:B:392:GLU:HA	1:B:397:PRO:HA	1.96	0.46
1:B:277:GLN:CD	1:B:277:GLN:H	2.18	0.46
1:A:605:ASP:OD2	2:C:804:THR:HG21	2.16	0.46
3:D:1628:GLN:HG3	3:D:1649:GLN:H	1.81	0.46
1:A:24:LEU:HD22	1:A:654:PHE:HE1	1.80	0.46
2:C:1107:LEU:O	2:C:1117:PHE:HE1	1.98	0.46
1:A:150:TYR:CZ	1:A:156:VAL:HG13	2.51	0.46
1:A:524:ARG:HB2	1:A:527:THR:HB	1.98	0.46
3:D:1580:ALA:HB1	3:D:1591:ALA:O	2.15	0.46
3:D:1498:ARG:O	3:D:1502:GLU:HG2	2.16	0.46
2:C:1267:TYR:CZ	2:C:1307:ILE:HG12	2.50	0.46
3:D:1527:ASP:OD1	3:D:1527:ASP:N	2.45	0.46
3:F:1500:ASP:HB3	3:F:1538:PHE:HB2	1.98	0.46
3:F:1483:MET:CE	3:F:1483:MET:H	2.29	0.46
2:C:1318:ALA:HA	2:C:1321:THR:OG1	2.16	0.46
3:D:1669:VAL:HG21	3:D:1675:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LEU:HD12	1:B:40:GLY:O	2.16	0.46
3:D:1506:SER:O	3:D:1508:SER:OG	2.24	0.46
2:E:1067:ALA:HB2	2:E:1074:SER:HA	1.97	0.46
2:E:1322:THR:O	2:E:1322:THR:OG1	2.27	0.46
1:A:271:ILE:CD1	2:C:804:THR:HG22	2.46	0.46
2:E:1206:PRO:O	2:E:1210:LEU:N	2.38	0.46
1:B:640:GLY:CA	1:B:646:VAL:HG22	2.46	0.46
1:B:213:TRP:HB2	1:B:231:PHE:CE1	2.51	0.46
2:C:889:VAL:HA	2:C:890:PRO:HD3	1.81	0.46
1:B:605:ASP:OD2	2:E:804:THR:HG21	2.15	0.46
1:B:185:ARG:HH21	2:E:1351:ILE:HG21	1.81	0.46
1:B:333:LEU:HD22	1:B:362:PHE:CE1	2.51	0.46
2:C:830:PHE:HZ	2:C:858:TYR:CD1	2.29	0.46
1:A:506:TYR:CD2	1:A:520:ARG:HB3	2.51	0.46
3:D:1643:PHE:CE2	3:D:1677:LEU:HD13	2.51	0.46
2:E:1404:LYS:O	3:F:1466:VAL:HG13	2.15	0.46
2:E:1227:ASN:HB2	2:E:1284:GLN:HB3	1.98	0.46
2:E:1029:ASP:HA	2:E:1034:TRP:HE1	1.80	0.46
3:D:1602:LEU:HD22	3:D:1713:PRO:HB3	1.98	0.46
2:C:790:ASP:C	2:C:792:PHE:H	2.19	0.46
3:D:1466:VAL:HB	3:D:1494:PHE:HE2	1.81	0.46
2:C:965:ASP:HB2	2:C:1362:LEU:N	2.31	0.46
1:B:473:LEU:HB2	1:B:547:TYR:CE2	2.51	0.46
1:A:377:HIS:ND1	1:A:640:GLY:HA2	2.31	0.46
1:B:247:PRO:HA	1:B:264:LEU:HA	1.97	0.46
1:A:552:HIS:HA	1:A:553:PRO:HD3	1.76	0.46
2:E:846:PHE:HE2	2:E:904:THR:HG23	1.81	0.45
2:C:812:SER:HB3	2:C:820:CYS:HB3	1.98	0.45
2:E:1107:LEU:O	2:E:1117:PHE:HE1	1.98	0.45
1:B:40:GLY:HA2	1:B:518:MET:HE1	1.97	0.45
2:E:850:GLU:OE1	2:E:898:ALA:HB1	2.16	0.45
1:A:479:ASP:HB2	1:A:489:LEU:HD11	1.98	0.45
2:C:956:ARG:HH21	2:C:1369:LYS:NZ	2.13	0.45
1:B:490:ASN:OD1	1:B:490:ASN:N	2.48	0.45
1:B:70:PRO:HD2	1:B:90:PRO:HD3	1.97	0.45
1:A:185:ARG:NH2	2:C:1351:ILE:HG21	2.31	0.45
2:E:1216:ASN:O	2:E:1220:MET:HG3	2.16	0.45
1:B:467:SER:C	1:B:469:GLY:H	2.19	0.45
1:B:619:LEU:HA	1:B:623:LYS:HD2	1.99	0.45
2:C:1359:GLN:OE1	2:C:1360:PHE:N	2.49	0.45
2:C:850:GLU:OE1	2:C:898:ALA:HB1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1500:ASP:O	3:D:1504:LEU:HD23	2.15	0.45
2:C:813:LEU:HD12	2:C:813:LEU:HA	1.75	0.45
2:E:968:MET:SD	2:E:970:PRO:HD2	2.56	0.45
1:A:146:ASP:OD1	1:A:147:GLN:HG3	2.16	0.45
2:C:949:ASN:HB3	2:C:952:ASP:HB2	1.97	0.45
1:A:427:GLY:N	1:A:429:GLY:H	2.15	0.45
2:C:1370:VAL:HG12	2:C:1371:GLY:H	1.81	0.45
1:A:287:LEU:HD23	1:A:293:LYS:HG2	1.98	0.45
1:A:24:LEU:HD11	1:A:44:GLN:HE21	1.81	0.45
1:B:60:ASN:OD1	1:B:65:ASN:ND2	2.49	0.45
3:D:1655:LYS:HB2	3:D:1689:ASP:OD1	2.17	0.45
2:C:1023:ALA:HB2	2:C:1306:VAL:HG13	1.99	0.45
1:A:490:ASN:OD1	1:A:490:ASN:N	2.49	0.45
3:F:1578:LEU:HD23	3:F:1579:LEU:N	2.32	0.45
2:C:936:GLU:HG3	2:C:937:GLY:H	1.80	0.45
1:B:593:THR:O	2:E:791:ARG:HA	2.16	0.45
1:B:339:TYR:HB2	1:B:362:PHE:CE1	2.51	0.45
2:E:1012:GLU:O	2:E:1016:ILE:HG13	2.16	0.45
1:B:446:LEU:HB2	1:B:460:LEU:O	2.17	0.45
3:F:1688:LEU:HD13	3:F:1706:ASN:HB3	1.99	0.45
1:A:76:LEU:HA	1:A:76:LEU:HD12	1.62	0.45
2:E:1327:LEU:HA	2:E:1370:VAL:HG21	1.98	0.45
2:E:1370:VAL:HB	2:E:1372:GLY:H	1.81	0.45
3:D:1483:MET:H	3:D:1483:MET:CE	2.30	0.45
1:A:339:TYR:HB2	1:A:362:PHE:CZ	2.51	0.45
1:A:69:SER:OG	1:A:87:LEU:HD11	2.17	0.45
2:E:994:ALA:HB1	2:E:1033:GLN:NE2	2.32	0.45
3:D:1640:PHE:HA	3:D:1669:VAL:O	2.16	0.45
2:E:1198:TYR:CE1	2:E:1270:LEU:HB3	2.52	0.45
1:B:482:PRO:HA	1:B:483:PRO:HD2	1.72	0.45
1:A:34:GLY:HA3	1:A:138:ARG:HD2	1.99	0.45
1:A:70:PRO:HD2	1:A:90:PRO:HD3	1.98	0.45
1:B:143:LEU:HD12	1:B:228:SER:HA	1.98	0.45
3:F:1640:PHE:HA	3:F:1669:VAL:O	2.17	0.45
2:C:877:LEU:HB3	2:C:901:VAL:HG13	1.98	0.45
3:F:1500:ASP:O	3:F:1504:LEU:HD23	2.17	0.45
3:D:1563:GLU:O	3:D:1565:ARG:HG2	2.16	0.45
2:E:936:GLU:HG3	2:E:937:GLY:H	1.80	0.45
1:A:287:LEU:HD12	1:A:338:LEU:CD2	2.45	0.45
2:E:775:ARG:HB3	2:E:801:ASP:HB3	1.99	0.45
1:B:84:LEU:HD13	1:B:518:MET:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1198:TYR:O	2:E:1202:LEU:HB2	2.17	0.45
1:A:576:ASP:HB2	1:A:590:HIS:CE1	2.52	0.45
1:B:161:PHE:HD1	1:B:197:ILE:HG22	1.82	0.45
1:B:162:ALA:O	1:B:163:LEU:HD23	2.17	0.45
2:C:1180:GLY:HA3	2:C:1209:LEU:HD23	1.98	0.45
1:B:185:ARG:NH1	1:B:188:LYS:HD2	2.32	0.45
1:B:598:LEU:HA	2:E:788:THR:HA	1.99	0.45
1:A:664:ARG:HG2	1:A:665:LYS:H	1.81	0.45
1:A:245:ILE:HG23	1:A:266:ILE:HG12	1.99	0.45
3:F:1669:VAL:HG21	3:F:1675:LEU:HD12	1.99	0.45
2:E:1061:LYS:HB3	2:E:1065:SER:H	1.80	0.45
2:C:1198:TYR:O	2:C:1202:LEU:HB2	2.17	0.45
1:B:479:ASP:HB2	1:B:489:LEU:HD11	1.98	0.45
2:E:1267:TYR:CZ	2:E:1307:ILE:HG12	2.52	0.45
2:C:783:LEU:HD22	2:C:783:LEU:HA	1.67	0.45
1:B:254:THR:CG2	1:B:362:PHE:HB3	2.47	0.44
1:A:534:ASP:H	1:A:537:LEU:HB2	1.81	0.44
1:A:149:ILE:HA	1:A:232:GLU:O	2.17	0.44
1:B:58:LEU:HD12	1:B:58:LEU:HA	1.86	0.44
2:E:950:PRO:HB2	2:E:1373:ASN:OD1	2.17	0.44
1:B:384:PHE:O	1:B:435:ILE:HG12	2.17	0.44
2:E:1083:LEU:O	2:E:1087:SER:OG	2.19	0.44
2:C:846:PHE:HE2	2:C:904:THR:HG23	1.82	0.44
2:E:837:LEU:HD12	2:E:853:PRO:HG3	1.99	0.44
3:F:1607:GLN:HG3	3:F:1613:ARG:HH21	1.81	0.44
1:B:91:LEU:O	1:B:94:ALA:HB3	2.17	0.44
2:E:866:SER:O	2:E:916:ARG:HG3	2.17	0.44
1:A:271:ILE:HD12	2:C:804:THR:HG22	2.00	0.44
1:A:598:LEU:HA	2:C:788:THR:HA	1.99	0.44
1:A:104:ARG:HB3	1:A:105:GLY:H	1.58	0.44
2:C:1140:ALA:O	2:C:1144:PHE:HB2	2.17	0.44
3:F:1623:VAL:HG13	3:F:1687:GLY:H	1.83	0.44
3:F:1586:GLU:H	3:F:1586:GLU:HG2	1.55	0.44
1:B:121:LEU:HD12	1:B:123:ARG:NE	2.27	0.44
3:F:1628:GLN:HG3	3:F:1649:GLN:H	1.82	0.44
1:A:58:LEU:HB2	1:A:87:LEU:HD21	1.99	0.44
3:D:1665:ARG:HA	3:D:1665:ARG:HD3	1.46	0.44
3:D:1479:GLY:C	3:D:1481:SER:H	2.19	0.44
2:E:1015:MET:HE2	2:E:1056:ILE:HG12	1.99	0.44
2:E:870:SER:HA	2:E:871:PRO:HD3	1.62	0.44
1:A:352:MET:HG2	1:A:354:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ARG:NH1	1:A:188:LYS:HD2	2.32	0.44
1:A:59:ARG:HG2	1:A:67:PRO:HA	2.00	0.44
2:E:831:ARG:C	2:E:833:PHE:H	2.20	0.44
2:C:890:PRO:HD2	2:C:893:SER:HB2	2.00	0.44
1:B:185:ARG:NH2	2:E:1351:ILE:HG21	2.33	0.44
3:F:1596:PRO:HB3	3:F:1675:LEU:HG	1.99	0.44
3:D:1596:PRO:HB3	3:D:1675:LEU:HG	2.00	0.44
2:C:1198:TYR:HA	2:C:1271:HIS:HB2	1.98	0.44
3:D:1500:ASP:HB3	3:D:1538:PHE:HB2	1.98	0.44
3:F:1667:PHE:HE2	3:F:1685:ILE:HG21	1.82	0.44
2:E:1176:ASN:HA	2:E:1179:LEU:HD12	1.99	0.44
1:B:391:ARG:HD3	1:B:392:GLU:OE1	2.17	0.44
3:D:1551:PRO:HB2	3:D:1569:PHE:HD2	1.83	0.44
3:D:1578:LEU:HA	3:D:1579:LEU:HB2	2.00	0.44
1:B:567:CYS:HB3	2:E:820:CYS:HB2	1.88	0.44
1:B:614:LYS:CD	1:B:616:HIS:HB2	2.48	0.44
1:B:644:LEU:O	1:B:647:PHE:HB2	2.18	0.44
2:E:888:LEU:HD12	2:E:888:LEU:H	1.82	0.44
2:C:811:LEU:HD23	2:C:811:LEU:HA	1.62	0.44
2:C:794:ILE:N	1:B:75:THR:HG21	2.29	0.44
3:D:1643:PHE:CD2	3:D:1677:LEU:HD22	2.52	0.44
1:A:38:SER:CB	1:A:515:ILE:H	2.30	0.44
1:A:62:SER:HB2	2:C:1029:ASP:HA	2.00	0.44
1:B:433:ILE:HA	1:B:434:PRO:HD2	1.89	0.44
1:B:391:ARG:HA	1:B:398:ALA:H	1.83	0.43
1:A:271:ILE:HG13	2:C:804:THR:HA	2.00	0.43
1:A:666:ARG:HB3	1:A:667:LEU:H	1.46	0.43
3:D:1625:TYR:CG	3:D:1701:TYR:HE2	2.36	0.43
2:C:976:SER:HB2	2:C:1360:PHE:CG	2.53	0.43
2:E:994:ALA:HB1	2:E:1033:GLN:HE22	1.83	0.43
1:B:349:GLY:C	2:E:896:PRO:HD3	2.38	0.43
1:A:306:VAL:HG23	1:A:309:GLN:O	2.17	0.43
1:A:140:HIS:ND1	1:A:167:MET:SD	2.86	0.43
1:B:168:ARG:HB3	1:B:169:PRO:HD2	1.99	0.43
2:C:831:ARG:C	2:C:833:PHE:H	2.21	0.43
1:A:143:LEU:HD12	1:A:228:SER:HA	2.00	0.43
2:C:1228:LEU:HD22	2:C:1285:ALA:HA	2.01	0.43
1:B:575:VAL:HG12	1:B:579:LYS:HG2	2.00	0.43
1:B:252:ILE:O	1:B:363:VAL:HG23	2.18	0.43
1:A:58:LEU:HD12	1:A:58:LEU:HA	1.88	0.43
2:E:875:LEU:HD23	2:E:903:PRO:HA	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:954:ARG:HB3	2:C:960:ILE:HG12	2.00	0.43
2:C:1318:ALA:O	2:C:1321:THR:HB	2.18	0.43
1:A:25:LEU:HD12	1:A:40:GLY:O	2.18	0.43
2:C:1015:MET:HE2	2:C:1056:ILE:HG12	1.99	0.43
2:C:1293:GLY:HA2	2:C:1300:ARG:NH2	2.33	0.43
2:E:1386:VAL:HG22	2:E:1388:ASP:H	1.84	0.43
1:A:147:GLN:H	1:A:150:TYR:HH	1.66	0.43
1:A:66:VAL:HG13	1:A:67:PRO:HD2	1.99	0.43
3:D:1623:VAL:HG13	3:D:1687:GLY:H	1.82	0.43
2:C:1292:GLN:O	2:C:1295:PHE:HB2	2.18	0.43
1:A:389:LEU:HG	1:A:430:GLN:HA	2.00	0.43
1:B:348:PRO:HA	3:F:1521:HIS:CE1	2.53	0.43
3:D:1468:TYR:HH	3:D:1570:TYR:HH	1.62	0.43
1:B:390:VAL:CG1	1:B:425:THR:HG21	2.48	0.43
2:C:1182:LYS:O	2:C:1188:LEU:HD21	2.19	0.43
1:B:389:LEU:CB	1:B:391:ARG:HG3	2.44	0.43
1:B:567:CYS:HA	1:B:621:MET:HE2	2.00	0.43
1:B:598:LEU:HD13	2:E:813:LEU:HB3	2.00	0.43
1:A:22:ARG:NH1	1:A:658:ASP:HB2	2.33	0.43
2:E:1000:VAL:HG11	2:E:1028:LEU:HG	2.00	0.43
1:B:591:LEU:HD21	1:B:601:LEU:HD11	2.00	0.43
2:C:781:ASN:OD1	2:C:782:TRP:N	2.51	0.43
1:A:546:PHE:HB3	1:A:555:ALA:HB2	2.01	0.43
1:B:574:SER:OG	1:B:590:HIS:HB2	2.18	0.43
1:A:391:ARG:HD3	1:A:392:GLU:OE1	2.19	0.43
2:E:830:PHE:CZ	2:E:858:TYR:CD1	3.02	0.43
3:D:1665:ARG:NH1	3:D:1699:PRO:HD2	2.33	0.43
2:C:843:VAL:HG11	2:C:931:LEU:HD11	2.00	0.43
2:E:1140:ALA:O	2:E:1144:PHE:HB2	2.18	0.43
3:D:1626:GLY:HA2	3:D:1685:ILE:O	2.19	0.43
1:A:583:ASN:HD22	2:C:831:ARG:HD3	1.84	0.43
3:F:1725:ALA:HA	3:F:1728:ALA:HB3	2.00	0.43
3:F:1689:ASP:N	3:F:1689:ASP:OD2	2.50	0.43
1:B:42:GLN:HG2	1:B:43:LEU:H	1.83	0.43
1:B:666:ARG:HB3	1:B:667:LEU:H	1.47	0.43
1:B:245:ILE:HD11	1:B:356:GLU:C	2.40	0.43
3:F:1524:LEU:HB2	3:F:1526:PHE:CE1	2.42	0.43
2:E:1191:HIS:O	2:E:1195:ILE:HG22	2.18	0.43
2:E:766:LEU:O	2:E:767:ILE:HD13	2.18	0.43
3:D:1468:TYR:OH	3:D:1570:TYR:OH	2.33	0.43
2:E:819:LEU:HD22	2:E:820:CYS:N	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:843:VAL:HG11	2:E:931:LEU:HD11	2.01	0.43
3:D:1607:GLN:HG3	3:D:1613:ARG:HH21	1.83	0.43
2:E:1126:ARG:NH1	2:E:1129:GLN:OE1	2.50	0.43
2:E:1198:TYR:HA	2:E:1271:HIS:HB2	2.00	0.43
1:B:583:ASN:HD22	2:E:831:ARG:HD3	1.84	0.43
2:E:1048:LEU:HD12	2:E:1048:LEU:HA	1.80	0.43
1:B:352:MET:HG2	1:B:354:GLU:OE2	2.18	0.42
1:A:287:LEU:O	1:A:338:LEU:HB3	2.19	0.42
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.71	0.42
2:C:1405:GLY:HA3	3:D:1466:VAL:HG22	2.00	0.42
1:A:142:PHE:C	1:A:143:LEU:HD23	2.39	0.42
1:A:145:THR:OG1	1:A:150:TYR:OH	2.28	0.42
2:E:1000:VAL:HB	2:E:1028:LEU:HD11	2.01	0.42
2:C:986:LEU:HD13	2:C:1350:GLN:HE22	1.84	0.42
3:D:1586:GLU:HG2	3:D:1586:GLU:H	1.60	0.42
2:E:1329:VAL:HA	2:E:1367:ASN:O	2.18	0.42
2:E:965:ASP:HB2	2:E:1362:LEU:CA	2.49	0.42
1:B:76:LEU:HA	1:B:76:LEU:HD12	1.65	0.42
1:A:348:PRO:HB3	3:D:1523:LEU:CD1	2.48	0.42
2:E:790:ASP:C	2:E:792:PHE:H	2.23	0.42
1:A:510:LEU:HD11	1:A:652:LEU:HG	2.01	0.42
1:B:146:ASP:HB2	1:B:157:ARG:O	2.19	0.42
2:E:1079:THR:HG22	2:E:1103:THR:HG23	2.01	0.42
2:C:1079:THR:HG22	2:C:1103:THR:HG23	2.01	0.42
2:E:807:GLU:HG3	2:E:826:GLN:OE1	2.20	0.42
2:C:1216:ASN:O	2:C:1220:MET:HG3	2.19	0.42
1:A:473:LEU:HB2	1:A:547:TYR:HE2	1.83	0.42
2:E:778:PHE:N	2:E:779:PRO:HD3	2.35	0.42
1:B:46:VAL:HA	1:B:47:PRO:HD3	1.71	0.42
1:B:534:ASP:H	1:B:537:LEU:HB2	1.83	0.42
1:B:102:LEU:HD22	1:B:103:LEU:H	1.84	0.42
1:B:146:ASP:HB3	1:B:150:TYR:OH	2.19	0.42
2:C:1386:VAL:HG22	2:C:1388:ASP:H	1.84	0.42
1:A:574:SER:OG	1:A:590:HIS:HB2	2.19	0.42
2:C:981:THR:HG22	2:C:1355:GLU:HB2	2.01	0.42
2:C:889:VAL:CG2	2:C:895:ARG:HB2	2.41	0.42
1:A:485:VAL:HA	1:A:533:VAL:CG1	2.48	0.42
2:E:1358:LEU:O	2:E:1359:GLN:HB2	2.19	0.42
2:E:1159:GLU:HA	2:E:1162:GLU:HB2	2.01	0.42
1:B:423:GLN:HG2	1:B:424:ASN:N	2.34	0.42
2:E:1228:LEU:HD22	2:E:1285:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:GLU:OE1	1:B:352:MET:N	2.53	0.42
2:E:1331:LEU:O	2:E:1341:SER:HA	2.20	0.42
3:F:1723:GLN:CD	3:F:1723:GLN:H	2.23	0.42
2:C:1022:LEU:O	2:C:1025:SER:HB3	2.20	0.42
3:D:1501:LEU:HA	3:D:1501:LEU:HD23	1.74	0.42
2:C:1329:VAL:HA	2:C:1367:ASN:O	2.18	0.42
2:E:889:VAL:HA	2:E:890:PRO:HD3	1.87	0.42
1:B:598:LEU:HB3	2:E:788:THR:HG22	2.01	0.42
1:A:269:ARG:HG3	1:A:274:LYS:C	2.40	0.42
2:C:950:PRO:HB2	2:C:1373:ASN:OD1	2.19	0.42
2:C:1191:HIS:O	2:C:1195:ILE:HG22	2.20	0.42
1:A:247:PRO:HA	1:A:264:LEU:HA	2.02	0.42
2:E:1196:THR:O	2:E:1200:LEU:HD12	2.20	0.42
1:A:382:ALA:HB1	1:A:383:PRO:HD2	2.01	0.42
1:B:319:PHE:HA	1:B:319:PHE:HD1	1.75	0.42
2:C:958:LEU:HA	2:C:958:LEU:HD23	1.91	0.42
1:B:244:LYS:HD3	1:B:244:LYS:HA	1.83	0.42
3:D:1704:ASP:OD2	3:D:1704:ASP:N	2.53	0.42
1:A:598:LEU:HB3	2:C:788:THR:HG22	2.01	0.42
1:A:337:ARG:HA	1:A:337:ARG:HD3	1.80	0.42
1:A:31:VAL:O	1:A:134:PHE:HA	2.19	0.42
2:E:877:LEU:HB3	2:E:901:VAL:HG13	2.00	0.42
2:C:775:ARG:HB3	2:C:801:ASP:HB3	2.02	0.42
3:F:1602:LEU:HD22	3:F:1713:PRO:HB3	2.01	0.42
2:C:774:VAL:HB	2:C:926:ALA:HB3	2.02	0.42
2:E:1221:ALA:HA	2:E:1229:TYR:CD1	2.54	0.42
1:A:573:LEU:HD11	2:C:810:GLY:HA3	2.01	0.42
3:F:1666:ASN:ND2	3:F:1694:ASP:OD2	2.52	0.42
3:D:1723:GLN:CD	3:D:1723:GLN:H	2.23	0.42
2:E:777:PHE:O	2:E:801:ASP:HB2	2.20	0.42
2:E:1061:LYS:HB3	2:E:1065:SER:N	2.34	0.42
2:E:886:GLN:HE21	2:E:886:GLN:HB3	1.70	0.42
1:A:245:ILE:HD11	1:A:356:GLU:C	2.40	0.42
2:E:845:ARG:HD2	2:E:846:PHE:CZ	2.55	0.42
3:D:1667:PHE:CE2	3:D:1685:ILE:HG21	2.55	0.42
3:D:1493:GLY:O	3:D:1543:GLU:HG3	2.19	0.42
2:E:1186:GLY:O	2:E:1216:ASN:ND2	2.53	0.42
1:B:576:ASP:HB2	1:B:590:HIS:CE1	2.55	0.42
2:C:857:ASN:OD1	2:C:859:LEU:HB2	2.20	0.42
1:A:627:ALA:O	1:A:630:SER:OG	2.22	0.42
2:C:1331:LEU:HD23	2:C:1331:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1132:LEU:O	2:E:1137:GLU:HG2	2.20	0.42
2:C:790:ASP:O	2:C:792:PHE:N	2.50	0.41
1:B:232:GLU:OE1	1:B:614:LYS:HB3	2.20	0.41
1:B:150:TYR:OH	1:B:156:VAL:HG13	2.20	0.41
1:B:59:ARG:CG	1:B:67:PRO:HA	2.50	0.41
1:B:524:ARG:HB2	1:B:527:THR:HB	2.01	0.41
2:C:1196:THR:O	2:C:1200:LEU:HD12	2.20	0.41
3:F:1479:GLY:C	3:F:1481:SER:H	2.22	0.41
2:E:1325:ARG:HG3	2:E:1348:ASN:HB2	2.02	0.41
2:C:795:LEU:HA	2:C:795:LEU:HD23	1.79	0.41
3:D:1702:LEU:HD12	3:D:1702:LEU:HA	1.83	0.41
2:E:1084:LYS:HE3	2:E:1151:HIS:NE2	2.35	0.41
1:A:597:ALA:HB1	2:C:813:LEU:O	2.20	0.41
2:C:845:ARG:HD2	2:C:846:PHE:CZ	2.55	0.41
2:E:1182:LYS:O	2:E:1188:LEU:HD21	2.19	0.41
2:C:960:ILE:HG23	2:C:961:PRO:HD2	2.01	0.41
1:B:269:ARG:HH21	1:B:275:PRO:HG3	1.85	0.41
2:C:866:SER:O	2:C:916:ARG:HG3	2.19	0.41
3:D:1623:VAL:HG11	3:D:1686:MET:HB3	2.03	0.41
2:E:1004:LEU:O	2:E:1021:THR:OG1	2.25	0.41
2:C:1132:LEU:HD21	2:C:1141:LEU:HB2	2.02	0.41
1:B:37:LEU:HD12	1:B:39:VAL:HG22	2.02	0.41
2:C:1072:ARG:HA	2:C:1072:ARG:HD3	1.79	0.41
3:F:1597:ARG:HD2	3:F:1597:ARG:HA	1.86	0.41
1:B:42:GLN:HE22	1:B:546:PHE:HZ	1.66	0.41
1:B:654:PHE:O	1:B:660:TRP:HA	2.20	0.41
1:A:47:PRO:O	1:A:49:GLY:N	2.54	0.41
2:C:1206:PRO:O	2:C:1210:LEU:N	2.41	0.41
3:F:1621:PRO:CG	3:F:1623:VAL:HG23	2.50	0.41
2:E:965:ASP:HB2	2:E:1362:LEU:N	2.34	0.41
2:E:1096:SER:HB3	2:E:1099:LYS:HD2	2.02	0.41
1:B:505:TYR:HE2	1:B:527:THR:HG21	1.84	0.41
2:E:949:ASN:HB3	2:E:952:ASP:HB2	2.02	0.41
3:F:1625:TYR:HB2	3:F:1627:PHE:CZ	2.55	0.41
3:F:1468:TYR:CE1	3:F:1490:LEU:HD22	2.54	0.41
3:D:1608:ASP:CG	3:D:1610:ASP:HB2	2.40	0.41
1:A:436:ILE:HD13	1:A:436:ILE:HA	1.89	0.41
2:E:1359:GLN:OE1	2:E:1360:PHE:N	2.52	0.41
2:E:960:ILE:HG23	2:E:961:PRO:HD2	2.01	0.41
2:E:1162:GLU:O	2:E:1165:LYS:HB3	2.21	0.41
2:C:1399:ILE:HG21	3:D:1556:LEU:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1607:GLN:HG3	3:F:1613:ARG:NH2	2.35	0.41
1:A:57:PHE:CE1	1:A:59:ARG:HD2	2.55	0.41
3:D:1725:ALA:HA	3:D:1728:ALA:HB3	2.02	0.41
2:E:781:ASN:OD1	2:E:782:TRP:N	2.54	0.41
1:A:33:LEU:HD13	1:A:33:LEU:HA	1.81	0.41
1:B:287:LEU:HD13	1:B:288:ASP:N	2.36	0.41
1:A:591:LEU:HD21	1:A:601:LEU:HD11	2.02	0.41
2:C:984:ASP:HA	2:C:985:PRO:HD2	1.93	0.41
1:A:465:PRO:HA	1:A:466:PRO:HD3	2.00	0.41
1:A:582:ARG:HB2	1:A:585:GLU:OE2	2.21	0.41
2:E:1007:PRO:HG3	2:E:1052:GLY:HA2	2.03	0.41
1:A:380:PRO:HD3	1:A:465:PRO:HG2	2.03	0.41
1:B:41:VAL:HG12	1:B:83:ALA:O	2.19	0.41
1:A:352:MET:CE	2:C:838:ARG:HG3	2.50	0.41
2:E:1061:LYS:HE3	2:E:1099:LYS:HG2	2.02	0.41
2:E:1005:ARG:O	2:E:1048:LEU:HD21	2.20	0.41
1:B:406:SER:HB2	1:B:420:ASP:OD1	2.20	0.41
3:F:1530:PRO:CG	3:F:1534:GLU:HB2	2.50	0.41
1:B:436:ILE:HD13	1:B:436:ILE:HA	1.90	0.41
2:C:797:LEU:HD23	2:C:797:LEU:HA	1.76	0.41
1:A:373:LYS:HB3	1:A:387:GLN:HB3	2.02	0.41
1:B:287:LEU:HD23	1:B:293:LYS:HG2	2.02	0.41
2:C:768:ASP:O	2:C:769:GLU:HB3	2.21	0.41
1:B:376:ARG:O	1:B:377:HIS:HB2	2.19	0.41
2:E:941:ARG:HB2	2:E:1381:LEU:HD11	2.03	0.41
2:E:1119:ASP:HA	2:E:1120:PRO:HD2	1.98	0.41
2:C:1012:GLU:O	2:C:1016:ILE:HG13	2.20	0.41
1:B:180:ASN:HB2	1:B:213:TRP:CE2	2.56	0.41
1:A:103:LEU:HD22	2:C:1316:TRP:CZ3	2.56	0.41
2:C:1004:LEU:O	2:C:1021:THR:OG1	2.23	0.41
1:A:384:PHE:O	1:A:435:ILE:HG12	2.21	0.41
2:E:1022:LEU:O	2:E:1025:SER:HB3	2.21	0.41
1:A:91:LEU:O	1:A:94:ALA:HB3	2.21	0.41
1:B:245:ILE:HD11	1:B:356:GLU:HB3	2.03	0.41
1:A:238:LEU:HA	1:A:239:PRO:HD2	1.82	0.41
3:D:1714:SER:N	3:D:1717:LEU:HB2	2.36	0.41
2:C:978:VAL:HG13	2:C:1381:LEU:O	2.20	0.41
3:F:1643:PHE:CE2	3:F:1677:LEU:HD13	2.55	0.41
2:C:766:LEU:O	2:C:767:ILE:HD13	2.20	0.41
1:A:475:ILE:HD13	1:A:543:PHE:CE1	2.56	0.41
2:C:1331:LEU:O	2:C:1341:SER:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:823:THR:HA	2:E:824:PRO:HD3	1.88	0.41
2:C:792:PHE:CZ	1:B:77:SER:HB2	2.55	0.40
1:A:123:ARG:HH22	1:A:657:GLY:HA3	1.86	0.40
3:D:1666:ASN:ND2	3:D:1694:ASP:OD2	2.54	0.40
2:C:994:ALA:HB1	2:C:1033:GLN:NE2	2.36	0.40
1:B:506:TYR:CE2	1:B:520:ARG:HD2	2.55	0.40
3:D:1714:SER:H	3:D:1717:LEU:HB2	1.86	0.40
2:C:1061:LYS:HE3	2:C:1099:LYS:HG2	2.03	0.40
1:A:267:GLN:HG2	1:A:309:GLN:HG2	2.02	0.40
2:C:1325:ARG:HG3	2:C:1348:ASN:HB2	2.03	0.40
3:F:1704:ASP:OD2	3:F:1704:ASP:N	2.54	0.40
3:D:1651:LEU:HD22	3:D:1651:LEU:HA	1.94	0.40
1:B:44:GLN:OE1	1:B:548:TYR:CD1	2.74	0.40
3:F:1665:ARG:HD3	3:F:1665:ARG:HA	1.45	0.40
3:D:1625:TYR:HE1	3:D:1685:ILE:HG22	1.86	0.40
1:A:168:ARG:HB3	1:A:169:PRO:HD2	2.02	0.40
2:C:1358:LEU:O	2:C:1359:GLN:HB2	2.21	0.40
1:B:502:PHE:CE1	1:B:523:LYS:HD2	2.56	0.40
2:C:1412:GLU:HG3	3:D:1549:VAL:CG1	2.52	0.40
2:C:1165:LYS:O	2:C:1169:GLU:HG2	2.22	0.40
1:A:213:TRP:HB2	1:A:231:PHE:CE1	2.56	0.40
1:B:180:ASN:HB2	1:B:213:TRP:CZ2	2.56	0.40
1:A:473:LEU:HB2	1:A:547:TYR:CE2	2.57	0.40
3:F:1608:ASP:CG	3:F:1610:ASP:HB2	2.41	0.40
2:E:1293:GLY:HA2	2:E:1300:ARG:NH2	2.37	0.40
1:B:597:ALA:CB	2:E:814:SER:HB3	2.47	0.40
1:B:33:LEU:HA	1:B:33:LEU:HD13	1.84	0.40
1:B:254:THR:HG21	1:B:333:LEU:HB3	2.01	0.40
2:E:848:GLN:CD	2:E:848:GLN:N	2.74	0.40
2:E:1331:LEU:HD23	2:E:1366:ILE:HA	2.04	0.40
1:B:377:HIS:HD1	1:B:640:GLY:HA2	1.84	0.40
3:F:1656:ASP:OD1	3:F:1699:PRO:HG2	2.21	0.40
2:C:1061:LYS:HB3	2:C:1065:SER:N	2.36	0.40
3:D:1623:VAL:HG11	3:D:1686:MET:HG2	2.03	0.40
3:F:1530:PRO:HG3	3:F:1534:GLU:HB2	2.04	0.40
1:B:131:ASN:OD1	2:E:1035:SER:HA	2.22	0.40
3:D:1486:ALA:HB3	3:D:1524:LEU:HD12	2.03	0.40
1:A:46:VAL:HA	1:A:47:PRO:HD3	1.70	0.40
2:E:813:LEU:HD13	2:E:819:LEU:HD23	2.03	0.40
3:F:1493:GLY:HA3	3:F:1544:VAL:HG13	2.02	0.40
2:E:1061:LYS:H	2:E:1061:LYS:HZ3	1.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1132:LEU:O	2:C:1137:GLU:HG2	2.22	0.40
1:B:131:ASN:O	1:B:132:LEU:HD23	2.21	0.40
1:A:644:LEU:O	1:A:647:PHE:HB2	2.21	0.40
2:C:1168:VAL:O	2:C:1172:ILE:HG12	2.21	0.40
3:F:1623:VAL:HG11	3:F:1686:MET:HB3	2.03	0.40
2:E:1006:LEU:HA	2:E:1007:PRO:HD2	1.87	0.40
1:B:147:GLN:OE1	2:E:780:GLU:HB3	2.21	0.40
3:F:1493:GLY:O	3:F:1543:GLU:HG3	2.21	0.40
2:E:1019:ALA:N	2:E:1020:PRO:HD2	2.37	0.40
1:B:573:LEU:HD11	2:E:810:GLY:HA3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1135:ASN:OD1	1:B:20:LYS:N[1_655]	2.07	0.13

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	649/656 (99%)	611 (94%)	36 (6%)	2 (0%)	46 83
1	B	649/656 (99%)	612 (94%)	35 (5%)	2 (0%)	46 83
2	C	628/690 (91%)	573 (91%)	53 (8%)	2 (0%)	46 83
2	E	628/690 (91%)	573 (91%)	53 (8%)	2 (0%)	46 83
3	D	279/291 (96%)	242 (87%)	37 (13%)	0	100 100
3	F	279/291 (96%)	241 (86%)	38 (14%)	0	100 100
All	All	3112/3274 (95%)	2852 (92%)	252 (8%)	8 (0%)	46 83

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	1228	LEU
1	A	63	ARG
1	B	63	ARG
2	E	1228	LEU
2	C	791	ARG
2	E	791	ARG
1	A	453	PRO
1	B	453	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	557/562 (99%)	467 (84%)	90 (16%)	3	22
1	B	557/562 (99%)	462 (83%)	95 (17%)	2	19
2	C	524/575 (91%)	436 (83%)	88 (17%)	2	20
2	E	524/575 (91%)	436 (83%)	88 (17%)	2	20
3	D	240/249 (96%)	194 (81%)	46 (19%)	2	14
3	F	240/249 (96%)	197 (82%)	43 (18%)	2	17
All	All	2642/2772 (95%)	2192 (83%)	450 (17%)	2	20

All (450) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	55	SER
1	A	56	VAL
1	A	57	PHE
1	A	62	SER
1	A	73	ASP
1	A	79	GLU
1	A	88	GLN
1	A	101	GLN
1	A	102	LEU
1	A	117	LEU

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Mol	Chain	Res	Type
1	A	124	THR
1	A	126	ASN
1	A	130	ILE
1	A	133	LEU
1	A	145	THR
1	A	159	ARG
1	A	172	ASP
1	A	176	VAL
1	A	182	HIS
1	A	184	LEU
1	A	193	MET
1	A	195	SER
1	A	201	ASP
1	A	203	VAL
1	A	207	ILE
1	A	218	ARG
1	A	221	ASP
1	A	223	LEU
1	A	226	ASN
1	A	238	LEU
1	A	240	ASN
1	A	245	ILE
1	A	246	THR
1	A	254	THR
1	A	255	VAL
1	A	262	MET
1	A	265	ASP
1	A	271	ILE
1	A	277	GLN
1	A	288	ASP
1	A	303	THR
1	A	306	VAL
1	A	319	PHE
1	A	336	LEU
1	A	337	ARG
1	A	340	VAL
1	A	347	SER
1	A	351	GLU
1	A	357	LEU
1	A	360	TRP
1	A	363	VAL
1	A	371	LEU

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Mol	Chain	Res	Type
1	A	372	SER
1	A	376	ARG
1	A	378	LEU
1	A	390	VAL
1	A	401	ILE
1	A	410	SER
1	A	411	SER
1	A	418	VAL
1	A	419	GLN
1	A	436	ILE
1	A	439	GLN
1	A	446	LEU
1	A	452	SER
1	A	454	HIS
1	A	457	ILE
1	A	460	LEU
1	A	479	ASP
1	A	481	ARG
1	A	490	ASN
1	A	520	ARG
1	A	527	THR
1	A	530	SER
1	A	535	HIS
1	A	551	ASP
1	A	576	ASP
1	A	589	LEU
1	A	595	SER
1	A	596	LEU
1	A	598	LEU
1	A	617	LYS
1	A	635	CYS
1	A	642	SER
1	A	654	PHE
1	A	660	TRP
1	A	662	LEU
1	A	664	ARG
1	A	667	LEU
2	C	759	GLU
2	C	765	ASP
2	C	766	LEU
2	C	767	ILE
2	C	774	VAL

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Mol	Chain	Res	Type
2	C	775	ARG
2	C	777	PHE
2	C	783	LEU
2	C	785	ARG
2	C	793	GLN
2	C	796	THR
2	C	798	TRP
2	C	801	ASP
2	C	828	ARG
2	C	829	VAL
2	C	833	PHE
2	C	836	HIS
2	C	837	LEU
2	C	838	ARG
2	C	845	ARG
2	C	848	GLN
2	C	849	LEU
2	C	850	GLU
2	C	864	THR
2	C	876	CYS
2	C	877	LEU
2	C	888	LEU
2	C	893	SER
2	C	895	ARG
2	C	916	ARG
2	C	919	PHE
2	C	931	LEU
2	C	939	ILE
2	C	944	LEU
2	C	949	ASN
2	C	951	LEU
2	C	953	HIS
2	C	964	SER
2	C	965	ASP
2	C	971	ASP
2	C	977	TYR
2	C	987	ASP
2	C	992	GLU
2	C	995	LEU
2	C	1005	ARG
2	C	1015	MET
2	C	1029	ASP

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Mol	Chain	Res	Type
2	C	1031	THR
2	C	1032	GLU
2	C	1035	SER
2	C	1036	THR
2	C	1037	LEU
2	C	1041	THR
2	C	1060	ARG
2	C	1103	THR
2	C	1136	ASP
2	C	1139	VAL
2	C	1162	GLU
2	C	1200	LEU
2	C	1202	LEU
2	C	1203	THR
2	C	1210	LEU
2	C	1226	ASP
2	C	1227	ASN
2	C	1267	TYR
2	C	1273	LEU
2	C	1275	HIS
2	C	1281	MET
2	C	1304	ASP
2	C	1327	LEU
2	C	1328	ASN
2	C	1341	SER
2	C	1342	HIS
2	C	1347	ASN
2	C	1348	ASN
2	C	1357	GLU
2	C	1367	ASN
2	C	1370	VAL
2	C	1378	LEU
2	C	1387	LEU
2	C	1393	THR
2	C	1396	ASP
2	C	1399	ILE
2	C	1401	VAL
2	C	1402	THR
2	C	1406	HIS
2	C	1410	THR
2	C	1411	MET
3	D	1465	ARG

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Mol	Chain	Res	Type
3	D	1468	TYR
3	D	1477	LYS
3	D	1480	LEU
3	D	1481	SER
3	D	1483	MET
3	D	1497	LEU
3	D	1500	ASP
3	D	1505	THR
3	D	1509	ASP
3	D	1512	VAL
3	D	1524	LEU
3	D	1527	ASP
3	D	1538	PHE
3	D	1541	VAL
3	D	1543	GLU
3	D	1544	VAL
3	D	1548	LEU
3	D	1549	VAL
3	D	1550	GLN
3	D	1556	LEU
3	D	1557	TYR
3	D	1577	ARG
3	D	1584	SER
3	D	1587	VAL
3	D	1590	CYS
3	D	1592	GLU
3	D	1606	LEU
3	D	1608	ASP
3	D	1612	TYR
3	D	1620	TYR
3	D	1627	PHE
3	D	1629	VAL
3	D	1632	LEU
3	D	1642	LEU
3	D	1651	LEU
3	D	1665	ARG
3	D	1673	CYS
3	D	1674	ARG
3	D	1684	LEU
3	D	1686	MET
3	D	1693	TYR
3	D	1721	THR

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Mol	Chain	Res	Type
3	D	1730	LEU
3	D	1731	ASN
3	D	1733	PHE
1	B	37	LEU
1	B	55	SER
1	B	56	VAL
1	B	57	PHE
1	B	62	SER
1	B	73	ASP
1	B	80	ARG
1	B	88	GLN
1	B	101	GLN
1	B	102	LEU
1	B	103	LEU
1	B	117	LEU
1	B	124	THR
1	B	126	ASN
1	B	130	ILE
1	B	133	LEU
1	B	145	THR
1	B	159	ARG
1	B	172	ASP
1	B	176	VAL
1	B	182	HIS
1	B	184	LEU
1	B	193	MET
1	B	195	SER
1	B	201	ASP
1	B	203	VAL
1	B	207	ILE
1	B	218	ARG
1	B	221	ASP
1	B	223	LEU
1	B	226	ASN
1	B	238	LEU
1	B	240	ASN
1	B	245	ILE
1	B	254	THR
1	B	255	VAL
1	B	262	MET
1	B	264	LEU
1	B	265	ASP

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Mol	Chain	Res	Type
1	B	271	ILE
1	B	277	GLN
1	B	288	ASP
1	B	303	THR
1	B	306	VAL
1	B	319	PHE
1	B	336	LEU
1	B	337	ARG
1	B	340	VAL
1	B	347	SER
1	B	351	GLU
1	B	357	LEU
1	B	360	TRP
1	B	363	VAL
1	B	371	LEU
1	B	372	SER
1	B	376	ARG
1	B	378	LEU
1	B	390	VAL
1	B	401	ILE
1	B	410	SER
1	B	411	SER
1	B	418	VAL
1	B	419	GLN
1	B	436	ILE
1	B	439	GLN
1	B	446	LEU
1	B	452	SER
1	B	454	HIS
1	B	457	ILE
1	B	460	LEU
1	B	479	ASP
1	B	481	ARG
1	B	490	ASN
1	B	519	ASN
1	B	520	ARG
1	B	527	THR
1	B	530	SER
1	B	535	HIS
1	B	544	VAL
1	B	551	ASP
1	B	576	ASP

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Mol	Chain	Res	Type
1	B	589	LEU
1	B	595	SER
1	B	596	LEU
1	B	598	LEU
1	B	617	LYS
1	B	635	CYS
1	B	642	SER
1	B	644	LEU
1	B	654	PHE
1	B	660	TRP
1	B	662	LEU
1	B	663	SER
1	B	664	ARG
1	B	667	LEU
2	E	759	GLU
2	E	765	ASP
2	E	766	LEU
2	E	767	ILE
2	E	774	VAL
2	E	777	PHE
2	E	783	LEU
2	E	785	ARG
2	E	793	GLN
2	E	796	THR
2	E	798	TRP
2	E	801	ASP
2	E	828	ARG
2	E	829	VAL
2	E	833	PHE
2	E	836	HIS
2	E	837	LEU
2	E	838	ARG
2	E	845	ARG
2	E	848	GLN
2	E	849	LEU
2	E	850	GLU
2	E	864	THR
2	E	876	CYS
2	E	877	LEU
2	E	888	LEU
2	E	893	SER
2	E	895	ARG

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Mol	Chain	Res	Type
2	E	904	THR
2	E	916	ARG
2	E	919	PHE
2	E	931	LEU
2	E	939	ILE
2	E	944	LEU
2	E	949	ASN
2	E	951	LEU
2	E	953	HIS
2	E	964	SER
2	E	965	ASP
2	E	971	ASP
2	E	977	TYR
2	E	987	ASP
2	E	992	GLU
2	E	995	LEU
2	E	1005	ARG
2	E	1029	ASP
2	E	1031	THR
2	E	1032	GLU
2	E	1035	SER
2	E	1036	THR
2	E	1037	LEU
2	E	1041	THR
2	E	1060	ARG
2	E	1103	THR
2	E	1136	ASP
2	E	1139	VAL
2	E	1162	GLU
2	E	1200	LEU
2	E	1202	LEU
2	E	1203	THR
2	E	1210	LEU
2	E	1226	ASP
2	E	1227	ASN
2	E	1228	LEU
2	E	1267	TYR
2	E	1273	LEU
2	E	1275	HIS
2	E	1281	MET
2	E	1304	ASP
2	E	1327	LEU

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Mol	Chain	Res	Type
2	E	1328	ASN
2	E	1341	SER
2	E	1342	HIS
2	E	1347	ASN
2	E	1348	ASN
2	E	1357	GLU
2	E	1367	ASN
2	E	1370	VAL
2	E	1378	LEU
2	E	1387	LEU
2	E	1393	THR
2	E	1396	ASP
2	E	1399	ILE
2	E	1401	VAL
2	E	1402	THR
2	E	1406	HIS
2	E	1410	THR
2	E	1411	MET
3	F	1465	ARG
3	F	1468	TYR
3	F	1477	LYS
3	F	1480	LEU
3	F	1481	SER
3	F	1483	MET
3	F	1497	LEU
3	F	1500	ASP
3	F	1505	THR
3	F	1509	ASP
3	F	1512	VAL
3	F	1524	LEU
3	F	1527	ASP
3	F	1538	PHE
3	F	1541	VAL
3	F	1543	GLU
3	F	1544	VAL
3	F	1548	LEU
3	F	1549	VAL
3	F	1550	GLN
3	F	1556	LEU
3	F	1557	TYR
3	F	1577	ARG
3	F	1584	SER

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Mol	Chain	Res	Type
3	F	1587	VAL
3	F	1590	CYS
3	F	1606	LEU
3	F	1608	ASP
3	F	1612	TYR
3	F	1620	TYR
3	F	1627	PHE
3	F	1629	VAL
3	F	1632	LEU
3	F	1642	LEU
3	F	1651	LEU
3	F	1665	ARG
3	F	1673	CYS
3	F	1674	ARG
3	F	1684	LEU
3	F	1693	TYR
3	F	1721	THR
3	F	1731	ASN
3	F	1733	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
2	C	1350	GLN
1	B	65	ASN
1	B	240	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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(Å^2)	Q<0.9
1	A	651/656 (99%)	-0.27	2 (0%) 94 92	56, 110, 166, 213	0
1	B	651/656 (99%)	-0.42	0 100 100	50, 91, 145, 171	0
2	C	632/690 (91%)	0.08	16 (2%) 61 50	53, 176, 238, 259	0
2	E	632/690 (91%)	-0.09	12 (1%) 70 60	71, 129, 202, 253	0
3	D	281/291 (96%)	-0.19	4 (1%) 78 69	49, 128, 202, 253	0
3	F	281/291 (96%)	-0.23	3 (1%) 82 75	85, 135, 211, 255	0
All	All	3128/3274 (95%)	-0.18	37 (1%) 81 73	49, 118, 218, 259	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1744	VAL	5.7
2	E	1370	VAL	4.5
2	E	957	THR	4.4
2	E	1371	GLY	4.2
2	E	1369	LYS	3.7
2	C	1371	GLY	3.7
3	D	1743	GLN	3.6
2	C	957	THR	3.4
2	C	1228	LEU	3.0
2	C	1257	ALA	3.0
2	E	958	LEU	3.0
2	C	763	GLU	3.0
2	C	1370	VAL	2.9
3	F	1719	ARG	2.8
2	C	988	THR	2.8
2	C	1297	GLY	2.7
2	E	967	ASN	2.7
2	E	1367	ASN	2.7
3	F	1716	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	990	GLY	2.7
2	C	1336	ARG	2.7
2	C	1360	PHE	2.6
2	E	948	LEU	2.4
2	E	1330	THR	2.4
3	F	1615	LYS	2.4
2	C	989	LEU	2.4
1	A	409	VAL	2.3
2	E	956	ARG	2.3
1	A	444	LEU	2.3
2	C	1187	LEU	2.2
2	C	1067	ALA	2.2
2	C	1372	GLY	2.2
3	D	1740	GLN	2.1
3	D	1615	LYS	2.1
2	E	1368	VAL	2.1
2	C	1066	TYR	2.1
2	E	1336	ARG	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.