Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 06:26 AM GMT

PDB ID	:	2WYR
Title	:	3-D STRUCTURE OF PHTET1-12S, DODECAMER IN THE ASYMMETRIC UNIT
Authors	:	Vellieux, F.M.D.; Dura, M.A.; Franzetti, B.
Deposited on	:	2009-11-20
Resolution	:	2.25 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:

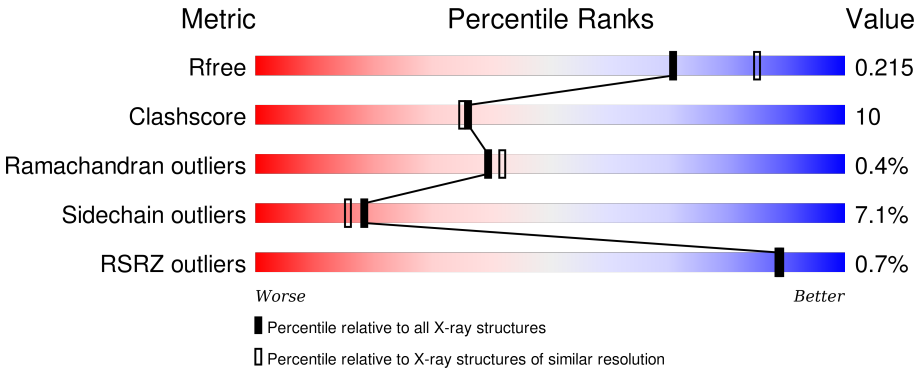
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.25 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	332	% 80% 15%
1	B	332	78% 17%
1	C	332	% 80% 17%
1	D	332	72% 21% 5%
1	E	332	78% 16%

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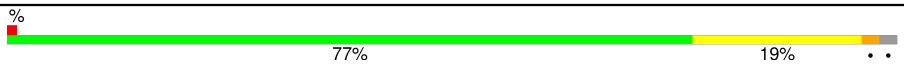
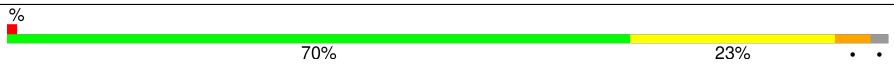
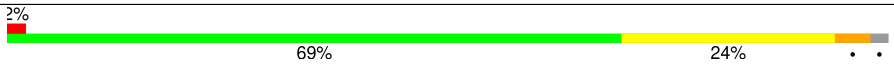
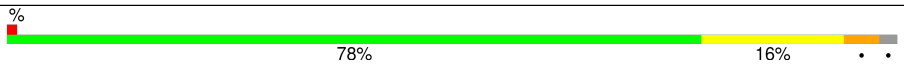
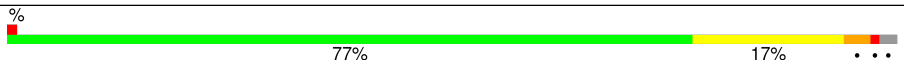
Mol	Chain	Length	Quality of chain
1	F	332	
1	G	332	
1	H	332	
1	I	332	
1	J	332	
1	K	332	
1	L	332	

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	CO	B	1663	-	-	-	X
2	CO	B	1664	-	-	-	X
2	CO	C	1995	-	-	-	X
2	CO	E	2657	-	-	-	X
2	CO	F	2988	-	-	-	X
2	CO	G	3319	-	-	-	X
2	CO	J	4312	-	-	-	X
2	CO	K	4643	-	-	-	X
2	CO	L	4974	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 32303 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 COBALT-ACTIVATED PEPTIDASE TET1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	5	0
			2582	1665	426	485	6			
1	B	325	Total	C	N	O	S	0	5	0
			2579	1666	426	480	7			
1	C	326	Total	C	N	O	S	0	2	0
			2568	1656	428	478	6			
1	D	325	Total	C	N	O	S	0	2	0
			2560	1653	423	478	6			
1	E	326	Total	C	N	O	S	0	3	0
			2574	1662	425	481	6			
1	F	324	Total	C	N	O	S	0	2	0
			2554	1648	424	477	5			
1	G	325	Total	C	N	O	S	0	1	0
			2554	1648	422	478	6			
1	H	326	Total	C	N	O	S	0	4	0
			2579	1664	430	479	6			
1	I	325	Total	C	N	O	S	0	0	0
			2545	1640	422	477	6			
1	J	326	Total	C	N	O	S	0	1	0
			2560	1651	425	478	6			
1	K	325	Total	C	N	O	S	0	3	0
			2565	1656	423	480	6			
1	L	325	Total	C	N	O	S	0	1	0
			2553	1645	425	477	6			

- Molecule 2 is COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	2	Total	Co	0	0
			2	2		
2	J	2	Total	Co	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Co 2 2	0	0
2	K	2	Total Co 2 2	0	0
2	E	2	Total Co 2 2	0	0
2	H	2	Total Co 2 2	0	0
2	B	2	Total Co 2 2	0	0
2	I	2	Total Co 2 2	0	0
2	C	2	Total Co 2 2	0	0
2	A	2	Total Co 2 2	0	0
2	L	2	Total Co 2 2	0	0
2	F	2	Total Co 2 2	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	140	Total O 140 140	0	0
3	B	122	Total O 122 122	0	0
3	C	146	Total O 146 146	0	0
3	D	125	Total O 125 125	0	0
3	E	143	Total O 143 143	0	0
3	F	110	Total O 110 110	0	0
3	G	142	Total O 142 142	0	0
3	H	110	Total O 110 110	0	0
3	I	84	Total O 84 84	0	0

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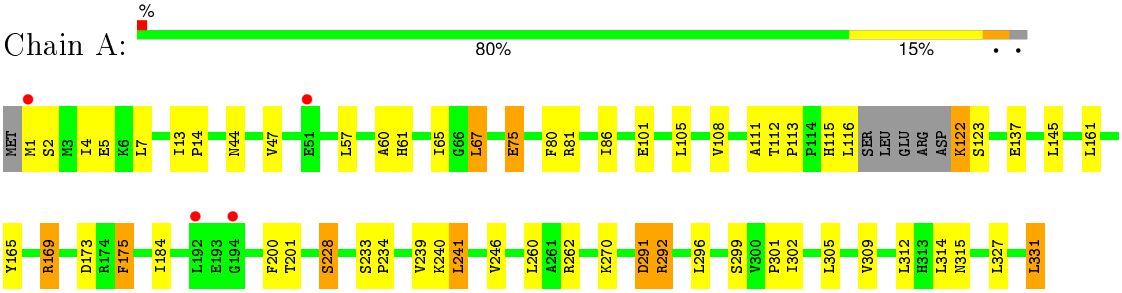
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	135	Total O 135 135	0	0
3	K	122	Total O 122 122	0	0
3	L	127	Total O 127 127	0	0

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.

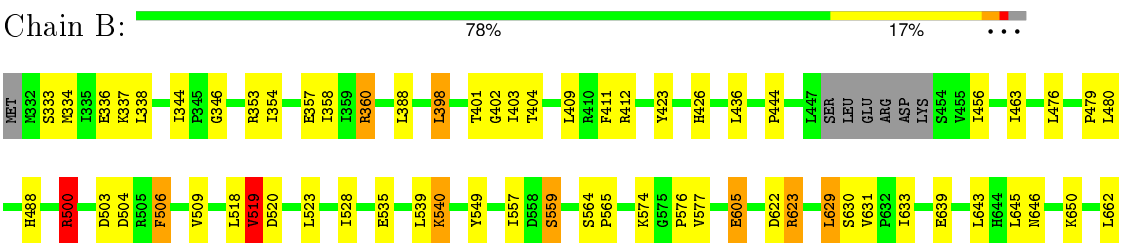
- Molecule 1: COBALT-ACTIVATED PEPTIDASE TET1

Chain A:



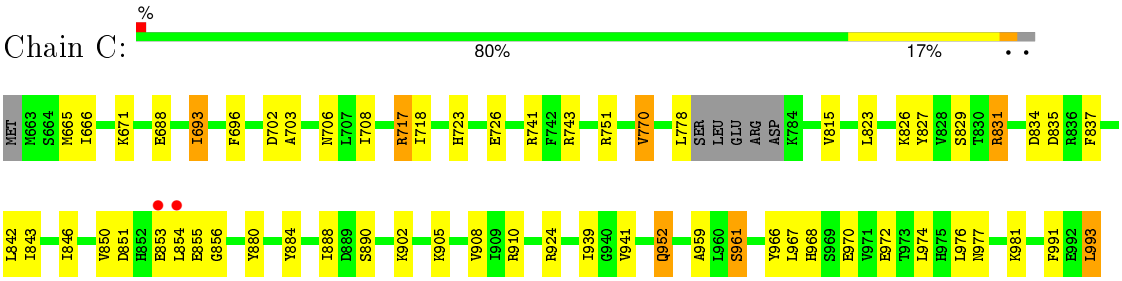
- Molecule 1: COBALT-ACTIVATED PEPTIDASE TET1

Chain B:



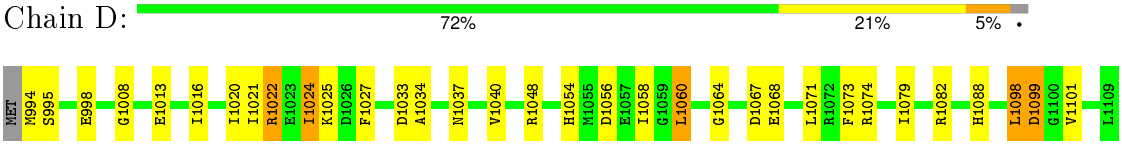
- Molecule 1: COBALT-ACTIVATED PEPTIDASE TET1

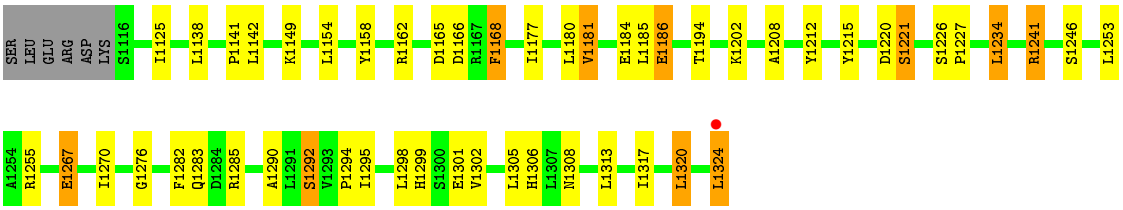
Chain C:



- Molecule 1: COBALT-ACTIVATED PEPTIDASE TET1

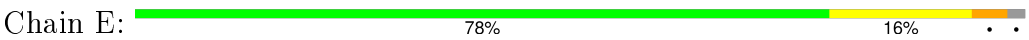
Chain D:

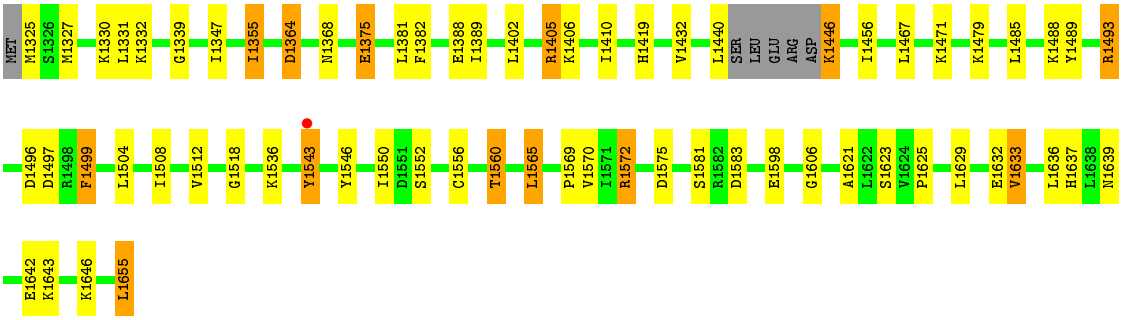




• Molecule 1: COBALT-ACTIVATED PEPTIDASE TET1

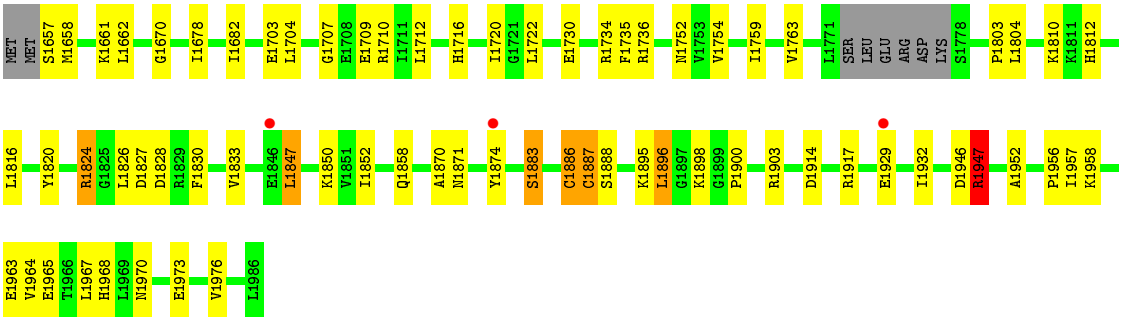
Chain E:





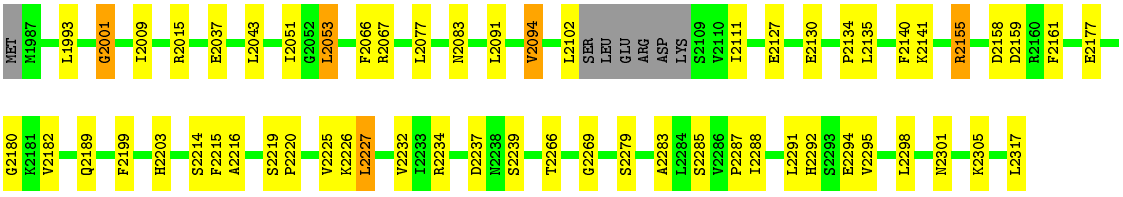
• Molecule 1: COBALT-ACTIVATED PEPTIDASE TET1

Chain F:



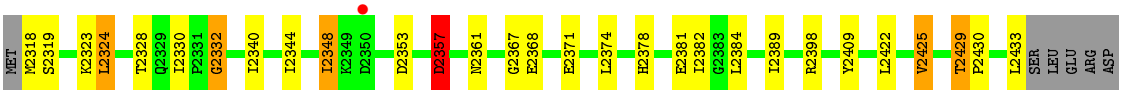
• Molecule 1: COBALT-ACTIVATED PEPTIDASE TET1

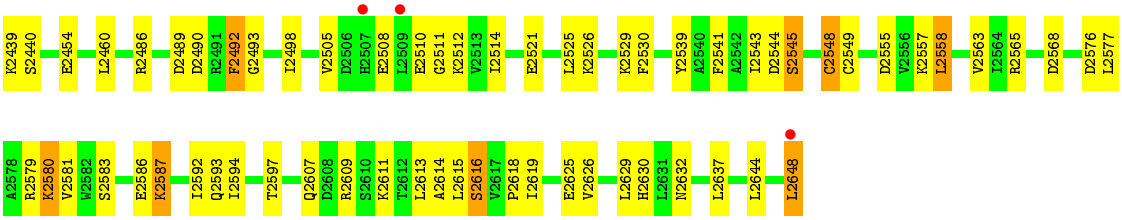
Chain G:

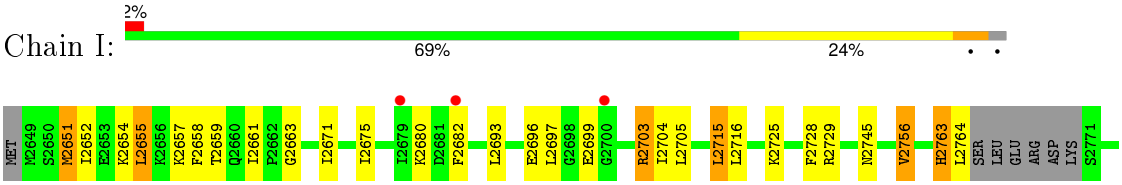


• Molecule 1: COBALT-ACTIVATED PEPTIDASE TET1

Chain H:

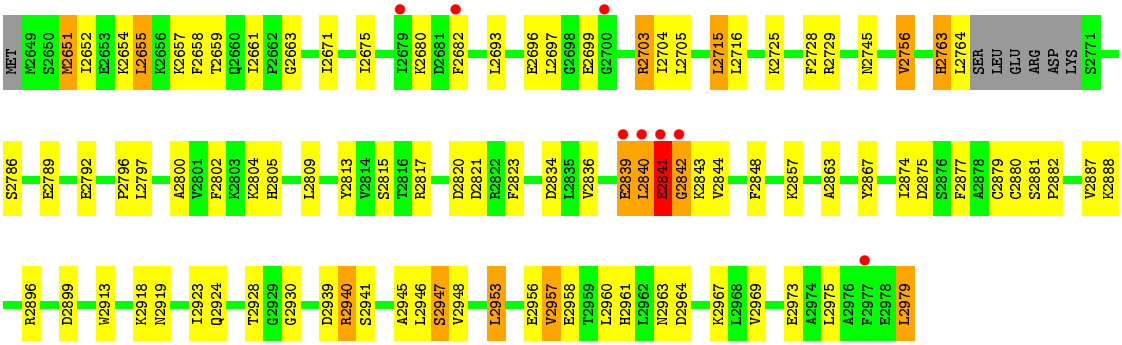






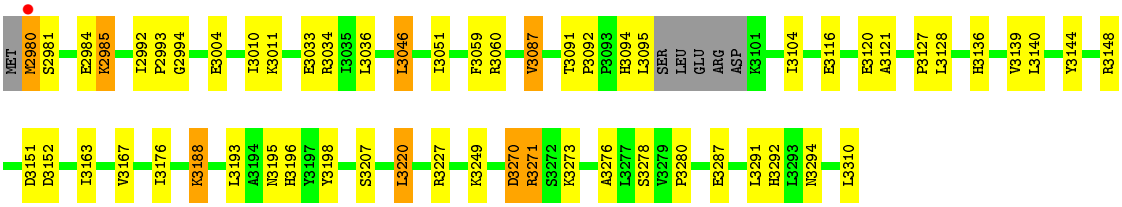
• Molecule 1: COBALT-ACTIVATED PEPTIDASE TET1

Chain I:



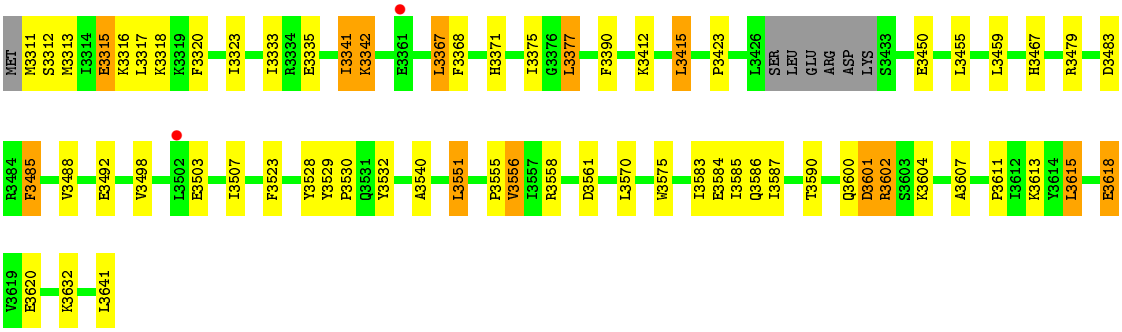
• Molecule 1: COBALT-ACTIVATED PEPTIDASE TET1

Chain J:



• Molecule 1: COBALT-ACTIVATED PEPTIDASE TET1

Chain K:



• Molecule 1: COBALT-ACTIVATED PEPTIDASE TET1

Chain L:


MET M3642 S3643 K3647 L3648 I3668 I3672 K3673 D3674 F3675 K3679 A3682 E3692 E3695 H3702 I3713 L3719 R3722 R3730 L3746 V3749 T3753 P3754 L3757 SER LEU GLU ARG ASP LYS S3764 I3773 E3781 L3784 E3785 P3789 L3790 K3805
R3810 D3814 R3815 F3816 V3829 D3830 H3831 E3832 L3833 I3838 K3850 Y3863 S3869 C3872 C3873 S3874 P3875 K3881 L3882 P3886 V3887 I3888 R3889 S3898 R3899 D3900 K3911 E3915 I3918 D3932 R3933 S3934 A3938 V3941 P3942 I3943 K3944 Y3945 L3946 H3947 S3948 E3949 V3950 E3951
T3952 L3953 N3956 D3957 L3958 E3959 K3960 L3972

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	113.26Å 205.22Å 113.49Å 90.00° 100.78° 90.00°	Depositor
Resolution (Å)	49.68 – 2.25 49.68 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.68-2.25) 99.8 (49.68-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.17 (at 2.25Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.170 , 0.220 0.163 , 0.215	Depositor DCC
R_{free} test set	12086 reflections (5.01%)	DCC
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.6	EDS
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 241311 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	32303	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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

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

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	0.39	0/2641	0.60	1/3559 (0.0%)
1	B	0.39	0/2639	0.61	1/3558 (0.0%)
1	C	0.42	0/2618	0.61	0/3527
1	D	0.40	0/2611	0.61	0/3521
1	E	0.42	0/2628	0.62	1/3543 (0.0%)
1	F	0.36	0/2605	0.60	1/3514 (0.0%)
1	G	0.44	0/2602	0.66	1/3510 (0.0%)
1	H	0.38	0/2635	0.62	1/3549 (0.0%)
1	I	0.36	0/2589	0.60	1/3491 (0.0%)
1	J	0.42	0/2607	0.62	0/3513
1	K	0.39	0/2619	0.61	1/3532 (0.0%)
1	L	0.41	0/2600	0.61	1/3505 (0.0%)
All	All	0.40	0/31394	0.61	9/42322 (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	1
1	C	0	1
1	F	0	1
1	H	0	1
1	J	0	1
1	L	0	1
All	All	0	6

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1493	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	F	1887	CYS	CA-CB-SG	-5.97	103.25	114.00
1	A	169	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	B	500	ARG	NE-CZ-NH1	-5.73	117.44	120.30
1	H	2580	LYS	N-CA-C	-5.59	95.90	111.00
1	G	2155	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	K	3415	LEU	CA-CB-CG	5.38	127.68	115.30
1	L	3810	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	I	2821	ASP	N-CA-C	5.07	124.69	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	SER	Peptide
1	C	961	SER	Peptide
1	F	1886	CYS	Peptide
1	H	2548	CYS	Peptide
1	J	3278	SER	Peptide
1	L	3833	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	2582	0	2642	38	0
1	B	2579	0	2642	61	0
1	C	2568	0	2631	48	0
1	D	2560	0	2614	80	0
1	E	2574	0	2631	54	0
1	F	2554	0	2605	50	0
1	G	2554	0	2601	41	0
1	H	2579	0	2650	73	0
1	I	2545	0	2592	75	0
1	J	2560	0	2618	39	0
1	K	2565	0	2618	43	0
1	L	2553	0	2605	55	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	140	0	0	4	0
3	B	122	0	0	3	0
3	C	146	0	0	5	0
3	D	125	0	0	8	0
3	E	143	0	0	3	0
3	F	110	0	0	5	0
3	G	142	0	0	4	0
3	H	110	0	0	6	0
3	I	84	0	0	4	0
3	J	135	0	0	1	0
3	K	122	0	0	2	0
3	L	127	0	0	5	0
All	All	32303	0	31449	598	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 10.

All (598) 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:D:1220:ASP:O	1:D:1292:SER:HB3	1.43	1.18
1:I:2841:GLU:N	1:I:2842:GLY:HA3	1.56	1.10
1:B:559:SER:HB3	1:B:633:ILE:HD12	1.40	1.04
1:I:2875:ASP:O	1:I:2947:SER:HB3	1.57	1.03
1:B:334[A]:MET:HA	1:B:334[A]:MET:HE3	1.43	0.98
1:L:3810:ARG:HH12	1:L:3951:GLU:CD	1.69	0.96
1:I:2841:GLU:H	1:I:2842:GLY:HA3	1.31	0.96
1:L:3882:LEU:HD22	1:L:3942:PRO:HB2	1.47	0.95
1:B:622:ASP:HB3	1:B:623:ARG:HE	1.30	0.95
1:L:3869:SER:HB3	1:L:3943:ILE:HD12	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:LEU:HD22	1:A:301:PRO:HB2	1.48	0.94
1:F:1896:LEU:HD22	1:F:1956:PRO:HB2	1.46	0.94
1:K:3551:LEU:HD22	1:K:3611:PRO:HB2	1.49	0.94
1:G:2214:SER:HB3	1:G:2288:ILE:HD12	1.49	0.94
1:F:1824:ARG:HH12	1:F:1965:GLU:CD	1.75	0.89
1:K:3601:ASP:HB3	1:K:3602:ARG:HE	1.35	0.88
1:D:1099:ASP:HB3	3:D:5054:HOH:O	1.76	0.86
1:G:2227:LEU:HD22	1:G:2287:PRO:HB2	1.58	0.86
1:I:2817:ARG:HB2	1:I:2956:GLU:HA	1.61	0.81
1:H:2510:GLU:HB3	1:H:2511:GLY:HA2	1.59	0.81
1:E:1633:VAL:CG2	1:H:2425:VAL:HG22	2.11	0.81
1:D:1302:VAL:HG22	1:J:3087:VAL:HG22	1.62	0.80
1:G:2216:ALA:HB2	1:G:2291:LEU:HD12	1.64	0.80
1:H:2581:VAL:N	3:H:5089:HOH:O	2.14	0.79
1:I:2867:TYR:HE1	1:I:2940:ARG:HB2	1.47	0.78
1:A:228:SER:HB3	1:A:302:ILE:HD12	1.67	0.76
1:L:3810:ARG:NE	3:L:5077:HOH:O	2.18	0.76
1:I:2840:LEU:HG	1:I:2841:GLU:H	1.50	0.76
1:A:292:ARG:HG2	1:A:292:ARG:HH11	1.50	0.76
1:I:2682:PHE:O	1:I:2836:VAL:HG21	1.85	0.76
1:F:1824:ARG:NH2	3:F:5066:HOH:O	2.19	0.76
1:E:1493:ARG:HB2	1:E:1632:GLU:HA	1.68	0.76
1:G:2295:VAL:HG22	1:L:3749:VAL:HG22	1.68	0.75
1:B:333:SER:OG	1:B:336:GLU:HG3	1.86	0.74
1:H:2583:SER:O	1:H:2587[B]:LYS:HG2	1.88	0.73
1:F:1870:ALA:O	1:F:1947:ARG:NH2	2.21	0.73
1:C:854:LEU:HD12	1:C:854:LEU:O	1.88	0.73
1:B:622:ASP:HB3	1:B:623:ARG:NE	2.03	0.72
1:D:1162:ARG:HB2	1:D:1301:GLU:HA	1.71	0.72
1:D:1298:LEU:HD12	1:J:3094:HIS:CE1	2.24	0.72
1:B:518:LEU:O	1:B:519:VAL:HG12	1.91	0.71
1:I:2963:ASN:HD21	1:I:2967:LYS:NZ	1.88	0.71
1:A:122[A]:LYS:HD2	1:A:123:SER:H	1.54	0.71
1:L:3831:HIS:O	1:L:3833:LEU:HD13	1.90	0.70
1:L:3810:ARG:NH2	3:L:5077:HOH:O	2.24	0.70
1:B:354:ILE:HD12	1:B:354:ILE:H	1.56	0.70
1:B:346:GLY:HA3	1:B:354:ILE:HD11	1.73	0.69
1:G:2301:ASN:OD1	1:G:2305:LYS:HE3	1.91	0.69
1:D:1298:LEU:HD13	1:D:1299:HIS:CD2	2.28	0.69
1:J:3220:LEU:HD22	1:J:3280:PRO:HB2	1.75	0.69
1:D:1234:LEU:HD22	1:D:1294:PRO:HB2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3450:GLU:H	1:K:3450:GLU:CD	1.98	0.67
1:I:2703:ARG:CZ	1:I:2841:GLU:HG2	2.25	0.67
1:D:1221:SER:HB3	1:D:1295:ILE:HD12	1.75	0.67
1:I:2867:TYR:CE1	1:I:2940:ARG:HB2	2.28	0.67
1:K:3601:ASP:CB	1:K:3602:ARG:HE	2.07	0.67
1:F:1824:ARG:HB2	1:F:1963:GLU:HA	1.77	0.66
1:D:1181:VAL:N	3:D:5089:HOH:O	2.27	0.66
1:A:101:GLU:HG3	3:A:5048:HOH:O	1.95	0.66
1:I:2699:GLU:H	1:I:2840:LEU:HD12	1.60	0.66
1:F:1947:ARG:HA	1:K:3523:PHE:CE1	2.30	0.66
1:D:1027:PHE:HB2	3:D:5025:HOH:O	1.95	0.66
1:I:2841:GLU:H	1:I:2842:GLY:CA	2.08	0.66
1:D:1022:ARG:O	1:D:1025[B]:LYS:HE2	1.96	0.66
1:H:2563:VAL:HG23	1:H:2618:PRO:HD3	1.78	0.65
1:D:1226:SER:HB2	1:D:1227:PRO:HD2	1.77	0.65
1:F:1824:ARG:NE	3:F:5066:HOH:O	2.28	0.65
1:E:1382:PHE:HD2	1:E:1550:ILE:HD11	1.61	0.65
1:E:1440:LEU:CD1	1:H:2548:CYS:O	2.45	0.65
1:A:291:ASP:HB3	1:A:292:ARG:NH1	2.13	0.64
1:D:1212[B]:TYR:HE1	1:D:1285:ARG:HH21	1.45	0.64
1:I:2839:GLU:HG2	1:I:2840:LEU:N	2.12	0.64
1:C:854:LEU:HD23	1:C:991:PHE:CE2	2.33	0.64
1:G:2295:VAL:O	1:G:2295:VAL:CG1	2.46	0.64
1:G:2295:VAL:HG12	1:G:2295:VAL:O	1.98	0.64
1:C:902[B]:LYS:HB3	1:C:905:LYS:HD2	1.80	0.64
3:G:5071:HOH:O	1:L:3944:LYS:HD2	1.98	0.64
1:G:2155:ARG:HB2	1:G:2294:GLU:HA	1.81	0.63
1:E:1637:HIS:CE1	1:E:1639:ASN:HB2	2.33	0.63
1:D:1024:ILE:HA	3:D:5025:HOH:O	1.97	0.63
1:D:1067:ASP:HB2	1:D:1068:GLU:OE2	1.98	0.63
1:H:2558:LEU:HD22	1:H:2618:PRO:HB2	1.81	0.63
1:I:2841:GLU:N	1:I:2842:GLY:CA	2.42	0.63
1:B:506:PHE:CZ	1:B:631:VAL:HG12	2.34	0.63
1:G:2111:ILE:N	1:G:2111:ILE:HD12	2.14	0.62
1:J:3292:HIS:HE1	1:J:3294:ASN:HD22	1.46	0.62
1:B:334[A]:MET:CE	1:B:509:VAL:HG11	2.28	0.62
1:J:3195:ASN:O	1:J:3196:HIS:HB2	2.00	0.62
1:L:3643:SER:O	1:L:3647:LYS:HG3	2.00	0.62
1:C:666:ILE:HD11	1:C:976:LEU:HD11	1.80	0.62
1:G:2295:VAL:HG11	1:L:3749:VAL:HG13	1.82	0.62
1:H:2544:ASP:O	1:H:2616:SER:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1048:ARG:NH1	1:D:1186:GLU:O	2.33	0.62
1:L:3810:ARG:CZ	3:L:5077:HOH:O	2.46	0.62
1:A:115:HIS:CE1	1:C:967:LEU:HD12	2.34	0.62
1:C:902[A]:LYS:HB2	1:C:905:LYS:HD2	1.82	0.61
1:G:2015:ARG:HD3	3:G:5023:HOH:O	2.00	0.61
1:K:3311:MET:SD	1:K:3315:GLU:HG2	2.40	0.61
1:I:2704:ILE:HD11	1:I:2979:LEU:HB3	1.82	0.61
1:F:1883:SER:HB3	1:F:1957:ILE:HD12	1.81	0.61
1:A:67:LEU:HG	1:A:80:PHE:CD1	2.35	0.61
1:J:3270:ASP:HB3	1:J:3271:ARG:HG3	1.81	0.61
1:C:855:GLU:HA	1:C:856:GLY:O	2.01	0.61
1:I:2839:GLU:HG2	1:I:2840:LEU:H	1.66	0.61
1:I:2875:ASP:O	1:I:2947:SER:CB	2.43	0.61
1:K:3583:ILE:HD11	1:K:3632[A]:LYS:HG3	1.82	0.61
1:L:3695:GLU:HG2	1:L:3838:ILE:HD11	1.80	0.61
1:G:2111:ILE:HD11	1:L:3730:ARG:NH1	2.16	0.60
1:K:3479:ARG:HB2	1:K:3618:GLU:HA	1.83	0.60
1:E:1639:ASN:O	1:E:1643[B]:LYS:HE3	2.01	0.60
1:G:2111:ILE:H	1:G:2111:ILE:HD12	1.67	0.60
1:G:2214:SER:CB	1:G:2288:ILE:HD12	2.28	0.59
1:K:3540:ALA:HB2	1:K:3615:LEU:HD12	1.84	0.59
1:K:3600:GLN:HE22	1:L:3850:LYS:HE3	1.67	0.59
1:I:2839:GLU:CG	1:I:2840:LEU:N	2.65	0.59
1:D:1016:ILE:HD12	1:D:1016:ILE:H	1.67	0.59
1:C:910:ARG:HB3	1:C:959:ALA:HB3	1.84	0.59
1:E:1572:ARG:HB3	1:E:1621:ALA:HB3	1.84	0.59
1:C:696:PHE:O	1:C:850:VAL:HG21	2.02	0.59
1:B:643:LEU:C	1:B:643:LEU:HD12	2.23	0.59
1:G:2219:SER:HB2	1:G:2220:PRO:HD2	1.85	0.59
1:J:3291:LEU:HD12	1:J:3291:LEU:C	2.23	0.59
1:K:3450:GLU:N	1:K:3450:GLU:CD	2.56	0.59
1:D:1212[B]:TYR:HE1	1:D:1285:ARG:NH2	2.00	0.59
1:F:1678:ILE:O	1:F:1682:ILE:HG13	2.03	0.58
1:C:856:GLY:N	3:C:5092:HOH:O	2.35	0.58
1:D:1034:ALA:HB1	1:H:2611:LYS:HE2	1.85	0.58
1:C:967:LEU:HD13	1:C:968:HIS:CD2	2.38	0.58
1:G:2295:VAL:CG2	1:L:3749:VAL:HG22	2.32	0.58
1:E:1633:VAL:HG23	1:H:2425:VAL:HG22	1.85	0.58
3:E:5051:HOH:O	1:H:2625:GLU:HG2	2.02	0.58
1:D:1283:GLN:HE22	1:I:2857:LYS:NZ	2.01	0.58
1:D:1033:ASP:OD2	1:D:1037:ASN:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:884:TYR:CD2	1:C:993:LEU:HD13	2.38	0.58
1:B:334[A]:MET:HA	1:B:334[A]:MET:CE	2.27	0.58
1:C:723:HIS:NE2	1:C:835:ASP:HB2	2.17	0.58
1:H:2580:LYS:O	1:H:2581:VAL:HB	2.04	0.58
1:F:1824:ARG:CZ	3:F:5066:HOH:O	2.51	0.58
1:F:1968:HIS:CE1	1:F:1970:ASN:HB3	2.39	0.58
1:A:105:LEU:HD21	1:A:145:LEU:HB3	1.86	0.57
1:C:974:LEU:HD12	1:C:974:LEU:C	2.25	0.57
1:D:1180:LEU:O	1:D:1181:VAL:HG12	2.05	0.57
1:H:2486:ARG:HB2	1:H:2625:GLU:HA	1.86	0.57
1:I:2651:MET:HE2	1:I:2652:ILE:H	1.69	0.57
1:L:3889:ARG:HB3	1:L:3938:ALA:HB3	1.87	0.57
1:A:292:ARG:HG2	1:A:292:ARG:NH1	2.20	0.57
1:F:1903:ARG:HB3	1:F:1952:ALA:HB3	1.87	0.57
1:B:480:LEU:HD11	1:C:939:ILE:HG12	1.86	0.56
1:F:1658:MET:CE	1:F:1833:VAL:HG11	2.35	0.56
1:I:2963:ASN:HD21	1:I:2967:LYS:HZ2	1.52	0.56
1:C:977:ASN:HD21	1:C:981:LYS:HZ1	1.51	0.56
1:H:2367:GLY:O	1:H:2368:GLU:HG3	2.05	0.56
1:F:1886:CYS:SG	1:F:1887:CYS:N	2.79	0.56
1:I:2840:LEU:HG	1:I:2841:GLU:N	2.20	0.56
1:K:3583:ILE:CD1	1:K:3632[A]:LYS:HG3	2.36	0.56
1:E:1419:HIS:HB3	1:E:1479:LYS:HD2	1.88	0.56
1:B:540:LYS:HG3	1:C:952:GLN:NE2	2.20	0.56
1:E:1446:LYS:N	1:E:1446:LYS:HE3	2.21	0.56
1:F:1932:ILE:HG12	1:K:3459:LEU:HD11	1.87	0.56
1:L:3882:LEU:CD2	1:L:3942:PRO:HB2	2.30	0.56
1:C:855:GLU:C	3:C:5092:HOH:O	2.43	0.56
1:L:3898:SER:HB3	3:L:5101:HOH:O	2.06	0.56
1:G:2134:PRO:O	1:G:2135:LEU:HB2	2.06	0.56
1:F:1816:LEU:HB2	1:F:1820:TYR:HB2	1.87	0.56
1:I:2699:GLU:N	1:I:2840:LEU:HD12	2.20	0.55
1:K:3601:ASP:HB3	1:K:3602:ARG:NE	2.14	0.55
1:E:1382:PHE:CD2	1:E:1550:ILE:HD11	2.41	0.55
1:E:1581:SER:OG	1:E:1583[B]:ASP:OD1	2.24	0.55
1:C:855:GLU:HB3	1:C:856:GLY:HA2	1.88	0.55
1:C:977:ASN:HD21	1:C:981:LYS:NZ	2.03	0.55
1:J:3163:ILE:O	1:J:3167:VAL:HG13	2.06	0.55
1:B:488:HIS:CE1	1:K:3467:HIS:CE1	2.95	0.55
1:H:2563:VAL:CG2	1:H:2618:PRO:HD3	2.36	0.55
1:I:2817:ARG:NH2	3:I:5049:HOH:O	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2094:VAL:HG22	1:L:3950:VAL:CG1	2.37	0.55
1:K:3507:ILE:HD13	1:K:3528:TYR:CD2	2.41	0.55
1:H:2615:LEU:HD13	1:H:2637:LEU:HD11	1.89	0.54
1:D:1186:GLU:HA	1:D:1186:GLU:OE1	2.07	0.54
1:D:1320:LEU:O	1:D:1324:LEU:HB2	2.07	0.54
1:L:3643:SER:HB2	3:L:5007:HOH:O	2.06	0.54
1:A:75:GLU:HG2	3:A:5025:HOH:O	2.07	0.54
1:E:1432:VAL:CG1	1:H:2626:VAL:HB	2.37	0.54
1:E:1633:VAL:CG2	1:H:2425:VAL:CG2	2.84	0.54
1:L:3832:GLU:O	1:L:3833:LEU:HD12	2.08	0.54
1:I:2796:PRO:O	1:I:2797:LEU:HB2	2.08	0.54
1:J:3227:ARG:HB3	1:J:3276:ALA:HB3	1.90	0.54
1:D:1234:LEU:CD2	1:D:1294:PRO:HB2	2.38	0.53
1:D:1021:ILE:O	1:D:1025[A]:LYS:HB2	2.08	0.53
1:F:1900:PRO:HD2	1:F:1929:GLU:O	2.08	0.53
1:K:3555:PRO:HD2	1:K:3584:GLU:O	2.08	0.53
1:E:1364:ASP:HB2	1:E:1368:ASN:HB2	1.90	0.53
1:H:2344:ILE:HG23	1:H:2498:ILE:HD11	1.89	0.53
1:J:3270:ASP:HB3	1:J:3271:ARG:CG	2.38	0.53
1:I:2953:LEU:HB2	3:I:5075:HOH:O	2.08	0.53
1:D:1298:LEU:CD1	1:D:1299:HIS:CD2	2.90	0.53
1:B:639:GLU:HG2	3:K:5039:HOH:O	2.07	0.53
1:I:2655:LEU:O	1:I:2659:THR:HG23	2.08	0.53
1:D:1098:LEU:HD21	1:D:1138:LEU:HB3	1.90	0.53
1:D:1027:PHE:O	1:D:1181:VAL:HG21	2.09	0.53
1:J:3033:GLU:HG2	1:J:3176:ILE:HD11	1.90	0.53
1:H:2545:SER:HB3	1:H:2619:ILE:HD12	1.90	0.53
1:D:1058:ILE:HG12	1:D:1162:ARG:NH2	2.24	0.53
1:H:2389:ILE:HD12	1:H:2460:LEU:HG	1.91	0.53
1:C:842:LEU:HD21	1:C:888:ILE:HG13	1.90	0.53
1:H:2510:GLU:CB	1:H:2511:GLY:HA2	2.32	0.53
3:G:5128:HOH:O	1:L:3754:PRO:HG3	2.08	0.53
1:H:2644:LEU:O	1:H:2648:LEU:HB2	2.09	0.53
1:B:409:LEU:HB2	1:B:463:ILE:HB	1.91	0.53
1:L:3953:LEU:HD12	1:L:3953:LEU:C	2.29	0.53
1:B:518:LEU:C	1:B:520:ASP:H	2.11	0.52
1:I:2961:HIS:CE1	1:I:2963:ASN:HB3	2.44	0.52
1:A:122[A]:LYS:HD2	1:A:123:SER:N	2.23	0.52
1:H:2558:LEU:CD2	1:H:2618:PRO:HB2	2.39	0.52
1:L:3675:PHE:O	1:L:3829:VAL:HG21	2.09	0.52
1:B:401:THR:HG22	1:C:941:VAL:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2371:GLU:HA	1:H:2512:LYS:HB3	1.91	0.52
1:G:2037:GLU:O	1:G:2180:GLY:HA2	2.10	0.52
1:A:327:LEU:O	1:A:331:LEU:HB2	2.09	0.52
1:C:977:ASN:ND2	1:C:981:LYS:NZ	2.58	0.52
1:H:2324:LEU:O	1:H:2328:THR:HG23	2.09	0.52
1:B:564:SER:HB2	1:B:565:PRO:HD2	1.90	0.52
1:B:357:GLU:HA	1:B:360:ARG:HD2	1.90	0.52
1:F:1763:VAL:CG1	1:I:2957:VAL:HG22	2.39	0.52
1:L:3956:ASN:OD1	1:L:3960:LYS:HE3	2.09	0.52
1:B:540:LYS:HG3	1:C:952:GLN:CD	2.29	0.52
1:C:831:ARG:HG2	1:C:970:GLU:HA	1.92	0.52
1:I:2671:ILE:HD12	1:I:2671:ILE:N	2.25	0.52
1:I:2671:ILE:O	1:I:2675:ILE:HG13	2.10	0.52
1:D:1298:LEU:CD1	1:J:3094:HIS:CE1	2.92	0.52
1:E:1440:LEU:HD11	1:H:2548:CYS:O	2.08	0.52
1:G:2001:GLY:HA3	1:G:2009:ILE:CD1	2.40	0.52
1:K:3532:TYR:CD1	1:K:3570:LEU:HD13	2.45	0.52
1:D:1142:LEU:CD1	1:H:2594:ILE:HG12	2.40	0.52
1:I:2675:ILE:HD13	1:I:2848:PHE:CD2	2.45	0.52
1:A:233:SER:HB2	1:A:234:PRO:HD2	1.91	0.52
1:E:1467:LEU:O	1:E:1471:LYS:HE3	2.10	0.52
1:D:1154:LEU:HB2	1:D:1158:TYR:HB2	1.92	0.52
1:J:3127:PRO:O	1:J:3128:LEU:HB2	2.09	0.52
1:E:1565:LEU:HD22	1:E:1625:PRO:HB2	1.91	0.51
1:I:2863:ALA:HB1	1:I:2940:ARG:NH1	2.26	0.51
1:J:3193:LEU:O	1:J:3195:ASN:O	2.28	0.51
1:C:823:LEU:HB2	1:C:827:TYR:HB2	1.93	0.51
1:D:1141:PRO:O	1:D:1142:LEU:HB2	2.11	0.51
1:D:994:MET:HG3	1:D:998:GLU:HB2	1.91	0.51
1:D:1024:ILE:C	3:D:5025:HOH:O	2.48	0.51
1:B:479:PRO:O	1:B:480:LEU:HB2	2.10	0.51
1:F:1658:MET:HE2	1:F:1833:VAL:HG11	1.91	0.51
1:H:2340:ILE:O	1:H:2344:ILE:HG13	2.10	0.51
1:K:3558:ARG:HB3	1:K:3607:ALA:HB3	1.92	0.51
1:I:2919:ASN:N	1:I:2919:ASN:HD22	2.09	0.51
1:L:3810:ARG:NH1	1:L:3951:GLU:OE2	2.35	0.51
1:H:2543:ILE:HD12	1:H:2615:LEU:HD11	1.93	0.51
1:D:1168:PHE:C	1:D:1168:PHE:CD1	2.83	0.51
1:A:315[A]:ASN:ND2	3:A:5136:HOH:O	2.43	0.51
1:D:1302:VAL:CG1	1:D:1302:VAL:O	2.59	0.51
1:B:557:ILE:HD12	1:B:629:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1406:LYS:HD2	1:E:1410:ILE:HB	1.92	0.51
1:G:2083:ASN:HD21	1:G:2141:LYS:HE2	1.75	0.51
1:H:2577:LEU:O	1:H:2580:LYS:O	2.28	0.51
1:E:1405:ARG:HG2	1:E:1406:LYS:N	2.26	0.51
1:H:2615:LEU:CD1	1:H:2637:LEU:HD11	2.41	0.50
1:D:1142:LEU:HD11	1:H:2594:ILE:HG12	1.93	0.50
1:B:646:ASN:HD21	1:B:650:LYS:HE3	1.76	0.50
1:I:2896:ARG:HB3	1:I:2945:ALA:HB3	1.92	0.50
1:G:2077:LEU:HD23	1:G:2140:PHE:HZ	1.76	0.50
1:F:1958:LYS:O	1:F:1965:GLU:HA	2.11	0.50
1:B:623:ARG:N	1:B:623:ARG:HD2	2.27	0.50
1:H:2539:TYR:CD1	1:H:2577:LEU:HD13	2.46	0.50
1:F:1870:ALA:HB1	1:F:1947:ARG:NH2	2.26	0.50
1:D:1082:ARG:NH1	1:J:3104:ILE:HD11	2.26	0.50
1:J:3195:ASN:O	1:J:3196:HIS:CB	2.59	0.50
1:H:2382:ILE:HG12	1:H:2486:ARG:NH2	2.27	0.50
1:I:2693:LEU:HB3	1:I:2848:PHE:HB2	1.92	0.50
1:B:577:VAL:HG13	1:B:630:SER:HB2	1.94	0.50
1:K:3556:VAL:HG13	1:K:3586:GLN:HB2	1.94	0.50
1:D:995:SER:OG	1:D:998:GLU:HG3	2.12	0.50
1:L:3668:ILE:O	1:L:3672:ILE:HG13	2.10	0.50
1:L:3932:ASP:HB3	1:L:3933:ARG:HG2	1.94	0.50
1:H:2548:CYS:SG	1:H:2549:CYS:N	2.85	0.50
1:B:334[A]:MET:HE2	1:B:509:VAL:HG11	1.94	0.49
1:F:1722:LEU:HG	1:F:1735:PHE:CD1	2.47	0.49
1:E:1347:ILE:HD12	1:E:1347:ILE:H	1.77	0.49
1:A:312:LEU:HD12	1:A:312:LEU:C	2.32	0.49
1:H:2580:LYS:HA	3:H:5089:HOH:O	2.13	0.49
1:D:1283:GLN:NE2	1:I:2857:LYS:NZ	2.60	0.49
1:A:161:LEU:HB2	1:A:165:TYR:HB2	1.94	0.49
1:L:3888:ILE:HB	1:L:3918:ILE:HG13	1.93	0.49
1:B:398:LEU:HG	1:B:411:PHE:CD1	2.48	0.49
1:B:518:LEU:O	1:B:520:ASP:N	2.44	0.49
1:E:1504:LEU:O	1:E:1508:ILE:HG13	2.13	0.49
1:D:1088:HIS:CD2	1:J:3136:HIS:HB2	2.48	0.49
1:D:1202:LYS:NZ	1:H:2607:GLN:HE22	2.11	0.49
1:B:423:TYR:CE1	1:B:456:ILE:HD12	2.47	0.49
1:I:2840:LEU:CG	1:I:2841:GLU:N	2.76	0.49
1:B:346:GLY:HA3	1:B:354:ILE:CD1	2.42	0.49
1:K:3311:MET:HG2	1:K:3312:SER:H	1.78	0.49
1:I:2715:LEU:HG	1:I:2728:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1964:VAL:CG1	1:I:2756:VAL:HG22	2.43	0.49
1:I:2671:ILE:HD12	1:I:2671:ILE:H	1.78	0.48
1:B:353[B]:ARG:HB2	3:B:5018:HOH:O	2.12	0.48
1:E:1440:LEU:HD12	1:H:2548:CYS:O	2.11	0.48
1:H:2615:LEU:C	1:H:2615:LEU:HD12	2.34	0.48
1:E:1636:LEU:C	1:E:1636:LEU:HD12	2.33	0.48
1:H:2615:LEU:HD12	1:H:2615:LEU:O	2.13	0.48
1:F:1734:ARG:NH1	3:F:5025:HOH:O	2.43	0.48
1:G:2295:VAL:CG1	1:L:3749:VAL:HG13	2.44	0.48
1:E:1339:GLY:HA3	1:E:1347:ILE:CD1	2.44	0.48
1:H:2371:GLU:HG2	1:H:2514:ILE:HD11	1.96	0.48
1:I:2918:LYS:HD2	3:I:5082:HOH:O	2.14	0.48
1:E:1633:VAL:HG22	1:H:2425:VAL:CG2	2.44	0.48
1:D:1283:GLN:HE22	1:I:2857:LYS:HZ3	1.62	0.48
1:D:1064:GLY:HA3	3:H:5076:HOH:O	2.13	0.48
1:J:3051:ILE:HG21	1:J:3121:ALA:HB3	1.95	0.48
1:I:2786:SER:OG	1:I:2789:GLU:HG3	2.12	0.48
1:B:646:ASN:ND2	1:B:650:LYS:HE3	2.28	0.48
1:G:2053:LEU:HG	1:G:2066:PHE:CD1	2.49	0.48
1:D:1313:LEU:O	1:D:1317:ILE:HG13	2.13	0.48
1:H:2629:LEU:HD12	1:H:2629:LEU:C	2.35	0.47
1:B:336:GLU:HB3	3:B:5014:HOH:O	2.13	0.47
1:D:1016:ILE:O	1:D:1020:ILE:HG13	2.14	0.47
1:L:3863:TYR:CD2	1:L:3972:LEU:HD13	2.49	0.47
1:L:3810:ARG:NH1	1:L:3951:GLU:CD	2.52	0.47
1:B:500:ARG:HB2	1:B:639:GLU:HA	1.97	0.47
1:K:3371:HIS:NE2	1:K:3483:ASP:HB2	2.30	0.47
1:H:2568:ASP:HA	1:H:2597:THR:O	2.14	0.47
1:L:3874:SER:HB2	1:L:3875:PRO:HD2	1.97	0.47
1:D:1060:LEU:HG	1:D:1073:PHE:CD1	2.50	0.47
1:D:1302:VAL:CG2	1:J:3087:VAL:HG22	2.39	0.47
1:B:506:PHE:C	1:B:506:PHE:CD1	2.87	0.47
1:E:1375:GLU:O	1:E:1518:GLY:HA2	2.15	0.47
1:C:693:ILE:CD1	1:C:843:ILE:HG23	2.45	0.47
1:C:703:ALA:HB1	1:J:3273:LYS:HE3	1.96	0.47
1:I:2658:PHE:HA	1:I:2661:ILE:HD12	1.96	0.47
1:C:974:LEU:O	1:C:974:LEU:HD12	2.14	0.47
1:D:1270:ILE:HG12	1:I:2797:LEU:HD11	1.95	0.47
1:H:2544:ASP:O	1:H:2616:SER:CB	2.63	0.47
1:J:3104:ILE:N	1:J:3104:ILE:HD12	2.30	0.47
1:F:1812:HIS:CE1	1:I:2805:HIS:CE1	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1546:TYR:CD2	1:E:1655:LEU:HD13	2.50	0.47
1:G:2234:ARG:HB3	1:G:2283:ALA:HB3	1.96	0.47
1:D:1165:ASP:HA	1:D:1166:ASP:HA	1.64	0.47
1:E:1402:LEU:HB2	1:E:1456:ILE:HB	1.96	0.47
1:B:334[A]:MET:HE1	1:B:509:VAL:CG1	2.45	0.46
1:C:967:LEU:CD1	1:C:968:HIS:CD2	2.98	0.46
1:E:1432:VAL:HG11	1:H:2626:VAL:HB	1.96	0.46
1:E:1556:CYS:HA	1:E:1560:THR:HG21	1.98	0.46
1:A:115:HIS:O	1:A:116:LEU:HD23	2.15	0.46
1:G:2094:VAL:HG22	1:L:3950:VAL:HG12	1.95	0.46
1:F:1826:LEU:HD13	1:F:1967:LEU:HG	1.97	0.46
1:H:2332:GLY:O	1:H:2381:GLU:HG2	2.15	0.46
1:D:1302:VAL:CG1	1:J:3087:VAL:HG13	2.46	0.46
1:I:2957:VAL:HG13	1:I:2957:VAL:O	2.15	0.46
1:K:3313:MET:HE1	1:K:3488:VAL:HG11	1.97	0.46
1:K:3529[B]:TYR:CE1	1:K:3602:ARG:NH2	2.83	0.46
1:B:564:SER:HB2	1:B:565:PRO:CD	2.46	0.46
1:L:3831:HIS:O	1:L:3832:GLU:C	2.54	0.46
1:A:233:SER:HB2	1:A:234:PRO:CD	2.46	0.46
1:A:239:VAL:O	1:A:240:LYS:HD3	2.15	0.46
1:G:2225:VAL:O	1:G:2226:LYS:HD2	2.16	0.46
1:D:1267:GLU:HB3	3:D:5108:HOH:O	2.16	0.46
1:B:334[A]:MET:HE1	1:B:509:VAL:HG11	1.96	0.46
1:E:1504:LEU:HD21	1:E:1550:ILE:HD13	1.97	0.46
1:B:557:ILE:HD12	1:B:629:LEU:CD1	2.45	0.46
1:E:1355:ILE:HA	1:E:1355:ILE:HD12	1.77	0.46
1:D:1220:ASP:OD1	1:D:1221:SER:N	2.42	0.46
1:F:1709:GLU:HG2	1:F:1852:ILE:HD11	1.98	0.46
1:K:3604:LYS:HE3	1:L:3682:ALA:HB1	1.98	0.46
1:I:2913:TRP:CZ3	1:I:2923:ILE:HG23	2.51	0.46
1:J:3104:ILE:HD12	1:J:3104:ILE:H	1.81	0.45
1:E:1339:GLY:HA3	1:E:1347:ILE:HD11	1.97	0.45
1:H:2489:ASP:HA	1:H:2490:ASP:HA	1.68	0.45
3:E:5131:HOH:O	1:H:2430:PRO:HG3	2.15	0.45
1:L:3810:ARG:HB2	1:L:3949:GLU:HA	1.98	0.45
1:J:3292:HIS:HE1	1:J:3294:ASN:ND2	2.12	0.45
1:C:908:VAL:HG13	1:C:961:SER:HB2	1.98	0.45
1:J:3148:ARG:HB2	1:J:3287:GLU:HA	1.99	0.45
1:C:834:ASP:HB2	1:C:890:SER:OG	2.16	0.45
1:K:3333:ILE:HD12	1:K:3333:ILE:H	1.81	0.45
1:D:1208:ALA:HA	1:D:1282:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:VAL:CG2	1:A:301:PRO:HG3	2.47	0.45
1:G:2015:ARG:O	1:G:2015:ARG:HG2	2.16	0.45
1:K:3587:ILE:HG12	1:L:3790:LEU:HD11	1.99	0.45
1:E:1496:ASP:HB2	1:E:1552:SER:OG	2.17	0.45
1:L:3946:LEU:O	1:L:3947:HIS:HB2	2.16	0.45
1:H:2580:LYS:O	1:H:2581:VAL:CB	2.64	0.45
1:H:2330:ILE:CG2	1:H:2340:ILE:HD13	2.47	0.45
1:L:3789:PRO:O	1:L:3790:LEU:HB2	2.15	0.45
1:I:2745:ASN:O	1:I:2800:ALA:HA	2.17	0.45
1:J:3116:GLU:HG2	1:J:3120:GLU:OE1	2.17	0.45
1:B:334[A]:MET:CA	1:B:334[A]:MET:HE3	2.31	0.45
1:D:1298:LEU:O	1:D:1299:HIS:HB2	2.17	0.45
1:L:3941:VAL:HG22	1:L:3957:ASP:CB	2.46	0.45
1:D:1149:LYS:HG2	1:D:1162:ARG:HB3	1.98	0.45
1:D:1024:ILE:CA	3:D:5025:HOH:O	2.60	0.45
1:H:2378:HIS:CB	1:H:2521:GLU:HB2	2.47	0.45
1:H:2615:LEU:HD13	1:H:2637:LEU:CD1	2.47	0.44
1:H:2348:ILE:HD13	1:H:2498:ILE:HG12	1.99	0.44
1:D:1054:HIS:NE2	1:D:1166:ASP:HB2	2.31	0.44
1:H:2630:HIS:CE1	1:H:2632[A]:ASN:HB2	2.52	0.44
1:D:1040:VAL:HG11	1:D:1177:ILE:HD13	1.98	0.44
1:I:2874:ILE:CD1	1:I:2946:LEU:HD11	2.46	0.44
1:H:2565:ARG:HB3	1:H:2614:ALA:HB3	1.99	0.44
1:G:2291:LEU:O	1:G:2292:HIS:HB2	2.16	0.44
1:E:1493:ARG:HA	1:E:1493:ARG:HD2	1.86	0.44
1:F:1947:ARG:N	1:F:1947:ARG:HD2	2.32	0.44
1:D:1058:ILE:HD12	1:D:1079:ILE:HG12	2.00	0.44
1:D:1270:ILE:HG12	1:I:2797:LEU:CD1	2.48	0.44
1:A:4:ILE:HD11	1:A:314:LEU:HD11	1.99	0.44
1:F:1707:GLY:O	1:F:1850:LYS:HD2	2.17	0.44
1:C:902[B]:LYS:HB3	1:C:905:LYS:CD	2.44	0.44
1:A:309:VAL:CG1	1:C:770:VAL:HG22	2.48	0.44
1:B:436:LEU:HD11	1:B:476:LEU:HB3	1.99	0.44
1:G:2199:PHE:CE2	1:G:2203:HIS:CE1	3.05	0.44
1:I:2654:LYS:O	1:I:2657:LYS:HB3	2.17	0.44
1:F:1847:LEU:HD12	1:F:1847:LEU:HA	1.88	0.44
1:C:842:LEU:O	1:C:846:ILE:HG13	2.17	0.44
1:L:3915:GLU:HG3	1:L:3960:LYS:NZ	2.32	0.44
1:D:1241:ARG:HB3	1:D:1290:ALA:HB3	1.99	0.44
1:D:1071:LEU:HB2	1:D:1125:ILE:HB	1.99	0.44
1:B:337:LYS:HB3	1:B:337:LYS:HE2	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3188:LYS:HD2	1:J:3188:LYS:HA	1.73	0.44
1:J:3046:LEU:HG	1:J:3059:PHE:CD1	2.52	0.44
1:E:1536:LYS:NZ	3:E:5100:HOH:O	2.50	0.44
1:C:726:GLU:HB2	1:C:831:ARG:HH21	1.81	0.44
1:E:1339:GLY:O	1:E:1388:GLU:HG2	2.18	0.44
1:F:1716:HIS:NE2	1:F:1828:ASP:HB2	2.33	0.44
1:A:175:PHE:CD1	1:A:175:PHE:C	2.91	0.44
1:I:2975:LEU:O	1:I:2979:LEU:HB2	2.18	0.44
1:F:1678:ILE:N	1:F:1678:ILE:HD12	2.32	0.44
1:C:851:ASP:HB2	3:C:5091:HOH:O	2.18	0.44
1:H:2525:LEU:O	1:H:2529:LYS:HG3	2.17	0.44
1:F:1824:ARG:NH1	1:F:1965:GLU:CD	2.57	0.44
1:F:1827:ASP:HA	1:F:1828:ASP:HA	1.72	0.44
1:D:1215:TYR:CD1	1:D:1253:LEU:HD13	2.53	0.44
1:E:1485:LEU:HB2	1:E:1489:TYR:HB2	1.99	0.44
1:I:2948:VAL:HG22	1:I:2964:ASP:HB3	1.99	0.44
1:H:2510:GLU:HA	1:H:2511:GLY:O	2.16	0.44
1:E:1569:PRO:HD2	1:E:1598:GLU:O	2.18	0.44
1:F:1871:ASN:HD21	1:L:3932:ASP:CG	2.21	0.44
1:B:557:ILE:CD1	1:B:629:LEU:CD1	2.96	0.43
1:I:2809:LEU:HB2	1:I:2813:TYR:HB2	2.00	0.43
1:G:2234:ARG:HD3	1:G:2237:ASP:HB3	2.00	0.43
1:A:65:ILE:HD12	1:A:86:ILE:HG12	2.00	0.43
1:D:1226:SER:HB2	1:D:1227:PRO:CD	2.46	0.43
1:A:61:HIS:NE2	1:A:173:ASP:HB2	2.33	0.43
1:I:2716:LEU:HD11	1:I:2797:LEU:HA	2.00	0.43
1:I:2899:ASP:HA	1:I:2928:THR:O	2.19	0.43
1:F:1973:GLU:O	1:F:1976:VAL:HG22	2.19	0.43
1:G:2189:GLN:NE2	3:G:5089:HOH:O	2.51	0.43
1:K:3377:LEU:HG	1:K:3390:PHE:CD1	2.54	0.43
1:L:3810:ARG:HA	1:L:3810:ARG:HH11	1.84	0.43
1:I:2655:LEU:HA	1:I:2655:LEU:HD12	1.90	0.43
1:E:1496:ASP:HA	1:E:1497:ASP:HA	1.76	0.43
1:L:3941:VAL:HG22	1:L:3957:ASP:HB3	2.00	0.43
3:B:5112:HOH:O	1:K:3423:PRO:HG3	2.19	0.43
1:B:576:PRO:HD2	1:B:605:GLU:O	2.18	0.43
1:I:2899:ASP:HB2	1:I:2930:GLY:O	2.18	0.43
1:H:2319:SER:O	1:H:2323:LYS:HG3	2.19	0.43
1:A:270:LYS:HB2	1:A:270:LYS:HE3	1.70	0.43
1:C:718:ILE:HD11	1:C:993:LEU:HB3	2.00	0.43
1:F:1752:ASN:HD21	1:F:1810:LYS:HE2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3341:ILE:HD12	1:K:3341:ILE:HA	1.74	0.43
1:I:2834:ASP:HB2	1:I:2973:GLU:OE2	2.19	0.43
1:I:2703:ARG:NH1	1:I:2841:GLU:HG2	2.33	0.43
1:J:3291:LEU:HD12	1:J:3291:LEU:O	2.19	0.43
1:I:2874:ILE:HD12	1:I:2946:LEU:HD11	2.00	0.43
1:B:403:ILE:HG22	1:B:404:THR:O	2.19	0.43
1:K:3367:LEU:HB2	1:K:3530:PRO:HG3	2.00	0.42
1:I:2881:SER:HB2	1:I:2882:PRO:HD2	2.01	0.42
1:C:671:LYS:HE2	1:C:688:GLU:OE2	2.19	0.42
1:B:444:PRO:HG3	3:K:5113:HOH:O	2.17	0.42
1:F:1657:SER:O	1:F:1661:LYS:HG3	2.20	0.42
1:D:1302:VAL:HG13	1:J:3087:VAL:CG1	2.49	0.42
1:E:1569:PRO:HD3	1:E:1643[B]:LYS:HB2	2.00	0.42
1:F:1888:SER:OG	1:I:2764:LEU:HD22	2.19	0.42
1:L:3702:HIS:NE2	1:L:3814:ASP:HB2	2.35	0.42
1:E:1499:PHE:CD1	1:E:1499:PHE:C	2.91	0.42
1:J:3140:LEU:HB2	1:J:3144:TYR:HB2	2.00	0.42
1:F:1730:GLU:N	1:F:1730:GLU:CD	2.73	0.42
1:C:717:ARG:NH1	3:C:5092:HOH:O	2.38	0.42
1:B:426:HIS:CD2	1:K:3467:HIS:HB2	2.55	0.42
1:L:3872:CYS:HA	1:L:3873:CYS:HA	1.80	0.42
1:A:13:ILE:HA	1:A:14:PRO:HD3	1.81	0.42
1:A:111:ALA:O	1:C:966:TYR:HA	2.19	0.42
1:I:2696:GLU:O	1:I:2697:LEU:HD23	2.20	0.42
1:G:2158:ASP:HA	1:G:2159:ASP:HA	1.72	0.42
1:J:3091:THR:HA	1:J:3092:PRO:HD3	1.85	0.42
1:D:1306:HIS:CE1	1:D:1308:ASN:HB2	2.55	0.42
1:B:528:ILE:HD13	1:B:549:TYR:CD2	2.55	0.42
1:K:3485:PHE:C	1:K:3485:PHE:CD1	2.92	0.42
1:E:1389:ILE:HG12	1:E:1493:ARG:NH2	2.34	0.42
1:I:2877:PHE:CE1	1:I:2928:THR:HB	2.54	0.42
1:F:1858:GLN:NE2	3:F:5068:HOH:O	2.52	0.42
1:H:2409:TYR:OH	1:H:2429:THR:HG22	2.20	0.42
1:A:315[B]:ASN:ND2	3:A:5136:HOH:O	2.52	0.42
1:B:402:GLY:C	1:B:403:ILE:HD12	2.39	0.42
1:H:2357:ASP:HB2	1:H:2361:ASN:HB2	2.01	0.42
1:J:2981:SER:HB2	3:J:5010:HOH:O	2.19	0.42
1:H:2580:LYS:CA	3:H:5089:HOH:O	2.68	0.42
1:D:1058:ILE:HG12	1:D:1162:ARG:HH21	1.84	0.42
1:K:3313:MET:CE	1:K:3488:VAL:HG11	2.50	0.42
1:B:503:ASP:HA	1:B:504:ASP:HA	1.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ILE:O	1:B:358:ILE:HG13	2.19	0.42
1:D:1013:GLU:OE2	1:D:1056:ASP:HB3	2.19	0.42
1:J:3151:ASP:HA	1:J:3152:ASP:HA	1.81	0.42
1:C:665:MET:HG2	3:C:5140:HOH:O	2.19	0.42
1:B:334[B]:MET:HE3	1:B:645:LEU:HD22	2.02	0.41
1:L:3887:VAL:CG2	1:L:3942:PRO:HG3	2.50	0.41
1:F:1670:GLY:HA3	1:F:1678:ILE:HD13	2.01	0.41
1:H:2378:HIS:HB3	1:H:2521:GLU:HB2	2.02	0.41
1:H:2357:ASP:OD1	1:H:2530:PHE:HE2	2.01	0.41
1:F:1803:PRO:O	1:F:1804:LEU:HB2	2.20	0.41
1:A:44:ASN:OD1	1:A:201:THR:HA	2.20	0.41
1:K:3561:ASP:HA	1:K:3590:THR:O	2.20	0.41
1:K:3320:PHE:HA	1:K:3323:ILE:HD12	2.03	0.41
1:C:902[A]:LYS:HB2	1:C:905:LYS:CD	2.47	0.41
1:E:1364:ASP:OD2	1:E:1368:ASN:HB2	2.20	0.41
1:B:500:ARG:HH11	1:B:500:ARG:HD2	1.65	0.41
1:J:3051:ILE:HD12	1:J:3051:ILE:N	2.35	0.41
1:J:2981:SER:O	1:J:2985[A]:LYS:HD3	2.20	0.41
1:J:2992:ILE:HA	1:J:2993:PRO:HD3	1.88	0.41
1:F:1703:GLU:O	1:F:1704:LEU:HD23	2.20	0.41
1:K:3311:MET:CG	1:K:3312:SER:H	2.33	0.41
1:L:3886:PRO:HD2	1:L:3915:GLU:O	2.21	0.41
1:I:2887:VAL:O	1:I:2888:LYS:HD3	2.20	0.41
1:D:1099:ASP:OD1	1:J:3139:VAL:O	2.38	0.41
1:E:1632:GLU:HG2	3:H:5036:HOH:O	2.21	0.41
1:H:2630:HIS:CE1	1:H:2632[B]:ASN:HB2	2.55	0.41
1:G:2215:PHE:CE1	1:G:2266:THR:HB	2.56	0.41
1:A:60:ALA:O	1:A:200:PHE:HA	2.21	0.41
1:F:1824:ARG:HH11	1:F:1824:ARG:HA	1.85	0.41
1:D:1008:GLY:HA3	1:D:1016:ILE:CD1	2.51	0.41
1:D:1283:GLN:NE2	1:I:2857:LYS:HZ3	2.17	0.41
1:L:3713:ILE:HD12	1:L:3784:LEU:HG	2.03	0.41
1:I:2802:PHE:O	1:I:2804:LYS:HG3	2.21	0.41
1:H:2592:ILE:HG12	1:H:2593:GLN:N	2.36	0.41
1:A:112:THR:HA	1:A:113:PRO:HD3	1.92	0.41
1:I:2960:LEU:C	1:I:2960:LEU:HD12	2.41	0.41
1:I:2879:CYS:HA	1:I:2880:CYS:HA	1.80	0.41
1:L:3719:LEU:HB2	1:L:3773:ILE:HB	2.01	0.41
1:F:1871:ASN:ND2	1:L:3932:ASP:CG	2.74	0.41
1:E:1327:MET:HA	1:E:1330:LYS:NZ	2.35	0.41
1:G:2239:SER:HB3	1:G:2269:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2295:VAL:CG1	1:L:3749:VAL:CG1	2.99	0.41
1:G:2111:ILE:CD1	1:G:2111:ILE:H	2.34	0.41
1:D:1016:ILE:N	1:D:1016:ILE:HD12	2.32	0.41
1:B:643:LEU:HD12	1:B:643:LEU:O	2.20	0.41
1:F:1886:CYS:O	1:I:2764:LEU:CD1	2.69	0.41
1:B:564:SER:CB	1:B:565:PRO:CD	2.99	0.41
1:E:1467:LEU:HA	1:E:1467:LEU:HD23	1.85	0.41
1:C:708:ILE:HG21	1:C:880:TYR:OH	2.20	0.41
1:H:2579[A]:ARG:HD2	3:H:5084:HOH:O	2.20	0.41
1:C:829:SER:HA	1:C:972:GLU:O	2.20	0.41
1:G:2298:LEU:C	1:G:2298:LEU:HD12	2.41	0.41
1:D:1305:LEU:C	1:D:1305:LEU:HD12	2.42	0.41
1:F:1895:LYS:HB3	1:F:1898:LYS:HD2	2.02	0.41
1:E:1575:ASP:HB2	1:E:1606:GLY:O	2.21	0.41
1:I:2725:LYS:NZ	3:I:5016:HOH:O	2.54	0.41
1:F:1754:VAL:HG13	1:F:1759:ILE:CD1	2.50	0.41
1:I:2815:SER:HA	1:I:2958:GLU:O	2.21	0.41
1:L:3881:LYS:HB3	1:L:3881:LYS:HE2	1.77	0.41
1:K:3415:LEU:HD11	1:K:3455:LEU:HB3	2.02	0.41
1:A:291:ASP:CB	1:A:292:ARG:NH1	2.84	0.41
1:B:540:LYS:HA	1:B:540:LYS:HD2	1.75	0.41
1:H:2543:ILE:CD1	1:H:2615:LEU:HD11	2.51	0.41
1:E:1565:LEU:CD2	1:E:1625:PRO:HB2	2.50	0.41
1:B:344:ILE:CG2	1:B:353[B]:ARG:HB3	2.51	0.41
1:E:1570:VAL:HG13	1:E:1623:SER:HB2	2.02	0.41
1:B:574:LYS:HA	1:B:574:LYS:HD2	1.92	0.41
1:D:1008:GLY:HA3	1:D:1016:ILE:HD11	2.03	0.40
1:J:2980:MET:HA	1:J:2984:GLU:OE2	2.21	0.40
1:D:1246:SER:HB3	1:D:1276:GLY:HA3	2.02	0.40
1:H:2576:ASP:OD1	1:H:2577:LEU:N	2.54	0.40
1:H:2541:PHE:HA	1:H:2613:LEU:O	2.20	0.40
1:G:2111:ILE:CD1	1:G:2111:ILE:N	2.84	0.40
1:C:831:ARG:HA	1:C:831:ARG:HD2	1.74	0.40
1:C:702:ASP:OD2	1:C:706:ASN:HB2	2.21	0.40
1:A:2:SER:OG	1:A:5:GLU:HG3	2.22	0.40
1:A:122[A]:LYS:NZ	1:C:751:ARG:HH12	2.20	0.40
1:D:1180:LEU:HB3	3:D:5089:HOH:O	2.21	0.40
1:D:1037:ASN:OD1	1:D:1194:THR:HA	2.20	0.40
1:L:3753:THR:HA	1:L:3754:PRO:HD3	2.00	0.40
1:K:3367:LEU:HD22	1:K:3368:PHE:N	2.37	0.40
1:K:3613:LYS:O	1:K:3620:GLU:HA	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:2555:ASP:O	1:H:2557[A]:LYS:HG2	2.22	0.40
1:A:47:VAL:HG11	1:A:184:ILE:HD13	2.04	0.40
1:A:260:LEU:HD23	1:A:296:LEU:HB2	2.03	0.40
1:G:2127:GLU:O	1:G:2130:GLU:HG2	2.22	0.40
1:H:2492:PHE:CG	1:H:2493:GLY:N	2.89	0.40
1:K:3575:TRP:CZ3	1:K:3585:ILE:HG23	2.56	0.40
1:B:535:GLU:HA	1:B:539:LEU:HA	2.03	0.40
1:G:2161:PHE:C	1:G:2161:PHE:CD1	2.95	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	326/332 (98%)	316 (97%)	10 (3%)	0	100	100
1	B	326/332 (98%)	308 (94%)	17 (5%)	1 (0%)	46	51
1	C	324/332 (98%)	310 (96%)	14 (4%)	0	100	100
1	D	323/332 (97%)	307 (95%)	15 (5%)	1 (0%)	46	51
1	E	325/332 (98%)	314 (97%)	11 (3%)	0	100	100
1	F	322/332 (97%)	311 (97%)	10 (3%)	1 (0%)	46	51
1	G	322/332 (97%)	313 (97%)	8 (2%)	1 (0%)	46	51
1	H	326/332 (98%)	309 (95%)	14 (4%)	3 (1%)	21	17
1	I	321/332 (97%)	297 (92%)	18 (6%)	6 (2%)	10	4
1	J	323/332 (97%)	312 (97%)	10 (3%)	1 (0%)	46	51
1	K	324/332 (98%)	308 (95%)	15 (5%)	1 (0%)	46	51
1	L	322/332 (97%)	305 (95%)	16 (5%)	1 (0%)	46	51
All	All	3884/3984 (98%)	3710 (96%)	158 (4%)	16 (0%)	39	42

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	519	VAL
1	I	2841	GLU
1	K	3342	LYS
1	F	1947	ARG
1	I	2842	GLY
1	H	2508	GLU
1	I	2763	HIS
1	I	2820	ASP
1	L	3832	GLU
1	H	2357	ASP
1	I	2680	LYS
1	D	1181	VAL
1	I	2663	GLY
1	G	2001	GLY
1	H	2332	GLY
1	J	2994	GLY

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	278/279 (100%)	259 (93%)	19 (7%)	20 17
1	B	277/279 (99%)	262 (95%)	15 (5%)	27 27
1	C	275/279 (99%)	261 (95%)	14 (5%)	29 30
1	D	274/279 (98%)	255 (93%)	19 (7%)	19 17
1	E	276/279 (99%)	254 (92%)	22 (8%)	15 11
1	F	273/279 (98%)	259 (95%)	14 (5%)	29 30
1	G	273/279 (98%)	258 (94%)	15 (6%)	27 26
1	H	277/279 (99%)	251 (91%)	26 (9%)	11 7
1	I	272/279 (98%)	248 (91%)	24 (9%)	12 9
1	J	274/279 (98%)	254 (93%)	20 (7%)	17 14
1	K	275/279 (99%)	253 (92%)	22 (8%)	15 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	L	273/279 (98%)	248 (91%)	25 (9%)	11 8
All	All	3297/3348 (98%)	3062 (93%)	235 (7%)	18 16

All (235) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	LEU
1	A	57	LEU
1	A	67	LEU
1	A	75	GLU
1	A	81	ARG
1	A	108	VAL
1	A	122[A]	LYS
1	A	122[B]	LYS
1	A	137	GLU
1	A	169	ARG
1	A	175	PHE
1	A	228	SER
1	A	241	LEU
1	A	262	ARG
1	A	291	ASP
1	A	292	ARG
1	A	305	LEU
1	A	331	LEU
1	B	338	LEU
1	B	360	ARG
1	B	388	LEU
1	B	398	LEU
1	B	412	ARG
1	B	500	ARG
1	B	506	PHE
1	B	519	VAL
1	B	523	LEU
1	B	540	LYS
1	B	559	SER
1	B	605	GLU
1	B	623	ARG
1	B	629	LEU
1	B	662	LEU
1	C	693	ILE
1	C	717	ARG

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Mol	Chain	Res	Type
1	C	741	ARG
1	C	743	ARG
1	C	770	VAL
1	C	778	LEU
1	C	815	VAL
1	C	826	LYS
1	C	831	ARG
1	C	837	PHE
1	C	853	GLU
1	C	924	ARG
1	C	952	GLN
1	C	993	LEU
1	D	1022	ARG
1	D	1024	ILE
1	D	1060	LEU
1	D	1074	ARG
1	D	1098	LEU
1	D	1099	ASP
1	D	1101	VAL
1	D	1168	PHE
1	D	1184	GLU
1	D	1185	LEU
1	D	1186	GLU
1	D	1221	SER
1	D	1234	LEU
1	D	1241	ARG
1	D	1255	ARG
1	D	1267	GLU
1	D	1292	SER
1	D	1320	LEU
1	D	1324	LEU
1	E	1325	MET
1	E	1331	LEU
1	E	1332	LYS
1	E	1355	ILE
1	E	1364	ASP
1	E	1375	GLU
1	E	1381	LEU
1	E	1405	ARG
1	E	1446	LYS
1	E	1488	LYS
1	E	1499	PHE

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Mol	Chain	Res	Type
1	E	1512	VAL
1	E	1543[A]	TYR
1	E	1543[B]	TYR
1	E	1560	THR
1	E	1565	LEU
1	E	1572	ARG
1	E	1629	LEU
1	E	1633	VAL
1	E	1642	GLU
1	E	1646	LYS
1	E	1655	LEU
1	F	1662	LEU
1	F	1710	ARG
1	F	1712	LEU
1	F	1720	ILE
1	F	1736	ARG
1	F	1824	ARG
1	F	1830	PHE
1	F	1847	LEU
1	F	1883	SER
1	F	1896	LEU
1	F	1914	ASP
1	F	1917	ARG
1	F	1946	ASP
1	F	1947	ARG
1	G	1993	LEU
1	G	2043	LEU
1	G	2051	ILE
1	G	2053	LEU
1	G	2067	ARG
1	G	2091	LEU
1	G	2094	VAL
1	G	2102	LEU
1	G	2177	GLU
1	G	2182	VAL
1	G	2227	LEU
1	G	2232	VAL
1	G	2279	SER
1	G	2285	SER
1	G	2317	LEU
1	H	2318	MET
1	H	2324	LEU

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Mol	Chain	Res	Type
1	H	2348	ILE
1	H	2353	ASP
1	H	2357	ASP
1	H	2374	LEU
1	H	2384	LEU
1	H	2398	ARG
1	H	2422	LEU
1	H	2425	VAL
1	H	2429	THR
1	H	2433	LEU
1	H	2439	LYS
1	H	2440	SER
1	H	2454	GLU
1	H	2492	PHE
1	H	2505	VAL
1	H	2526	LYS
1	H	2545	SER
1	H	2558	LEU
1	H	2586	GLU
1	H	2587[A]	LYS
1	H	2587[B]	LYS
1	H	2609	ARG
1	H	2616	SER
1	H	2648	LEU
1	I	2651	MET
1	I	2655	LEU
1	I	2703	ARG
1	I	2705	LEU
1	I	2715	LEU
1	I	2729	ARG
1	I	2756	VAL
1	I	2763	HIS
1	I	2792	GLU
1	I	2823	PHE
1	I	2839	GLU
1	I	2840	LEU
1	I	2841	GLU
1	I	2843	LYS
1	I	2844	VAL
1	I	2924	GLN
1	I	2939	ASP
1	I	2940	ARG

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Mol	Chain	Res	Type
1	I	2941	SER
1	I	2947	SER
1	I	2953	LEU
1	I	2957	VAL
1	I	2969	VAL
1	I	2979	LEU
1	J	2980	MET
1	J	2985[A]	LYS
1	J	2985[B]	LYS
1	J	3004	GLU
1	J	3010	ILE
1	J	3011	LYS
1	J	3034	ARG
1	J	3036	LEU
1	J	3046	LEU
1	J	3060	ARG
1	J	3087	VAL
1	J	3095	LEU
1	J	3188	LYS
1	J	3198	TYR
1	J	3207	SER
1	J	3220	LEU
1	J	3249	LYS
1	J	3270	ASP
1	J	3271	ARG
1	J	3310	LEU
1	K	3315	GLU
1	K	3316	LYS
1	K	3317	LEU
1	K	3318	LYS
1	K	3335	GLU
1	K	3341	ILE
1	K	3342	LYS
1	K	3367	LEU
1	K	3375	ILE
1	K	3377	LEU
1	K	3412	LYS
1	K	3485	PHE
1	K	3492	GLU
1	K	3498	VAL
1	K	3503	GLU
1	K	3551	LEU

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Mol	Chain	Res	Type
1	K	3556	VAL
1	K	3601	ASP
1	K	3602	ARG
1	K	3615	LEU
1	K	3618	GLU
1	K	3641	LEU
1	L	3648	LEU
1	L	3679	LYS
1	L	3692	GLU
1	L	3722	ARG
1	L	3746	LEU
1	L	3749	VAL
1	L	3781	GLU
1	L	3785	GLU
1	L	3805	LYS
1	L	3810	ARG
1	L	3816	PHE
1	L	3831	HIS
1	L	3832	GLU
1	L	3869	SER
1	L	3882	LEU
1	L	3889	ARG
1	L	3900	ASP
1	L	3911	LYS
1	L	3933	ARG
1	L	3934	SER
1	L	3941	VAL
1	L	3946	LEU
1	L	3956	ASN
1	L	3959	GLU
1	L	3972	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	HIS
1	A	221	GLN
1	A	290	GLN
1	B	488	HIS
1	B	534	GLN
1	B	552	GLN
1	B	621	GLN

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Mol	Chain	Res	Type
1	B	646	ASN
1	C	883	GLN
1	C	952	GLN
1	C	977	ASN
1	D	1209	ASN
1	D	1283	GLN
1	E	1527	GLN
1	E	1614	GLN
1	F	1667	GLN
1	F	1752	ASN
1	F	1812	HIS
1	F	1858	GLN
1	F	1876	GLN
1	F	1945	GLN
1	G	2083	ASN
1	G	2143	HIS
1	G	2189	GLN
1	G	2203	HIS
1	G	2207	GLN
1	H	2520	GLN
1	H	2538	GLN
1	H	2607	GLN
1	I	2745	ASN
1	I	2805	HIS
1	I	2838	HIS
1	I	2851	GLN
1	I	2869	GLN
1	I	2919	ASN
1	I	2963	ASN
1	J	3182	GLN
1	J	3200	GLN
1	J	3269	GLN
1	J	3294	ASN
1	K	3407	ASN
1	K	3467	HIS
1	K	3513	GLN
1	K	3531	GLN
1	K	3600	GLN
1	L	3798	HIS
1	L	3844	GLN
1	L	3862	GLN

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

Of 24 ligands modelled in this entry, 24 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	326/332 (98%)	-0.40	4 (1%) 81 82	17, 29, 58, 83	0
1	B	325/332 (97%)	-0.44	0 100 100	18, 32, 60, 85	0
1	C	326/332 (98%)	-0.48	2 (0%) 90 90	15, 28, 53, 82	0
1	D	325/332 (97%)	-0.41	1 (0%) 94 95	20, 35, 60, 83	0
1	E	326/332 (98%)	-0.51	1 (0%) 94 95	19, 29, 51, 73	0
1	F	324/332 (97%)	-0.33	3 (0%) 85 86	24, 35, 62, 81	0
1	G	325/332 (97%)	-0.47	0 100 100	17, 27, 48, 70	0
1	H	326/332 (98%)	-0.34	4 (1%) 81 82	23, 36, 62, 85	0
1	I	325/332 (97%)	-0.20	8 (2%) 61 64	25, 41, 70, 94	0
1	J	326/332 (98%)	-0.47	1 (0%) 94 95	19, 28, 53, 74	0
1	K	325/332 (97%)	-0.34	2 (0%) 90 90	20, 33, 57, 81	0
1	L	325/332 (97%)	-0.53	3 (0%) 85 86	16, 29, 53, 78	1 (0%)
All	All	3904/3984 (97%)	-0.41	29 (0%) 89 89	15, 32, 59, 94	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	2840	LEU	3.6
1	E	1543[A]	TYR	3.5
1	H	2509	LEU	3.4
1	C	853	GLU	3.3
1	C	854	LEU	3.3
1	I	2700	GLY	3.1
1	I	2841	GLU	2.9
1	I	2679	ILE	2.9
1	I	2842	GLY	2.8
1	K	3502	LEU	2.8
1	A	194	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	2980	MET	2.6
1	A	1	MET	2.5
1	I	2839	GLU	2.4
1	H	2507	HIS	2.4
1	D	1324	LEU	2.4
1	I	2977	PHE	2.3
1	A	192	LEU	2.2
1	L	3674	ASP	2.2
1	F	1929	GLU	2.2
1	A	51	GLU	2.1
1	F	1874[A]	TYR	2.1
1	F	1846	GLU	2.1
1	I	2682	PHE	2.1
1	H	2648	LEU	2.1
1	H	2350	ASP	2.0
1	K	3361	GLU	2.0
1	L	3833	LEU	2.0
1	L	3673	LYS	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, 95^{th} 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	CO	G	3319	1/1	1.00	0.12	4.77	24,24,24,24	0
2	CO	J	4312	1/1	0.99	0.14	3.73	23,23,23,23	0
2	CO	F	2988	1/1	1.00	0.13	3.21	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CO	E	2657	1/1	1.00	0.12	3.02	27,27,27,27	0
2	CO	B	1663	1/1	0.98	0.12	2.99	30,30,30,30	0
2	CO	B	1664	1/1	0.98	0.12	2.84	25,25,25,25	0
2	CO	C	1995	1/1	1.00	0.13	2.51	22,22,22,22	0
2	CO	L	4974	1/1	0.99	0.12	2.45	23,23,23,23	0
2	CO	K	4643	1/1	1.00	0.12	2.33	26,26,26,26	0
2	CO	K	4642	1/1	0.98	0.13	1.72	35,35,35,35	0
2	CO	H	3650	1/1	0.99	0.12	1.51	29,29,29,29	0
2	CO	J	4311	1/1	0.99	0.12	1.01	28,28,28,28	0
2	CO	A	1333	1/1	0.99	0.13	0.99	24,24,24,24	0
2	CO	H	3649	1/1	0.98	0.12	0.78	39,39,39,39	0
2	CO	G	3318	1/1	1.00	0.11	0.67	27,27,27,27	0
2	CO	D	2326	1/1	0.99	0.11	0.54	28,28,28,28	0
2	CO	I	3980	1/1	0.98	0.12	0.22	38,38,38,38	0
2	CO	E	2656	1/1	0.98	0.10	0.17	30,30,30,30	0
2	CO	A	1332	1/1	0.99	0.11	0.06	28,28,28,28	0
2	CO	F	2987	1/1	0.99	0.09	-0.22	35,35,35,35	0
2	CO	I	3981	1/1	0.99	0.13	-0.31	33,33,33,33	0
2	CO	C	1994	1/1	1.00	0.10	-0.35	30,30,30,30	0
2	CO	L	4973	1/1	1.00	0.09	-0.37	29,29,29,29	0
2	CO	D	2325	1/1	0.98	0.08	-1.09	35,35,35,35	0

6.5 Other polymers

There are no such residues in this entry.