Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:12 AM GMT

PDB ID	:	3HKB
Title	:	Tubulin: RB3 Stathmin-like domain complex
Authors	:	Dorleans, A.; Gigant, B.; Ravelli, R.B.G.; Mailliet, P.; Mikol, V.; Knossow, M.
Deposited on	:	2009-05-23
Resolution	:	3.65 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:

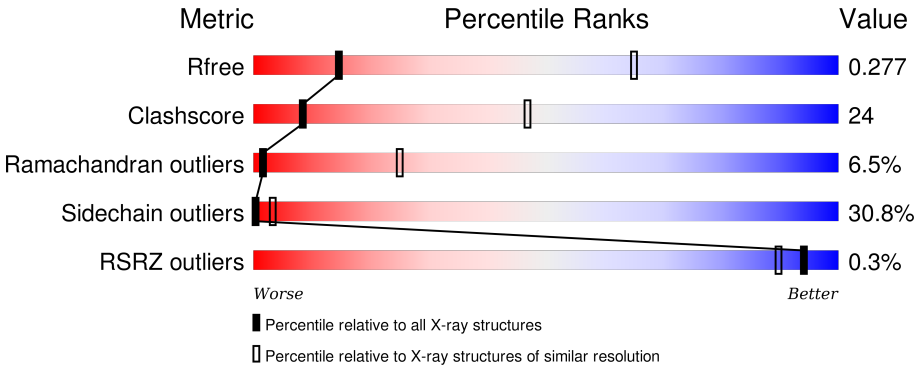
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.65 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	1010 (3.82-3.50)
Clashscore	102246	1125 (3.82-3.50)
Ramachandran outliers	100387	1079 (3.82-3.50)
Sidechain outliers	100360	1078 (3.82-3.50)
RSRZ outliers	91569	1017 (3.82-3.50)

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	451	46% 33% 14% • 5%
1	C	451	% 49% 33% 11% • 5%
2	B	445	40% 35% 17% • 6%
2	D	445	41% 37% 15% • 6%
3	E	142	% 47% 26% 13% • 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14125 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	0	0	0
			3307	2100	560	626	21			
1	C	428	Total	C	N	O	S	0	0	0
			3296	2095	557	623	21			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3249	2044	548	633	24			
2	D	419	Total	C	N	O	S	0	0	0
			3240	2038	546	632	24			

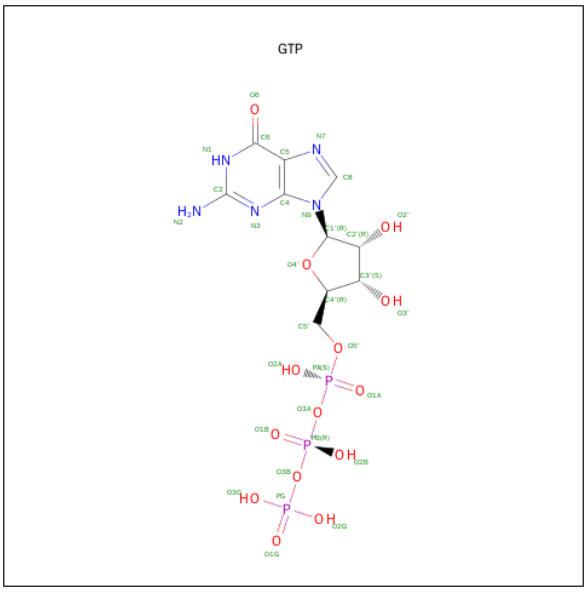
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			911	552	171	183	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	EXPRESSION TAG	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

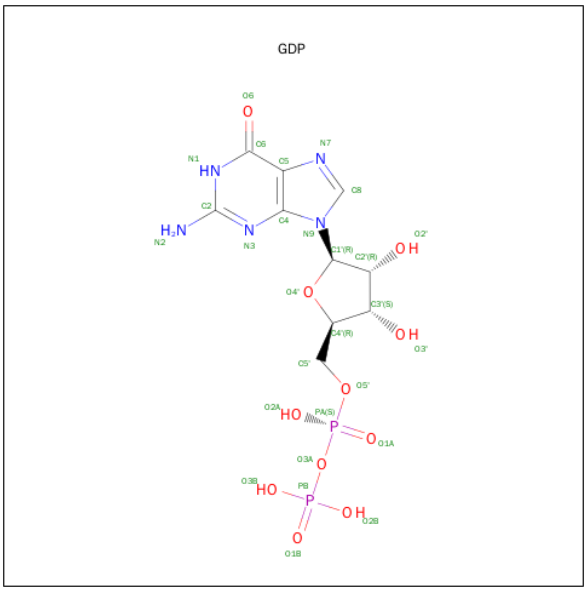


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



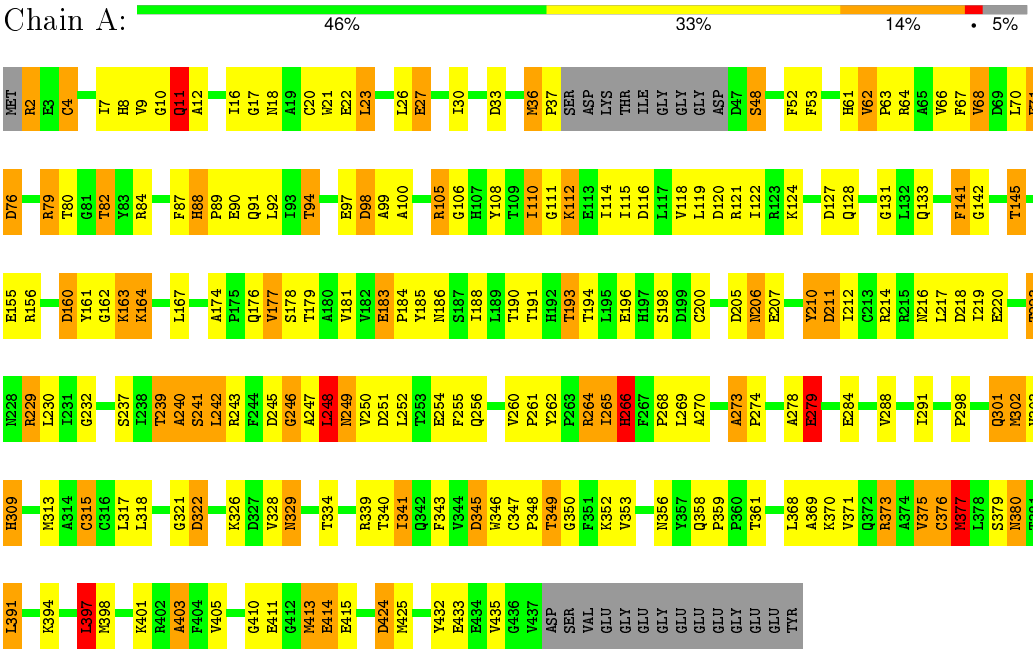
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
6	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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.

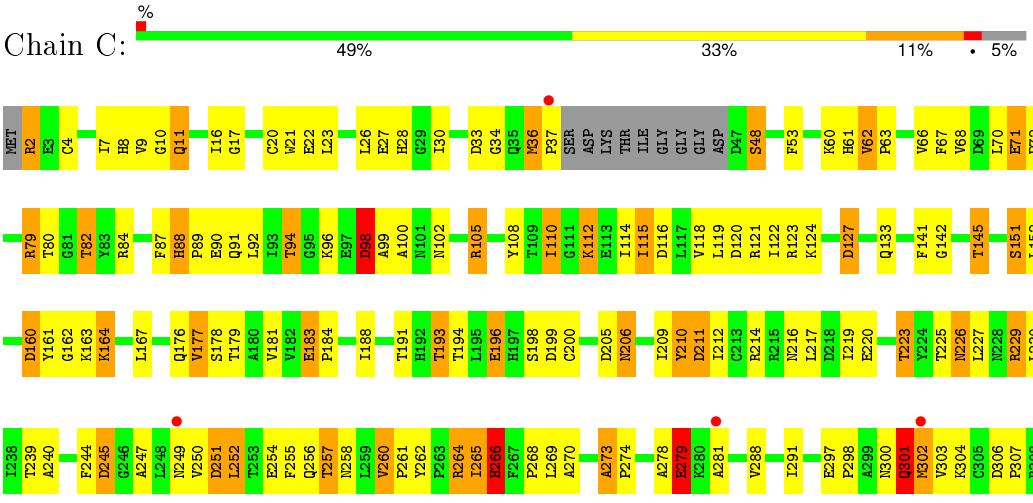
- Molecule 1: Tubulin alpha chain

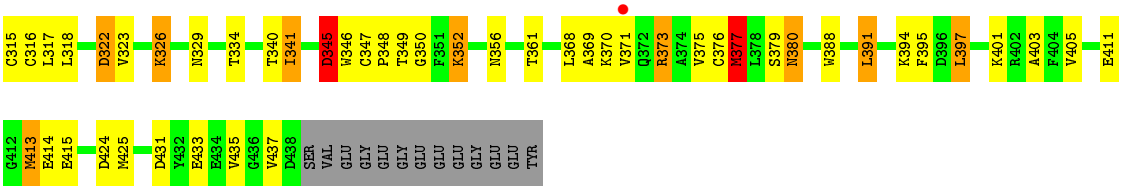
Chain A:



- Molecule 1: Tubulin alpha chain

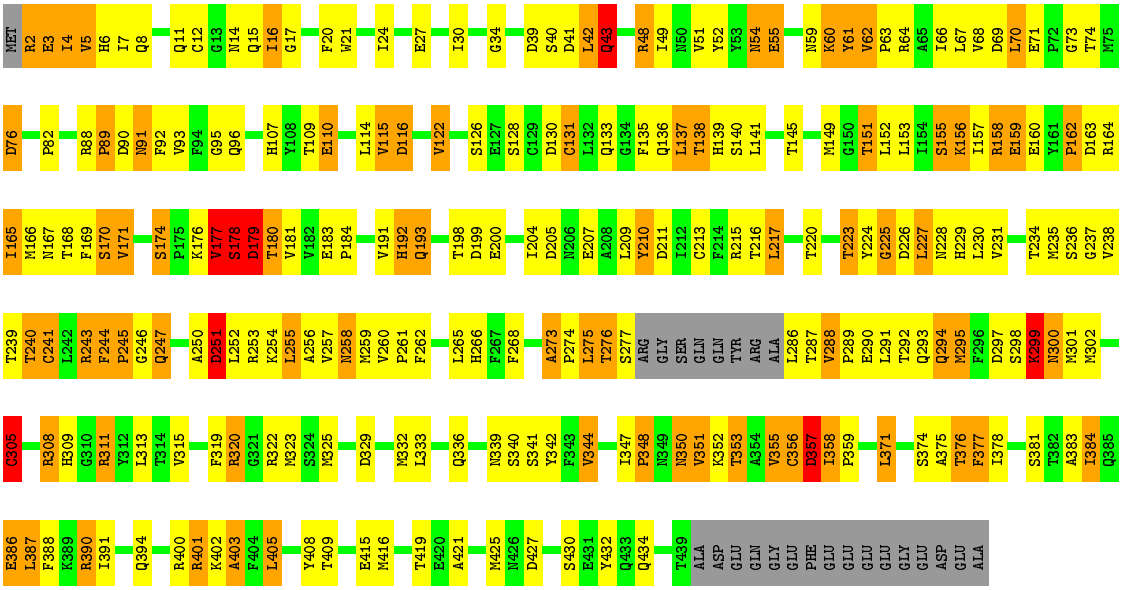
Chain C:





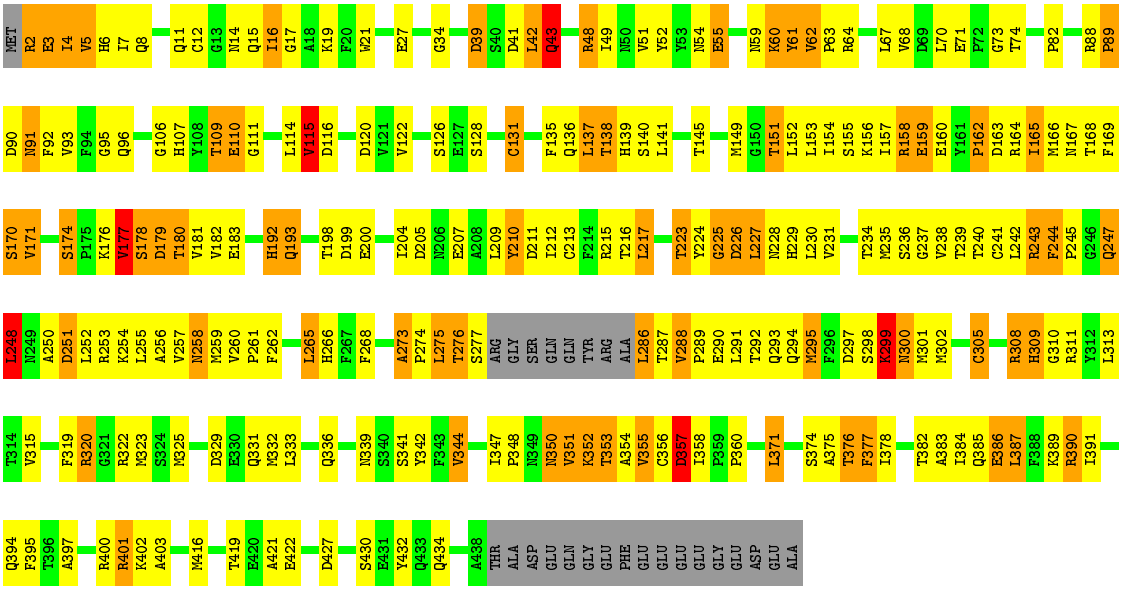
• Molecule 2: Tubulin beta chain

Chain B:



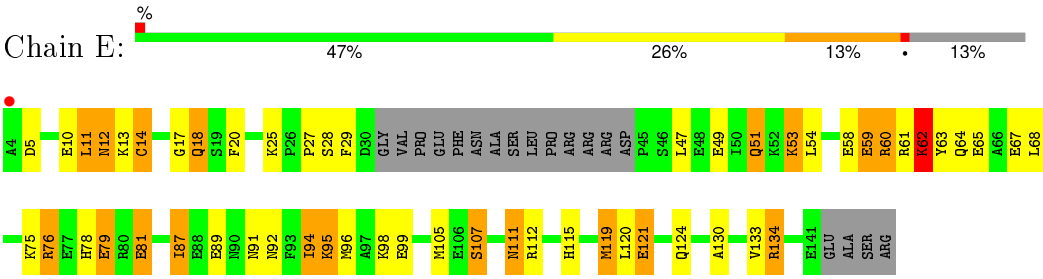
• Molecule 2: Tubulin beta chain

Chain D:



• Molecule 3: Stathmin-4

Chain E:


%
47%
26%
13%
13%
A4 D5 E10 L11 N12 K13 C14 G17 Q18 S19 F20 K25 P26 P27 S28 F29 D30 GLY VAL PRO GLU PHE ASN ALA SER LEU PRO ARG ARG ARG ASP P45 S46 L47 E48 F49 I50 Q51 K52 K53 L54 E58 E59 R60 R61 K62 Y63 Q64 E65 A66 E67 L68 L69 K70 H71 L72
K75 R76 E77 H78 E79 R80 E81 I87 E88 E89 N90 N91 N92 F93 I94 K95 M96 A97 K98 E99 M105 E106 S107 N111 R112 H115 M119 L120 E121 Q124 A130 V133 R134 E141 GLU ALA SER ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	328.83Å 328.83Å 53.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.65 24.87 – 3.65	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-3.65) 96.4 (24.87-3.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.27 (at 3.64Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.213 , 0.254 0.244 , 0.277	Depositor DCC
R_{free} test set	1812 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	150.2	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 141.0	EDS
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 36513 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	14125	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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: GDP, GTP, MG

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	0.66	0/3384	0.90	9/4601 (0.2%)
1	C	0.53	0/3373	0.85	10/4588 (0.2%)
2	B	0.56	0/3321	0.86	11/4509 (0.2%)
2	D	0.59	0/3312	0.88	9/4498 (0.2%)
3	E	0.55	0/919	0.79	1/1234 (0.1%)
All	All	0.58	0/14309	0.87	40/19430 (0.2%)

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
2	B	0	2
2	D	0	1
All	All	0	5

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	120	ASP	CB-CG-OD2	8.69	126.12	118.30
1	A	120	ASP	CB-CG-OD2	8.50	125.95	118.30
1	A	160	ASP	CB-CG-OD2	7.20	124.78	118.30
2	D	357	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	76	ASP	CB-CG-OD2	6.78	124.40	118.30
2	B	427	ASP	CB-CG-OD2	6.75	124.37	118.30
1	C	160	ASP	CB-CG-OD2	6.64	124.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	211	ASP	CB-CG-OD2	6.25	123.93	118.30
2	D	120	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	211	ASP	CB-CG-OD2	6.21	123.89	118.30
2	D	248	LEU	CA-CB-CG	6.17	129.49	115.30
2	D	427	ASP	CB-CG-OD2	6.17	123.85	118.30
1	A	266	HIS	CB-CA-C	-6.15	98.11	110.40
2	B	116	ASP	CB-CG-OD2	6.14	123.83	118.30
2	D	251	ASP	CB-CG-OD2	6.14	123.83	118.30
2	D	179	ASP	CB-CG-OD2	6.13	123.81	118.30
1	A	397	LEU	CA-CB-CG	6.13	129.39	115.30
1	C	266	HIS	CB-CA-C	-6.09	98.22	110.40
2	B	357	ASP	CB-CG-OD2	5.86	123.57	118.30
2	B	179	ASP	CB-CG-OD2	5.76	123.48	118.30
1	C	397	LEU	CA-CB-CG	5.64	128.28	115.30
2	B	69	ASP	CB-CG-OD2	5.52	123.27	118.30
2	B	255	LEU	CA-CB-CG	5.49	127.92	115.30
1	A	33	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	345	ASP	CB-CG-OD2	5.41	123.17	118.30
1	C	431	ASP	CB-CG-OD2	5.40	123.16	118.30
1	C	127	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	424	ASP	CB-CG-OD2	5.32	123.09	118.30
3	E	5	ASP	CB-CG-OD2	5.31	123.08	118.30
2	B	41	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	33	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	218	ASP	CB-CG-OD2	5.18	122.96	118.30
2	B	251	ASP	CB-CG-OD2	5.17	122.95	118.30
2	D	39	ASP	CB-CG-OD2	5.12	122.90	118.30
2	B	297	ASP	CB-CG-OD2	5.11	122.90	118.30
2	D	255	LEU	CA-CB-CG	5.11	127.04	115.30
2	B	130	ASP	CB-CG-OD2	5.09	122.89	118.30
2	D	41	ASP	CB-CG-OD2	5.06	122.86	118.30
2	B	76	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	76	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	HIS	Peptide
2	B	162	PRO	Peptide
2	B	178	SER	Peptide
1	C	266	HIS	Peptide

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Mol	Chain	Res	Type	Group
2	D	162	PRO	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	3307	0	3182	160	0
1	C	3296	0	3158	140	0
2	B	3249	0	3069	183	0
2	D	3240	0	3056	175	0
3	E	911	0	792	40	0
4	A	32	0	12	3	0
4	C	32	0	12	2	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	1	0
6	D	28	0	12	3	0
All	All	14125	0	13305	660	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 24.

All (660) 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)
2:B:180:THR:HA	1:C:352:LYS:NZ	1.68	1.08
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.84	1.08
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.84	1.07
2:D:251:ASP:HB3	2:D:254:LYS:HB2	1.35	1.04
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.89	1.03
2:B:140:SER:HA	2:B:171:VAL:HG23	1.42	1.02
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.43	1.01
2:B:273:ALA:HB1	2:B:274:PRO:HD3	1.43	1.00
2:D:273:ALA:HB1	2:D:274:PRO:HD3	1.39	1.00
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.46	0.98
1:C:273:ALA:CB	1:C:274:PRO:HD3	1.93	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:HD21	4:A:600:GTP:HN22	1.11	0.98
1:C:278:ALA:O	1:C:279:GLU:HB3	1.63	0.97
2:D:244:PHE:HB3	2:D:245:PRO:HD3	1.46	0.97
2:D:140:SER:HA	2:D:171:VAL:HG23	1.45	0.96
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.29	0.96
1:A:278:ALA:O	1:A:279:GLU:HB3	1.64	0.96
2:B:216:THR:HG21	2:B:299:LYS:HD3	1.47	0.96
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.31	0.94
2:D:54:ASN:HD22	2:D:64:ARG:HD3	1.33	0.93
1:C:199:ASP:HB3	1:C:256:GLN:HE22	1.32	0.93
1:A:133:GLN:HE21	1:A:252:LEU:HG	1.34	0.92
2:B:158:ARG:O	2:B:159:GLU:HB2	1.69	0.92
2:D:158:ARG:O	2:D:159:GLU:HB2	1.68	0.91
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.35	0.90
2:D:273:ALA:CB	2:D:274:PRO:CD	2.50	0.90
1:A:322:ASP:O	1:A:373:ARG:NH1	2.04	0.90
2:D:2:ARG:HD3	2:D:131:CYS:SG	2.13	0.89
2:B:180:THR:HA	1:C:352:LYS:HZ2	1.38	0.88
2:B:273:ALA:CB	2:B:274:PRO:CD	2.52	0.87
2:B:2:ARG:HD3	2:B:131:CYS:SG	2.15	0.87
3:E:11:LEU:O	3:E:12:ASN:HB3	1.76	0.85
1:C:79:ARG:HH22	1:C:94:THR:HG21	1.40	0.85
2:D:223:THR:HB	2:D:225:GLY:H	1.40	0.85
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.41	0.85
2:B:54:ASN:HD22	2:B:64:ARG:HD3	1.40	0.84
2:D:251:ASP:CB	2:D:254:LYS:HB2	2.08	0.83
1:A:273:ALA:HB3	1:A:274:PRO:CD	2.07	0.83
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.60	0.83
2:B:180:THR:HA	1:C:352:LYS:HZ1	1.39	0.82
1:C:322:ASP:O	1:C:373:ARG:NH1	2.12	0.82
2:B:244:PHE:HB3	2:B:245:PRO:HD3	1.60	0.81
1:A:347:CYS:O	3:E:27:PRO:HA	1.80	0.81
1:C:229:ARG:HH11	1:C:229:ARG:HG2	1.44	0.81
1:C:206:ASN:HD21	4:C:600:GTP:HN22	1.27	0.81
2:D:244:PHE:HB3	2:D:245:PRO:CD	2.10	0.80
2:B:223:THR:HB	2:B:225:GLY:H	1.46	0.80
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.15	0.80
1:C:244:PHE:O	1:C:245:ASP:HB2	1.80	0.80
1:A:79:ARG:NH2	1:A:94:THR:HG21	1.95	0.79
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.47	0.79
1:A:273:ALA:CB	1:A:375:VAL:H	1.96	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ALA:CB	1:A:274:PRO:CD	2.58	0.79
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.64	0.79
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.64	0.79
2:B:251:ASP:HB3	2:B:254:LYS:HB2	1.64	0.79
2:D:114:LEU:HB3	2:D:149:MET:HE2	1.63	0.78
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.65	0.78
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.18	0.78
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.13	0.78
1:A:133:GLN:NE2	1:A:252:LEU:H	1.79	0.78
2:D:216:THR:HG21	2:D:299:LYS:HD3	1.66	0.78
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.66	0.78
2:D:311:ARG:HE	2:D:344:VAL:HG23	1.48	0.78
1:C:100:ALA:HB1	2:D:253:ARG:HG2	1.66	0.78
2:D:273:ALA:HB2	2:D:375:ALA:H	1.47	0.77
1:A:270:ALA:HB3	1:A:302:MET:HE2	1.67	0.77
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.67	0.77
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.14	0.77
2:D:238:VAL:HG13	2:D:378:ILE:HD11	1.66	0.76
1:C:8:HIS:CD2	1:C:17:GLY:HA3	2.20	0.76
2:D:229:HIS:CE1	2:D:277:SER:HB3	2.21	0.76
1:C:79:ARG:NH2	1:C:94:THR:HG21	2.01	0.76
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.67	0.75
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.25	0.75
1:C:273:ALA:CB	1:C:274:PRO:CD	2.63	0.75
1:C:273:ALA:CB	1:C:375:VAL:H	1.99	0.75
2:D:332:MET:HG3	2:D:353:THR:HG21	1.69	0.75
2:B:273:ALA:HB2	2:B:375:ALA:H	1.51	0.75
2:B:180:THR:CA	1:C:352:LYS:HZ2	1.99	0.74
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.16	0.74
1:C:142:GLY:HA3	1:C:183:GLU:HG3	1.70	0.74
1:C:270:ALA:O	1:C:302:MET:HB2	1.88	0.74
2:D:165:ILE:HD11	2:D:252:LEU:HG	1.70	0.73
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.69	0.73
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.69	0.73
2:D:2:ARG:O	2:D:3:GLU:HB2	1.87	0.73
1:A:133:GLN:NE2	1:A:252:LEU:HG	2.02	0.73
2:D:260:VAL:HG11	2:D:266:HIS:HB3	1.69	0.73
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.30	0.72
1:A:273:ALA:HB1	1:A:274:PRO:HD3	1.71	0.72
3:E:89:GLU:HA	3:E:92:ASN:HB2	1.70	0.72
3:E:67:GLU:C	3:E:69:LEU:H	1.91	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:ASN:ND2	2:D:64:ARG:HD3	2.05	0.72
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.72	0.72
2:B:220:THR:CG2	1:C:326:LYS:HG3	2.19	0.72
1:A:206:ASN:HD21	4:A:600:GTP:N2	1.87	0.71
1:A:133:GLN:OE1	1:A:251:ASP:HB2	1.90	0.71
2:B:165:ILE:HD11	2:B:252:LEU:HG	1.70	0.71
2:D:70:LEU:HA	2:D:95:GLY:HA3	1.71	0.71
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.55	0.71
1:C:266:HIS:O	1:C:268:PRO:HD3	1.90	0.71
2:D:223:THR:HB	2:D:225:GLY:N	2.04	0.71
2:B:114:LEU:O	2:B:116:ASP:N	2.24	0.71
1:C:262:TYR:HB2	1:C:265:ILE:HD13	1.72	0.71
1:A:273:ALA:HB2	1:A:375:VAL:H	1.56	0.70
1:C:179:THR:HG22	2:D:248:LEU:HB2	1.73	0.70
2:B:244:PHE:HB3	2:B:245:PRO:CD	2.21	0.70
1:A:270:ALA:O	1:A:302:MET:HB2	1.91	0.70
1:A:266:HIS:O	1:A:268:PRO:HD3	1.92	0.70
2:D:114:LEU:O	2:D:116:ASP:N	2.25	0.69
2:D:244:PHE:CB	2:D:245:PRO:CD	2.70	0.69
2:B:229:HIS:CE1	2:B:277:SER:HB3	2.27	0.69
2:D:319:PHE:HB2	2:D:355:VAL:HG12	1.74	0.69
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.75	0.69
1:C:229:ARG:HH11	1:C:229:ARG:CG	2.04	0.69
1:C:179:THR:O	2:D:352:LYS:HE2	1.92	0.69
2:B:153:LEU:O	2:B:157:ILE:HG12	1.93	0.69
2:D:5:VAL:HG22	2:D:135:PHE:CD2	2.27	0.68
1:A:88:HIS:HB2	1:A:91:GLN:NE2	2.08	0.68
2:D:158:ARG:O	2:D:159:GLU:CB	2.42	0.68
2:B:2:ARG:O	2:B:3:GLU:HB2	1.91	0.68
2:B:241:CYS:HB2	2:B:250:ALA:HB2	1.76	0.68
1:C:167:LEU:HD13	1:C:252:LEU:HD11	1.74	0.68
2:B:332:MET:HG3	2:B:353:THR:HG21	1.75	0.68
1:C:264:ARG:NH2	1:C:424:ASP:OD1	2.28	0.67
2:B:223:THR:HB	2:B:225:GLY:N	2.09	0.67
1:C:70:LEU:HD13	1:C:145:THR:CB	2.25	0.67
1:C:206:ASN:HD21	4:C:600:GTP:N2	1.93	0.66
2:B:301:MET:SD	2:B:377:PHE:HE2	2.18	0.66
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.31	0.66
2:B:180:THR:CA	1:C:352:LYS:NZ	2.53	0.66
2:B:260:VAL:HG11	2:B:266:HIS:HB3	1.78	0.66
1:A:70:LEU:HD13	1:A:145:THR:HB	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:HIS:HB2	1:C:91:GLN:NE2	2.11	0.65
1:C:133:GLN:NE2	1:C:252:LEU:HB2	2.11	0.65
1:C:249:ASN:HB3	1:C:255:PHE:CD2	2.32	0.65
2:D:27:GLU:OE2	2:D:320:ARG:NH2	2.30	0.65
1:C:70:LEU:HD13	1:C:145:THR:HB	1.79	0.65
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.79	0.65
2:B:158:ARG:O	2:B:159:GLU:CB	2.44	0.65
1:A:264:ARG:NH2	1:A:424:ASP:OD1	2.28	0.65
1:A:66:VAL:HG11	1:A:122:ILE:HG12	1.79	0.65
3:E:61:ARG:O	3:E:63:TYR:N	2.30	0.64
2:B:54:ASN:ND2	2:B:64:ARG:HD3	2.12	0.64
2:D:200:GLU:HB3	2:D:268:PHE:CE1	2.33	0.64
2:D:301:MET:SD	2:D:377:PHE:HE2	2.19	0.64
1:A:229:ARG:CG	1:A:229:ARG:HH11	2.08	0.64
1:A:71:GLU:HG3	1:A:73:THR:OG1	1.98	0.64
2:D:2:ARG:CD	2:D:131:CYS:SG	2.87	0.63
1:C:167:LEU:HD13	1:C:252:LEU:CD1	2.27	0.63
1:A:99:ALA:CB	1:A:145:THR:HG22	2.29	0.63
1:C:377:MET:HG3	1:C:377:MET:O	1.99	0.63
1:C:249:ASN:HB3	1:C:255:PHE:HD2	1.63	0.63
1:C:191:THR:HG23	1:C:425:MET:CE	2.28	0.63
2:B:292:THR:HA	2:B:295:MET:HE3	1.80	0.63
1:C:273:ALA:HB1	1:C:274:PRO:HD3	1.78	0.62
2:D:244:PHE:CB	2:D:245:PRO:HD3	2.25	0.62
1:C:121:ARG:HH11	1:C:121:ARG:HG3	1.64	0.62
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.34	0.62
1:A:223:THR:O	1:A:227:LEU:HD13	1.99	0.62
2:D:54:ASN:HD22	2:D:64:ARG:CD	2.08	0.62
2:B:7:ILE:O	2:B:137:LEU:HA	2.00	0.62
1:C:177:VAL:O	1:C:177:VAL:HG13	1.99	0.62
1:A:241:SER:HB2	1:A:249:ASN:O	2.00	0.62
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.35	0.61
2:B:6:HIS:CE1	2:B:8:GLN:HB2	2.35	0.61
2:B:311:ARG:HE	2:B:344:VAL:HG23	1.65	0.61
1:C:317:LEU:HD23	1:C:377:MET:HB2	1.81	0.61
2:B:287:THR:HG22	2:B:290:GLU:HB2	1.82	0.61
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.82	0.61
1:C:177:VAL:O	1:C:177:VAL:CG1	2.48	0.61
2:D:151:THR:HB	2:D:193:GLN:HG2	1.82	0.61
1:C:435:VAL:HG12	1:C:435:VAL:O	2.00	0.61
1:A:121:ARG:HH11	1:A:121:ARG:HG3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:GLY:HA2	3:E:14:CYS:SG	2.41	0.61
1:C:273:ALA:HB2	1:C:375:VAL:H	1.66	0.61
1:A:70:LEU:HD13	1:A:145:THR:CB	2.31	0.61
1:C:179:THR:HA	2:D:248:LEU:HD12	1.83	0.61
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.82	0.61
1:C:70:LEU:HD12	1:C:70:LEU:N	2.16	0.60
1:A:317:LEU:HD23	1:A:377:MET:HB2	1.84	0.60
1:A:145:THR:HG23	4:A:600:GTP:O2B	2.00	0.60
1:A:179:THR:O	2:B:352:LYS:HE2	2.02	0.60
2:B:27:GLU:OE2	2:B:320:ARG:NH2	2.34	0.60
2:D:153:LEU:O	2:D:157:ILE:HG12	2.01	0.60
3:E:61:ARG:C	3:E:63:TYR:H	2.04	0.60
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.36	0.59
2:B:145:THR:HG22	6:B:600:GDP:O3B	2.02	0.59
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.37	0.59
2:D:287:THR:HG22	2:D:290:GLU:HB2	1.83	0.59
2:D:5:VAL:HG22	2:D:135:PHE:HD2	1.66	0.59
2:D:383:ALA:O	2:D:386:GLU:HB2	2.02	0.59
2:B:224:TYR:O	2:B:228:ASN:ND2	2.35	0.59
1:A:2:ARG:HA	1:A:2:ARG:NH1	2.16	0.59
2:B:169:PHE:CE2	2:B:235:MET:HG2	2.38	0.59
2:D:223:THR:CB	2:D:225:GLY:H	2.13	0.59
2:D:48:ARG:HH22	2:D:250:ALA:HB1	1.66	0.59
2:B:54:ASN:HD22	2:B:64:ARG:CD	2.13	0.59
1:C:191:THR:HG23	1:C:425:MET:HE3	1.85	0.59
1:C:114:ILE:O	1:C:118:VAL:HG23	2.02	0.59
2:B:291:LEU:HD21	2:B:375:ALA:CB	2.32	0.59
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.08	0.59
2:B:59:ASN:O	2:B:60:LYS:O	2.21	0.58
1:A:262:TYR:HB2	1:A:265:ILE:HD13	1.84	0.58
2:B:114:LEU:HB3	2:B:149:MET:HE2	1.84	0.58
2:B:14:ASN:HD22	2:B:67:LEU:HD23	1.68	0.58
2:D:7:ILE:O	2:D:137:LEU:HA	2.04	0.58
1:A:151:SER:OG	1:A:193:THR:HB	2.04	0.58
1:C:256:GLN:C	1:C:258:ASN:N	2.55	0.58
2:B:48:ARG:HH22	2:B:246:GLY:HA3	1.67	0.58
1:C:79:ARG:HH22	1:C:94:THR:CG2	2.13	0.58
2:B:229:HIS:HE1	2:B:276:THR:O	1.86	0.57
1:A:177:VAL:HG13	1:A:177:VAL:O	2.04	0.57
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.38	0.57
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:51:GLN:C	3:E:53:LYS:H	2.07	0.57
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.84	0.57
2:D:4:ILE:HD11	2:D:52:TYR:CE2	2.39	0.57
2:B:4:ILE:HD11	2:B:52:TYR:CE2	2.39	0.57
2:D:224:TYR:O	2:D:228:ASN:ND2	2.38	0.57
1:C:100:ALA:CB	2:D:253:ARG:HG2	2.34	0.57
2:D:198:THR:OG1	2:D:266:HIS:CE1	2.58	0.57
2:D:48:ARG:NH2	2:D:250:ALA:HB1	2.20	0.57
2:B:319:PHE:HB2	2:B:355:VAL:HG12	1.85	0.57
3:E:61:ARG:C	3:E:63:TYR:N	2.59	0.57
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.67	0.56
3:E:17:GLY:O	3:E:18:GLN:HB2	2.03	0.56
2:B:200:GLU:OE2	2:B:255:LEU:HD12	2.05	0.56
2:B:2:ARG:CD	2:B:131:CYS:SG	2.92	0.56
2:B:5:VAL:HG22	2:B:135:PHE:HD2	1.70	0.56
2:B:200:GLU:HB3	2:B:268:PHE:CE1	2.40	0.56
2:D:141:LEU:HD13	2:D:170:SER:HB3	1.86	0.56
3:E:11:LEU:O	3:E:12:ASN:CB	2.52	0.56
2:B:229:HIS:CE1	2:B:276:THR:O	2.58	0.56
1:A:191:THR:HG23	1:A:425:MET:CE	2.35	0.56
2:D:180:THR:HG22	2:D:182:VAL:HG22	1.86	0.56
2:B:357:ASP:OD2	2:B:357:ASP:N	2.38	0.56
1:C:99:ALA:CB	1:C:145:THR:HG22	2.36	0.56
2:B:174:SER:O	2:B:178:SER:HB3	2.06	0.56
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.88	0.56
1:C:273:ALA:HB3	1:C:375:VAL:H	1.71	0.56
2:D:88:ARG:O	2:D:91:ASN:HB2	2.05	0.56
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.88	0.55
2:D:336:GLN:OE1	2:D:351:VAL:HG11	2.05	0.55
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.88	0.55
2:D:295:MET:HG2	2:D:295:MET:O	2.06	0.55
2:B:88:ARG:O	2:B:91:ASN:HB2	2.07	0.55
2:D:89:PRO:O	2:D:92:PHE:HD1	1.89	0.55
2:D:224:TYR:OH	6:D:600:GDP:H2'	2.07	0.55
2:B:205:ASP:OD1	2:B:207:GLU:HB3	2.07	0.55
2:D:261:PRO:HB2	2:D:262:PHE:CD1	2.41	0.55
1:C:96:LYS:HD3	2:D:131:CYS:HB2	1.89	0.54
2:B:401:ARG:HG3	2:B:401:ARG:NH1	2.22	0.54
2:B:250:ALA:O	2:B:251:ASP:HB2	2.08	0.54
1:A:36:MET:HG3	1:A:36:MET:O	2.06	0.54
1:A:250:VAL:HG22	1:A:250:VAL:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.89	0.54
1:C:53:PHE:HD2	1:C:61:HIS:O	1.90	0.54
1:A:114:ILE:O	1:A:118:VAL:HG23	2.07	0.54
1:A:247:ALA:HB2	3:E:12:ASN:CG	2.28	0.54
3:E:67:GLU:C	3:E:69:LEU:N	2.61	0.54
2:B:383:ALA:O	2:B:386:GLU:HB2	2.08	0.53
1:C:66:VAL:HG11	1:C:122:ILE:HG12	1.89	0.53
1:A:410:GLY:HA2	3:E:64:GLN:HE22	1.73	0.53
1:C:229:ARG:NH1	1:C:229:ARG:HG2	2.20	0.53
2:D:136:GLN:HB3	2:D:167:ASN:HB3	1.90	0.53
2:B:336:GLN:OE1	2:B:351:VAL:HG11	2.09	0.53
2:D:174:SER:HB2	2:D:207:GLU:HB2	1.90	0.53
2:D:192:HIS:CD2	2:D:421:ALA:HA	2.44	0.53
2:B:401:ARG:HG3	2:B:401:ARG:HH11	1.73	0.53
2:D:205:ASP:OD1	2:D:207:GLU:HB3	2.09	0.53
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.91	0.53
2:D:200:GLU:HA	2:D:266:HIS:HB2	1.90	0.53
1:A:398:MET:HG3	2:B:348:PRO:HD3	1.90	0.53
1:C:88:HIS:O	1:C:91:GLN:HG2	2.09	0.53
1:A:100:ALA:HB1	2:B:253:ARG:HG2	1.90	0.53
2:D:305:CYS:HB3	2:D:386:GLU:HB3	1.90	0.53
2:D:292:THR:HA	2:D:295:MET:HE3	1.90	0.53
2:B:20:PHE:O	2:B:24:ILE:HG23	2.09	0.53
1:A:249:ASN:N	1:A:254:GLU:OE1	2.42	0.53
1:A:398:MET:HG3	2:B:348:PRO:CD	2.39	0.52
2:B:210:TYR:HD1	2:B:210:TYR:C	2.12	0.52
2:B:89:PRO:O	2:B:92:PHE:HD1	1.91	0.52
2:B:274:PRO:C	2:B:275:LEU:HG	2.29	0.52
2:D:234:THR:O	2:D:238:VAL:HG23	2.10	0.52
2:D:51:VAL:HG12	2:D:52:TYR:CD1	2.45	0.52
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.44	0.52
2:D:6:HIS:CE1	2:D:8:GLN:HB2	2.45	0.52
2:B:342:TYR:HD2	2:B:342:TYR:N	2.07	0.52
2:B:14:ASN:ND2	2:B:67:LEU:HD23	2.24	0.52
1:A:211:ASP:OD1	1:A:304:LYS:HE3	2.08	0.52
2:D:217:LEU:HD21	2:D:276:THR:HB	1.92	0.52
2:D:342:TYR:HD2	2:D:342:TYR:N	2.07	0.52
2:B:8:GLN:OE1	2:B:67:LEU:HD23	2.10	0.52
2:B:210:TYR:CD1	2:B:210:TYR:C	2.83	0.52
3:E:76:ARG:C	3:E:78:HIS:H	2.14	0.52
1:A:229:ARG:HG2	1:A:229:ARG:NH1	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:THR:HB	2:B:193:GLN:HG2	1.92	0.52
1:A:88:HIS:O	1:A:91:GLN:HG2	2.10	0.52
1:A:8:HIS:CD2	1:A:17:GLY:CA	2.92	0.52
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.91	0.52
2:D:336:GLN:OE1	2:D:351:VAL:CG1	2.58	0.52
1:A:210:TYR:CE1	1:A:214:ARG:HD3	2.45	0.52
1:A:87:PHE:N	1:A:87:PHE:CD2	2.77	0.52
1:A:377:MET:O	1:A:377:MET:HG3	2.08	0.52
1:A:105:ARG:HD2	1:A:411:GLU:OE1	2.10	0.52
1:C:256:GLN:C	1:C:258:ASN:H	2.11	0.51
3:E:12:ASN:OD1	3:E:12:ASN:C	2.49	0.51
2:B:234:THR:O	2:B:238:VAL:HG23	2.10	0.51
2:D:210:TYR:HD1	2:D:210:TYR:C	2.13	0.51
1:C:102:ASN:OD1	1:C:105:ARG:HB2	2.11	0.51
2:D:8:GLN:OE1	2:D:67:LEU:HD23	2.10	0.51
2:B:166:MET:HB2	2:B:199:ASP:OD1	2.10	0.51
2:D:274:PRO:C	2:D:275:LEU:HG	2.31	0.51
2:D:166:MET:HB2	2:D:199:ASP:OD1	2.09	0.51
2:D:342:TYR:N	2:D:342:TYR:CD2	2.79	0.51
1:C:346:TRP:HZ2	1:C:435:VAL:CG1	2.22	0.51
2:B:401:ARG:CG	2:B:401:ARG:HH11	2.23	0.51
1:A:64:ARG:HG3	1:A:64:ARG:HH11	1.75	0.51
2:D:229:HIS:HE1	2:D:276:THR:O	1.93	0.51
3:E:60:ARG:HG3	3:E:60:ARG:HH11	1.76	0.51
2:B:213:CYS:HA	2:B:217:LEU:HB2	1.92	0.51
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.91	0.51
2:B:198:THR:OG1	2:B:266:HIS:CE1	2.64	0.51
1:A:291:ILE:HD12	1:A:375:VAL:CG2	2.41	0.50
1:C:121:ARG:HG3	1:C:121:ARG:NH1	2.26	0.50
2:B:88:ARG:NH1	2:B:91:ASN:OD1	2.45	0.50
2:B:223:THR:CB	2:B:225:GLY:H	2.20	0.50
1:A:186:ASN:O	1:A:190:THR:HG22	2.11	0.50
2:B:342:TYR:CD2	2:B:342:TYR:N	2.79	0.50
2:D:256:ALA:O	2:D:260:VAL:HG22	2.10	0.50
2:D:292:THR:HA	2:D:295:MET:CE	2.41	0.50
2:D:210:TYR:CD1	2:D:210:TYR:C	2.84	0.50
3:E:60:ARG:NH1	3:E:60:ARG:HG3	2.26	0.50
2:B:70:LEU:CA	2:B:95:GLY:HA3	2.38	0.50
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.92	0.50
2:D:265:LEU:HB3	2:D:432:TYR:CE2	2.45	0.50
1:A:239:THR:O	1:A:242:LEU:N	2.38	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ASP:HB2	1:C:303:VAL:HA	1.94	0.50
2:B:251:ASP:O	2:B:253:ARG:N	2.42	0.50
2:B:295:MET:HG2	2:B:295:MET:O	2.10	0.50
1:A:306:ASP:O	1:A:309:HIS:HB3	2.12	0.50
1:C:260:VAL:CG2	1:C:260:VAL:O	2.60	0.50
2:B:192:HIS:CD2	2:B:421:ALA:HA	2.47	0.50
2:B:336:GLN:OE1	2:B:351:VAL:CG1	2.59	0.50
2:B:141:LEU:HD13	2:B:170:SER:HB3	1.92	0.50
1:C:115:ILE:HG13	1:C:152:LEU:HD23	1.94	0.50
2:D:174:SER:O	2:D:178:SER:HB3	2.12	0.49
2:B:387:LEU:O	2:B:390:ARG:HG3	2.12	0.49
3:E:130:ALA:HB1	3:E:134:ARG:HH12	1.76	0.49
1:A:298:PRO:HA	1:A:301:GLN:NE2	2.26	0.49
1:A:53:PHE:HD2	1:A:61:HIS:O	1.95	0.49
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.94	0.49
2:D:16:ILE:HG12	2:D:231:VAL:HG11	1.94	0.49
2:D:4:ILE:O	2:D:4:ILE:HG12	2.12	0.49
1:A:435:VAL:HG12	1:A:435:VAL:O	2.12	0.49
2:B:256:ALA:O	2:B:260:VAL:HG22	2.13	0.49
1:C:264:ARG:O	1:C:265:ILE:C	2.51	0.49
2:D:14:ASN:HD22	2:D:67:LEU:HD23	1.77	0.49
2:B:156:LYS:HE3	3:E:76:ARG:NE	2.28	0.49
1:A:329:ASN:ND2	3:E:20:PHE:CE1	2.80	0.49
1:A:273:ALA:HB3	1:A:375:VAL:H	1.77	0.49
2:B:4:ILE:HD11	2:B:52:TYR:CZ	2.48	0.49
2:D:311:ARG:NE	2:D:344:VAL:HG23	2.23	0.49
2:B:200:GLU:HA	2:B:266:HIS:HB2	1.95	0.49
1:A:167:LEU:HD22	1:A:252:LEU:HD22	1.94	0.48
2:D:52:TYR:CE1	2:D:243:ARG:HD3	2.48	0.48
1:A:397:LEU:CD2	2:B:348:PRO:HG3	2.43	0.48
1:A:181:VAL:H	2:B:258:ASN:HD21	1.59	0.48
2:D:200:GLU:HG2	2:D:268:PHE:HE1	1.78	0.48
1:A:177:VAL:O	1:A:177:VAL:CG1	2.62	0.48
1:C:36:MET:O	1:C:36:MET:HG3	2.14	0.48
1:C:265:ILE:HG22	1:C:265:ILE:O	2.13	0.48
1:A:2:ARG:HB2	1:A:131:GLY:O	2.13	0.48
3:E:94:ILE:O	3:E:98:LYS:N	2.45	0.48
2:D:107:HIS:O	2:D:152:LEU:HD22	2.13	0.48
1:C:260:VAL:O	1:C:260:VAL:HG23	2.12	0.48
2:B:211:ASP:O	2:B:215:ARG:N	2.36	0.48
1:C:211:ASP:OD1	1:C:304:LYS:HE3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.94	0.48
1:A:70:LEU:N	1:A:70:LEU:HD12	2.29	0.48
1:A:223:THR:HB	1:A:226:ASN:H	1.78	0.48
2:D:4:ILE:HD11	2:D:52:TYR:CZ	2.49	0.48
1:C:212:ILE:O	1:C:216:ASN:HB2	2.14	0.48
1:A:346:TRP:HE3	1:A:346:TRP:O	1.96	0.48
2:D:5:VAL:CG2	2:D:135:PHE:HD2	2.27	0.48
2:B:244:PHE:CB	2:B:245:PRO:CD	2.89	0.48
1:A:121:ARG:HG3	1:A:121:ARG:NH1	2.28	0.48
2:D:395:PHE:CE2	2:D:422:GLU:HB2	2.49	0.47
2:D:126:SER:C	2:D:128:SER:H	2.16	0.47
1:A:388:TRP:HA	1:A:388:TRP:CE3	2.49	0.47
1:A:62:VAL:HA	1:A:63:PRO:HD3	1.82	0.47
2:D:59:ASN:O	2:D:60:LYS:O	2.31	0.47
1:C:88:HIS:H	1:C:91:GLN:NE2	2.12	0.47
2:D:320:ARG:HA	2:D:356:CYS:O	2.14	0.47
1:C:223:THR:O	1:C:227:LEU:HD13	2.13	0.47
2:D:204:ILE:HD13	2:D:231:VAL:HG13	1.95	0.47
2:D:231:VAL:HG12	2:D:235:MET:HE2	1.97	0.47
2:B:114:LEU:HB3	2:B:149:MET:CE	2.44	0.47
2:D:239:THR:O	2:D:242:LEU:N	2.45	0.47
2:B:292:THR:HA	2:B:295:MET:CE	2.43	0.47
2:D:88:ARG:NH1	2:D:91:ASN:OD1	2.48	0.47
1:A:30:ILE:HA	1:A:36:MET:HB3	1.95	0.47
1:C:313:MET:HG2	1:C:380:ASN:O	2.15	0.47
2:B:315:VAL:HG13	2:B:377:PHE:HD1	1.79	0.47
1:A:313:MET:HE1	1:A:382:THR:HG22	1.96	0.47
2:B:4:ILE:O	2:B:4:ILE:HG12	2.15	0.47
2:B:70:LEU:HD11	2:B:149:MET:HE3	1.97	0.47
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.97	0.47
2:B:107:HIS:O	2:B:152:LEU:HD22	2.15	0.47
1:A:317:LEU:CD2	1:A:377:MET:HB2	2.45	0.46
2:D:169:PHE:CD2	2:D:235:MET:HG2	2.50	0.46
1:C:264:ARG:O	1:C:266:HIS:N	2.48	0.46
1:A:298:PRO:O	1:A:301:GLN:HB2	2.15	0.46
1:C:395:PHE:CD2	1:C:395:PHE:C	2.87	0.46
1:C:28:HIS:CE1	1:C:244:PHE:CZ	3.04	0.46
1:C:317:LEU:CD2	1:C:377:MET:HB2	2.45	0.46
1:C:244:PHE:O	1:C:245:ASP:CB	2.57	0.46
2:D:259:MET:HB3	2:D:268:PHE:CZ	2.51	0.46
2:D:14:ASN:ND2	2:D:67:LEU:HD23	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:401:ARG:NH1	2:D:401:ARG:HG3	2.29	0.46
1:C:376:CYS:O	1:C:377:MET:C	2.54	0.46
1:A:97:GLU:HG3	1:A:98:ASP:N	2.31	0.46
2:D:114:LEU:HB3	2:D:149:MET:CE	2.38	0.46
2:D:145:THR:HG22	6:D:600:GDP:O3B	2.16	0.46
2:D:11:GLN:HG3	2:D:74:THR:CG2	2.41	0.46
2:D:138:THR:CG2	2:D:169:PHE:HB2	2.43	0.46
2:D:178:SER:HB2	2:D:183:GLU:OE1	2.15	0.46
2:D:177:VAL:CG1	2:D:177:VAL:O	2.64	0.46
1:C:71:GLU:HG3	1:C:73:THR:OG1	2.15	0.46
2:D:225:GLY:O	2:D:227:LEU:N	2.41	0.46
2:B:115:VAL:HG12	2:B:116:ASP:N	2.30	0.46
2:B:259:MET:HB3	2:B:268:PHE:CZ	2.51	0.45
1:A:190:THR:O	1:A:193:THR:N	2.49	0.45
1:A:212:ILE:O	1:A:216:ASN:HB2	2.16	0.45
1:C:210:TYR:CE1	1:C:214:ARG:HD3	2.51	0.45
2:D:291:LEU:HD21	2:D:375:ALA:CB	2.46	0.45
2:D:54:ASN:ND2	2:D:64:ARG:HH11	2.14	0.45
2:D:229:HIS:CE1	2:D:276:THR:O	2.69	0.45
2:D:401:ARG:HH11	2:D:401:ARG:CG	2.29	0.45
1:A:7:ILE:HG21	1:A:153:LEU:HD11	1.98	0.45
1:A:315:CYS:SG	1:A:377:MET:CE	3.05	0.45
2:B:70:LEU:C	2:B:95:GLY:HA3	2.37	0.45
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.29	0.45
2:B:48:ARG:NH2	2:B:246:GLY:HA3	2.30	0.45
1:A:397:LEU:HD23	2:B:348:PRO:HG3	1.97	0.45
3:E:94:ILE:HG22	3:E:95:LYS:H	1.81	0.45
2:B:308:ARG:HH11	2:B:308:ARG:CG	2.29	0.45
3:E:67:GLU:O	3:E:69:LEU:N	2.45	0.45
1:A:105:ARG:HG2	1:A:110:ILE:HG22	1.99	0.45
1:C:152:LEU:HA	1:C:155:GLU:HG3	1.98	0.45
3:E:119:MET:O	3:E:119:MET:HG3	2.12	0.45
2:D:298:SER:C	2:D:300:ASN:H	2.19	0.45
1:A:247:ALA:HB2	3:E:12:ASN:OD1	2.16	0.45
1:C:251:ASP:OD1	1:C:252:LEU:N	2.49	0.45
1:A:376:CYS:O	1:A:377:MET:C	2.55	0.45
1:A:377:MET:HA	1:A:377:MET:HE3	1.98	0.45
1:A:99:ALA:HB3	1:A:145:THR:HG22	1.99	0.45
2:D:16:ILE:HG22	2:D:17:GLY:N	2.32	0.45
2:B:62:VAL:CG2	2:B:62:VAL:O	2.64	0.45
2:D:308:ARG:HH11	2:D:308:ARG:CG	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:VAL:CG1	2:B:177:VAL:O	2.65	0.45
2:D:265:LEU:HB3	2:D:432:TYR:CZ	2.52	0.45
2:D:297:ASP:HB3	2:D:300:ASN:HB2	1.99	0.45
2:B:110:GLU:H	2:B:110:GLU:HG2	1.64	0.45
1:A:242:LEU:HD21	1:A:255:PHE:HE2	1.82	0.45
1:C:223:THR:HB	1:C:226:ASN:H	1.80	0.45
2:D:177:VAL:O	2:D:177:VAL:HG12	2.16	0.45
1:C:67:PHE:HB2	1:C:92:LEU:HD22	1.99	0.45
2:D:274:PRO:HG2	2:D:286:LEU:HD13	1.99	0.44
1:A:239:THR:O	1:A:240:ALA:C	2.54	0.44
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.99	0.44
2:D:212:ILE:CD1	2:D:215:ARG:HH22	2.31	0.44
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.99	0.44
1:C:388:TRP:CE3	1:C:388:TRP:HA	2.52	0.44
1:C:2:ARG:HA	1:C:2:ARG:NH1	2.32	0.44
1:A:88:HIS:H	1:A:91:GLN:NE2	2.15	0.44
2:D:225:GLY:C	2:D:227:LEU:H	2.21	0.44
2:D:114:LEU:HD23	2:D:149:MET:HE1	1.99	0.44
3:E:107:SER:O	3:E:111:ASN:HB2	2.17	0.44
1:C:87:PHE:N	1:C:87:PHE:CD2	2.85	0.44
2:D:385:GLN:HE21	2:D:389:LYS:HE3	1.81	0.44
1:A:273:ALA:HB2	1:A:375:VAL:N	2.27	0.44
2:D:12:CYS:SG	6:D:600:GDP:C4	3.11	0.44
2:D:315:VAL:HG13	2:D:377:PHE:HD1	1.82	0.44
1:C:34:GLY:O	1:C:61:HIS:HB2	2.18	0.44
1:A:375:VAL:HG12	1:A:376:CYS:H	1.83	0.44
3:E:94:ILE:CG2	3:E:95:LYS:N	2.80	0.44
2:D:211:ASP:O	2:D:215:ARG:N	2.36	0.44
2:B:178:SER:HB2	2:B:183:GLU:OE1	2.17	0.44
2:D:55:GLU:HB3	2:D:61:TYR:CD2	2.53	0.44
2:B:52:TYR:CE1	2:B:243:ARG:HD3	2.53	0.44
1:C:209:ILE:HD11	1:C:302:MET:SD	2.57	0.44
2:D:351:VAL:O	2:D:351:VAL:HG22	2.17	0.44
2:B:156:LYS:HE3	3:E:76:ARG:HE	1.82	0.44
2:D:357:ASP:N	2:D:357:ASP:OD2	2.48	0.44
1:C:281:ALA:HB2	1:C:369:ALA:HB1	1.99	0.43
1:A:229:ARG:CG	1:A:229:ARG:NH1	2.78	0.43
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.66	0.43
1:A:414:GLU:N	3:E:60:ARG:HH21	2.16	0.43
1:A:306:ASP:O	1:A:309:HIS:CB	2.66	0.43
1:A:11:GLN:CG	1:A:12:ALA:N	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ARG:O	1:A:266:HIS:CD2	2.70	0.43
1:A:313:MET:HG2	1:A:380:ASN:O	2.17	0.43
2:D:115:VAL:HG12	2:D:116:ASP:N	2.33	0.43
1:A:163:LYS:O	1:A:164:LYS:C	2.57	0.43
1:A:321:GLY:HA2	1:A:359:PRO:HA	2.00	0.43
2:B:403:ALA:C	2:B:405:LEU:H	2.22	0.43
2:B:288:VAL:HB	2:B:289:PRO:HD3	2.00	0.43
1:A:191:THR:HG23	1:A:425:MET:HE3	2.00	0.43
1:A:87:PHE:H	1:A:87:PHE:HD2	1.66	0.43
2:B:155:SER:O	3:E:76:ARG:NH2	2.52	0.43
2:B:171:VAL:HA	2:B:204:ILE:O	2.18	0.43
1:C:36:MET:HG2	1:C:61:HIS:CD2	2.54	0.43
1:A:141:PHE:HD2	1:A:141:PHE:HA	1.69	0.43
2:D:247:GLN:CD	2:D:354:ALA:HB1	2.38	0.43
2:B:179:ASP:C	1:C:352:LYS:HE3	2.39	0.43
2:D:308:ARG:O	2:D:310:GLY:N	2.52	0.43
1:C:108:TYR:CE1	1:C:413:MET:HG3	2.54	0.43
2:B:66:ILE:HD11	2:B:122:VAL:HA	1.99	0.43
1:C:298:PRO:O	1:C:301:GLN:HB2	2.18	0.43
2:B:225:GLY:C	2:B:227:LEU:H	2.22	0.43
2:D:231:VAL:HG12	2:D:235:MET:CE	2.49	0.43
1:C:133:GLN:HE21	1:C:252:LEU:HG	1.84	0.43
1:C:70:LEU:N	1:C:70:LEU:CD1	2.81	0.43
2:D:320:ARG:NH1	2:D:360:PRO:HG3	2.33	0.43
2:B:191:VAL:CG1	2:B:425:MET:HG3	2.47	0.43
2:D:387:LEU:O	2:D:390:ARG:HG3	2.19	0.43
1:A:68:VAL:HG11	1:A:118:VAL:CG2	2.49	0.43
1:C:151:SER:OG	1:C:193:THR:HB	2.19	0.43
2:B:298:SER:C	2:B:300:ASN:H	2.22	0.43
2:B:240:THR:HG21	2:B:320:ARG:CZ	2.49	0.43
1:A:394:LYS:HG3	2:B:348:PRO:HG2	2.01	0.43
1:C:161:TYR:HB3	1:C:164:LYS:HG3	2.01	0.43
1:C:164:LYS:H	1:C:164:LYS:HG2	1.70	0.42
1:C:347:CYS:HB3	1:C:348:PRO:HD2	2.00	0.42
1:A:248:LEU:HD23	1:A:248:LEU:HA	1.92	0.42
1:A:88:HIS:CD2	1:A:89:PRO:HD2	2.55	0.42
1:C:260:VAL:HA	1:C:261:PRO:HD3	1.93	0.42
1:C:297:GLU:HA	1:C:298:PRO:HD2	1.92	0.42
1:A:349:THR:OG1	3:E:25:LYS:N	2.51	0.42
1:C:391:LEU:HA	1:C:391:LEU:HD12	1.83	0.42
2:D:3:GLU:CG	2:D:64:ARG:NH2	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:GLU:HG3	2:D:64:ARG:NH2	2.35	0.42
2:B:114:LEU:HD23	2:B:149:MET:HE1	2.00	0.42
1:A:264:ARG:O	1:A:266:HIS:N	2.52	0.42
2:D:288:VAL:HB	2:D:289:PRO:HD3	2.02	0.42
1:C:30:ILE:HA	1:C:36:MET:HB3	2.00	0.42
2:B:136:GLN:HB3	2:B:167:ASN:HB3	2.01	0.42
2:D:110:GLU:HG2	2:D:110:GLU:H	1.65	0.42
1:C:346:TRP:HE3	1:C:346:TRP:O	2.01	0.42
1:C:249:ASN:HA	1:C:255:PHE:HA	2.00	0.42
2:B:305:CYS:HB3	2:B:386:GLU:HB3	2.01	0.42
3:E:76:ARG:HD3	3:E:79:GLU:OE1	2.19	0.42
2:D:401:ARG:HG3	2:D:401:ARG:HH11	1.85	0.42
1:A:152:LEU:HD11	3:E:54:LEU:HD22	2.01	0.42
1:A:264:ARG:O	1:A:265:ILE:C	2.57	0.42
2:B:183:GLU:N	2:B:184:PRO:HD2	2.34	0.42
1:A:36:MET:HA	1:A:37:PRO:HD3	1.88	0.42
1:A:108:TYR:CE1	1:A:413:MET:HG3	2.53	0.42
2:D:141:LEU:HA	2:D:141:LEU:HD12	1.79	0.42
2:D:192:HIS:HD2	2:D:421:ALA:HA	1.83	0.42
1:C:105:ARG:HD2	1:C:411:GLU:OE1	2.19	0.42
2:B:403:ALA:O	2:B:405:LEU:N	2.53	0.42
2:B:247:GLN:HE21	2:B:247:GLN:H	1.66	0.42
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.73	0.42
1:A:185:TYR:OH	1:A:403:ALA:HB3	2.19	0.42
2:B:320:ARG:HA	2:B:356:CYS:O	2.20	0.42
2:B:16:ILE:HG22	2:B:17:GLY:N	2.34	0.42
2:B:42:LEU:O	2:B:43:GLN:C	2.57	0.42
3:E:121:GLU:HG3	3:E:121:GLU:O	2.17	0.42
2:B:179:ASP:O	1:C:352:LYS:HE3	2.20	0.42
1:C:346:TRP:CZ2	1:C:435:VAL:HG13	2.39	0.42
1:A:265:ILE:O	1:A:265:ILE:HG22	2.20	0.42
2:D:382:THR:HG22	2:D:432:TYR:HD2	1.84	0.42
1:C:181:VAL:H	2:D:258:ASN:HD21	1.67	0.42
2:D:226:ASP:OD1	2:D:226:ASP:N	2.53	0.42
2:D:394:GLN:O	2:D:397:ALA:HB3	2.19	0.42
1:C:291:ILE:HD12	1:C:375:VAL:CG2	2.49	0.42
1:C:8:HIS:HE1	1:C:21:TRP:HE1	1.68	0.42
2:B:7:ILE:HG22	2:B:137:LEU:HD13	2.02	0.42
1:C:7:ILE:HG21	1:C:153:LEU:HD11	2.01	0.42
1:A:358:GLN:HA	1:A:359:PRO:HD3	1.84	0.42
2:B:294:GLN:HG3	2:B:300:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HA	1:A:155:GLU:HG3	2.02	0.42
1:A:174:ALA:CB	1:A:207:GLU:HB2	2.49	0.42
2:D:42:LEU:O	2:D:43:GLN:C	2.58	0.42
1:A:270:ALA:HB3	1:A:302:MET:CE	2.45	0.41
1:C:105:ARG:HG2	1:C:110:ILE:HG22	2.02	0.41
2:B:66:ILE:HD13	2:B:122:VAL:HG12	2.03	0.41
2:B:381:SER:O	2:B:384:ILE:HB	2.20	0.41
2:B:4:ILE:HG22	2:B:133:GLN:CB	2.50	0.41
3:E:58:GLU:O	3:E:62:LYS:HB2	2.20	0.41
2:B:265:LEU:HB3	2:B:432:TYR:CE2	2.54	0.41
1:A:79:ARG:HH12	1:A:94:THR:HG22	1.85	0.41
1:A:23:LEU:HD23	1:A:27:GLU:OE1	2.20	0.41
1:A:346:TRP:HZ2	1:A:435:VAL:CG1	2.31	0.41
2:D:151:THR:O	2:D:154:ILE:HG12	2.21	0.41
1:A:64:ARG:HG3	1:A:64:ARG:NH1	2.34	0.41
1:A:181:VAL:HG23	2:B:258:ASN:ND2	2.35	0.41
2:B:408:TYR:O	2:B:409:THR:C	2.59	0.41
2:B:169:PHE:CD2	2:B:235:MET:HG2	2.54	0.41
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.03	0.41
2:D:239:THR:O	2:D:240:THR:C	2.58	0.41
1:A:67:PHE:HB2	1:A:92:LEU:HD22	2.03	0.41
1:A:79:ARG:HH12	1:A:94:THR:CG2	2.33	0.41
2:B:51:VAL:HG12	2:B:52:TYR:CD1	2.56	0.41
1:C:188:ILE:HD12	1:C:425:MET:HG3	2.01	0.41
1:A:210:TYR:HE1	1:A:214:ARG:HH11	1.68	0.41
1:A:260:VAL:HA	1:A:261:PRO:HD3	1.91	0.41
1:A:328:VAL:HG11	1:A:353:VAL:HG11	2.02	0.41
2:B:401:ARG:CG	2:B:401:ARG:NH1	2.83	0.41
1:C:123:ARG:HD2	1:C:161:TYR:OH	2.20	0.41
2:D:106:GLY:O	2:D:111:GLY:HA3	2.21	0.41
1:C:98:ASP:OD2	2:D:251:ASP:OD1	2.39	0.41
1:C:322:ASP:O	1:C:323:VAL:HG23	2.21	0.41
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.80	0.41
1:A:174:ALA:HB1	1:A:207:GLU:HB2	2.03	0.41
2:B:211:ASP:HB3	2:B:215:ARG:NH1	2.35	0.41
2:B:358:ILE:HA	2:B:359:PRO:HD3	1.87	0.41
2:B:55:GLU:HB3	2:B:61:TYR:CD2	2.56	0.41
1:C:196:GLU:H	1:C:196:GLU:HG3	1.59	0.41
2:D:62:VAL:O	2:D:62:VAL:CG2	2.68	0.41
1:C:306:ASP:O	1:C:309:HIS:HB3	2.20	0.41
2:B:12:CYS:HB3	2:B:140:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.39	0.41
1:C:8:HIS:CD2	1:C:17:GLY:CA	2.98	0.41
2:D:5:VAL:CG2	2:D:135:PHE:CD2	3.02	0.41
2:B:177:VAL:HG12	2:B:177:VAL:O	2.21	0.41
2:D:308:ARG:NH1	2:D:308:ARG:HG3	2.35	0.41
2:B:388:PHE:HB3	2:B:425:MET:HE2	2.02	0.41
1:A:106:GLY:O	1:A:111:GLY:HA3	2.21	0.41
1:C:88:HIS:CD2	1:C:89:PRO:HD2	2.57	0.41
2:B:225:GLY:O	2:B:227:LEU:N	2.45	0.41
2:B:239:THR:O	2:B:241:CYS:N	2.53	0.41
1:A:142:GLY:CA	1:A:183:GLU:HG3	2.45	0.41
1:A:205:ASP:CB	1:A:303:VAL:HA	2.50	0.41
3:E:87:ILE:O	3:E:91:ASN:HB2	2.21	0.41
2:B:126:SER:C	2:B:128:SER:H	2.23	0.41
2:B:20:PHE:HD2	2:B:235:MET:HB3	1.85	0.40
2:B:239:THR:O	2:B:240:THR:C	2.59	0.40
3:E:111:ASN:HA	3:E:111:ASN:HD22	1.62	0.40
1:C:306:ASP:HA	1:C:307:PRO:HD3	1.75	0.40
1:C:273:ALA:HB2	1:C:375:VAL:N	2.35	0.40
1:A:52:PHE:HE1	1:A:242:LEU:HD12	1.86	0.40
2:B:2:ARG:NH1	2:B:133:GLN:HA	2.37	0.40
1:C:167:LEU:CD1	1:C:252:LEU:CD1	2.98	0.40
1:A:394:LYS:HG3	2:B:348:PRO:CG	2.51	0.40
1:C:20:CYS:HB3	1:C:232:GLY:HA2	2.04	0.40
2:B:76:ASP:N	2:B:76:ASP:OD1	2.55	0.40
2:B:231:VAL:HG12	2:B:235:MET:HE2	2.03	0.40
2:D:223:THR:HB	2:D:225:GLY:CA	2.51	0.40
3:E:78:HIS:HA	3:E:81:GLU:HB2	2.03	0.40
1:C:298:PRO:C	1:C:300:ASN:H	2.25	0.40
2:D:240:THR:HG21	2:D:320:ARG:CZ	2.52	0.40
2:B:287:THR:O	2:B:288:VAL:HB	2.22	0.40
1:C:36:MET:HA	1:C:37:PRO:HD3	1.93	0.40
1:A:20:CYS:HB3	1:A:232:GLY:HA2	2.02	0.40
3:E:59:GLU:OE1	3:E:59:GLU:HA	2.12	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	423/451 (94%)	357 (84%)	41 (10%)	25 (6%)	2	27
1	C	424/451 (94%)	356 (84%)	42 (10%)	26 (6%)	2	26
2	B	416/445 (94%)	326 (78%)	60 (14%)	30 (7%)	1	21
2	D	415/445 (93%)	325 (78%)	62 (15%)	28 (7%)	1	24
3	E	120/142 (84%)	91 (76%)	21 (18%)	8 (7%)	1	24
All	All	1798/1934 (93%)	1455 (81%)	226 (13%)	117 (6%)	1	25

All (117) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	48	SER
1	A	72	PRO
1	A	73	THR
1	A	82	THR
1	A	264	ARG
1	A	265	ILE
1	A	273	ALA
1	A	345	ASP
1	A	403	ALA
2	B	3	GLU
2	B	43	GLN
2	B	60	LYS
2	B	62	VAL
2	B	82	PRO
2	B	115	VAL
2	B	163	ASP
2	B	244	PHE
2	B	251	ASP
2	B	273	ALA
2	B	276	THR

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Mol	Chain	Res	Type
2	B	288	VAL
2	B	348	PRO
2	B	371	LEU
1	C	11	GLN
1	C	48	SER
1	C	72	PRO
1	C	73	THR
1	C	82	THR
1	C	245	ASP
1	C	264	ARG
1	C	265	ILE
1	C	273	ALA
1	C	345	ASP
1	C	403	ALA
1	C	437	VAL
2	D	3	GLU
2	D	43	GLN
2	D	60	LYS
2	D	62	VAL
2	D	82	PRO
2	D	115	VAL
2	D	163	ASP
2	D	244	PHE
2	D	273	ALA
2	D	276	THR
2	D	288	VAL
2	D	348	PRO
2	D	371	LEU
3	E	18	GLN
3	E	29	PHE
3	E	49	GLU
1	A	18	ASN
1	A	162	GLY
1	A	240	ALA
1	A	279	GLU
1	A	350	GLY
1	A	377	MET
2	B	34	GLY
2	B	73	GLY
2	B	159	GLU
2	B	299	LYS
2	B	403	ALA

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Mol	Chain	Res	Type
1	C	98	ASP
1	C	162	GLY
1	C	279	GLU
1	C	350	GLY
1	C	377	MET
2	D	73	GLY
2	D	159	GLU
2	D	299	LYS
2	D	309	HIS
2	D	403	ALA
3	E	12	ASN
3	E	62	LYS
3	E	68	LEU
1	A	248	LEU
2	B	217	LEU
2	B	226	ASP
2	B	245	PRO
2	B	322	ARG
1	C	164	LYS
2	D	34	GLY
2	D	89	PRO
2	D	217	LEU
2	D	226	ASP
2	D	402	LYS
3	E	47	LEU
2	B	89	PRO
2	B	162	PRO
2	B	240	THR
2	B	402	LYS
1	C	10	GLY
1	C	112	LYS
1	C	240	ALA
1	C	247	ALA
1	C	257	THR
1	C	341	ILE
2	D	109	THR
2	D	162	PRO
2	D	322	ARG
1	A	10	GLY
1	A	112	LYS
1	A	164	LYS
1	A	309	HIS

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Mol	Chain	Res	Type
1	A	341	ILE
2	B	305	CYS
2	D	225	GLY
1	A	4	CYS
2	B	225	GLY
1	C	301	GLN
3	E	95	LYS
2	B	177	VAL
2	D	177	VAL
1	A	348	PRO
1	A	246	GLY
1	C	62	VAL

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	349/378 (92%)	241 (69%)	108 (31%)	0	3
1	C	345/378 (91%)	240 (70%)	105 (30%)	0	3
2	B	349/383 (91%)	243 (70%)	106 (30%)	0	3
2	D	348/383 (91%)	246 (71%)	102 (29%)	0	4
3	E	79/126 (63%)	47 (60%)	32 (40%)	0	1
All	All	1470/1648 (89%)	1017 (69%)	453 (31%)	0	3

All (453) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	4	CYS
1	A	9	VAL
1	A	11	GLN
1	A	16	ILE
1	A	22	GLU
1	A	23	LEU

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Mol	Chain	Res	Type
1	A	26	LEU
1	A	27	GLU
1	A	36	MET
1	A	48	SER
1	A	62	VAL
1	A	68	VAL
1	A	71	GLU
1	A	73	THR
1	A	74	VAL
1	A	76	ASP
1	A	79	ARG
1	A	80	THR
1	A	82	THR
1	A	84	ARG
1	A	88	HIS
1	A	90	GLU
1	A	94	THR
1	A	98	ASP
1	A	105	ARG
1	A	110	ILE
1	A	112	LYS
1	A	115	ILE
1	A	116	ASP
1	A	119	LEU
1	A	124	LYS
1	A	127	ASP
1	A	128	GLN
1	A	141	PHE
1	A	145	THR
1	A	151	SER
1	A	153	LEU
1	A	156	ARG
1	A	160	ASP
1	A	163	LYS
1	A	176	GLN
1	A	177	VAL
1	A	178	SER
1	A	183	GLU
1	A	193	THR
1	A	194	THR
1	A	196	GLU
1	A	198	SER

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Mol	Chain	Res	Type
1	A	200	CYS
1	A	206	ASN
1	A	210	TYR
1	A	217	LEU
1	A	219	ILE
1	A	220	GLU
1	A	223	THR
1	A	224	TYR
1	A	225	THR
1	A	226	ASN
1	A	229	ARG
1	A	230	LEU
1	A	237	SER
1	A	239	THR
1	A	241	SER
1	A	242	LEU
1	A	245	ASP
1	A	248	LEU
1	A	249	ASN
1	A	256	GLN
1	A	269	LEU
1	A	279	GLU
1	A	284	GLU
1	A	288	VAL
1	A	301	GLN
1	A	302	MET
1	A	315	CYS
1	A	318	LEU
1	A	322	ASP
1	A	326	LYS
1	A	329	ASN
1	A	334	THR
1	A	339	ARG
1	A	340	THR
1	A	341	ILE
1	A	343	PHE
1	A	345	ASP
1	A	349	THR
1	A	352	LYS
1	A	356	ASN
1	A	361	THR
1	A	368	LEU

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Mol	Chain	Res	Type
1	A	370	LYS
1	A	371	VAL
1	A	373	ARG
1	A	375	VAL
1	A	376	CYS
1	A	377	MET
1	A	379	SER
1	A	380	ASN
1	A	391	LEU
1	A	397	LEU
1	A	401	LYS
1	A	405	VAL
1	A	413	MET
1	A	414	GLU
1	A	415	GLU
1	A	432	TYR
1	A	433	GLU
2	B	2	ARG
2	B	4	ILE
2	B	5	VAL
2	B	15	GLN
2	B	16	ILE
2	B	30	ILE
2	B	39	ASP
2	B	40	SER
2	B	42	LEU
2	B	43	GLN
2	B	48	ARG
2	B	49	ILE
2	B	54	ASN
2	B	55	GLU
2	B	61	TYR
2	B	68	VAL
2	B	70	LEU
2	B	71	GLU
2	B	90	ASP
2	B	91	ASN
2	B	93	VAL
2	B	96	GLN
2	B	109	THR
2	B	110	GLU
2	B	122	VAL

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Mol	Chain	Res	Type
2	B	131	CYS
2	B	137	LEU
2	B	138	THR
2	B	139	HIS
2	B	151	THR
2	B	155	SER
2	B	156	LYS
2	B	158	ARG
2	B	160	GLU
2	B	164	ARG
2	B	165	ILE
2	B	168	THR
2	B	170	SER
2	B	171	VAL
2	B	174	SER
2	B	176	LYS
2	B	177	VAL
2	B	178	SER
2	B	179	ASP
2	B	180	THR
2	B	181	VAL
2	B	192	HIS
2	B	193	GLN
2	B	209	LEU
2	B	210	TYR
2	B	223	THR
2	B	227	LEU
2	B	230	LEU
2	B	236	SER
2	B	241	CYS
2	B	243	ARG
2	B	247	GLN
2	B	257	VAL
2	B	258	ASN
2	B	275	LEU
2	B	286	LEU
2	B	293	GLN
2	B	294	GLN
2	B	295	MET
2	B	299	LYS
2	B	300	ASN
2	B	302	MET

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Mol	Chain	Res	Type
2	B	305	CYS
2	B	308	ARG
2	B	309	HIS
2	B	311	ARG
2	B	313	LEU
2	B	320	ARG
2	B	323	MET
2	B	325	MET
2	B	329	ASP
2	B	333	LEU
2	B	339	ASN
2	B	340	SER
2	B	341	SER
2	B	344	VAL
2	B	350	ASN
2	B	351	VAL
2	B	353	THR
2	B	355	VAL
2	B	356	CYS
2	B	357	ASP
2	B	358	ILE
2	B	371	LEU
2	B	374	SER
2	B	376	THR
2	B	377	PHE
2	B	384	ILE
2	B	386	GLU
2	B	387	LEU
2	B	390	ARG
2	B	391	ILE
2	B	394	GLN
2	B	400	ARG
2	B	401	ARG
2	B	405	LEU
2	B	415	GLU
2	B	416	MET
2	B	419	THR
2	B	430	SER
2	B	434	GLN
1	C	2	ARG
1	C	4	CYS
1	C	9	VAL

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Mol	Chain	Res	Type
1	C	11	GLN
1	C	16	ILE
1	C	22	GLU
1	C	23	LEU
1	C	26	LEU
1	C	27	GLU
1	C	36	MET
1	C	48	SER
1	C	60	LYS
1	C	62	VAL
1	C	68	VAL
1	C	71	GLU
1	C	73	THR
1	C	74	VAL
1	C	76	ASP
1	C	79	ARG
1	C	80	THR
1	C	82	THR
1	C	84	ARG
1	C	88	HIS
1	C	90	GLU
1	C	94	THR
1	C	98	ASP
1	C	105	ARG
1	C	110	ILE
1	C	112	LYS
1	C	115	ILE
1	C	116	ASP
1	C	119	LEU
1	C	124	LYS
1	C	127	ASP
1	C	141	PHE
1	C	145	THR
1	C	151	SER
1	C	153	LEU
1	C	155	GLU
1	C	156	ARG
1	C	160	ASP
1	C	163	LYS
1	C	176	GLN
1	C	177	VAL
1	C	178	SER

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Mol	Chain	Res	Type
1	C	183	GLU
1	C	193	THR
1	C	194	THR
1	C	196	GLU
1	C	198	SER
1	C	200	CYS
1	C	206	ASN
1	C	210	TYR
1	C	217	LEU
1	C	219	ILE
1	C	220	GLU
1	C	223	THR
1	C	225	THR
1	C	226	ASN
1	C	229	ARG
1	C	230	LEU
1	C	237	SER
1	C	239	THR
1	C	250	VAL
1	C	251	ASP
1	C	252	LEU
1	C	254	GLU
1	C	257	THR
1	C	260	VAL
1	C	269	LEU
1	C	279	GLU
1	C	288	VAL
1	C	301	GLN
1	C	302	MET
1	C	313	MET
1	C	315	CYS
1	C	316	CYS
1	C	318	LEU
1	C	322	ASP
1	C	326	LYS
1	C	329	ASN
1	C	334	THR
1	C	340	THR
1	C	341	ILE
1	C	345	ASP
1	C	349	THR
1	C	352	LYS

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Mol	Chain	Res	Type
1	C	356	ASN
1	C	361	THR
1	C	368	LEU
1	C	370	LYS
1	C	371	VAL
1	C	373	ARG
1	C	377	MET
1	C	379	SER
1	C	380	ASN
1	C	391	LEU
1	C	394	LYS
1	C	397	LEU
1	C	401	LYS
1	C	405	VAL
1	C	413	MET
1	C	414	GLU
1	C	415	GLU
1	C	433	GLU
2	D	2	ARG
2	D	4	ILE
2	D	5	VAL
2	D	15	GLN
2	D	16	ILE
2	D	19	LYS
2	D	39	ASP
2	D	42	LEU
2	D	43	GLN
2	D	48	ARG
2	D	49	ILE
2	D	55	GLU
2	D	61	TYR
2	D	68	VAL
2	D	71	GLU
2	D	90	ASP
2	D	91	ASN
2	D	93	VAL
2	D	96	GLN
2	D	109	THR
2	D	110	GLU
2	D	115	VAL
2	D	122	VAL
2	D	131	CYS

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Mol	Chain	Res	Type
2	D	137	LEU
2	D	138	THR
2	D	139	HIS
2	D	151	THR
2	D	155	SER
2	D	156	LYS
2	D	158	ARG
2	D	160	GLU
2	D	164	ARG
2	D	165	ILE
2	D	168	THR
2	D	170	SER
2	D	171	VAL
2	D	174	SER
2	D	176	LYS
2	D	177	VAL
2	D	178	SER
2	D	179	ASP
2	D	180	THR
2	D	181	VAL
2	D	192	HIS
2	D	193	GLN
2	D	209	LEU
2	D	210	TYR
2	D	223	THR
2	D	227	LEU
2	D	230	LEU
2	D	236	SER
2	D	241	CYS
2	D	243	ARG
2	D	247	GLN
2	D	248	LEU
2	D	257	VAL
2	D	258	ASN
2	D	265	LEU
2	D	275	LEU
2	D	286	LEU
2	D	293	GLN
2	D	294	GLN
2	D	295	MET
2	D	299	LYS
2	D	300	ASN

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Mol	Chain	Res	Type
2	D	302	MET
2	D	305	CYS
2	D	308	ARG
2	D	309	HIS
2	D	313	LEU
2	D	320	ARG
2	D	323	MET
2	D	325	MET
2	D	329	ASP
2	D	331	GLN
2	D	333	LEU
2	D	339	ASN
2	D	341	SER
2	D	344	VAL
2	D	350	ASN
2	D	351	VAL
2	D	352	LYS
2	D	353	THR
2	D	355	VAL
2	D	357	ASP
2	D	358	ILE
2	D	371	LEU
2	D	374	SER
2	D	376	THR
2	D	377	PHE
2	D	384	ILE
2	D	386	GLU
2	D	387	LEU
2	D	390	ARG
2	D	391	ILE
2	D	400	ARG
2	D	401	ARG
2	D	416	MET
2	D	419	THR
2	D	430	SER
2	D	434	GLN
3	E	10	GLU
3	E	11	LEU
3	E	13	LYS
3	E	14	CYS
3	E	28	SER
3	E	51	GLN

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Mol	Chain	Res	Type
3	E	53	LYS
3	E	59	GLU
3	E	60	ARG
3	E	62	LYS
3	E	65	GLU
3	E	70	LYS
3	E	72	LEU
3	E	75	LYS
3	E	76	ARG
3	E	79	GLU
3	E	81	GLU
3	E	87	ILE
3	E	94	ILE
3	E	96	MET
3	E	99	GLU
3	E	105	MET
3	E	107	SER
3	E	111	ASN
3	E	112	ARG
3	E	115	HIS
3	E	119	MET
3	E	120	LEU
3	E	121	GLU
3	E	124	GLN
3	E	133	VAL
3	E	134	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	50	ASN
1	A	61	HIS
1	A	88	HIS
1	A	91	GLN
1	A	133	GLN
1	A	139	HIS
1	A	176	GLN
1	A	206	ASN
1	A	216	ASN
1	A	258	ASN
1	A	266	HIS

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Mol	Chain	Res	Type
1	A	301	GLN
1	A	380	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	15	GLN
2	B	54	ASN
2	B	136	GLN
2	B	206	ASN
2	B	229	HIS
2	B	247	GLN
2	B	258	ASN
2	B	266	HIS
2	B	294	GLN
2	B	350	ASN
2	B	380	ASN
2	B	385	GLN
2	B	436	GLN
1	C	8	HIS
1	C	50	ASN
1	C	61	HIS
1	C	88	HIS
1	C	91	GLN
1	C	133	GLN
1	C	139	HIS
1	C	176	GLN
1	C	197	HIS
1	C	206	ASN
1	C	216	ASN
1	C	256	GLN
1	C	258	ASN
1	C	266	HIS
1	C	380	ASN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	15	GLN
2	D	54	ASN
2	D	136	GLN
2	D	229	HIS
2	D	258	ASN
2	D	266	HIS

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Mol	Chain	Res	Type
2	D	294	GLN
2	D	339	ASN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
2	D	436	GLN
3	E	64	GLN
3	E	108	ASN
3	E	111	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GTP	A	600	-	25,34,34	1.03	3 (12%)	34,54,54	1.96	9 (26%)
6	GDP	B	600	-	23,30,30	0.97	1 (4%)	30,47,47	1.76	6 (20%)
4	GTP	C	600	-	25,34,34	0.97	1 (4%)	34,54,54	1.60	6 (17%)
6	GDP	D	600	-	23,30,30	1.02	1 (4%)	30,47,47	1.92	9 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	A	600	-	-	0/18/38/38	0/3/3/3
6	GDP	B	600	-	-	0/12/32/32	0/3/3/3
4	GTP	C	600	-	-	0/18/38/38	0/3/3/3
6	GDP	D	600	-	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	600	GTP	O4'-C4'	-2.13	1.40	1.45
4	A	600	GTP	C6-N1	2.58	1.37	1.33
4	A	600	GTP	C2-N1	2.62	1.40	1.35
6	B	600	GDP	C6-N1	2.75	1.38	1.33
4	C	600	GTP	C6-N1	3.04	1.38	1.33
6	D	600	GDP	C6-N1	3.06	1.38	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	600	GDP	N3-C2-N1	-5.36	119.28	127.44
4	C	600	GTP	N3-C2-N1	-4.99	119.85	127.44
6	B	600	GDP	N3-C2-N1	-4.81	120.12	127.44
4	A	600	GTP	N3-C2-N1	-4.57	120.48	127.44
4	A	600	GTP	PB-O3B-PG	-3.85	119.77	132.67
4	A	600	GTP	C5-C6-N1	-3.72	118.50	123.59
6	B	600	GDP	C2'-C1'-N9	-3.64	108.73	114.29
4	A	600	GTP	PA-O3A-PB	-3.59	122.64	132.73
6	B	600	GDP	PA-O3A-PB	-3.59	120.64	132.67
6	D	600	GDP	C5-C6-N1	-3.29	119.09	123.59
6	D	600	GDP	PA-O3A-PB	-2.96	122.75	132.67
4	C	600	GTP	PB-O3B-PG	-2.95	122.79	132.67
4	C	600	GTP	PA-O3A-PB	-2.90	124.60	132.73
6	B	600	GDP	C5-C6-N1	-2.66	119.95	123.59
4	C	600	GTP	C5-C6-N1	-2.65	119.96	123.59
6	D	600	GDP	C2'-C1'-N9	-2.51	110.46	114.29
6	D	600	GDP	C4-C5-N7	-2.19	107.47	109.48
4	A	600	GTP	O5'-C5'-C4'	-2.06	101.53	109.12
4	A	600	GTP	C4'-O4'-C1'	2.03	111.95	109.72
6	B	600	GDP	O4'-C1'-N9	2.07	112.42	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	600	GTP	N2-C2-N1	2.26	120.94	117.20
6	D	600	GDP	N2-C2-N1	2.35	121.09	117.20
6	D	600	GDP	C4'-O4'-C1'	2.43	112.39	109.72
6	D	600	GDP	C2'-C3'-C4'	2.56	107.88	102.61
6	B	600	GDP	C6-N1-C2	2.61	119.56	115.94
4	A	600	GTP	N2-C2-N1	2.73	121.71	117.20
4	C	600	GTP	C6-N1-C2	2.75	119.76	115.94
6	D	600	GDP	C6-N1-C2	3.34	120.57	115.94
4	A	600	GTP	C6-N1-C2	3.36	120.61	115.94
4	A	600	GTP	C2'-C1'-N9	4.11	120.58	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GTP	3	0
6	B	600	GDP	1	0
4	C	600	GTP	2	0
6	D	600	GDP	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	427/451 (94%)	-0.11	0 100 100	57, 61, 64, 70	0
1	C	428/451 (94%)	-0.08	5 (1%) 81 66	57, 61, 65, 76	0
2	B	420/445 (94%)	-0.17	0 100 100	59, 62, 71, 87	0
2	D	419/445 (94%)	-0.21	0 100 100	59, 62, 72, 87	0
3	E	124/142 (87%)	-0.42	1 (0%) 87 76	47, 62, 73, 80	0
All	All	1818/1934 (94%)	-0.16	6 (0%) 94 90	47, 61, 68, 87	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	PRO	5.4
3	E	4	ALA	2.9
1	C	302	MET	2.3
1	C	371	VAL	2.2
1	C	281	ALA	2.1
1	C	249	ASN	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
4	GTP	C	600	32/32	0.93	0.14	-0.94	53,56,57,57	0
6	GDP	D	600	28/28	0.92	0.14	-1.03	55,58,63,63	0
5	MG	C	601	1/1	0.97	0.17	-1.18	40,40,40,40	0
4	GTP	A	600	32/32	0.96	0.17	-1.27	53,59,62,63	0
5	MG	A	601	1/1	0.99	0.18	-1.41	40,40,40,40	0
6	GDP	B	600	28/28	0.92	0.12	-1.42	48,51,59,60	0

6.5 Other polymers

There are no such residues in this entry.