Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:12 AM GMT

PDB ID	:	3HKD
Title	:	Tubulin-TN16 : 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	:	3.70 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:

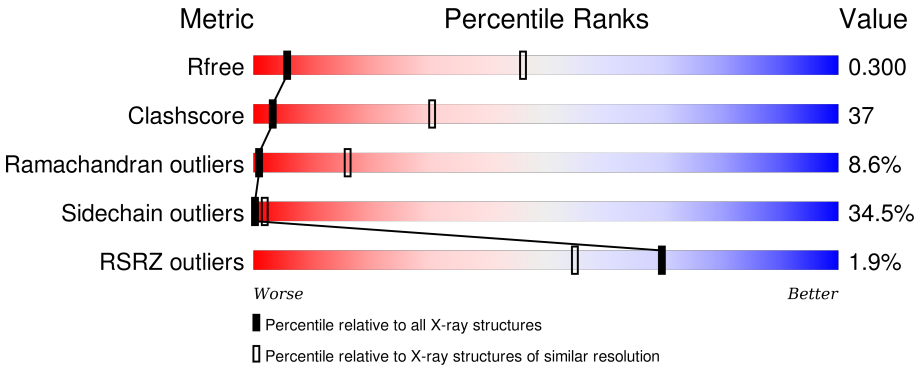
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.70 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	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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	40% 37% 15% • 5%
1	C	451	3% 39% 38% 16% • 5%
2	B	445	2% 31% 42% 18% • 6%
2	D	445	2% 27% 40% 24% • •
3	E	142	31% 39% 15% • 13%

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
6	GDP	B	600	-	-	X	-
6	GDP	D	600	-	-	X	-
7	N16	D	700	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14223 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	428	Total	C	N	O	S	0	0	0
			3300	2097	557	625	21			
1	C	429	Total	C	N	O	S	0	0	0
			3286	2084	554	627	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
			3251	2046	547	633	25			
2	D	427	Total	C	N	O	S	0	0	0
			3297	2071	559	643	24			

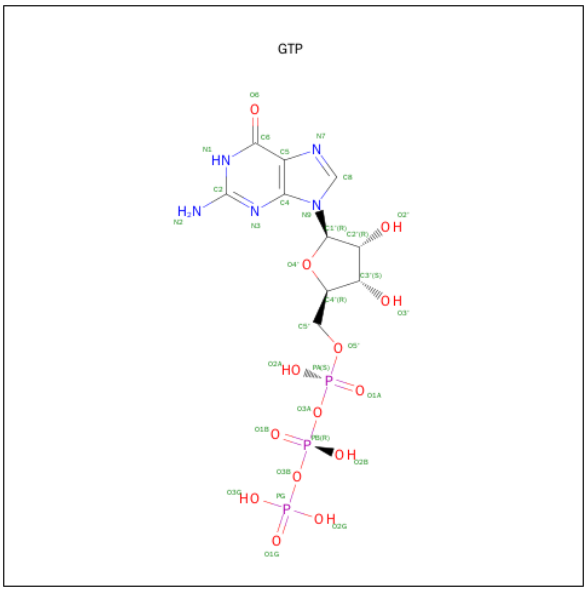
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			920	557	174	184	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: $C_{10}H_{16}N_5O_{14}P_3$).

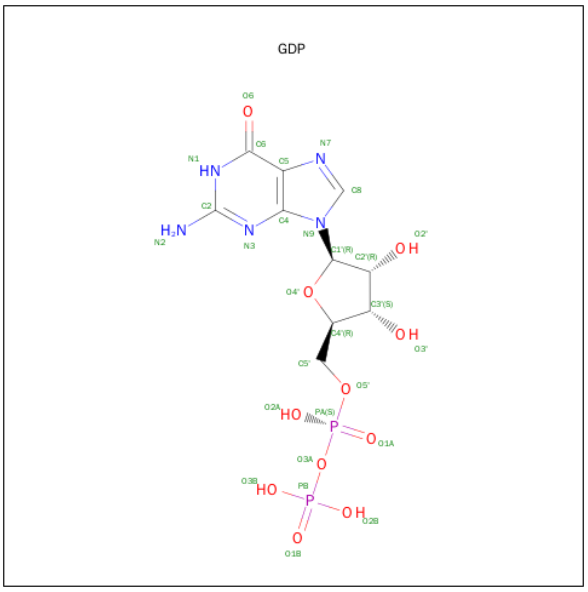


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 32 10 5 14 3	0	0
4	C	1	Total C N O P 32 10 5 14 3	0	0

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

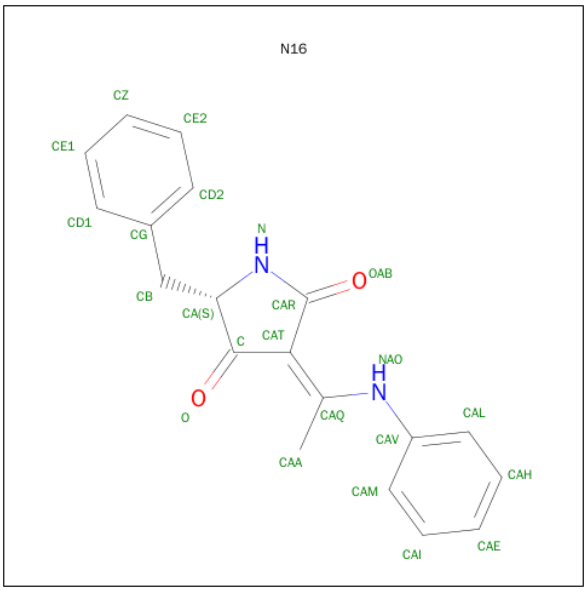
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

- 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		

- Molecule 7 is (3Z,5S)-5-BENZYL-3-[1-(PHENYLAMINO)ETHYLIDENE]PYRROLIDINE-2,4-DIONE (three-letter code: N16) (formula: $C_{19}H_{18}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			23	19	2	2		

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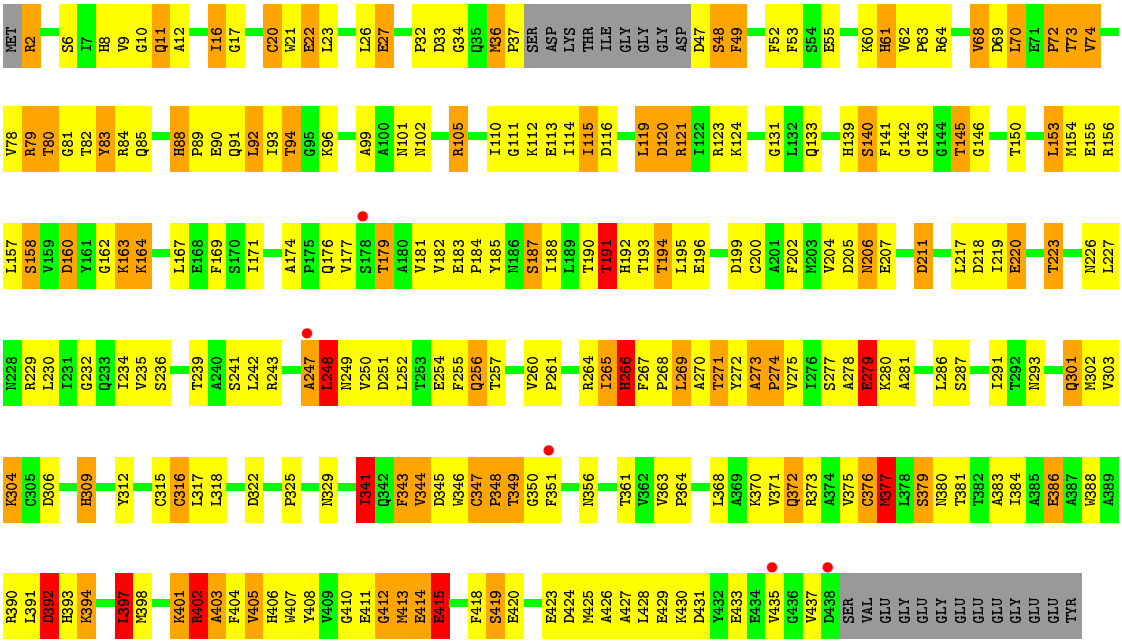
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	D	1	Total	C	N	O	0	0
			23	19	2	2		

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.

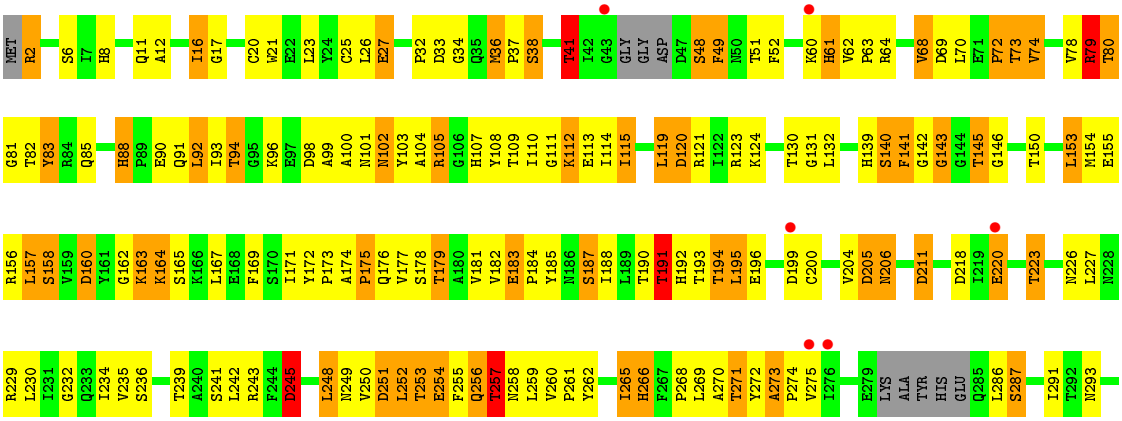
- Molecule 1: Tubulin alpha chain

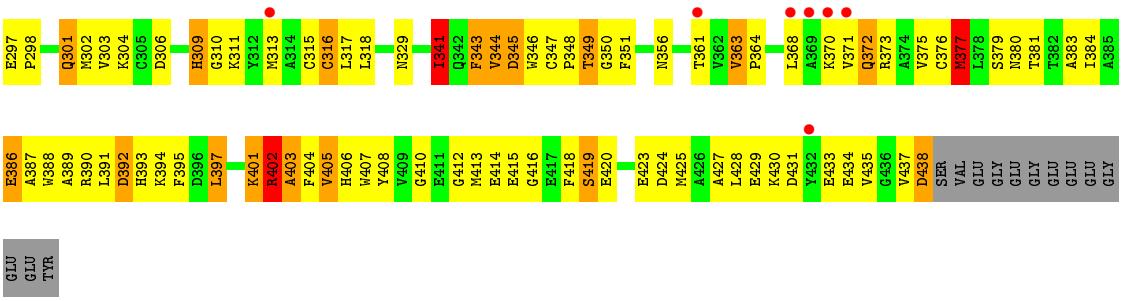
Chain A:



- Molecule 1: Tubulin alpha chain

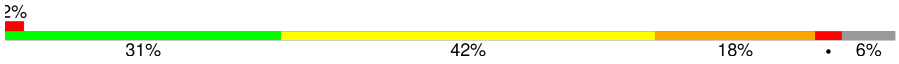
Chain C:

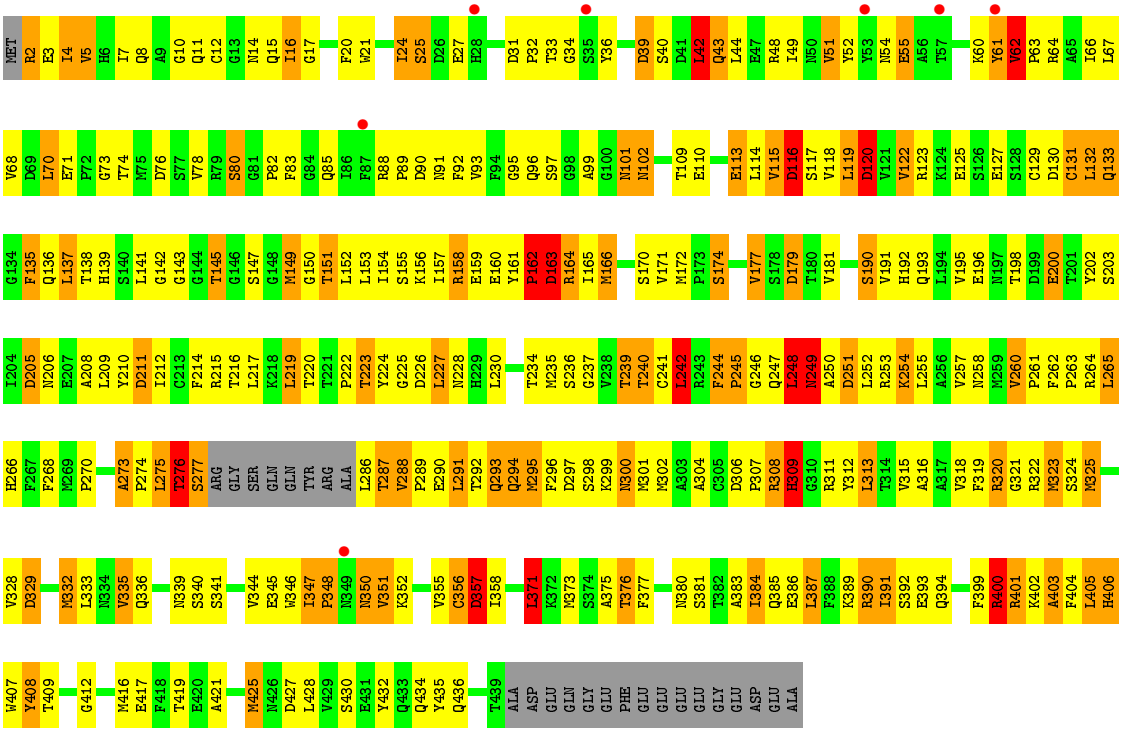




• Molecule 2: Tubulin beta chain

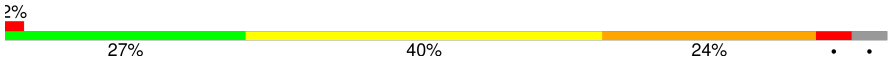
Chain B:

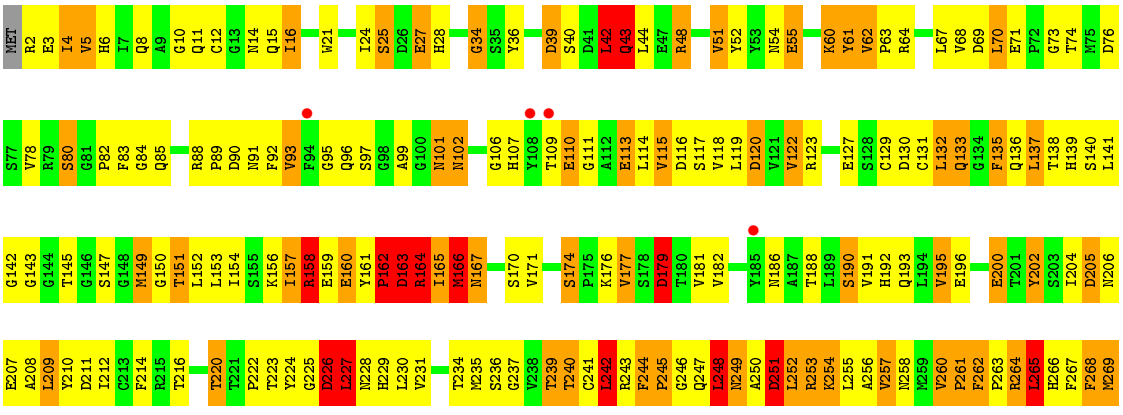


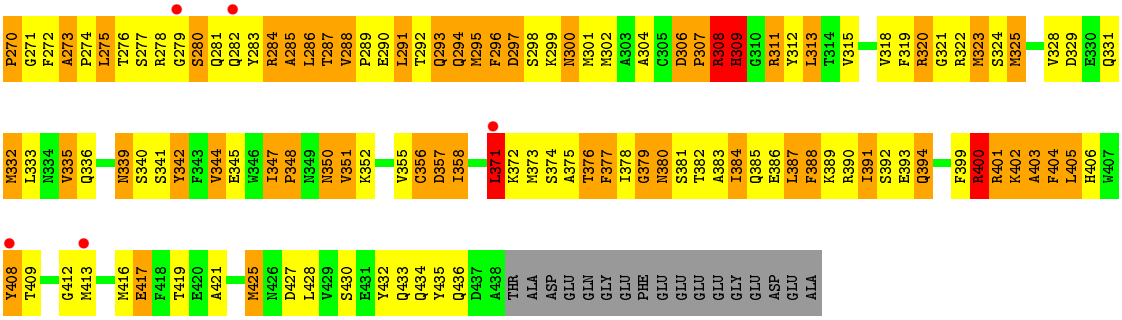


• Molecule 2: Tubulin beta chain

Chain D:

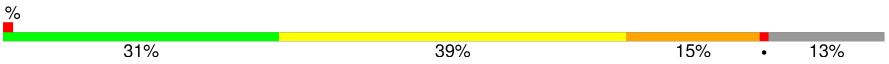


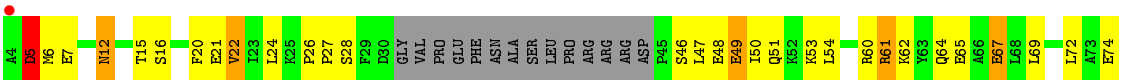


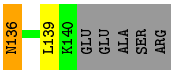


- Molecule 3: Stathmin-4

Chain E:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	328.53Å 328.53Å 54.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.70 48.55 – 3.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (20.00-3.70) 98.4 (48.55-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.209 , 0.264 0.264 , 0.300	Depositor DCC
R_{free} test set	1839 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	152.5	Xtriage
Anisotropy	0.181	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 1.5	EDS
Estimated twinning fraction	0.127 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 36232 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14223	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.01% 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, N16

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	0.69	0/3377	0.94	19/4593 (0.4%)
1	C	0.61	0/3360	0.91	13/4572 (0.3%)
2	B	0.71	0/3323	0.96	13/4512 (0.3%)
2	D	1.04	10/3370 (0.3%)	1.09	21/4574 (0.5%)
3	E	0.74	0/928	0.89	2/1243 (0.2%)
All	All	0.78	10/14358 (0.1%)	0.97	68/19494 (0.3%)

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	2
1	C	0	3
2	B	0	3
2	D	0	4
3	E	0	1
All	All	0	13

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	379	GLY	C-O	8.38	1.37	1.23
2	D	200	GLU	CD-OE1	7.45	1.33	1.25
2	D	388	PHE	CD2-CE2	6.74	1.52	1.39
2	D	269	MET	C-O	5.92	1.34	1.23
2	D	377	PHE	CG-CD1	5.81	1.47	1.38
2	D	377	PHE	CG-CD2	5.65	1.47	1.38
2	D	388	PHE	CD1-CE1	5.61	1.50	1.39
2	D	377	PHE	CE1-CZ	5.30	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	202	TYR	CE2-CZ	5.21	1.45	1.38
2	D	200	GLU	CD-OE2	5.01	1.31	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	308	ARG	NE-CZ-NH1	10.29	125.44	120.30
2	D	297	ASP	CB-CG-OD2	8.41	125.87	118.30
1	A	248	LEU	CA-CB-CG	7.58	132.74	115.30
1	A	397	LEU	CA-CB-CG	7.52	132.59	115.30
2	D	164	ARG	NE-CZ-NH2	-7.50	116.55	120.30
2	D	357	ASP	CB-CG-OD2	7.49	125.04	118.30
1	C	211	ASP	CB-CG-OD2	7.44	125.00	118.30
2	D	308	ARG	NE-CZ-NH2	-7.43	116.58	120.30
2	D	164	ARG	NE-CZ-NH1	7.37	123.98	120.30
2	B	116	ASP	CB-CG-OD2	7.27	124.84	118.30
1	A	424	ASP	CB-CG-OD2	7.05	124.64	118.30
1	C	397	LEU	CA-CB-CG	6.98	131.35	115.30
1	C	269	LEU	CA-CB-CG	6.79	130.93	115.30
2	D	179	ASP	CB-CG-OD2	6.66	124.30	118.30
2	B	357	ASP	CB-CG-OD2	6.62	124.26	118.30
2	B	205	ASP	CB-CG-OD2	6.42	124.07	118.30
2	B	427	ASP	CB-CG-OD2	6.41	124.07	118.30
2	D	427	ASP	CB-CG-OD2	6.28	123.95	118.30
2	D	163	ASP	CB-CG-OD2	6.27	123.94	118.30
2	B	211	ASP	CB-CG-OD2	6.23	123.91	118.30
1	C	306	ASP	CB-CG-OD2	6.23	123.90	118.30
1	A	33	ASP	CB-CG-OD2	6.14	123.83	118.30
1	C	120	ASP	CB-CG-OD2	6.13	123.81	118.30
1	C	160	ASP	CB-CG-OD2	6.12	123.81	118.30
1	A	211	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	269	LEU	CA-CB-CG	5.90	128.86	115.30
2	D	226	ASP	CB-CG-OD2	5.88	123.59	118.30
2	D	69	ASP	CB-CG-OD2	5.87	123.58	118.30
1	C	205	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	33	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	116	ASP	CB-CG-OD2	5.75	123.47	118.30
2	B	120	ASP	CB-CG-OD2	5.73	123.46	118.30
1	A	218	ASP	CB-CG-OD2	5.72	123.45	118.30
2	B	163	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	160	ASP	CB-CG-OD2	5.70	123.43	118.30
2	B	242	LEU	CA-CB-CG	5.69	128.40	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	120	ASP	CB-CG-OD2	5.68	123.42	118.30
2	D	379	GLY	N-CA-C	5.68	127.30	113.10
2	D	371	LEU	CA-CB-CG	5.64	128.28	115.30
2	D	251	ASP	CB-CG-OD2	5.64	123.37	118.30
2	B	39	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	392	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	322	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	345	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	69	ASP	CB-CG-OD2	5.54	123.28	118.30
2	D	39	ASP	CB-CG-OD2	5.46	123.22	118.30
2	D	252	LEU	CB-CG-CD1	5.44	120.25	111.00
1	A	306	ASP	CB-CG-OD2	5.42	123.18	118.30
2	D	166	MET	CG-SD-CE	-5.37	91.60	100.20
1	A	20	CYS	CA-CB-SG	5.34	123.61	114.00
2	D	306	ASP	CB-CG-OD2	5.33	123.09	118.30
2	B	371	LEU	CA-CB-CG	5.32	127.53	115.30
1	C	424	ASP	CB-CG-OD2	5.29	123.06	118.30
2	D	158	ARG	NE-CZ-NH1	5.29	122.94	120.30
2	B	2	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	69	ASP	CB-CG-OD2	5.25	123.03	118.30
2	B	329	ASP	CB-CG-OD2	5.25	123.03	118.30
1	C	345	ASP	CB-CG-OD2	5.25	123.02	118.30
3	E	54	LEU	CA-CB-CG	5.23	127.33	115.30
1	C	245	ASP	CB-CG-OD2	5.21	122.99	118.30
2	B	297	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	266	HIS	CB-CA-C	-5.18	100.04	110.40
2	D	242	LEU	CA-CB-CG	5.17	127.20	115.30
3	E	127	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	120	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	218	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	376	CYS	N-CA-C	5.05	124.64	111.00
1	A	121	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	GLY	Peptide
1	A	266	HIS	Peptide
2	B	162	PRO	Peptide
2	B	248	LEU	Peptide
2	B	249	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	C	143	GLY	Peptide
1	C	266	HIS	Peptide
1	C	41	THR	Peptide
2	D	162	PRO	Peptide
2	D	248	LEU	Peptide
2	D	249	ASN	Peptide
2	D	262	PHE	Peptide
3	E	5	ASP	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	3300	0	3162	181	0
1	C	3286	0	3133	195	0
2	B	3251	0	3074	281	0
2	D	3297	0	3116	370	0
3	E	920	0	816	58	0
4	A	32	0	12	2	0
4	C	32	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	10	0
6	D	28	0	12	19	0
7	B	23	0	18	8	0
7	D	23	0	18	16	0
All	All	14223	0	13385	1033	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 37.

All (1033) 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)
3:E:119:MET:CE	3:E:119:MET:SD	2.02	1.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:96:MET:CE	3:E:96:MET:SD	2.05	1.44
2:D:140:SER:CB	6:D:600:GDP:H5'	1.59	1.31
2:D:387:LEU:O	2:D:390:ARG:HG2	1.31	1.26
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.16	1.14
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.22	1.13
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.27	1.12
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.80	1.11
2:B:142:GLY:O	6:B:600:GDP:H5'	1.52	1.10
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.22	1.09
2:D:223:THR:HB	2:D:225:GLY:H	1.16	1.08
2:D:140:SER:HB2	6:D:600:GDP:H5'	1.15	1.07
2:B:308:ARG:HH11	2:B:308:ARG:HG3	1.16	1.07
2:B:387:LEU:O	2:B:390:ARG:HG2	1.53	1.07
1:C:105:ARG:NH2	2:D:253:ARG:HH21	1.53	1.06
2:D:270:PRO:HD2	2:D:302:MET:HB2	1.33	1.05
2:D:135:PHE:HB2	2:D:166:MET:CE	1.87	1.05
2:D:319:PHE:HB2	2:D:355:VAL:HG12	1.39	1.04
2:B:223:THR:HB	2:B:225:GLY:H	1.16	1.04
2:D:171:VAL:HG12	2:D:206:ASN:HD21	1.23	1.04
2:D:133:GLN:HE21	2:D:252:LEU:HD22	1.21	1.03
2:B:401:ARG:NH2	1:C:434:GLU:O	1.90	1.03
3:E:118:ALA:O	3:E:122:ARG:NH1	1.91	1.02
1:A:105:ARG:HH22	2:B:253:ARG:HH21	1.02	1.01
2:D:171:VAL:HG12	2:D:206:ASN:ND2	1.74	1.01
2:B:319:PHE:HB2	2:B:355:VAL:HG12	1.44	1.00
2:D:287:THR:HG23	2:D:290:GLU:HB2	1.41	0.99
2:B:135:PHE:HB2	2:B:166:MET:CE	1.91	0.99
2:B:133:GLN:HE21	2:B:252:LEU:HD22	1.26	0.99
2:D:171:VAL:CG1	2:D:206:ASN:HD21	1.75	0.97
2:D:11:GLN:HG3	2:D:74:THR:HG21	1.44	0.97
1:C:206:ASN:HD21	4:C:600:GTP:N2	1.63	0.97
2:D:287:THR:CG2	2:D:290:GLU:HB2	1.94	0.97
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.95	0.95
2:D:262:PHE:HB2	2:D:265:LEU:HD11	1.48	0.95
1:C:404:PHE:HE1	2:D:347:ILE:HG21	1.28	0.94
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.96	0.94
2:D:242:LEU:HD11	7:D:700:N16:HD1	1.49	0.94
2:B:287:THR:HG23	2:B:290:GLU:HB2	1.49	0.94
1:C:206:ASN:HD21	4:C:600:GTP:HN22	0.94	0.94
2:B:5:VAL:HG22	2:B:135:PHE:HD2	1.32	0.93
2:B:262:PHE:HB2	2:B:265:LEU:HD11	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:200:GLU:HB3	2:D:268:PHE:CE1	2.03	0.93
2:B:273:ALA:HB3	2:B:274:PRO:CD	1.98	0.93
1:A:404:PHE:HE1	2:B:347:ILE:HG21	1.34	0.93
2:D:308:ARG:HG3	2:D:308:ARG:HH11	1.32	0.92
2:D:135:PHE:HB2	2:D:166:MET:HE1	1.49	0.92
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.51	0.92
1:A:70:LEU:HD12	1:A:145:THR:HB	1.52	0.92
2:D:229:HIS:CE1	2:D:277:SER:HB3	2.05	0.91
2:D:223:THR:CB	2:D:225:GLY:H	1.84	0.91
2:D:255:LEU:HG	7:D:700:N16:HAAA	1.51	0.90
2:D:391:ILE:HG13	2:D:392:SER:N	1.84	0.90
2:B:135:PHE:HB2	2:B:166:MET:HE1	1.53	0.90
2:B:403:ALA:O	2:B:405:LEU:N	2.04	0.90
2:B:171:VAL:HG12	2:B:206:ASN:ND2	1.87	0.90
1:C:105:ARG:HH22	2:D:253:ARG:HH21	0.89	0.89
1:C:273:ALA:CB	1:C:274:PRO:HD3	2.03	0.89
2:B:287:THR:CG2	2:B:290:GLU:HB2	2.02	0.89
1:C:105:ARG:HH22	2:D:253:ARG:NH2	1.70	0.88
2:D:248:LEU:HD11	7:D:700:N16:CAH	2.03	0.88
2:D:223:THR:HB	2:D:225:GLY:N	1.88	0.88
2:D:350:ASN:H	2:D:350:ASN:HD22	1.17	0.88
2:B:270:PRO:HD2	2:B:302:MET:HB2	1.56	0.87
2:B:220:THR:O	2:B:222:PRO:HD3	1.76	0.86
2:B:242:LEU:HD21	7:B:700:N16:HD1	1.56	0.86
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.57	0.86
1:C:70:LEU:HD12	1:C:145:THR:HB	1.58	0.86
2:D:5:VAL:HG22	2:D:135:PHE:HD2	1.42	0.85
1:A:278:ALA:O	1:A:279:GLU:HB3	1.77	0.85
2:D:162:PRO:HD2	2:D:163:ASP:HB2	1.57	0.84
2:B:273:ALA:CB	2:B:274:PRO:CD	2.55	0.84
1:C:206:ASN:ND2	4:C:600:GTP:HN22	1.75	0.84
2:D:200:GLU:HB3	2:D:268:PHE:HE1	1.43	0.84
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.60	0.84
1:C:315:CYS:SG	1:C:377:MET:CE	2.66	0.84
2:D:391:ILE:HG13	2:D:392:SER:H	1.39	0.83
2:D:99:ALA:HB1	2:D:145:THR:CG2	2.07	0.83
1:A:105:ARG:HH22	2:B:253:ARG:NH2	1.76	0.83
2:D:140:SER:CB	6:D:600:GDP:C5'	2.52	0.83
2:D:296:PHE:HE1	2:D:332:MET:CE	1.91	0.83
1:A:79:ARG:NH2	1:A:94:THR:HG21	1.94	0.83
2:B:223:THR:HB	2:B:225:GLY:N	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:292:THR:HA	2:D:295:MET:CE	2.09	0.82
2:D:220:THR:O	2:D:222:PRO:HD3	1.79	0.82
2:B:145:THR:HG23	6:B:600:GDP:O3B	1.79	0.82
2:D:224:TYR:O	2:D:228:ASN:ND2	2.12	0.82
2:B:99:ALA:HB1	2:B:145:THR:HG22	1.61	0.81
2:D:123:ARG:O	2:D:127:GLU:HB2	1.80	0.81
2:B:200:GLU:HB3	2:B:268:PHE:CE1	2.15	0.81
2:D:296:PHE:HE1	2:D:332:MET:HE3	1.44	0.81
2:B:171:VAL:CG1	2:B:206:ASN:HD21	1.94	0.80
1:A:206:ASN:HD21	4:A:600:GTP:HN22	1.26	0.80
2:B:99:ALA:HB1	2:B:145:THR:CG2	2.12	0.80
1:C:79:ARG:NH2	1:C:94:THR:HG21	1.96	0.80
2:D:250:ALA:HA	2:D:255:LEU:HD13	1.64	0.80
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.63	0.80
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.63	0.80
2:D:403:ALA:O	2:D:405:LEU:N	2.14	0.79
2:B:391:ILE:HG13	2:B:392:SER:N	1.95	0.79
2:D:151:THR:HB	2:D:193:GLN:HG2	1.65	0.79
1:C:315:CYS:SG	1:C:377:MET:HE2	2.21	0.79
2:B:123:ARG:O	2:B:127:GLU:HB2	1.83	0.79
1:C:41:THR:HG21	1:C:61:HIS:HE1	1.48	0.78
1:C:343:PHE:CD1	1:C:349:THR:HG22	2.18	0.78
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.08	0.78
2:B:171:VAL:HG12	2:B:206:ASN:HD21	1.47	0.78
1:C:167:LEU:HD13	1:C:252:LEU:HD11	1.65	0.78
2:D:309:HIS:H	2:D:309:HIS:CD2	2.00	0.78
3:E:60:ARG:HH11	3:E:60:ARG:HB2	1.49	0.77
2:D:312:TYR:HD2	2:D:315:VAL:CG2	1.97	0.77
2:D:261:PRO:HG3	2:D:313:LEU:HD12	1.64	0.77
2:B:276:THR:HG23	2:B:277:SER:N	1.99	0.77
2:B:312:TYR:HE2	2:B:377:PHE:HZ	1.31	0.77
2:D:195:VAL:HG21	2:D:428:LEU:HD22	1.65	0.77
2:D:265:LEU:CB	2:D:432:TYR:CE2	2.69	0.76
1:C:404:PHE:CE1	2:D:347:ILE:HG21	2.17	0.76
1:A:273:ALA:HB3	1:A:274:PRO:CD	2.10	0.76
1:A:145:THR:HG23	4:A:600:GTP:O2B	1.85	0.76
2:B:308:ARG:NH1	2:B:308:ARG:HG3	1.95	0.76
2:D:255:LEU:HG	7:D:700:N16:CAA	2.15	0.76
1:C:153:LEU:HD13	1:C:157:LEU:HD11	1.68	0.75
2:D:248:LEU:HD11	7:D:700:N16:CAL	2.15	0.75
2:D:159:GLU:HB2	3:E:123:LEU:HD13	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:133:GLN:NE2	2:D:252:LEU:HD22	2.01	0.75
2:D:270:PRO:CD	2:D:302:MET:HB2	2.13	0.75
1:C:167:LEU:HD13	1:C:252:LEU:CD1	2.16	0.75
1:C:406:HIS:CG	2:D:263:PRO:HG3	2.21	0.75
2:B:276:THR:HG23	2:B:277:SER:H	1.49	0.75
2:D:179:ASP:N	2:D:179:ASP:OD1	2.19	0.75
1:C:265:ILE:HD12	1:C:265:ILE:H	1.52	0.75
2:D:298:SER:O	2:D:300:ASN:N	2.18	0.75
2:D:345:GLU:N	2:D:345:GLU:OE1	2.19	0.75
3:E:22:VAL:O	3:E:22:VAL:HG13	1.86	0.75
3:E:74:GLU:C	3:E:76:ARG:H	1.90	0.75
2:D:383:ALA:O	2:D:386:GLU:HB2	1.87	0.74
2:D:312:TYR:CD2	2:D:315:VAL:CG2	2.70	0.74
2:D:250:ALA:HA	2:D:255:LEU:CD1	2.17	0.74
2:D:298:SER:HA	2:D:301:MET:HG2	1.67	0.74
1:C:101:ASN:HD22	2:D:254:LYS:HG2	1.53	0.74
1:A:153:LEU:HD13	1:A:157:LEU:HD11	1.69	0.74
2:D:298:SER:C	2:D:300:ASN:H	1.90	0.74
2:B:292:THR:HA	2:B:295:MET:HE3	1.70	0.74
1:A:265:ILE:H	1:A:265:ILE:HD12	1.51	0.74
2:B:292:THR:HA	2:B:295:MET:CE	2.18	0.74
1:C:273:ALA:HB3	1:C:375:VAL:H	1.52	0.73
2:D:312:TYR:CD2	2:D:315:VAL:HG21	2.23	0.73
1:C:183:GLU:HB3	1:C:184:PRO:CD	2.18	0.72
2:B:151:THR:HB	2:B:193:GLN:HG2	1.71	0.72
2:D:387:LEU:O	2:D:390:ARG:CG	2.24	0.72
2:B:403:ALA:C	2:B:405:LEU:H	1.91	0.72
1:A:343:PHE:CD1	1:A:349:THR:HG22	2.23	0.72
2:D:51:VAL:HG13	2:D:52:TYR:CD1	2.24	0.72
1:C:315:CYS:SG	1:C:377:MET:HE1	2.28	0.72
2:B:147:SER:O	2:B:151:THR:OG1	2.05	0.72
2:D:140:SER:HB3	6:D:600:GDP:H5'	1.67	0.72
2:B:309:HIS:CD2	2:B:309:HIS:H	2.05	0.72
2:D:265:LEU:HB3	2:D:432:TYR:CE2	2.25	0.72
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.25	0.72
2:D:99:ALA:HB1	2:D:145:THR:HG22	1.71	0.71
2:B:224:TYR:O	2:B:228:ASN:ND2	2.20	0.71
1:A:181:VAL:H	2:B:258:ASN:ND2	1.87	0.71
2:D:276:THR:HG21	2:D:280:SER:CB	2.21	0.71
2:D:51:VAL:O	2:D:64:ARG:NH2	2.24	0.71
2:B:223:THR:CB	2:B:225:GLY:H	1.99	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:HD22	2:B:254:LYS:HG2	1.55	0.71
2:D:12:CYS:SG	6:D:600:GDP:C4	2.84	0.71
2:D:36:TYR:OH	2:D:40:SER:O	2.07	0.71
3:E:60:ARG:NH1	3:E:60:ARG:HB2	2.05	0.70
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.72	0.70
1:A:412:GLY:O	3:E:60:ARG:NH1	2.24	0.70
2:D:312:TYR:HE2	2:D:377:PHE:CZ	2.09	0.70
2:D:265:LEU:HB2	2:D:432:TYR:CE2	2.27	0.70
1:C:260:VAL:O	1:C:260:VAL:HG23	1.92	0.70
2:D:5:VAL:HG13	2:D:132:LEU:CD1	2.21	0.70
2:B:155:SER:CB	3:E:76:ARG:HH22	2.05	0.70
2:D:208:ALA:O	2:D:211:ASP:N	2.23	0.70
1:A:105:ARG:NH2	2:B:253:ARG:HH21	1.84	0.70
2:D:273:ALA:HB2	2:D:375:ALA:H	1.57	0.70
2:D:89:PRO:O	2:D:92:PHE:HD1	1.74	0.70
1:A:270:ALA:O	1:A:302:MET:HB2	1.92	0.70
2:D:295:MET:HG2	2:D:295:MET:O	1.92	0.69
2:D:312:TYR:HE2	2:D:377:PHE:HZ	1.41	0.69
1:C:256:GLN:C	1:C:258:ASN:H	1.96	0.69
2:B:200:GLU:HB3	2:B:268:PHE:HE1	1.55	0.69
1:C:256:GLN:C	1:C:258:ASN:N	2.44	0.69
2:D:292:THR:HA	2:D:295:MET:HE1	1.74	0.69
2:D:51:VAL:CG1	2:D:52:TYR:HD1	2.06	0.69
3:E:72:LEU:C	3:E:74:GLU:H	1.96	0.69
2:D:285:ALA:O	2:D:287:THR:HG22	1.93	0.69
2:B:296:PHE:HE1	2:B:332:MET:CE	2.06	0.69
1:A:99:ALA:CB	1:A:145:THR:HG22	2.22	0.68
2:D:273:ALA:CB	2:D:375:ALA:H	2.05	0.68
1:C:273:ALA:CB	1:C:375:VAL:H	2.06	0.68
2:D:202:TYR:OH	7:D:700:N16:HA	1.93	0.68
1:A:273:ALA:HB3	1:A:375:VAL:H	1.59	0.68
1:A:401:LYS:C	1:A:403:ALA:H	1.94	0.68
1:A:273:ALA:CB	1:A:274:PRO:CD	2.70	0.68
3:E:120:LEU:O	3:E:123:LEU:HB2	1.94	0.68
1:C:8:HIS:CD2	1:C:17:GLY:HA3	2.28	0.68
2:D:135:PHE:HZ	2:D:161:TYR:CD1	2.11	0.68
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.15	0.68
1:C:85:GLN:HA	1:C:85:GLN:HE21	1.59	0.68
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.75	0.68
2:B:151:THR:HG21	2:B:190:SER:HB3	1.75	0.68
2:D:135:PHE:CZ	2:D:161:TYR:CD1	2.82	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:384:ILE:HG22	2:D:432:TYR:CE1	2.30	0.67
2:B:54:ASN:HB2	2:B:64:ARG:HD3	1.76	0.67
2:B:401:ARG:O	1:C:262:TYR:OH	2.12	0.67
2:D:234:THR:HG21	2:D:302:MET:HG3	1.75	0.67
1:C:190:THR:HG23	1:C:191:THR:H	1.60	0.67
1:A:85:GLN:HA	1:A:85:GLN:HE21	1.59	0.67
1:A:411:GLU:O	3:E:61:ARG:NH1	2.26	0.67
2:B:179:ASP:N	2:B:179:ASP:OD1	2.28	0.67
2:B:135:PHE:HZ	2:B:161:TYR:CD1	2.13	0.66
2:B:250:ALA:HA	2:B:255:LEU:HD13	1.78	0.66
2:B:298:SER:C	2:B:300:ASN:H	1.99	0.66
2:D:140:SER:HB2	6:D:600:GDP:C5'	2.09	0.66
1:A:70:LEU:CD1	1:A:145:THR:HB	2.24	0.66
2:D:224:TYR:CE2	6:D:600:GDP:C4	2.84	0.66
2:D:224:TYR:OH	6:D:600:GDP:H2'	1.94	0.65
2:B:274:PRO:C	2:B:275:LEU:HG	2.16	0.65
2:D:350:ASN:HD22	2:D:350:ASN:N	1.89	0.65
2:B:133:GLN:HE21	2:B:252:LEU:CD2	2.07	0.65
2:B:89:PRO:O	2:B:92:PHE:HD1	1.78	0.65
2:D:252:LEU:HD13	7:D:700:N16:CD1	2.26	0.65
2:D:162:PRO:CD	2:D:163:ASP:HB2	2.24	0.65
2:B:312:TYR:HE2	2:B:377:PHE:CZ	2.12	0.65
2:D:171:VAL:CG1	2:D:206:ASN:ND2	2.47	0.65
2:B:2:ARG:N	2:B:133:GLN:OE1	2.29	0.65
1:A:404:PHE:CE1	2:B:347:ILE:HG21	2.24	0.65
2:D:412:GLY:O	3:E:133:VAL:HB	1.96	0.65
2:B:224:TYR:CE2	6:B:600:GDP:C4	2.84	0.65
2:D:306:ASP:C	2:D:308:ARG:H	1.99	0.65
2:D:229:HIS:ND1	2:D:277:SER:HB3	2.12	0.65
1:A:404:PHE:HE1	2:B:347:ILE:CG2	2.10	0.65
2:B:51:VAL:HG13	2:B:52:TYR:CD1	2.32	0.65
2:D:384:ILE:CG2	2:D:432:TYR:CE1	2.80	0.65
2:B:192:HIS:O	2:B:195:VAL:HG12	1.97	0.65
2:B:273:ALA:HB1	2:B:274:PRO:HD3	1.78	0.64
2:B:114:LEU:HB3	2:B:149:MET:HE1	1.78	0.64
1:C:187:SER:O	1:C:191:THR:HB	1.98	0.64
1:C:181:VAL:H	2:D:258:ASN:ND2	1.94	0.64
2:D:255:LEU:HG	7:D:700:N16:CAQ	2.28	0.64
1:A:133:GLN:NE2	1:A:252:LEU:HG	2.13	0.64
1:A:79:ARG:NH2	1:A:94:THR:CG2	2.60	0.64
2:D:154:ILE:HA	2:D:157:ILE:HB	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:HIS:CG	2:B:263:PRO:HG3	2.33	0.63
2:D:147:SER:O	2:D:151:THR:OG1	2.09	0.63
1:C:401:LYS:C	1:C:403:ALA:H	2.00	0.63
2:D:55:GLU:HB3	2:D:61:TYR:HD2	1.61	0.63
2:D:273:ALA:CB	2:D:274:PRO:CD	2.74	0.63
1:C:404:PHE:HE1	2:D:347:ILE:CG2	2.08	0.63
2:D:266:HIS:H	2:D:267:PHE:HD1	1.45	0.63
1:C:270:ALA:O	1:C:302:MET:HB2	1.99	0.63
2:B:135:PHE:CZ	2:B:161:TYR:CD1	2.87	0.63
1:A:34:GLY:O	1:A:61:HIS:HB2	1.98	0.63
2:B:298:SER:HA	2:B:301:MET:HG2	1.78	0.63
1:A:88:HIS:HB2	1:A:91:GLN:NE2	2.14	0.63
1:C:143:GLY:HA3	4:C:600:GTP:H5'	1.80	0.63
1:C:108:TYR:HB3	3:E:108:ASN:OD1	1.99	0.63
2:D:252:LEU:HD13	7:D:700:N16:HD1	1.79	0.63
2:B:412:GLY:HA3	3:E:86:ALA:HB2	1.80	0.63
2:D:245:PRO:HG2	2:D:246:GLY:H	1.64	0.63
2:B:345:GLU:OE1	2:B:345:GLU:N	2.32	0.63
3:E:84:GLN:C	3:E:86:ALA:H	2.02	0.62
3:E:118:ALA:O	3:E:122:ARG:CZ	2.47	0.62
2:D:292:THR:HA	2:D:295:MET:HE3	1.79	0.62
2:D:336:GLN:O	2:D:340:SER:HA	1.98	0.62
2:D:114:LEU:O	2:D:116:ASP:N	2.31	0.62
2:D:54:ASN:HB2	2:D:64:ARG:HD3	1.81	0.62
2:D:251:ASP:HB2	2:D:254:LYS:HB2	1.81	0.62
1:C:88:HIS:HB2	1:C:91:GLN:NE2	2.13	0.62
2:D:306:ASP:O	2:D:308:ARG:N	2.33	0.62
2:D:51:VAL:HG13	2:D:52:TYR:HD1	1.63	0.62
1:A:167:LEU:HD13	1:A:252:LEU:HD13	1.81	0.62
3:E:48:GLU:O	3:E:50:ILE:N	2.32	0.62
1:A:273:ALA:CB	1:A:375:VAL:H	2.13	0.62
1:C:256:GLN:O	1:C:259:LEU:N	2.32	0.62
1:C:79:ARG:NH2	1:C:94:THR:CG2	2.63	0.61
1:A:266:HIS:O	1:A:268:PRO:HD3	1.99	0.61
1:C:266:HIS:O	1:C:268:PRO:HD3	1.99	0.61
1:C:111:GLY:O	1:C:113:GLU:N	2.33	0.61
2:D:381:SER:O	2:D:384:ILE:HB	2.00	0.61
3:E:74:GLU:C	3:E:76:ARG:N	2.54	0.61
1:A:260:VAL:O	1:A:260:VAL:HG23	1.99	0.61
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.24	0.61
2:B:245:PRO:HB2	2:B:247:GLN:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:159:GLU:HB2	3:E:72:LEU:HD23	1.83	0.61
1:A:271:THR:HG23	1:A:301:GLN:HA	1.83	0.61
2:B:251:ASP:HB2	2:B:254:LYS:HB2	1.83	0.61
2:B:308:ARG:HH11	2:B:308:ARG:CG	2.05	0.61
2:D:2:ARG:NH1	2:D:133:GLN:HB2	2.16	0.61
2:B:155:SER:HB3	3:E:76:ARG:HH22	1.65	0.61
1:A:286:LEU:HD12	1:A:286:LEU:H	1.64	0.61
1:A:133:GLN:HE21	1:A:252:LEU:HG	1.66	0.60
1:A:249:ASN:HD22	1:A:254:GLU:HG2	1.66	0.60
2:B:131:CYS:O	2:B:131:CYS:SG	2.58	0.60
2:B:265:LEU:CB	2:B:432:TYR:CE2	2.84	0.60
1:A:256:GLN:HG3	1:A:260:VAL:CG2	2.31	0.60
2:D:242:LEU:HD11	7:D:700:N16:CD1	2.29	0.60
2:D:101:ASN:HD22	2:D:143:GLY:HA2	1.65	0.60
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.65	0.60
2:D:118:VAL:O	2:D:122:VAL:HG13	2.01	0.60
1:A:105:ARG:HD3	1:A:411:GLU:OE1	2.01	0.60
1:A:291:ILE:HD12	1:A:375:VAL:CG2	2.32	0.60
1:A:344:VAL:HG13	1:A:346:TRP:H	1.67	0.60
3:E:99:GLU:C	3:E:101:LEU:N	2.54	0.60
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.35	0.60
2:D:262:PHE:CE1	2:D:435:TYR:CZ	2.90	0.60
2:B:55:GLU:HB3	2:B:61:TYR:HD2	1.66	0.60
1:A:275:VAL:O	1:A:275:VAL:HG23	2.02	0.60
2:B:114:LEU:O	2:B:116:ASP:N	2.35	0.59
3:E:123:LEU:C	3:E:125:GLU:H	2.05	0.59
1:C:343:PHE:HD1	1:C:349:THR:HG22	1.67	0.59
2:B:245:PRO:HG3	2:B:247:GLN:HE21	1.67	0.59
2:D:70:LEU:HD11	2:D:149:MET:HG3	1.84	0.59
1:C:101:ASN:ND2	2:D:254:LYS:HG2	2.16	0.59
7:B:700:N16:HAA	7:B:700:N16:CAL	2.31	0.59
3:E:78:HIS:CD2	3:E:78:HIS:C	2.74	0.59
2:D:210:TYR:CE2	2:D:222:PRO:HG2	2.37	0.59
1:C:165:SER:OG	1:C:252:LEU:HD12	2.02	0.59
2:D:10:GLY:O	2:D:14:ASN:N	2.31	0.59
2:D:307:PRO:HB2	2:D:312:TYR:OH	2.03	0.59
3:E:78:HIS:O	3:E:81:GLU:HB2	2.03	0.59
2:B:195:VAL:HG21	2:B:428:LEU:HD22	1.83	0.59
2:B:296:PHE:HE1	2:B:332:MET:HE1	1.66	0.59
1:C:229:ARG:HG2	1:C:229:ARG:HH11	1.66	0.59
1:C:34:GLY:O	1:C:61:HIS:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4:ILE:HD11	2:D:136:GLN:HG2	1.85	0.59
2:D:276:THR:HG21	2:D:280:SER:HB3	1.84	0.59
2:D:358:ILE:HG23	2:D:358:ILE:O	2.01	0.59
2:D:403:ALA:C	2:D:405:LEU:H	2.05	0.59
2:D:42:LEU:O	2:D:44:LEU:N	2.36	0.59
2:B:306:ASP:O	2:B:308:ARG:N	2.36	0.58
2:D:262:PHE:CD1	2:D:435:TYR:CE1	2.91	0.58
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.18	0.58
2:D:309:HIS:N	2:D:309:HIS:CD2	2.70	0.58
2:D:265:LEU:HB2	2:D:432:TYR:OH	2.03	0.58
2:D:52:TYR:OH	2:D:239:THR:HG22	2.03	0.58
2:D:391:ILE:HA	2:D:394:GLN:NE2	2.18	0.58
2:D:192:HIS:CD2	2:D:421:ALA:CB	2.87	0.58
2:B:192:HIS:HD2	2:B:421:ALA:HA	1.68	0.58
1:C:177:VAL:O	1:C:177:VAL:HG13	2.03	0.58
1:C:72:PRO:O	1:C:74:VAL:N	2.36	0.58
2:D:332:MET:O	2:D:335:VAL:HG23	2.02	0.58
2:D:226:ASP:N	2:D:226:ASP:OD1	2.37	0.58
1:A:317:LEU:CD2	1:A:377:MET:HE3	2.32	0.58
2:D:205:ASP:OD1	2:D:207:GLU:HB3	2.02	0.58
2:D:313:LEU:HD13	2:D:347:ILE:HD11	1.86	0.58
1:C:190:THR:HG23	1:C:191:THR:N	2.18	0.58
2:D:295:MET:CG	2:D:377:PHE:HB2	2.34	0.58
2:D:200:GLU:OE2	2:D:268:PHE:HE1	1.87	0.58
2:D:192:HIS:HD2	2:D:421:ALA:CB	2.16	0.58
1:C:344:VAL:HG13	1:C:346:TRP:H	1.69	0.58
3:E:67:GLU:C	3:E:69:LEU:H	2.07	0.58
3:E:130:ALA:O	3:E:134:ARG:HD3	2.03	0.58
3:E:99:GLU:C	3:E:101:LEU:H	2.06	0.57
2:B:171:VAL:CG1	2:B:206:ASN:ND2	2.58	0.57
1:C:99:ALA:CB	1:C:145:THR:HG22	2.33	0.57
3:E:81:GLU:O	3:E:82:VAL:C	2.42	0.57
2:D:270:PRO:HD2	2:D:302:MET:CB	2.21	0.57
2:D:245:PRO:HB2	2:D:247:GLN:HG3	1.86	0.57
2:B:350:ASN:HD22	2:B:350:ASN:H	1.52	0.57
2:D:142:GLY:O	6:D:600:GDP:H5"	2.04	0.57
2:D:2:ARG:HH12	2:D:133:GLN:HA	1.67	0.57
2:B:384:ILE:HG22	2:B:432:TYR:CE1	2.39	0.57
2:D:350:ASN:H	2:D:350:ASN:ND2	1.96	0.57
1:C:271:THR:HG23	1:C:301:GLN:HA	1.87	0.57
2:D:265:LEU:HB2	2:D:432:TYR:HE2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:261:PRO:HG3	2:D:313:LEU:CD1	2.32	0.57
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.40	0.57
2:D:55:GLU:HB3	2:D:61:TYR:CD2	2.38	0.57
3:E:101:LEU:O	3:E:103:GLN:N	2.38	0.57
2:B:42:LEU:O	2:B:44:LEU:N	2.38	0.57
2:D:269:MET:HE1	2:D:307:PRO:HG3	1.86	0.57
2:B:2:ARG:CZ	2:B:133:GLN:HB2	2.35	0.57
2:B:158:ARG:O	2:B:159:GLU:HB3	2.04	0.57
2:D:351:VAL:HG22	2:D:351:VAL:O	2.05	0.57
2:B:2:ARG:NH1	2:B:133:GLN:HB2	2.20	0.57
2:B:306:ASP:C	2:B:308:ARG:H	2.08	0.56
2:B:210:TYR:CE2	2:B:222:PRO:HG2	2.39	0.56
2:B:76:ASP:O	2:B:80:SER:HB2	2.05	0.56
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.86	0.56
1:C:100:ALA:O	1:C:102:ASN:N	2.38	0.56
2:B:265:LEU:HB2	2:B:432:TYR:CE2	2.40	0.56
1:A:88:HIS:O	1:A:90:GLU:N	2.38	0.56
2:B:245:PRO:HG2	2:B:246:GLY:H	1.70	0.56
2:B:5:VAL:HG13	2:B:132:LEU:CD1	2.35	0.56
2:B:265:LEU:HB3	2:B:432:TYR:CE2	2.40	0.56
1:C:188:ILE:HG23	1:C:425:MET:HG3	1.86	0.56
2:B:21:TRP:CH2	2:B:63:PRO:HB3	2.41	0.56
1:C:20:CYS:HB3	1:C:232:GLY:HA2	1.87	0.56
1:A:397:LEU:HG	2:B:346:TRP:HA	1.87	0.56
2:D:320:ARG:HA	2:D:356:CYS:O	2.05	0.56
2:D:284:ARG:HD3	2:D:372:LYS:HD2	1.85	0.56
2:D:21:TRP:O	2:D:25:SER:HB2	2.05	0.56
2:D:224:TYR:CE2	6:D:600:GDP:C5	2.92	0.56
2:B:205:ASP:OD2	2:B:387:LEU:HD12	2.05	0.56
1:C:105:ARG:CZ	2:D:253:ARG:HH21	2.16	0.56
2:D:229:HIS:CE1	2:D:277:SER:CB	2.84	0.56
2:D:296:PHE:CE1	2:D:332:MET:CE	2.82	0.56
2:D:236:SER:O	2:D:240:THR:HG23	2.05	0.56
2:B:295:MET:CG	2:B:377:PHE:HB2	2.32	0.56
1:A:52:PHE:O	1:A:64:ARG:HB2	2.05	0.56
2:D:192:HIS:HD2	2:D:421:ALA:HA	1.71	0.56
2:B:208:ALA:O	2:B:211:ASP:N	2.38	0.56
2:B:101:ASN:HD22	2:B:143:GLY:HA2	1.70	0.56
1:A:315:CYS:SG	1:A:377:MET:HE1	2.46	0.56
1:A:22:GLU:HB2	1:A:83:TYR:HE1	1.71	0.56
1:C:68:VAL:HG12	1:C:93:ILE:HB	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:308:ARG:NH1	2:D:308:ARG:HG3	2.07	0.55
1:A:183:GLU:HB3	1:A:184:PRO:CD	2.33	0.55
2:D:2:ARG:CZ	2:D:133:GLN:HB2	2.35	0.55
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.70	0.55
2:B:21:TRP:O	2:B:25:SER:HB2	2.06	0.55
2:B:115:VAL:HG12	2:B:116:ASP:N	2.21	0.55
3:E:77:GLU:HG2	3:E:80:ARG:HB2	1.87	0.55
1:A:388:TRP:HA	1:A:388:TRP:CE3	2.41	0.55
2:B:118:VAL:O	2:B:122:VAL:HG13	2.06	0.55
3:E:120:LEU:HA	3:E:123:LEU:HD12	1.88	0.55
2:B:276:THR:CG2	2:B:277:SER:N	2.68	0.55
2:B:51:VAL:CG1	2:B:52:TYR:HD1	2.18	0.55
2:D:164:ARG:HE	2:D:164:ARG:HA	1.71	0.55
2:D:298:SER:C	2:D:300:ASN:N	2.57	0.55
2:B:261:PRO:HG3	2:B:313:LEU:HD12	1.87	0.55
2:B:55:GLU:HB3	2:B:61:TYR:CD2	2.42	0.55
2:B:110:GLU:O	2:B:113:GLU:HB3	2.07	0.55
2:D:114:LEU:HB3	2:D:149:MET:HE1	1.87	0.55
2:D:266:HIS:N	2:D:267:PHE:HD1	2.05	0.55
1:A:315:CYS:SG	1:A:377:MET:CE	2.95	0.55
2:B:10:GLY:O	2:B:14:ASN:N	2.37	0.55
2:D:406:HIS:HA	2:D:409:THR:HB	1.88	0.55
2:D:2:ARG:N	2:D:133:GLN:OE1	2.40	0.55
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.41	0.55
2:D:165:ILE:CG2	2:D:253:ARG:HH11	2.20	0.55
1:C:190:THR:CG2	1:C:191:THR:H	2.20	0.55
2:D:137:LEU:HD21	2:D:139:HIS:CE1	2.41	0.55
1:A:312:TYR:HE2	1:A:379:SER:HB3	1.72	0.55
1:A:72:PRO:O	1:A:74:VAL:N	2.39	0.54
3:E:84:GLN:C	3:E:86:ALA:N	2.60	0.54
1:C:427:ALA:O	1:C:430:LYS:HB3	2.08	0.54
1:C:286:LEU:HD12	1:C:286:LEU:H	1.72	0.54
1:C:70:LEU:CD1	1:C:145:THR:HB	2.35	0.54
2:B:309:HIS:CD2	2:B:309:HIS:N	2.75	0.54
2:B:51:VAL:HG13	2:B:52:TYR:HD1	1.72	0.54
2:B:391:ILE:HG13	2:B:392:SER:H	1.71	0.54
1:A:270:ALA:HB3	1:A:302:MET:HE2	1.87	0.54
1:A:154:MET:O	1:A:158:SER:HB2	2.07	0.54
2:D:48:ARG:NH1	2:D:242:LEU:O	2.40	0.54
2:B:234:THR:HG21	2:B:302:MET:HG3	1.89	0.54
2:B:273:ALA:CB	2:B:375:ALA:H	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:ND2	2:B:254:LYS:HG2	2.23	0.54
2:B:312:TYR:CD2	2:B:315:VAL:HG21	2.43	0.54
2:D:255:LEU:CG	7:D:700:N16:HAAA	2.31	0.54
2:D:4:ILE:HG23	2:D:51:VAL:HG22	1.89	0.54
1:C:80:THR:HG22	1:C:81:GLY:N	2.23	0.54
2:B:383:ALA:O	2:B:386:GLU:HB2	2.08	0.54
2:B:319:PHE:CB	2:B:355:VAL:HG12	2.29	0.54
2:D:384:ILE:CG2	2:D:432:TYR:HE1	2.21	0.54
2:B:270:PRO:CD	2:B:302:MET:HB2	2.35	0.54
2:B:64:ARG:HG3	2:B:125:GLU:OE1	2.08	0.54
1:A:8:HIS:CD2	1:A:17:GLY:CA	2.90	0.54
2:D:192:HIS:CD2	2:D:421:ALA:HB2	2.43	0.53
2:B:12:CYS:SG	6:B:600:GDP:C4	3.01	0.53
1:C:102:ASN:C	1:C:102:ASN:ND2	2.62	0.53
1:A:79:ARG:HH21	1:A:94:THR:HG21	1.73	0.53
1:A:187:SER:O	1:A:191:THR:HB	2.06	0.53
2:B:36:TYR:OH	2:B:40:SER:O	2.27	0.53
2:B:312:TYR:CD2	2:B:315:VAL:CG2	2.91	0.53
2:D:191:VAL:HG11	2:D:425:MET:CE	2.39	0.53
2:D:245:PRO:CG	2:D:246:GLY:H	2.21	0.53
2:D:242:LEU:CD1	7:D:700:N16:HD1	2.33	0.53
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.91	0.53
2:D:158:ARG:O	2:D:160:GLU:N	2.32	0.53
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.15	0.53
2:B:155:SER:HB2	3:E:76:ARG:HH22	1.74	0.53
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.42	0.53
1:C:291:ILE:HD12	1:C:375:VAL:CG2	2.38	0.53
1:A:351:PHE:HB2	3:E:22:VAL:HG12	1.91	0.53
2:D:158:ARG:HA	2:D:161:TYR:O	2.07	0.52
3:E:118:ALA:O	3:E:122:ARG:NH2	2.43	0.52
2:D:171:VAL:HG11	2:D:206:ASN:HD21	1.66	0.52
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.91	0.52
2:B:133:GLN:NE2	2:B:252:LEU:HB2	2.24	0.52
1:A:85:GLN:HA	1:A:85:GLN:NE2	2.22	0.52
2:D:11:GLN:HB3	6:D:600:GDP:O1A	2.09	0.52
2:D:12:CYS:SG	6:D:600:GDP:N3	2.83	0.52
2:D:265:LEU:CB	2:D:432:TYR:CZ	2.92	0.52
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.90	0.52
2:B:70:LEU:HD11	2:B:149:MET:HG3	1.92	0.52
2:D:151:THR:HG21	2:D:190:SER:HB3	1.92	0.52
2:D:226:ASP:O	2:D:227:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:HH11	1:A:229:ARG:HG2	1.75	0.52
2:B:239:THR:O	2:B:240:THR:C	2.48	0.52
1:C:383:ALA:O	1:C:386:GLU:HB2	2.10	0.52
2:D:296:PHE:CE1	2:D:332:MET:HE3	2.35	0.52
3:E:74:GLU:O	3:E:76:ARG:N	2.43	0.52
3:E:133:VAL:HA	3:E:136:ASN:HB3	1.92	0.52
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.92	0.52
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.45	0.52
2:B:177:VAL:HG12	2:B:177:VAL:O	2.10	0.52
2:B:70:LEU:C	2:B:95:GLY:HA3	2.31	0.51
1:C:102:ASN:HD22	1:C:103:TYR:N	2.08	0.51
2:B:2:ARG:HD2	2:B:131:CYS:SG	2.50	0.51
2:D:209:LEU:HD21	2:D:231:VAL:HG22	1.92	0.51
2:B:406:HIS:HA	2:B:409:THR:HB	1.91	0.51
2:D:224:TYR:CD2	6:D:600:GDP:C5	2.98	0.51
1:A:190:THR:HG23	1:A:191:THR:N	2.25	0.51
2:B:138:THR:O	2:B:139:HIS:HB3	2.11	0.51
2:B:295:MET:HG2	2:B:295:MET:O	2.11	0.51
2:D:153:LEU:O	2:D:157:ILE:N	2.43	0.51
2:D:150:GLY:HA2	2:D:153:LEU:HB2	1.91	0.51
2:D:383:ALA:O	2:D:386:GLU:CB	2.57	0.51
2:D:21:TRP:CH2	2:D:63:PRO:HB3	2.46	0.51
1:C:154:MET:O	1:C:158:SER:HB2	2.10	0.51
1:C:376:CYS:SG	1:C:376:CYS:O	2.69	0.51
1:C:387:ALA:HB2	1:C:390:ARG:HH12	1.75	0.51
2:D:145:THR:O	2:D:149:MET:HB2	2.10	0.51
2:B:224:TYR:CD2	6:B:600:GDP:C6	2.98	0.51
2:D:2:ARG:HD2	2:D:131:CYS:SG	2.51	0.51
2:B:248:LEU:O	2:B:249:ASN:HB3	2.09	0.51
2:B:102:ASN:OD1	2:B:102:ASN:C	2.48	0.51
2:D:402:LYS:HB3	2:D:405:LEU:HD22	1.92	0.51
2:B:245:PRO:CG	2:B:247:GLN:HE21	2.24	0.51
2:D:284:ARG:HB2	2:D:372:LYS:HE3	1.91	0.51
2:D:237:GLY:CA	2:D:376:THR:HG21	2.41	0.51
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.46	0.51
2:B:145:THR:O	2:B:149:MET:HB2	2.11	0.51
2:D:391:ILE:CG1	2:D:392:SER:N	2.68	0.51
2:B:171:VAL:HG11	2:B:206:ASN:HD21	1.73	0.51
2:B:296:PHE:CE1	2:B:332:MET:HE1	2.45	0.51
2:B:237:GLY:CA	2:B:376:THR:HG21	2.41	0.51
2:D:133:GLN:HE21	2:D:252:LEU:CD2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:253:ARG:O	2:D:254:LYS:C	2.49	0.51
1:A:88:HIS:O	1:A:91:GLN:N	2.40	0.51
1:C:48:SER:O	1:C:243:ARG:O	2.29	0.51
2:D:182:VAL:HG23	2:D:186:ASN:ND2	2.26	0.51
2:D:114:LEU:HD12	2:D:117:SER:HB2	1.92	0.51
2:D:287:THR:OG1	2:D:289:PRO:HD2	2.11	0.50
2:D:141:LEU:HA	2:D:147:SER:HB3	1.92	0.50
2:D:265:LEU:CB	2:D:432:TYR:OH	2.59	0.50
1:A:47:ASP:O	1:A:48:SER:HB2	2.12	0.50
2:B:7:ILE:O	2:B:137:LEU:HA	2.10	0.50
2:D:312:TYR:CE2	2:D:377:PHE:HZ	2.24	0.50
3:E:78:HIS:HA	3:E:81:GLU:OE2	2.10	0.50
2:D:164:ARG:HE	2:D:164:ARG:CA	2.21	0.50
1:A:179:THR:O	2:B:352:LYS:HG3	2.11	0.50
2:B:224:TYR:CE2	6:B:600:GDP:C5	2.99	0.50
1:C:431:ASP:O	1:C:435:VAL:HG23	2.12	0.50
2:D:52:TYR:OH	2:D:136:GLN:NE2	2.45	0.50
1:A:111:GLY:O	1:A:113:GLU:N	2.44	0.50
1:C:109:THR:HG21	3:E:112:ARG:NH2	2.27	0.50
1:C:191:THR:HG23	1:C:425:MET:CE	2.41	0.50
1:A:190:THR:HG23	1:A:191:THR:H	1.75	0.50
2:B:350:ASN:HD22	2:B:350:ASN:N	2.09	0.50
2:D:231:VAL:O	2:D:235:MET:HE2	2.12	0.50
2:B:114:LEU:HB3	2:B:149:MET:CE	2.41	0.50
2:B:255:LEU:HD23	7:B:700:N16:HB	1.94	0.50
2:B:200:GLU:OE2	2:B:268:PHE:HE1	1.94	0.50
3:E:72:LEU:C	3:E:74:GLU:N	2.64	0.50
1:C:190:THR:O	1:C:192:HIS:N	2.45	0.50
1:C:78:VAL:C	1:C:80:THR:H	2.15	0.50
1:C:12:ALA:HB3	1:C:140:SER:OG	2.12	0.50
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.94	0.50
2:D:202:TYR:CD1	2:D:202:TYR:N	2.79	0.50
1:A:181:VAL:N	2:B:258:ASN:ND2	2.59	0.50
2:D:231:VAL:HG12	2:D:235:MET:CE	2.42	0.50
2:B:287:THR:HG21	2:B:290:GLU:HB2	1.92	0.49
2:B:51:VAL:O	2:B:64:ARG:NH2	2.44	0.49
3:E:22:VAL:O	3:E:22:VAL:CG1	2.55	0.49
2:D:319:PHE:CB	2:D:355:VAL:HG12	2.27	0.49
1:C:401:LYS:C	1:C:403:ALA:N	2.66	0.49
1:A:312:TYR:CE2	1:A:379:SER:HB3	2.47	0.49
2:D:225:GLY:O	2:D:228:ASN:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.48	0.49
2:B:292:THR:C	2:B:294:GLN:H	2.14	0.49
1:C:90:GLU:O	1:C:121:ARG:CD	2.60	0.49
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.93	0.49
2:D:276:THR:HG21	2:D:280:SER:HB2	1.94	0.49
1:A:88:HIS:O	1:A:89:PRO:C	2.51	0.49
2:D:385:GLN:HG2	2:D:389:LYS:HD2	1.95	0.49
1:A:247:ALA:O	1:A:248:LEU:HB3	2.12	0.49
2:D:205:ASP:OD2	2:D:387:LEU:HD12	2.12	0.49
2:D:413:MET:HE1	2:D:417:GLU:OE2	2.13	0.49
3:E:49:GLU:HG3	3:E:49:GLU:O	2.11	0.49
1:A:177:VAL:O	1:A:177:VAL:HG13	2.13	0.49
1:A:376:CYS:SG	1:A:376:CYS:O	2.70	0.49
2:B:149:MET:O	2:B:152:LEU:HB3	2.13	0.49
2:B:261:PRO:HG2	2:B:262:PHE:H	1.78	0.49
2:D:275:LEU:O	2:D:276:THR:HB	2.11	0.49
1:C:253:THR:O	1:C:256:GLN:N	2.40	0.49
2:B:88:ARG:HB3	2:B:91:ASN:OD1	2.13	0.49
2:B:164:ARG:NH2	2:B:253:ARG:HH22	2.11	0.49
2:B:261:PRO:HG3	2:B:313:LEU:CD1	2.43	0.49
1:A:55:GLU:HG2	1:A:61:HIS:CE1	2.48	0.49
1:A:68:VAL:HG12	1:A:93:ILE:HB	1.94	0.49
1:A:420:GLU:HA	1:A:423:GLU:HG3	1.95	0.49
2:D:287:THR:HG21	2:D:290:GLU:HB2	1.88	0.48
2:B:255:LEU:HG	7:B:700:N16:CAQ	2.43	0.48
2:D:88:ARG:HB3	2:D:91:ASN:OD1	2.13	0.48
1:A:383:ALA:O	1:A:386:GLU:HB2	2.12	0.48
1:C:167:LEU:HD13	1:C:252:LEU:HD13	1.96	0.48
1:C:139:HIS:HD2	1:C:146:GLY:O	1.95	0.48
1:C:115:ILE:O	1:C:119:LEU:HB2	2.13	0.48
2:D:267:PHE:CD2	2:D:388:PHE:HZ	2.31	0.48
1:C:167:LEU:CD1	1:C:252:LEU:HD13	2.44	0.48
2:D:195:VAL:CG2	2:D:428:LEU:HD22	2.41	0.48
1:A:204:VAL:HG22	1:A:302:MET:CE	2.43	0.48
1:A:202:PHE:CE2	1:A:268:PRO:HG2	2.48	0.48
2:B:399:PHE:O	2:B:400:ARG:O	2.30	0.48
2:B:251:ASP:HB3	2:B:254:LYS:H	1.78	0.48
2:D:276:THR:CG2	2:D:277:SER:N	2.77	0.48
1:A:312:TYR:HE2	1:A:379:SER:CB	2.27	0.48
1:A:343:PHE:HD1	1:A:349:THR:HG22	1.76	0.48
1:C:8:HIS:CD2	1:C:17:GLY:CA	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:VAL:HG22	1:C:302:MET:CE	2.43	0.48
2:B:224:TYR:CD2	6:B:600:GDP:C5	3.02	0.48
2:D:307:PRO:HB2	2:D:312:TYR:CZ	2.49	0.48
1:A:278:ALA:HA	1:A:281:ALA:HB2	1.95	0.48
2:B:217:LEU:HB3	2:B:219:LEU:HG	1.95	0.48
1:A:6:SER:HB3	1:A:8:HIS:HE1	1.79	0.48
1:C:260:VAL:O	1:C:260:VAL:CG2	2.61	0.48
2:D:15:GLN:O	2:D:15:GLN:HG3	2.13	0.48
2:D:265:LEU:HB2	2:D:432:TYR:CZ	2.49	0.48
1:C:275:VAL:HG23	1:C:275:VAL:O	2.13	0.48
2:B:164:ARG:HE	2:B:164:ARG:HA	1.79	0.48
2:B:202:TYR:OH	7:B:700:N16:HA	2.14	0.48
1:C:181:VAL:N	2:D:258:ASN:ND2	2.62	0.48
2:B:102:ASN:OD1	2:B:102:ASN:O	2.31	0.48
2:D:251:ASP:HB2	2:D:254:LYS:HD3	1.96	0.48
2:B:141:LEU:HA	2:B:147:SER:HB3	1.94	0.48
1:A:182:VAL:HG22	1:A:182:VAL:O	2.14	0.48
1:A:53:PHE:CD1	1:A:53:PHE:N	2.81	0.48
2:D:205:ASP:OD1	2:D:207:GLU:CB	2.62	0.47
2:B:273:ALA:HB2	2:B:375:ALA:H	1.79	0.47
1:A:204:VAL:HG22	1:A:302:MET:HE1	1.95	0.47
1:A:190:THR:O	1:A:192:HIS:N	2.47	0.47
2:D:298:SER:CB	2:D:307:PRO:HD2	2.43	0.47
2:D:200:GLU:OE2	2:D:268:PHE:CE1	2.66	0.47
1:C:316:CYS:O	1:C:377:MET:HA	2.14	0.47
2:B:298:SER:O	2:B:300:ASN:N	2.45	0.47
2:B:408:TYR:O	2:B:409:THR:C	2.52	0.47
3:E:90:ASN:O	3:E:93:PHE:HB3	2.14	0.47
2:D:291:LEU:HD11	2:D:374:SER:HA	1.95	0.47
1:C:105:ARG:NH2	2:D:253:ARG:NH2	2.39	0.47
2:B:202:TYR:N	2:B:202:TYR:CD1	2.82	0.47
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.96	0.47
2:B:191:VAL:HG11	2:B:425:MET:CE	2.44	0.47
2:B:114:LEU:HD12	2:B:117:SER:HB2	1.95	0.47
1:C:391:LEU:O	1:C:392:ASP:C	2.52	0.47
2:D:177:VAL:O	2:D:177:VAL:HG12	2.14	0.47
2:B:357:ASP:OD2	2:B:357:ASP:N	2.46	0.47
2:D:262:PHE:CE1	2:D:435:TYR:CE1	3.03	0.47
1:C:317:LEU:CD2	1:C:377:MET:HE3	2.45	0.47
2:D:27:GLU:OE2	2:D:243:ARG:NH2	2.38	0.47
1:C:223:THR:O	1:C:227:LEU:HD13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:192:HIS:HD2	2:D:421:ALA:CA	2.28	0.47
1:A:6:SER:HB3	1:A:8:HIS:CE1	2.50	0.47
1:C:187:SER:HB2	1:C:391:LEU:HD21	1.97	0.47
1:A:133:GLN:CD	1:A:252:LEU:H	2.18	0.47
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.83	0.47
2:B:400:ARG:C	2:B:402:LYS:H	2.18	0.47
1:A:431:ASP:O	1:A:435:VAL:HG23	2.14	0.47
1:C:341:ILE:HD13	1:C:341:ILE:H	1.79	0.47
2:B:298:SER:C	2:B:300:ASN:N	2.68	0.47
1:A:256:GLN:HG3	1:A:260:VAL:HG22	1.96	0.47
2:B:7:ILE:HG22	2:B:137:LEU:HD13	1.96	0.47
2:D:207:GLU:O	2:D:211:ASP:HB2	2.15	0.47
2:D:200:GLU:HA	2:D:266:HIS:HB2	1.96	0.47
2:D:260:VAL:HG11	2:D:266:HIS:HB3	1.95	0.47
2:D:273:ALA:HB2	2:D:375:ALA:N	2.28	0.47
2:D:202:TYR:H	2:D:202:TYR:HD1	1.63	0.47
2:B:153:LEU:O	2:B:157:ILE:N	2.43	0.47
2:D:158:ARG:O	2:D:159:GLU:HB3	2.15	0.46
1:C:391:LEU:O	1:C:393:HIS:N	2.49	0.46
2:D:336:GLN:O	2:D:340:SER:CA	2.63	0.46
2:B:191:VAL:HG11	2:B:425:MET:HE2	1.96	0.46
1:C:372:GLN:HB2	1:C:373:ARG:HE	1.80	0.46
2:D:202:TYR:HE2	2:D:378:ILE:HG12	1.80	0.46
2:B:162:PRO:HD2	2:B:163:ASP:HB2	1.97	0.46
2:B:296:PHE:HE1	2:B:332:MET:HE3	1.79	0.46
1:A:316:CYS:O	1:A:377:MET:HA	2.14	0.46
2:B:154:ILE:HA	2:B:157:ILE:HB	1.97	0.46
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.49	0.46
1:C:163:LYS:O	1:C:164:LYS:C	2.53	0.46
2:B:407:TRP:CE2	1:C:257:THR:HA	2.51	0.46
2:B:321:GLY:O	2:B:323:MET:N	2.48	0.46
2:B:312:TYR:CE2	2:B:377:PHE:CZ	3.00	0.46
1:C:6:SER:HB3	1:C:8:HIS:CE1	2.50	0.46
3:E:119:MET:HA	3:E:122:ARG:NH2	2.31	0.46
2:D:115:VAL:HG12	2:D:116:ASP:N	2.29	0.46
2:D:226:ASP:O	2:D:227:LEU:CB	2.63	0.46
1:A:223:THR:O	1:A:227:LEU:HD13	2.16	0.46
2:D:255:LEU:HA	7:D:700:N16:HAAA	1.98	0.46
2:D:283:TYR:C	2:D:285:ALA:H	2.19	0.46
2:B:236:SER:O	2:B:240:THR:HG23	2.16	0.46
2:B:239:THR:HG22	7:B:700:N16:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:405:VAL:CG1	1:C:406:HIS:N	2.78	0.46
2:D:286:LEU:H	2:D:286:LEU:HG	1.38	0.46
2:D:251:ASP:HB3	2:D:254:LYS:H	1.79	0.46
2:D:4:ILE:CD1	2:D:136:GLN:HG2	2.46	0.46
1:A:190:THR:O	1:A:194:THR:HB	2.15	0.46
2:D:321:GLY:O	2:D:323:MET:N	2.49	0.46
2:B:312:TYR:HD2	2:B:315:VAL:CG2	2.29	0.46
2:D:76:ASP:O	2:D:80:SER:HB2	2.15	0.46
1:A:20:CYS:HB3	1:A:232:GLY:HA2	1.96	0.46
2:D:223:THR:HB	2:D:225:GLY:CA	2.44	0.46
2:B:122:VAL:CG2	2:B:123:ARG:N	2.79	0.46
2:B:142:GLY:O	6:B:600:GDP:C5'	2.43	0.46
1:A:317:LEU:HD23	1:A:377:MET:HE3	1.96	0.46
2:B:172:MET:CE	2:B:203:SER:HB3	2.46	0.46
2:B:205:ASP:HB2	2:B:304:ALA:H	1.80	0.46
1:C:142:GLY:HA3	1:C:183:GLU:HG3	1.98	0.46
1:A:115:ILE:O	1:A:119:LEU:HB2	2.15	0.46
1:A:12:ALA:HB3	1:A:140:SER:OG	2.16	0.46
2:D:149:MET:O	2:D:152:LEU:HB3	2.16	0.46
2:B:52:TYR:OH	2:B:136:GLN:NE2	2.49	0.46
2:D:413:MET:CE	2:D:417:GLU:OE2	2.64	0.46
1:A:163:LYS:O	1:A:164:LYS:C	2.54	0.46
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.72	0.46
1:A:341:ILE:H	1:A:341:ILE:HD13	1.81	0.46
2:D:264:ARG:O	2:D:265:LEU:C	2.55	0.45
1:C:251:ASP:OD1	1:C:252:LEU:N	2.50	0.45
2:B:4:ILE:HG23	2:B:51:VAL:HG22	1.97	0.45
1:A:260:VAL:O	1:A:260:VAL:CG2	2.64	0.45
3:E:77:GLU:HG2	3:E:80:ARG:CB	2.46	0.45
1:C:27:GLU:OE2	1:C:243:ARG:NH2	2.48	0.45
1:C:169:PHE:CE2	1:C:235:VAL:HG22	2.51	0.45
2:D:140:SER:OG	6:D:600:GDP:H5'	2.12	0.45
1:C:102:ASN:HD21	1:C:104:ALA:HB3	1.81	0.45
2:B:265:LEU:HB2	2:B:432:TYR:HE2	1.80	0.45
1:A:401:LYS:C	1:A:403:ALA:N	2.61	0.45
2:D:351:VAL:O	2:D:351:VAL:CG2	2.64	0.45
2:D:231:VAL:HG12	2:D:235:MET:HE2	1.97	0.45
1:C:248:LEU:HD22	1:C:249:ASN:H	1.81	0.45
2:B:12:CYS:SG	6:B:600:GDP:N3	2.89	0.45
2:D:51:VAL:CG1	2:D:52:TYR:CD1	2.89	0.45
1:C:256:GLN:O	1:C:258:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:TYR:CD1	1:A:418:PHE:HE2	2.34	0.45
2:B:198:THR:OG1	2:B:266:HIS:CE1	2.69	0.45
2:B:260:VAL:HG11	2:B:266:HIS:HB3	1.98	0.45
2:D:99:ALA:CB	2:D:145:THR:CG2	2.89	0.45
2:B:308:ARG:HD2	2:B:308:ARG:HA	1.76	0.45
1:A:8:HIS:HD2	1:A:17:GLY:HA3	1.80	0.45
1:C:190:THR:O	1:C:194:THR:HB	2.16	0.45
1:C:229:ARG:HD3	1:C:363:VAL:HG21	1.99	0.45
2:B:16:ILE:HG22	2:B:17:GLY:N	2.32	0.45
2:B:172:MET:HG2	2:B:387:LEU:HD21	1.97	0.45
7:B:700:N16:CAA	7:B:700:N16:CAL	2.94	0.45
1:C:79:ARG:HD3	1:C:92:LEU:HD13	1.99	0.45
1:C:41:THR:CG2	1:C:61:HIS:HE1	2.24	0.45
1:C:139:HIS:CG	1:C:150:THR:HG21	2.51	0.45
1:C:2:ARG:HB2	1:C:131:GLY:O	2.16	0.45
1:C:273:ALA:CB	1:C:274:PRO:CD	2.76	0.45
3:E:123:LEU:C	3:E:125:GLU:N	2.70	0.45
2:B:381:SER:O	2:B:384:ILE:HB	2.16	0.45
1:C:185:TYR:CD1	1:C:418:PHE:HE2	2.35	0.45
2:D:192:HIS:O	2:D:195:VAL:HG12	2.16	0.45
1:C:85:GLN:HA	1:C:85:GLN:NE2	2.27	0.45
3:E:101:LEU:O	3:E:104:LYS:N	2.47	0.45
1:C:309:HIS:ND1	1:C:310:GLY:N	2.64	0.45
2:B:20:PHE:HD2	2:B:235:MET:HB3	1.80	0.45
2:B:20:PHE:O	2:B:24:ILE:HG23	2.16	0.45
1:C:103:TYR:O	1:C:104:ALA:C	2.54	0.45
2:D:308:ARG:HH21	2:D:339:ASN:HD21	1.64	0.45
2:B:403:ALA:C	2:B:405:LEU:N	2.54	0.45
1:C:317:LEU:HD23	1:C:377:MET:HE3	1.99	0.45
1:C:49:PHE:C	1:C:49:PHE:CD2	2.90	0.45
2:D:223:THR:CG2	2:D:225:GLY:H	2.29	0.45
2:D:5:VAL:HG22	2:D:135:PHE:CD2	2.34	0.45
3:E:76:ARG:O	3:E:79:GLU:HB2	2.17	0.45
2:B:248:LEU:HD23	2:B:248:LEU:HA	1.46	0.45
2:D:250:ALA:HA	2:D:255:LEU:HD11	1.95	0.45
2:B:4:ILE:HD11	2:B:136:GLN:HG2	1.99	0.45
2:B:407:TRP:NE1	1:C:257:THR:HA	2.32	0.45
1:C:153:LEU:HD13	1:C:157:LEU:CD1	2.44	0.44
1:C:153:LEU:HA	1:C:153:LEU:HD23	1.84	0.44
2:B:192:HIS:CD2	2:B:421:ALA:CB	3.00	0.44
2:D:245:PRO:CG	2:D:246:GLY:N	2.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:THR:O	1:C:83:TYR:CG	2.69	0.44
2:D:325:MET:HA	2:D:328:VAL:HG23	1.99	0.44
1:A:408:TYR:C	1:A:410:GLY:N	2.69	0.44
2:D:289:PRO:HA	2:D:331:GLN:NE2	2.31	0.44
2:D:313:LEU:HD23	2:D:382:THR:CG2	2.47	0.44
2:B:239:THR:O	2:B:241:CYS:N	2.50	0.44
1:C:167:LEU:CD1	1:C:252:LEU:CD1	2.91	0.44
2:D:282:GLN:HG3	2:D:286:LEU:HD21	1.98	0.44
2:D:404:PHE:H	2:D:404:PHE:HD1	1.66	0.44
2:D:145:THR:HG23	6:D:600:GDP:O3B	2.17	0.44
2:D:174:SER:HB2	2:D:390:ARG:NH2	2.32	0.44
2:B:118:VAL:O	2:B:119:LEU:C	2.54	0.44
2:D:165:ILE:HD11	2:D:167:ASN:ND2	2.33	0.44
1:A:309:HIS:ND1	1:A:309:HIS:C	2.71	0.44
2:D:306:ASP:C	2:D:308:ARG:N	2.68	0.44
2:D:229:HIS:HE1	2:D:277:SER:HB3	1.72	0.44
1:A:174:ALA:HB1	1:A:207:GLU:HB2	1.99	0.44
1:A:169:PHE:CE2	1:A:235:VAL:HG22	2.51	0.44
2:D:224:TYR:CD2	6:D:600:GDP:C6	3.06	0.44
2:B:174:SER:HB2	2:B:390:ARG:NH2	2.32	0.44
1:A:394:LYS:HG2	2:B:348:PRO:HB3	1.99	0.44
1:C:68:VAL:CG1	1:C:93:ILE:HB	2.48	0.44
2:B:8:GLN:OE1	2:B:67:LEU:HD23	2.17	0.44
2:B:150:GLY:HA2	2:B:153:LEU:HB2	1.98	0.44
1:C:408:TYR:C	1:C:410:GLY:N	2.69	0.44
1:A:2:ARG:HB2	1:A:131:GLY:O	2.17	0.44
2:D:384:ILE:HG22	2:D:432:TYR:CD1	2.52	0.44
2:D:239:THR:O	2:D:240:THR:C	2.56	0.44
2:B:332:MET:O	2:B:335:VAL:HG23	2.18	0.44
2:D:245:PRO:CB	2:D:247:GLN:HG3	2.47	0.44
2:D:237:GLY:HA2	2:D:376:THR:HG21	2.00	0.44
1:A:372:GLN:HG2	1:A:372:GLN:H	1.42	0.44
2:D:252:LEU:CD1	7:D:700:N16:CD1	2.95	0.44
2:D:358:ILE:O	2:D:358:ILE:CG2	2.66	0.44
1:C:428:LEU:C	1:C:430:LYS:N	2.70	0.44
2:D:311:ARG:HG2	2:D:342:TYR:HD2	1.82	0.44
2:D:403:ALA:C	2:D:405:LEU:N	2.67	0.44
1:C:260:VAL:HA	1:C:261:PRO:HD3	1.84	0.44
2:D:28:HIS:HA	2:D:43:GLN:HB3	2.00	0.44
1:A:205:ASP:CB	1:A:303:VAL:HA	2.48	0.44
1:A:277:SER:O	1:A:280:LYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ILE:HD13	1:C:171:ILE:HD11	2.00	0.44
2:B:224:TYR:OH	6:B:600:GDP:H2'	2.18	0.43
2:D:292:THR:C	2:D:294:GLN:H	2.21	0.43
2:D:379:GLY:O	2:D:381:SER:N	2.51	0.43
1:C:184:PRO:O	1:C:185:TYR:C	2.57	0.43
1:A:239:THR:OG1	1:A:243:ARG:NH1	2.50	0.43
1:A:205:ASP:HB3	1:A:303:VAL:HA	2.00	0.43
1:C:52:PHE:O	1:C:64:ARG:HB2	2.19	0.43
1:C:183:GLU:O	1:C:184:PRO:C	2.54	0.43
1:A:315:CYS:SG	1:A:377:MET:HE2	2.58	0.43
1:C:420:GLU:HA	1:C:423:GLU:HG3	1.99	0.43
1:C:402:ARG:O	1:C:403:ALA:C	2.56	0.43
2:D:174:SER:OG	2:D:176:LYS:N	2.51	0.43
1:C:100:ALA:O	1:C:102:ASN:HB3	2.18	0.43
1:C:270:ALA:HB3	1:C:302:MET:HE2	2.00	0.43
2:B:320:ARG:HA	2:B:356:CYS:O	2.18	0.43
1:A:304:LYS:O	1:A:390:ARG:NH1	2.51	0.43
1:A:80:THR:HG22	1:A:81:GLY:N	2.34	0.43
2:D:107:HIS:O	2:D:152:LEU:HD22	2.19	0.43
1:C:105:ARG:HH12	2:D:253:ARG:NH2	2.16	0.43
1:C:234:ILE:HG12	1:C:272:TYR:HB2	2.00	0.43
1:C:395:PHE:C	1:C:395:PHE:CD2	2.91	0.43
1:A:49:PHE:CD2	1:A:49:PHE:C	2.92	0.43
2:B:262:PHE:CE1	2:B:435:TYR:CZ	3.06	0.43
2:D:55:GLU:HG3	2:D:55:GLU:H	1.57	0.43
2:B:177:VAL:CG1	2:B:177:VAL:O	2.65	0.43
1:A:68:VAL:CG1	1:A:93:ILE:HB	2.48	0.43
1:C:49:PHE:HD2	1:C:49:PHE:C	2.22	0.43
1:A:82:THR:O	1:A:83:TYR:CG	2.72	0.43
1:A:188:ILE:HG23	1:A:425:MET:HG3	2.00	0.43
1:A:425:MET:O	1:A:426:ALA:C	2.56	0.43
1:C:407:TRP:CD2	2:D:257:VAL:HG22	2.53	0.43
1:A:217:LEU:HB3	1:A:219:ILE:HG12	2.00	0.43
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.78	0.43
1:C:100:ALA:CB	2:D:253:ARG:HG2	2.49	0.43
1:C:190:THR:CG2	1:C:191:THR:N	2.81	0.43
1:C:90:GLU:O	1:C:121:ARG:HD3	2.19	0.43
1:A:419:SER:O	1:A:423:GLU:HG2	2.19	0.43
1:C:70:LEU:HD12	1:C:145:THR:CB	2.41	0.43
1:A:391:LEU:O	1:A:392:ASP:C	2.57	0.43
1:A:391:LEU:HB3	1:A:392:ASP:H	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:248:LEU:HD23	2:D:248:LEU:HA	1.53	0.42
2:B:316:ALA:HB1	7:B:700:N16:CAM	2.49	0.42
2:B:55:GLU:HG3	2:B:55:GLU:H	1.56	0.42
2:B:211:ASP:O	2:B:215:ARG:HG2	2.19	0.42
2:D:164:ARG:NE	2:D:164:ARG:CA	2.82	0.42
2:D:16:ILE:HG23	2:D:235:MET:CE	2.49	0.42
2:D:311:ARG:HH21	2:D:344:VAL:CG2	2.32	0.42
1:C:407:TRP:CG	2:D:257:VAL:HG22	2.54	0.42
1:A:407:TRP:CD2	2:B:257:VAL:HG22	2.54	0.42
1:A:36:MET:HA	1:A:37:PRO:HD3	1.89	0.42
1:A:267:PHE:CD1	1:A:267:PHE:N	2.87	0.42
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.01	0.42
2:D:265:LEU:HB3	2:D:432:TYR:CZ	2.52	0.42
1:A:185:TYR:OH	1:A:403:ALA:HB3	2.19	0.42
1:C:6:SER:HB3	1:C:8:HIS:HE1	1.83	0.42
1:C:389:ALA:HA	1:C:392:ASP:HB2	2.01	0.42
1:A:247:ALA:HB1	3:E:12:ASN:HB3	2.01	0.42
2:B:336:GLN:O	2:B:340:SER:HA	2.19	0.42
1:C:250:VAL:HG22	1:C:250:VAL:O	2.19	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.18	0.42
2:D:297:ASP:OD1	2:D:298:SER:N	2.52	0.42
2:B:401:ARG:HH11	2:B:401:ARG:CG	2.32	0.42
2:D:288:VAL:HB	2:D:289:PRO:HD3	2.01	0.42
1:A:79:ARG:HD3	1:A:92:LEU:HD13	2.02	0.42
1:A:90:GLU:O	1:A:121:ARG:HD3	2.19	0.42
1:A:372:GLN:HB2	1:A:373:ARG:HE	1.84	0.42
2:D:5:VAL:HG23	2:D:6:HIS:N	2.34	0.42
2:D:308:ARG:HD2	2:D:308:ARG:HA	1.78	0.42
1:C:191:THR:O	1:C:195:LEU:HB3	2.20	0.42
2:D:177:VAL:CG1	2:D:177:VAL:O	2.67	0.42
1:C:179:THR:O	2:D:352:LYS:HG3	2.19	0.42
2:B:15:GLN:O	2:B:15:GLN:HG3	2.18	0.42
1:A:428:LEU:C	1:A:430:LYS:N	2.73	0.42
3:E:116:LEU:O	3:E:119:MET:HB3	2.19	0.42
2:D:70:LEU:HA	2:D:95:GLY:HA3	2.00	0.42
2:D:165:ILE:CG2	2:D:253:ARG:NH1	2.82	0.42
1:C:183:GLU:CB	1:C:184:PRO:CD	2.91	0.42
1:A:70:LEU:HD12	1:A:145:THR:CB	2.34	0.42
1:C:119:LEU:HD22	1:C:156:ARG:NH2	2.35	0.42
2:D:102:ASN:OD1	2:D:102:ASN:O	2.37	0.42
2:B:2:ARG:CB	2:B:131:CYS:SG	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:ILE:HA	2:B:348:PRO:HD3	1.81	0.42
1:C:406:HIS:CD2	2:D:263:PRO:HG3	2.53	0.42
2:D:51:VAL:CG1	2:D:52:TYR:N	2.83	0.42
1:C:402:ARG:HD3	1:C:402:ARG:HA	1.89	0.42
2:B:245:PRO:CG	2:B:246:GLY:H	2.25	0.42
1:C:239:THR:OG1	1:C:243:ARG:NH1	2.53	0.42
1:A:348:PRO:HA	3:E:27:PRO:HD3	2.01	0.42
1:C:102:ASN:C	1:C:102:ASN:HD22	2.23	0.42
2:B:5:VAL:HG13	2:B:132:LEU:HD11	2.01	0.42
2:B:384:ILE:CG2	2:B:432:TYR:CE1	3.02	0.42
2:D:151:THR:HA	2:D:154:ILE:HG12	2.02	0.42
1:C:372:GLN:HG2	1:C:372:GLN:H	1.47	0.42
1:C:178:SER:HB3	2:D:352:LYS:NZ	2.35	0.42
1:C:291:ILE:HD12	1:C:375:VAL:HG23	2.00	0.42
1:C:79:ARG:H	1:C:79:ARG:HG2	1.40	0.42
1:A:88:HIS:C	1:A:90:GLU:N	2.71	0.42
2:D:245:PRO:HG2	2:D:246:GLY:N	2.32	0.42
1:C:416:GLY:O	1:C:419:SER:HB2	2.20	0.42
1:A:325:PRO:HB3	3:E:20:PHE:CE2	2.54	0.42
2:B:118:VAL:O	2:B:120:ASP:N	2.53	0.42
2:B:172:MET:HE2	2:B:203:SER:HA	2.02	0.42
1:A:402:ARG:HD2	1:A:415:GLU:OE2	2.20	0.42
1:A:402:ARG:O	1:A:403:ALA:C	2.58	0.42
2:B:51:VAL:CG1	2:B:52:TYR:N	2.83	0.42
1:C:204:VAL:HG22	1:C:302:MET:HE1	2.02	0.42
2:B:44:LEU:HA	2:B:49:ILE:HB	2.02	0.42
2:D:385:GLN:HE21	2:D:389:LYS:CD	2.32	0.42
2:B:292:THR:HA	2:B:295:MET:HE1	1.99	0.42
2:D:296:PHE:HE1	2:D:332:MET:HE1	1.81	0.42
1:A:119:LEU:HD22	1:A:156:ARG:HH21	1.85	0.42
1:A:174:ALA:CB	1:A:207:GLU:HB2	2.50	0.42
2:D:133:GLN:HG3	2:D:252:LEU:HD23	2.00	0.41
2:D:269:MET:HA	2:D:270:PRO:HD3	1.93	0.41
2:D:158:ARG:C	2:D:160:GLU:H	2.19	0.41
1:A:153:LEU:HD13	1:A:157:LEU:CD1	2.46	0.41
1:A:402:ARG:HA	1:A:402:ARG:HD3	1.80	0.41
3:E:84:GLN:O	3:E:86:ALA:N	2.53	0.41
1:C:111:GLY:O	1:C:112:LYS:C	2.57	0.41
2:D:110:GLU:O	2:D:113:GLU:HB3	2.20	0.41
2:D:401:ARG:CG	2:D:401:ARG:HH11	2.33	0.41
1:C:103:TYR:HH	1:C:107:HIS:HD1	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:255:LEU:HD23	7:D:700:N16:HB	2.01	0.41
2:D:5:VAL:CG2	2:D:135:PHE:HD2	2.23	0.41
2:D:384:ILE:HA	2:D:384:ILE:HD13	1.89	0.41
1:C:391:LEU:HA	1:C:391:LEU:HD12	1.92	0.41
2:D:406:HIS:CD2	2:D:406:HIS:C	2.92	0.41
2:D:408:TYR:O	2:D:409:THR:C	2.58	0.41
2:D:176:LYS:HD2	2:D:207:GLU:OE2	2.20	0.41
1:C:251:ASP:O	1:C:255:PHE:CB	2.68	0.41
1:C:36:MET:HA	1:C:37:PRO:HD3	1.90	0.41
2:D:433:GLN:OE1	2:D:433:GLN:HA	2.20	0.41
2:B:116:ASP:O	2:B:120:ASP:OD1	2.38	0.41
1:A:398:MET:HG3	2:B:348:PRO:HD3	2.02	0.41
2:D:400:ARG:C	2:D:402:LYS:H	2.22	0.41
1:A:234:ILE:HG12	1:A:272:TYR:HB2	2.02	0.41
6:D:600:GDP:C8	6:D:600:GDP:C3'	3.03	0.41
1:C:287:SER:O	1:C:291:ILE:HG12	2.20	0.41
2:B:306:ASP:C	2:B:308:ARG:N	2.72	0.41
2:B:2:ARG:HB3	2:B:131:CYS:SG	2.60	0.41
1:C:98:ASP:OD1	1:C:99:ALA:N	2.52	0.41
2:B:151:THR:CG2	2:B:190:SER:HB3	2.47	0.41
2:D:204:ILE:HG22	2:D:209:LEU:HD22	2.01	0.41
1:A:139:HIS:CG	1:A:150:THR:HG21	2.55	0.41
2:B:31:ASP:O	2:B:33:THR:N	2.54	0.41
2:B:164:ARG:CA	2:B:164:ARG:HE	2.32	0.41
2:D:8:GLN:OE1	2:D:14:ASN:ND2	2.54	0.41
1:A:347:CYS:O	1:A:348:PRO:C	2.59	0.41
1:A:16:ILE:HD13	1:A:171:ILE:HD11	2.02	0.41
1:C:174:ALA:HA	1:C:175:PRO:HD2	1.63	0.41
2:B:351:VAL:HG22	2:B:351:VAL:O	2.20	0.41
2:D:34:GLY:HA2	2:D:60:LYS:HE2	2.03	0.41
2:D:224:TYR:HE2	6:D:600:GDP:C4	2.34	0.41
1:C:100:ALA:O	1:C:101:ASN:C	2.58	0.41
1:A:10:GLY:O	1:A:11:GLN:C	2.59	0.41
1:C:297:GLU:HA	1:C:298:PRO:HD2	1.79	0.41
6:D:600:GDP:H8	6:D:600:GDP:H3'	1.86	0.41
2:D:5:VAL:HG13	2:D:132:LEU:HD11	2.01	0.41
3:E:76:ARG:C	3:E:78:HIS:H	2.24	0.41
2:D:245:PRO:HG3	2:D:247:GLN:HE21	1.85	0.41
2:B:245:PRO:CB	2:B:247:GLN:HG3	2.50	0.41
2:B:70:LEU:HD12	2:B:145:THR:HB	2.03	0.41
2:D:253:ARG:O	2:D:256:ALA:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:ARG:HG3	2:B:401:ARG:NH1	2.36	0.41
2:B:163:ASP:HB3	2:B:164:ARG:HG2	2.02	0.41
2:D:262:PHE:O	2:D:264:ARG:O	2.38	0.41
2:D:399:PHE:O	2:D:400:ARG:O	2.39	0.41
2:B:217:LEU:HD11	2:B:276:THR:HB	2.02	0.41
2:D:240:THR:O	2:D:243:ARG:N	2.53	0.41
1:A:405:VAL:CG1	1:A:406:HIS:N	2.84	0.41
2:D:209:LEU:HD12	2:D:209:LEU:HA	1.87	0.41
1:C:178:SER:HB3	2:D:352:LYS:HZ3	1.85	0.41
3:E:107:SER:O	3:E:111:ASN:HB2	2.21	0.41
1:A:413:MET:HG2	1:A:414:GLU:H	1.84	0.41
2:B:325:MET:HA	2:B:328:VAL:HG23	2.03	0.41
2:D:67:LEU:O	2:D:93:VAL:HG23	2.20	0.41
2:D:205:ASP:HB2	2:D:304:ALA:H	1.86	0.41
2:B:99:ALA:CB	2:B:145:THR:CG2	2.93	0.41
2:B:253:ARG:O	2:B:254:LYS:C	2.58	0.41
2:B:135:PHE:HB2	2:B:166:MET:HE2	1.89	0.41
2:B:242:LEU:N	2:B:242:LEU:HD23	2.36	0.41
1:A:249:ASN:H	1:A:254:GLU:CD	2.24	0.41
2:D:138:THR:O	2:D:139:HIS:HB3	2.21	0.41
1:C:119:LEU:HD22	1:C:156:ARG:HH21	1.86	0.41
1:C:182:VAL:HG22	1:C:182:VAL:O	2.21	0.41
2:B:70:LEU:CA	2:B:95:GLY:HA3	2.51	0.40
1:A:427:ALA:O	1:A:430:LYS:HB3	2.21	0.40
1:A:84:ARG:HB3	1:A:84:ARG:HE	1.78	0.40
2:D:271:GLY:HA2	2:D:302:MET:HG2	2.02	0.40
1:A:153:LEU:HA	1:A:153:LEU:HD23	1.82	0.40
1:A:317:LEU:HD21	1:A:377:MET:HE3	2.03	0.40
1:C:36:MET:SD	1:C:38:SER:HB2	2.61	0.40
2:B:385:GLN:HG2	2:B:389:LYS:HD2	2.02	0.40
2:B:118:VAL:C	2:B:120:ASP:N	2.75	0.40
2:D:2:ARG:NH2	2:D:251:ASP:O	2.54	0.40
2:D:255:LEU:HD11	7:D:700:N16:HAL	2.03	0.40
3:E:84:GLN:HA	3:E:87:ILE:HG22	2.02	0.40
2:B:8:GLN:OE1	2:B:14:ASN:ND2	2.54	0.40
1:A:139:HIS:HD2	1:A:146:GLY:O	2.04	0.40
1:A:391:LEU:O	1:A:393:HIS:N	2.54	0.40
1:C:345:ASP:OD2	1:C:438:ASP:HB2	2.21	0.40
2:D:347:ILE:HA	2:D:348:PRO:HD3	1.72	0.40
1:A:264:ARG:O	1:A:266:HIS:N	2.55	0.40
1:A:260:VAL:HA	1:A:261:PRO:HD3	1.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:LEU:O	2:D:43:GLN:C	2.59	0.40
1:A:78:VAL:C	1:A:80:THR:H	2.24	0.40
2:B:2:ARG:HH12	2:B:133:GLN:HA	1.86	0.40
2:D:265:LEU:CB	2:D:432:TYR:HE2	2.22	0.40
1:C:265:ILE:HG22	1:C:265:ILE:O	2.21	0.40
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.21	0.40
1:A:22:GLU:HB2	1:A:83:TYR:CE1	2.55	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	424/451 (94%)	324 (76%)	72 (17%)	28 (7%)	1 24
1	C	423/451 (94%)	337 (80%)	54 (13%)	32 (8%)	1 19
2	B	416/445 (94%)	302 (73%)	80 (19%)	34 (8%)	1 17
2	D	425/445 (96%)	291 (68%)	88 (21%)	46 (11%)	0 10
3	E	119/142 (84%)	73 (61%)	30 (25%)	16 (13%)	0 6
All	All	1807/1934 (93%)	1327 (73%)	324 (18%)	156 (9%)	1 16

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	PRO
1	A	73	THR
1	A	112	LYS
1	A	265	ILE
1	A	341	ILE
1	A	348	PRO
1	A	377	MET

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Mol	Chain	Res	Type
1	A	392	ASP
1	A	403	ALA
1	A	437	VAL
2	B	42	LEU
2	B	43	GLN
2	B	62	VAL
2	B	73	GLY
2	B	82	PRO
2	B	163	ASP
2	B	227	LEU
2	B	245	PRO
2	B	273	ALA
2	B	288	VAL
2	B	299	LYS
2	B	371	LEU
2	B	400	ARG
2	B	404	PHE
1	C	72	PRO
1	C	73	THR
1	C	112	LYS
1	C	191	THR
1	C	257	THR
1	C	265	ILE
1	C	341	ILE
1	C	348	PRO
1	C	377	MET
1	C	392	ASP
1	C	403	ALA
1	C	437	VAL
2	D	43	GLN
2	D	62	VAL
2	D	73	GLY
2	D	82	PRO
2	D	162	PRO
2	D	163	ASP
2	D	245	PRO
2	D	251	ASP
2	D	288	VAL
2	D	299	LYS
2	D	380	ASN
2	D	400	ARG
3	E	49	GLU

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Mol	Chain	Res	Type
3	E	81	GLU
3	E	82	VAL
3	E	102	ALA
3	E	139	LEU
1	A	48	SER
1	A	83	TYR
1	A	162	GLY
1	A	164	LYS
1	A	191	THR
1	A	273	ALA
1	A	279	GLU
2	B	3	GLU
2	B	34	GLY
2	B	60	LYS
2	B	162	PRO
2	B	226	ASP
2	B	264	ARG
2	B	276	THR
2	B	309	HIS
2	B	348	PRO
1	C	83	TYR
1	C	162	GLY
1	C	164	LYS
1	C	253	THR
1	C	273	ALA
1	C	350	GLY
1	C	429	GLU
2	D	3	GLU
2	D	34	GLY
2	D	115	VAL
2	D	227	LEU
2	D	244	PHE
2	D	264	ARG
2	D	265	LEU
2	D	278	ARG
2	D	285	ALA
2	D	309	HIS
2	D	322	ARG
2	D	348	PRO
2	D	371	LEU
2	D	403	ALA
2	D	404	PHE

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Mol	Chain	Res	Type
3	E	12	ASN
3	E	26	PRO
3	E	28	SER
3	E	46	SER
3	E	75	LYS
3	E	124	GLN
1	A	32	PRO
1	A	247	ALA
1	A	350	GLY
1	A	415	GLU
1	A	429	GLU
2	B	115	VAL
2	B	240	THR
2	B	244	PHE
2	B	249	ASN
2	B	403	ALA
1	C	32	PRO
1	C	245	ASP
2	D	42	LEU
2	D	60	LYS
2	D	195	VAL
2	D	279	GLY
3	E	85	LYS
3	E	113	GLU
1	A	402	ARG
1	C	183	GLU
1	C	220	GLU
2	D	167	ASN
2	D	220	THR
2	D	226	ASP
2	D	240	THR
2	D	293	GLN
3	E	7	GLU
3	E	47	LEU
1	A	220	GLU
2	B	119	LEU
2	B	307	PRO
2	B	322	ARG
1	C	48	SER
1	C	79	ARG
1	C	141	PHE
1	C	351	PHE

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Mol	Chain	Res	Type
2	D	249	ASN
2	D	268	PHE
2	D	273	ALA
2	D	402	LYS
1	A	248	LEU
2	B	293	GLN
1	C	254	GLU
1	C	402	ARG
2	D	270	PRO
2	D	342	TYR
3	E	5	ASP
2	D	261	PRO
1	A	364	PRO
1	C	364	PRO
1	C	412	GLY
1	A	412	GLY
2	B	32	PRO
1	C	175	PRO
2	D	84	GLY
2	D	177	VAL
2	D	307	PRO
1	A	274	PRO
2	B	177	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	346/378 (92%)	243 (70%)	103 (30%)	0 3
1	C	344/378 (91%)	234 (68%)	110 (32%)	0 2
2	B	350/383 (91%)	224 (64%)	126 (36%)	0 1
2	D	353/383 (92%)	224 (64%)	129 (36%)	0 1
3	E	82/126 (65%)	41 (50%)	41 (50%)	0 0
All	All	1475/1648 (90%)	966 (66%)	509 (34%)	0 2

All (509) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	9	VAL
1	A	11	GLN
1	A	16	ILE
1	A	22	GLU
1	A	23	LEU
1	A	26	LEU
1	A	27	GLU
1	A	36	MET
1	A	49	PHE
1	A	60	LYS
1	A	61	HIS
1	A	62	VAL
1	A	68	VAL
1	A	70	LEU
1	A	73	THR
1	A	74	VAL
1	A	79	ARG
1	A	80	THR
1	A	88	HIS
1	A	92	LEU
1	A	94	THR
1	A	96	LYS
1	A	102	ASN
1	A	105	ARG
1	A	110	ILE
1	A	114	ILE
1	A	115	ILE
1	A	119	LEU
1	A	120	ASP
1	A	123	ARG
1	A	124	LYS
1	A	140	SER
1	A	141	PHE
1	A	145	THR
1	A	153	LEU
1	A	155	GLU
1	A	158	SER
1	A	160	ASP
1	A	163	LYS
1	A	176	GLN
1	A	179	THR

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Mol	Chain	Res	Type
1	A	187	SER
1	A	191	THR
1	A	193	THR
1	A	194	THR
1	A	195	LEU
1	A	196	GLU
1	A	199	ASP
1	A	200	CYS
1	A	206	ASN
1	A	211	ASP
1	A	220	GLU
1	A	223	THR
1	A	226	ASN
1	A	230	LEU
1	A	236	SER
1	A	241	SER
1	A	242	LEU
1	A	248	LEU
1	A	250	VAL
1	A	255	PHE
1	A	256	GLN
1	A	257	THR
1	A	269	LEU
1	A	271	THR
1	A	279	GLU
1	A	287	SER
1	A	293	ASN
1	A	301	GLN
1	A	304	LYS
1	A	309	HIS
1	A	316	CYS
1	A	318	LEU
1	A	329	ASN
1	A	341	ILE
1	A	343	PHE
1	A	344	VAL
1	A	347	CYS
1	A	349	THR
1	A	356	ASN
1	A	361	THR
1	A	363	VAL
1	A	368	LEU

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Mol	Chain	Res	Type
1	A	370	LYS
1	A	371	VAL
1	A	372	GLN
1	A	377	MET
1	A	379	SER
1	A	380	ASN
1	A	381	THR
1	A	384	ILE
1	A	386	GLU
1	A	394	LYS
1	A	397	LEU
1	A	401	LYS
1	A	402	ARG
1	A	405	VAL
1	A	413	MET
1	A	414	GLU
1	A	415	GLU
1	A	419	SER
1	A	433	GLU
2	B	4	ILE
2	B	5	VAL
2	B	16	ILE
2	B	24	ILE
2	B	25	SER
2	B	27	GLU
2	B	39	ASP
2	B	42	LEU
2	B	43	GLN
2	B	48	ARG
2	B	51	VAL
2	B	55	GLU
2	B	61	TYR
2	B	62	VAL
2	B	68	VAL
2	B	70	LEU
2	B	71	GLU
2	B	78	VAL
2	B	80	SER
2	B	83	PHE
2	B	85	GLN
2	B	90	ASP
2	B	93	VAL

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Mol	Chain	Res	Type
2	B	96	GLN
2	B	97	SER
2	B	101	ASN
2	B	102	ASN
2	B	109	THR
2	B	113	GLU
2	B	116	ASP
2	B	120	ASP
2	B	122	VAL
2	B	129	CYS
2	B	130	ASP
2	B	131	CYS
2	B	132	LEU
2	B	133	GLN
2	B	135	PHE
2	B	137	LEU
2	B	145	THR
2	B	149	MET
2	B	151	THR
2	B	156	LYS
2	B	158	ARG
2	B	160	GLU
2	B	163	ASP
2	B	164	ARG
2	B	165	ILE
2	B	166	MET
2	B	170	SER
2	B	174	SER
2	B	179	ASP
2	B	181	VAL
2	B	190	SER
2	B	196	GLU
2	B	200	GLU
2	B	209	LEU
2	B	212	ILE
2	B	214	PHE
2	B	216	THR
2	B	219	LEU
2	B	223	THR
2	B	227	LEU
2	B	230	LEU
2	B	239	THR

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Mol	Chain	Res	Type
2	B	242	LEU
2	B	244	PHE
2	B	248	LEU
2	B	251	ASP
2	B	254	LYS
2	B	260	VAL
2	B	265	LEU
2	B	275	LEU
2	B	276	THR
2	B	277	SER
2	B	286	LEU
2	B	287	THR
2	B	291	LEU
2	B	293	GLN
2	B	294	GLN
2	B	295	MET
2	B	300	ASN
2	B	308	ARG
2	B	309	HIS
2	B	311	ARG
2	B	313	LEU
2	B	318	VAL
2	B	320	ARG
2	B	323	MET
2	B	324	SER
2	B	325	MET
2	B	329	ASP
2	B	332	MET
2	B	333	LEU
2	B	335	VAL
2	B	339	ASN
2	B	341	SER
2	B	344	VAL
2	B	347	ILE
2	B	350	ASN
2	B	351	VAL
2	B	356	CYS
2	B	357	ASP
2	B	358	ILE
2	B	371	LEU
2	B	373	MET
2	B	376	THR

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Mol	Chain	Res	Type
2	B	380	ASN
2	B	384	ILE
2	B	387	LEU
2	B	390	ARG
2	B	391	ILE
2	B	393	GLU
2	B	394	GLN
2	B	400	ARG
2	B	401	ARG
2	B	405	LEU
2	B	406	HIS
2	B	408	TYR
2	B	416	MET
2	B	417	GLU
2	B	419	THR
2	B	425	MET
2	B	430	SER
2	B	434	GLN
2	B	436	GLN
1	C	2	ARG
1	C	11	GLN
1	C	16	ILE
1	C	23	LEU
1	C	25	CYS
1	C	26	LEU
1	C	27	GLU
1	C	36	MET
1	C	38	SER
1	C	41	THR
1	C	49	PHE
1	C	51	THR
1	C	60	LYS
1	C	61	HIS
1	C	62	VAL
1	C	68	VAL
1	C	73	THR
1	C	74	VAL
1	C	79	ARG
1	C	80	THR
1	C	88	HIS
1	C	92	LEU
1	C	94	THR

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Mol	Chain	Res	Type
1	C	96	LYS
1	C	102	ASN
1	C	105	ARG
1	C	110	ILE
1	C	114	ILE
1	C	115	ILE
1	C	119	LEU
1	C	120	ASP
1	C	123	ARG
1	C	124	LYS
1	C	130	THR
1	C	132	LEU
1	C	140	SER
1	C	141	PHE
1	C	145	THR
1	C	153	LEU
1	C	155	GLU
1	C	157	LEU
1	C	158	SER
1	C	160	ASP
1	C	163	LYS
1	C	176	GLN
1	C	179	THR
1	C	187	SER
1	C	191	THR
1	C	193	THR
1	C	194	THR
1	C	195	LEU
1	C	196	GLU
1	C	199	ASP
1	C	200	CYS
1	C	206	ASN
1	C	211	ASP
1	C	220	GLU
1	C	223	THR
1	C	226	ASN
1	C	230	LEU
1	C	236	SER
1	C	241	SER
1	C	242	LEU
1	C	245	ASP
1	C	248	LEU

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Mol	Chain	Res	Type
1	C	251	ASP
1	C	252	LEU
1	C	254	GLU
1	C	256	GLN
1	C	257	THR
1	C	271	THR
1	C	287	SER
1	C	293	ASN
1	C	301	GLN
1	C	304	LYS
1	C	309	HIS
1	C	311	LYS
1	C	313	MET
1	C	316	CYS
1	C	318	LEU
1	C	329	ASN
1	C	341	ILE
1	C	343	PHE
1	C	344	VAL
1	C	347	CYS
1	C	349	THR
1	C	356	ASN
1	C	361	THR
1	C	363	VAL
1	C	368	LEU
1	C	370	LYS
1	C	371	VAL
1	C	372	GLN
1	C	377	MET
1	C	379	SER
1	C	380	ASN
1	C	381	THR
1	C	384	ILE
1	C	386	GLU
1	C	394	LYS
1	C	397	LEU
1	C	401	LYS
1	C	402	ARG
1	C	405	VAL
1	C	413	MET
1	C	414	GLU
1	C	415	GLU

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Mol	Chain	Res	Type
1	C	419	SER
1	C	433	GLU
1	C	438	ASP
2	D	4	ILE
2	D	5	VAL
2	D	16	ILE
2	D	24	ILE
2	D	25	SER
2	D	27	GLU
2	D	39	ASP
2	D	42	LEU
2	D	43	GLN
2	D	48	ARG
2	D	51	VAL
2	D	55	GLU
2	D	61	TYR
2	D	62	VAL
2	D	68	VAL
2	D	70	LEU
2	D	71	GLU
2	D	78	VAL
2	D	80	SER
2	D	83	PHE
2	D	85	GLN
2	D	90	ASP
2	D	93	VAL
2	D	96	GLN
2	D	97	SER
2	D	101	ASN
2	D	102	ASN
2	D	109	THR
2	D	110	GLU
2	D	113	GLU
2	D	119	LEU
2	D	120	ASP
2	D	122	VAL
2	D	129	CYS
2	D	130	ASP
2	D	132	LEU
2	D	133	GLN
2	D	135	PHE
2	D	137	LEU

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Mol	Chain	Res	Type
2	D	149	MET
2	D	151	THR
2	D	156	LYS
2	D	157	ILE
2	D	158	ARG
2	D	160	GLU
2	D	163	ASP
2	D	164	ARG
2	D	165	ILE
2	D	166	MET
2	D	170	SER
2	D	174	SER
2	D	179	ASP
2	D	181	VAL
2	D	188	THR
2	D	190	SER
2	D	196	GLU
2	D	205	ASP
2	D	209	LEU
2	D	212	ILE
2	D	214	PHE
2	D	216	THR
2	D	227	LEU
2	D	230	LEU
2	D	239	THR
2	D	241	CYS
2	D	242	LEU
2	D	244	PHE
2	D	248	LEU
2	D	251	ASP
2	D	253	ARG
2	D	254	LYS
2	D	257	VAL
2	D	260	VAL
2	D	265	LEU
2	D	272	PHE
2	D	275	LEU
2	D	280	SER
2	D	281	GLN
2	D	284	ARG
2	D	286	LEU
2	D	287	THR

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Mol	Chain	Res	Type
2	D	291	LEU
2	D	293	GLN
2	D	294	GLN
2	D	295	MET
2	D	296	PHE
2	D	300	ASN
2	D	308	ARG
2	D	309	HIS
2	D	311	ARG
2	D	313	LEU
2	D	318	VAL
2	D	320	ARG
2	D	323	MET
2	D	324	SER
2	D	325	MET
2	D	329	ASP
2	D	332	MET
2	D	333	LEU
2	D	335	VAL
2	D	339	ASN
2	D	341	SER
2	D	344	VAL
2	D	347	ILE
2	D	350	ASN
2	D	351	VAL
2	D	356	CYS
2	D	357	ASP
2	D	358	ILE
2	D	371	LEU
2	D	373	MET
2	D	376	THR
2	D	380	ASN
2	D	384	ILE
2	D	387	LEU
2	D	391	ILE
2	D	393	GLU
2	D	394	GLN
2	D	400	ARG
2	D	401	ARG
2	D	405	LEU
2	D	408	TYR
2	D	416	MET

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Mol	Chain	Res	Type
2	D	417	GLU
2	D	419	THR
2	D	425	MET
2	D	430	SER
2	D	434	GLN
2	D	436	GLN
3	E	5	ASP
3	E	6	MET
3	E	15	THR
3	E	16	SER
3	E	21	GLU
3	E	22	VAL
3	E	24	LEU
3	E	51	GLN
3	E	53	LYS
3	E	61	ARG
3	E	62	LYS
3	E	64	GLN
3	E	65	GLU
3	E	67	GLU
3	E	76	ARG
3	E	77	GLU
3	E	78	HIS
3	E	80	ARG
3	E	81	GLU
3	E	84	GLN
3	E	87	ILE
3	E	89	GLU
3	E	91	ASN
3	E	92	ASN
3	E	94	ILE
3	E	96	MET
3	E	98	LYS
3	E	99	GLU
3	E	106	GLU
3	E	109	LYS
3	E	111	ASN
3	E	112	ARG
3	E	113	GLU
3	E	115	HIS
3	E	119	MET
3	E	122	ARG

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Mol	Chain	Res	Type
3	E	125	GLU
3	E	126	LYS
3	E	129	HIS
3	E	134	ARG
3	E	136	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	50	ASN
1	A	85	GLN
1	A	91	GLN
1	A	101	ASN
1	A	102	ASN
1	A	128	GLN
1	A	139	HIS
1	A	176	GLN
1	A	206	ASN
1	A	249	ASN
1	A	258	ASN
1	A	329	ASN
1	A	356	ASN
1	A	380	ASN
2	B	8	GLN
2	B	14	ASN
2	B	54	ASN
2	B	85	GLN
2	B	101	ASN
2	B	133	GLN
2	B	136	GLN
2	B	192	HIS
2	B	193	GLN
2	B	206	ASN
2	B	258	ASN
2	B	266	HIS
2	B	294	GLN
2	B	309	HIS
2	B	331	GLN
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN

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Mol	Chain	Res	Type
2	B	385	GLN
2	B	406	HIS
2	B	436	GLN
1	C	8	HIS
1	C	50	ASN
1	C	85	GLN
1	C	91	GLN
1	C	101	ASN
1	C	102	ASN
1	C	128	GLN
1	C	139	HIS
1	C	176	GLN
1	C	206	ASN
1	C	258	ASN
1	C	329	ASN
1	C	356	ASN
2	D	8	GLN
2	D	14	ASN
2	D	85	GLN
2	D	101	ASN
2	D	133	GLN
2	D	136	GLN
2	D	192	HIS
2	D	193	GLN
2	D	206	ASN
2	D	229	HIS
2	D	258	ASN
2	D	266	HIS
2	D	294	GLN
2	D	309	HIS
2	D	331	GLN
2	D	339	ASN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
2	D	394	GLN
2	D	406	HIS
2	D	436	GLN
3	E	78	HIS
3	E	90	ASN
3	E	91	ASN
3	E	111	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GTP	A	600	-	25,34,34	0.99	1 (4%)	34,54,54	1.57	4 (11%)
6	GDP	B	600	-	23,30,30	1.07	1 (4%)	30,47,47	1.72	4 (13%)
7	N16	B	700	-	25,25,25	1.40	3 (12%)	25,34,34	0.96	1 (4%)
4	GTP	C	600	-	25,34,34	0.99	1 (4%)	34,54,54	1.92	9 (26%)
6	GDP	D	600	-	23,30,30	1.04	1 (4%)	30,47,47	2.01	6 (20%)
7	N16	D	700	-	25,25,25	1.98	7 (28%)	25,34,34	1.55	5 (20%)

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
7	N16	B	700	-	-	0/12/28/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GTP	C	600	-	-	0/18/38/38	0/3/3/3
6	GDP	D	600	-	-	0/12/32/32	0/3/3/3
7	N16	D	700	-	-	0/12/28/28	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	N16	CAV-NAO	-5.04	1.32	1.41
7	D	700	N16	CAV-NAO	-4.35	1.33	1.41
7	B	700	N16	CAT-CAR	-2.18	1.40	1.47
7	D	700	N16	CA-C	2.02	1.56	1.53
7	D	700	N16	CAE-CAI	2.05	1.43	1.38
7	D	700	N16	CAL-CAV	2.14	1.42	1.39
7	D	700	N16	CD2-CG	2.52	1.44	1.38
4	A	600	GTP	C6-N1	2.84	1.38	1.33
4	C	600	GTP	C6-N1	2.90	1.38	1.33
6	B	600	GDP	C6-N1	3.08	1.38	1.33
7	B	700	N16	CAA-CAQ	3.16	1.54	1.50
6	D	600	GDP	C6-N1	3.55	1.39	1.33
7	D	700	N16	CB-CG	3.70	1.60	1.51
7	D	700	N16	CAA-CAQ	3.88	1.55	1.50

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	600	GDP	N3-C2-N1	-6.16	118.06	127.44
4	C	600	GTP	N3-C2-N1	-5.52	119.03	127.44
6	B	600	GDP	N3-C2-N1	-5.06	119.75	127.44
4	C	600	GTP	PB-O3B-PG	-4.99	115.92	132.67
4	A	600	GTP	N3-C2-N1	-4.58	120.47	127.44
6	D	600	GDP	C5-C6-N1	-4.19	117.87	123.59
6	D	600	GDP	C2'-C1'-N9	-3.97	108.22	114.29
4	A	600	GTP	PA-O3A-PB	-3.67	122.42	132.73
6	B	600	GDP	C5-C6-N1	-3.60	118.67	123.59
7	D	700	N16	CAT-CAQ-NAO	-3.40	113.55	119.18
4	A	600	GTP	PB-O3B-PG	-3.10	122.27	132.67
6	D	600	GDP	PA-O3A-PB	-2.87	123.04	132.67
7	D	700	N16	CAI-CAM-CAV	-2.71	116.27	119.72
6	B	600	GDP	C2'-C1'-N9	-2.63	110.28	114.29
7	D	700	N16	OAB-CAR-N	-2.62	121.62	126.00
4	A	600	GTP	C5-C6-N1	-2.48	120.20	123.59
4	C	600	GTP	C4-C5-N7	-2.46	107.22	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	600	GDP	C4-C5-N7	-2.34	107.33	109.48
4	C	600	GTP	PA-O3A-PB	-2.25	126.40	132.73
4	C	600	GTP	C4'-O4'-C1'	-2.23	107.27	109.72
4	C	600	GTP	C1'-N9-C4	-2.19	123.63	126.94
7	B	700	N16	CAV-NAO-CAQ	-2.04	124.39	128.25
4	C	600	GTP	C5-C6-N1	-2.02	120.82	123.59
7	D	700	N16	CAA-CAQ-NAO	2.24	122.06	118.44
7	D	700	N16	CAL-CAV-CAM	2.45	122.47	119.06
4	C	600	GTP	C6-N1-C2	2.91	119.98	115.94
4	C	600	GTP	C2'-C1'-N9	3.22	119.21	114.29
6	B	600	GDP	C6-N1-C2	3.60	120.94	115.94
6	D	600	GDP	C6-N1-C2	4.33	121.95	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 59 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	600	GTP	2	0
6	B	600	GDP	10	0
7	B	700	N16	8	0
4	C	600	GTP	4	0
6	D	600	GDP	19	0
7	D	700	N16	16	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	428/451 (94%)	-0.05	5 (1%) 81 68	39, 43, 44, 47	0
1	C	429/451 (95%)	0.05	13 (3%) 54 37	40, 43, 44, 52	0
2	B	420/445 (94%)	0.05	7 (1%) 73 58	41, 43, 45, 50	0
2	D	427/445 (95%)	0.04	9 (2%) 67 52	41, 43, 45, 48	0
3	E	123/142 (86%)	-0.29	1 (0%) 87 77	34, 43, 49, 53	0
All	All	1827/1934 (94%)	-0.00	35 (1%) 70 55	34, 43, 45, 53	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	369	ALA	3.7
1	C	361	THR	2.9
1	A	178	SER	2.9
1	A	351	PHE	2.7
2	D	109	THR	2.7
2	D	279	GLY	2.7
2	B	28	HIS	2.7
1	C	313	MET	2.6
1	C	370	LYS	2.6
2	D	413	MET	2.6
2	D	94	PHE	2.5
1	A	438	ASP	2.5
2	B	57	THR	2.4
1	C	432	TYR	2.4
1	A	435	VAL	2.4
1	C	60	LYS	2.3
2	B	35	SER	2.3
2	D	371	LEU	2.3
1	C	368	LEU	2.3
2	D	108	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	87	PHE	2.2
2	D	185	TYR	2.2
2	B	349	ASN	2.2
1	C	371	VAL	2.2
1	A	247	ALA	2.2
1	C	220	GLU	2.2
2	B	61	TYR	2.2
1	C	199	ASP	2.2
1	C	43	GLY	2.2
2	D	408	TYR	2.1
1	C	276	ILE	2.1
2	D	282	GLN	2.1
2	B	53	TYR	2.0
1	C	275	VAL	2.0
3	E	4	ALA	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
7	N16	D	700	23/23	0.87	0.34	0.79	79,83,85,85	0
5	MG	C	601	1/1	0.98	0.32	0.62	5,5,5,5	0
5	MG	A	601	1/1	0.97	0.30	0.62	5,5,5,5	0
4	GTP	C	600	32/32	0.93	0.27	0.41	24,32,36,37	0
6	GDP	B	600	28/28	0.88	0.28	0.40	34,42,49,50	0
7	N16	B	700	23/23	0.89	0.36	0.22	48,49,50,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GTP	A	600	32/32	0.96	0.29	-0.10	33,35,38,40	0
6	GDP	D	600	28/28	0.92	0.22	-0.55	40,49,56,57	0
5	MG	B	601	1/1	0.89	2.40	-	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.