Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 10:09 PM GMT

PDB ID	:	1SA0
Title	:	TUBULIN-COLCHICINE: STATHMIN-LIKE DOMAIN COMPLEX
Authors	:	Ravelli, R.B.; Gigant, B.; Curmi, P.A.; Jourdain, I.; Lachkar, S.; Sobel, A.; Knossow, M.
Deposited on	:	2004-02-06
Resolution	:	3.58 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 ⓘ symbol.

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

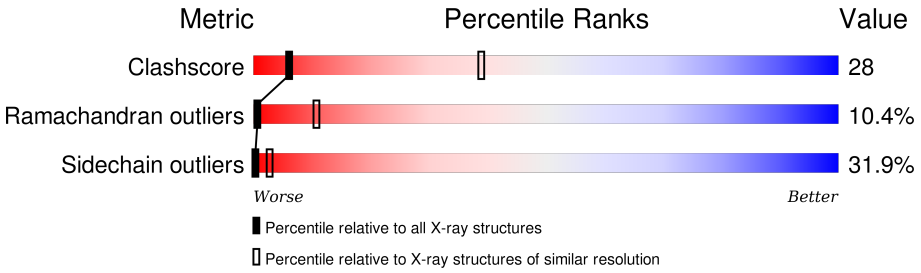
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.58 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))
Clashscore	102246	1026 (3.72-3.44)
Ramachandran outliers	100387	1028 (3.74-3.42)
Sidechain outliers	100360	1028 (3.74-3.42)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	451	43% 34% 14% • 5%
1	C	451	40% 37% 14% • 7%
2	B	445	36% 37% 18% • 6%
2	D	445	37% 34% 20% • 6%
3	E	142	49% 27% 11% 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
7	CN2	B	700	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14074 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
			3291	2091	555	624	21			
1	C	421	Total	C	N	O	S	0	0	0
			3220	2043	544	612	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	ILE	ALA	SEE REMARK 999	UNP P02550
C	265	ILE	ALA	SEE REMARK 999	UNP P02550

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	419	Total	C	N	O	S	0	0	0
			3236	2037	543	631	25			
2	D	419	Total	C	N	O	S	0	0	0
			3237	2037	544	631	25			

- 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
			907	549	170	183	5			

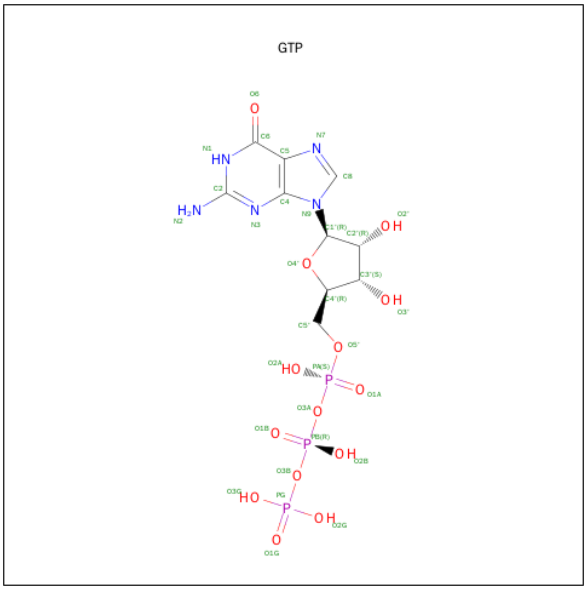
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	SEE REMARK 999	UNP P63043

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

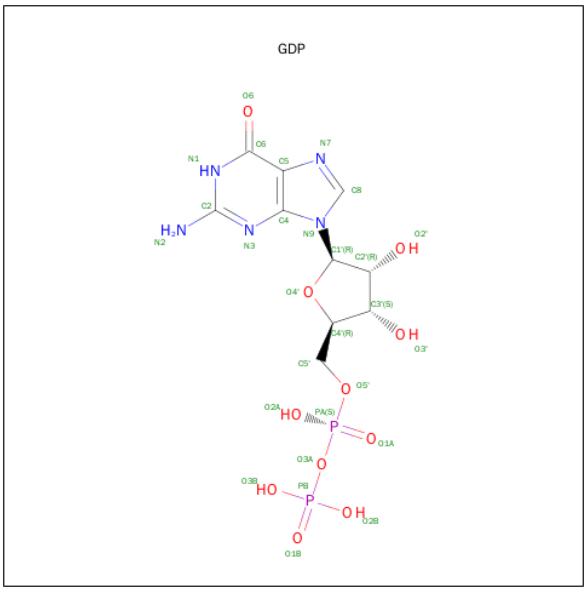
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

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



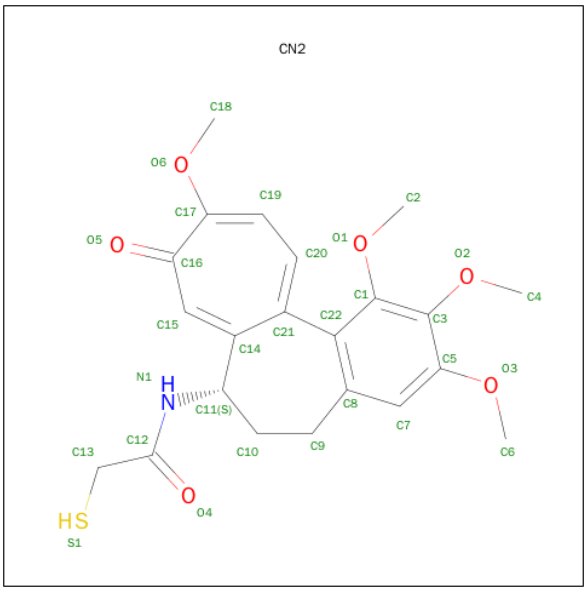
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 32 10 5 14 3	0	0
5	C	1	Total C N O P 32 10 5 14 3	0	0

- 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 2-MERCAPTO-N-[1,2,3,10-TETRAMETHOXY-9-OXO-5,6,7,9-TETRAHYDRO-BENZO[A]HEPTALEN-7-YL]ACETAMIDE (three-letter code: CN2) (formula: $C_{22}H_{25}NO_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			30	22	1	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	S	0	0
			30	22	1	6	1		

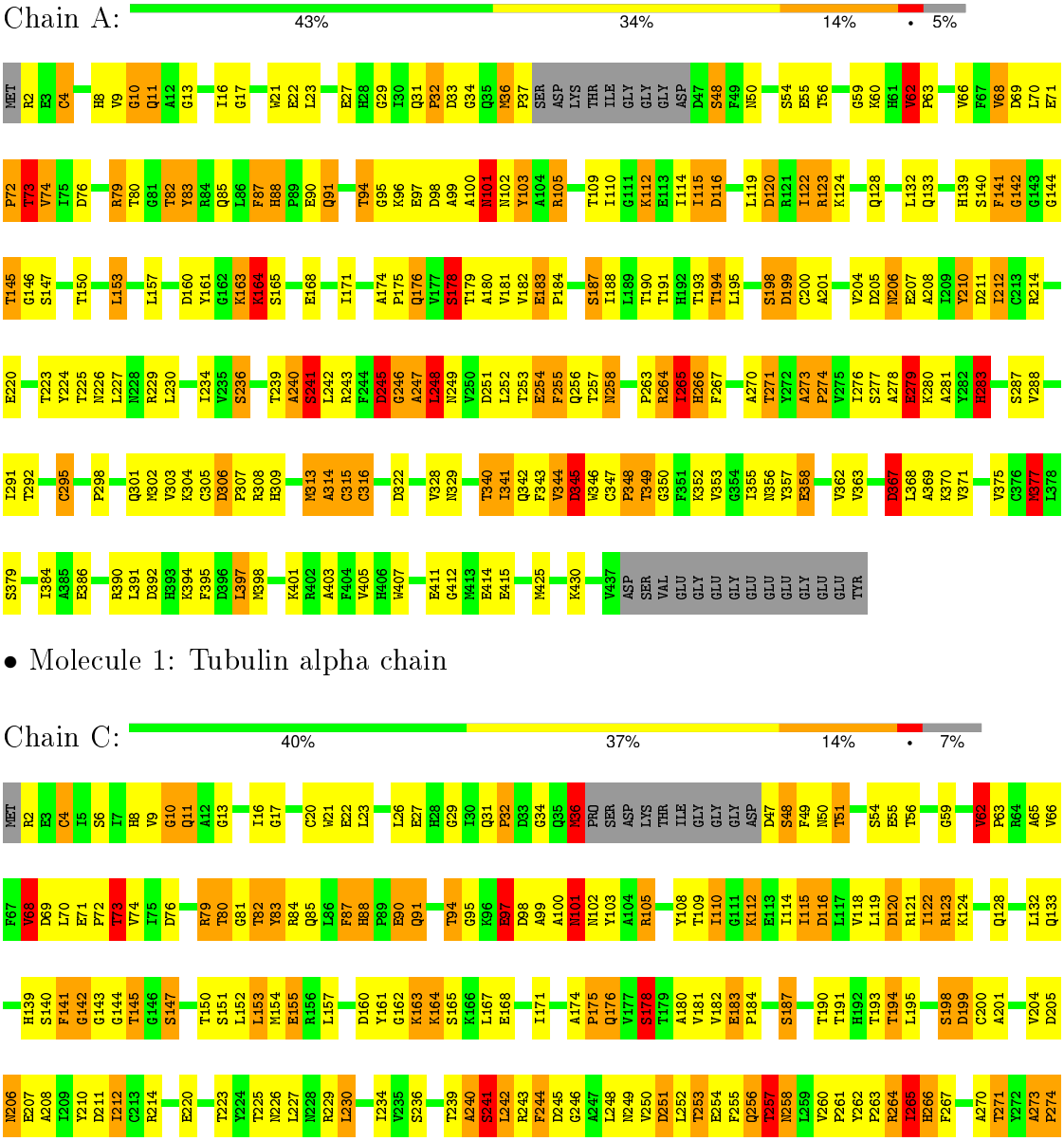
3 Residue-property plots (i)

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.

Note EDS was not executed.

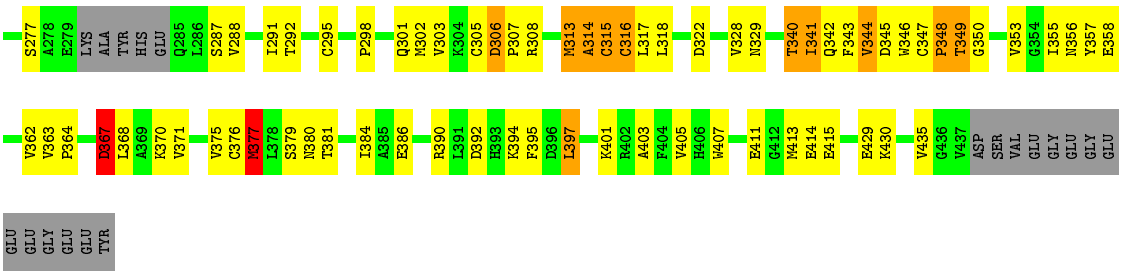
- Molecule 1: Tubulin alpha chain

Chain A:



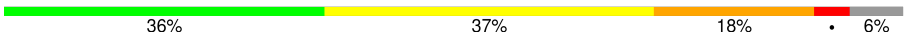
- Molecule 1: Tubulin alpha chain

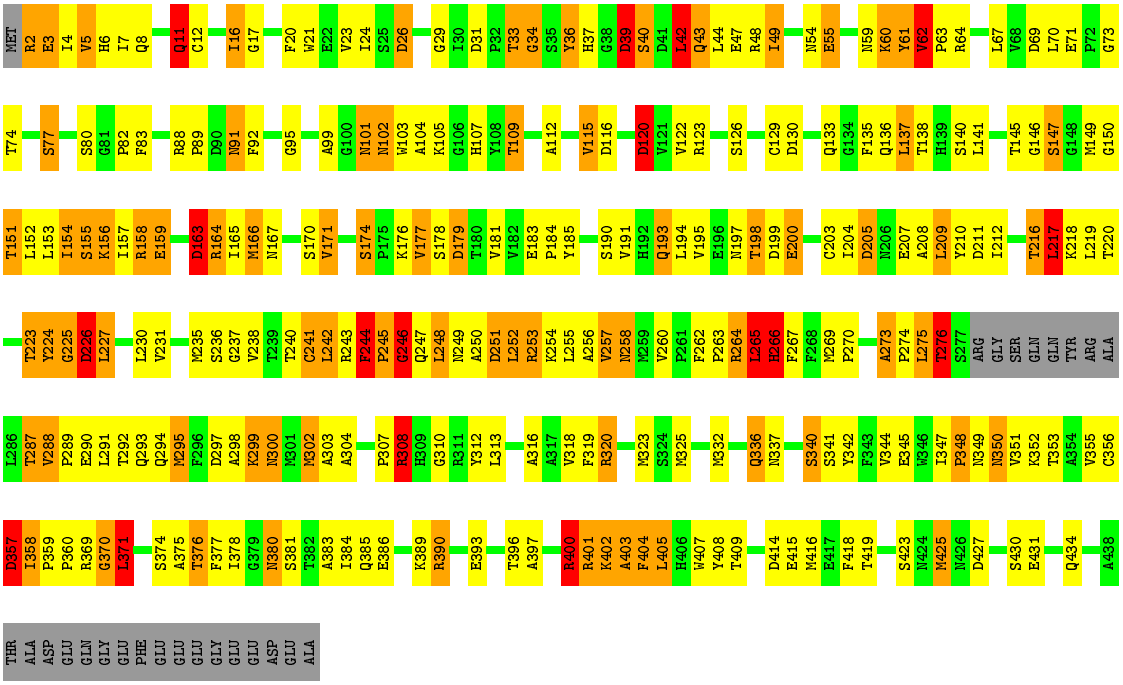
Chain C:



• Molecule 2: Tubulin beta chain

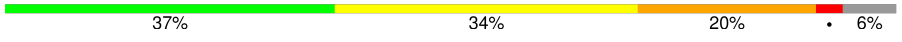
Chain B:

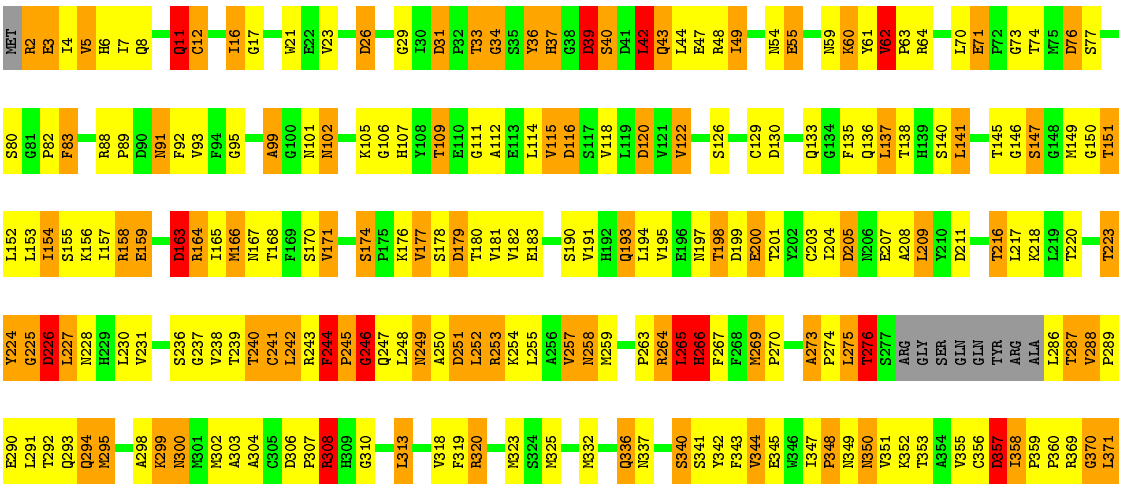


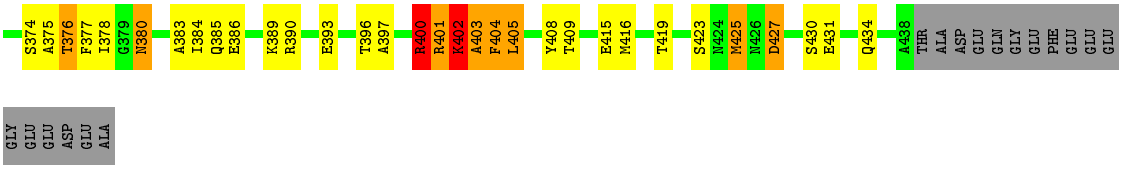


• Molecule 2: Tubulin beta chain

Chain D:

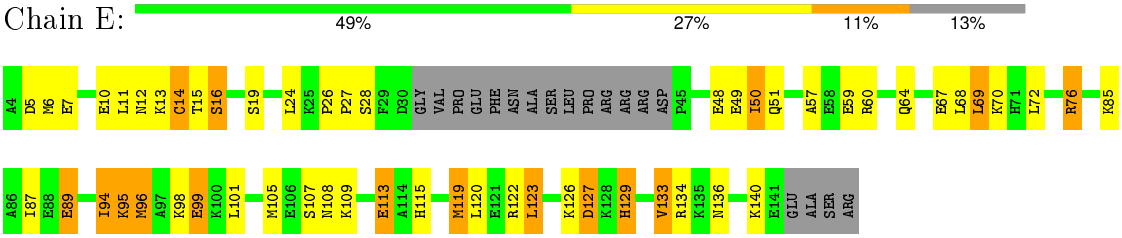






- Molecule 3: Stathmin 4

Chain E:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	328.69Å 328.69Å 54.68Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.58	Depositor
% Data completeness (in resolution range)	98.8 (20.00-3.58)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.232 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14074	wwPDB-VP
Average B, all atoms (Å^2)	83.0	wwPDB-VP

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, CN2

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	0.70	1/3368 (0.0%)	0.98	16/4581 (0.3%)
1	C	0.65	2/3292 (0.1%)	0.95	14/4479 (0.3%)
2	B	0.64	0/3308	1.01	20/4494 (0.4%)
2	D	0.61	0/3309	0.99	19/4494 (0.4%)
3	E	0.67	0/915	0.94	2/1230 (0.2%)
All	All	0.65	3/14192 (0.0%)	0.98	71/19278 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	97	GLU	CD-OE1	-6.64	1.18	1.25
1	A	97	GLU	CD-OE1	-5.52	1.19	1.25
1	C	97	GLU	CD-OE2	-5.36	1.19	1.25

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	160	ASP	CB-CG-OD2	7.19	124.77	118.30
2	B	116	ASP	CB-CG-OD2	7.16	124.75	118.30
2	B	205	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	120	ASP	CB-CG-OD2	6.98	124.58	118.30
2	D	205	ASP	CB-CG-OD2	6.84	124.45	118.30
1	A	322	ASP	CB-CG-OD2	6.83	124.45	118.30
2	D	163	ASP	CB-CG-OD2	6.83	124.44	118.30
1	C	160	ASP	CB-CG-OD2	6.79	124.41	118.30
1	C	244	PHE	N-CA-C	6.76	129.26	111.00
2	B	266	HIS	CB-CA-C	6.71	123.81	110.40
2	B	217	LEU	CA-CB-CG	-6.69	99.92	115.30
2	D	179	ASP	CB-CG-OD2	6.38	124.04	118.30
2	B	244	PHE	N-CA-C	6.33	128.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	116	ASP	CB-CG-OD2	6.27	123.94	118.30
1	A	97	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	A	397	LEU	CA-CB-CG	6.21	129.58	115.30
2	D	244	PHE	N-CA-C	6.15	127.61	111.00
1	C	397	LEU	CA-CB-CG	6.12	129.37	115.30
2	D	242	LEU	CA-CB-CG	6.11	129.36	115.30
2	D	26	ASP	CB-CG-OD2	6.07	123.77	118.30
1	A	76	ASP	CB-CG-OD2	6.03	123.72	118.30
1	C	120	ASP	CB-CG-OD2	5.92	123.63	118.30
2	D	357	ASP	CB-CG-OD2	5.91	123.62	118.30
1	C	116	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	95	GLY	N-CA-C	5.86	127.76	113.10
2	B	242	LEU	CA-CB-CG	5.83	128.70	115.30
2	D	266	HIS	CB-CA-C	5.80	122.01	110.40
2	B	179	ASP	CB-CG-OD2	5.79	123.51	118.30
2	B	199	ASP	CB-CG-OD2	5.76	123.48	118.30
1	C	76	ASP	CB-CG-OD2	5.74	123.47	118.30
1	C	142	GLY	N-CA-C	-5.73	98.77	113.10
1	C	95	GLY	N-CA-C	5.72	127.40	113.10
1	A	142	GLY	N-CA-C	-5.68	98.89	113.10
2	B	211	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	116	ASP	CB-CG-OD2	5.64	123.38	118.30
2	B	26	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	245	ASP	CB-CG-OD2	5.62	123.36	118.30
2	B	308	ARG	N-CA-C	-5.60	95.88	111.00
2	B	39	ASP	CB-CG-OD2	5.56	123.31	118.30
2	B	163	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	68	VAL	CB-CA-C	-5.51	100.94	111.40
2	B	297	ASP	CB-CG-OD2	5.49	123.24	118.30
2	D	427	ASP	CB-CG-OD2	5.47	123.22	118.30
2	B	226	ASP	CB-CG-OD2	5.40	123.16	118.30
2	D	211	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	345	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	97	GLU	OE1-CD-OE2	-5.38	116.85	123.30
2	D	199	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	322	ASP	CB-CG-OD2	5.36	123.13	118.30
2	B	246	GLY	N-CA-C	-5.32	99.81	113.10
1	C	36	MET	CG-SD-CE	5.31	108.70	100.20
1	C	68	VAL	CB-CA-C	-5.28	101.37	111.40
1	C	199	ASP	CB-CG-OD2	5.26	123.03	118.30
2	B	120	ASP	CB-CA-C	5.26	120.92	110.40
2	D	226	ASP	CB-CG-OD2	5.25	123.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	308	ARG	N-CA-C	-5.23	96.88	111.00
3	E	134	ARG	N-CA-C	-5.22	96.91	111.00
2	D	39	ASP	CB-CG-OD2	5.21	122.99	118.30
1	C	367	ASP	CB-CG-OD2	5.21	122.98	118.30
1	A	62	VAL	N-CA-C	5.19	125.01	111.00
2	D	306	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	367	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	199	ASP	CB-CG-OD2	5.15	122.94	118.30
2	B	69	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	392	ASP	CB-CG-OD2	5.08	122.87	118.30
2	B	414	ASP	CB-CG-OD2	5.05	122.84	118.30
2	D	31	ASP	CB-CG-OD2	5.05	122.84	118.30
2	D	246	GLY	N-CA-C	-5.04	100.49	113.10
2	D	163	ASP	N-CA-CB	-5.04	101.52	110.60
2	B	357	ASP	CB-CG-OD2	5.03	122.83	118.30
3	E	127	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3291	0	3155	159	0
1	C	3220	0	3074	180	0
2	B	3236	0	3058	215	0
2	D	3237	0	3060	217	0
3	E	907	0	781	31	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	32	0	12	4	0
5	C	32	0	12	2	0
6	B	28	0	12	2	0
6	D	28	0	12	1	0
7	B	30	0	23	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	30	0	23	8	0
All	All	14074	0	13222	773	0

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

All (773) 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:96:MET:SD	3:E:96:MET:CE	2.01	1.47
2:B:316:ALA:HB1	7:B:700:CN2:C2	1.55	1.36
2:B:316:ALA:CB	7:B:700:CN2:H21	1.70	1.20
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.22	1.15
1:C:198:SER:CB	1:C:265:ILE:HD11	1.78	1.13
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.21	1.12
1:A:198:SER:CB	1:A:265:ILE:HD11	1.81	1.11
1:A:198:SER:HB3	1:A:265:ILE:CD1	1.79	1.11
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.22	1.10
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.12	1.09
1:C:79:ARG:NH2	1:C:94:THR:HG21	1.68	1.09
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.26	1.09
1:A:79:ARG:NH2	1:A:94:THR:HG21	1.68	1.09
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.82	1.08
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.15	1.07
1:C:198:SER:HB3	1:C:265:ILE:CD1	1.85	1.05
1:C:273:ALA:CB	1:C:274:PRO:HD3	1.86	1.05
1:A:278:ALA:O	1:A:279:GLU:HB3	1.51	1.04
1:A:99:ALA:CB	1:A:145:THR:HG22	1.88	1.02
1:C:79:ARG:HH22	1:C:94:THR:CG2	1.73	1.01
2:D:48:ARG:HH12	2:D:245:PRO:HD2	1.22	1.01
1:C:79:ARG:HH22	1:C:94:THR:HG21	0.84	1.00
1:A:79:ARG:HH22	1:A:94:THR:HG21	0.84	0.99
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.92	0.98
2:B:48:ARG:HH12	2:B:245:PRO:HD2	1.26	0.98
1:A:79:ARG:HH22	1:A:94:THR:CG2	1.75	0.98
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.93	0.97
1:A:273:ALA:HB1	1:A:274:PRO:HD3	1.47	0.96
2:D:291:LEU:HD21	2:D:375:ALA:CB	1.96	0.96
1:C:99:ALA:CB	1:C:145:THR:HG22	1.93	0.95
7:B:700:CN2:H62	7:B:700:CN2:H43	1.48	0.92
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ALA:CB	1:C:375:VAL:H	1.82	0.92
1:A:273:ALA:CB	1:A:375:VAL:H	1.82	0.92
2:B:291:LEU:HD21	2:B:375:ALA:CB	2.00	0.92
1:A:273:ALA:HB2	1:A:375:VAL:H	1.35	0.92
2:B:332:MET:HG3	2:B:353:THR:HG21	1.52	0.90
2:B:336:GLN:OE1	2:B:351:VAL:HG11	1.71	0.90
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.53	0.90
2:D:247:GLN:HG2	2:D:248:LEU:H	1.37	0.89
1:A:133:GLN:HE21	1:A:252:LEU:HG	1.36	0.89
1:A:341:ILE:HG12	1:A:342:GLN:H	1.36	0.89
1:C:273:ALA:HB2	1:C:375:VAL:H	1.38	0.89
2:B:265:LEU:HD12	2:B:265:LEU:O	1.73	0.88
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.53	0.88
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.56	0.88
1:C:198:SER:HB3	1:C:265:ILE:HD11	0.89	0.87
2:D:332:MET:HG3	2:D:353:THR:HG21	1.55	0.87
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.56	0.87
1:C:273:ALA:HB1	1:C:274:PRO:HD3	1.57	0.87
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.56	0.87
2:D:308:ARG:HG3	2:D:308:ARG:HH11	1.39	0.86
2:B:316:ALA:CB	7:B:700:CN2:C2	2.38	0.86
1:A:273:ALA:CB	1:A:274:PRO:CD	2.52	0.86
1:A:100:ALA:O	1:A:101:ASN:HB2	1.72	0.86
1:A:341:ILE:HG12	1:A:342:GLN:N	1.87	0.86
2:D:336:GLN:OE1	2:D:351:VAL:HG11	1.74	0.85
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.55	0.84
1:C:178:SER:HB3	7:D:701:CN2:S1	2.17	0.84
1:A:316:CYS:O	1:A:377:MET:HA	1.78	0.83
1:A:386:GLU:O	1:A:390:ARG:HG3	1.77	0.83
2:D:265:LEU:O	2:D:265:LEU:HD12	1.78	0.83
1:C:386:GLU:O	1:C:390:ARG:HG3	1.78	0.83
1:C:273:ALA:CB	1:C:274:PRO:CD	2.57	0.83
2:B:36:TYR:OH	2:B:40:SER:O	1.96	0.83
2:B:48:ARG:NH1	2:B:245:PRO:HD2	1.94	0.82
1:A:70:LEU:HD23	1:A:110:ILE:HG23	1.59	0.82
1:C:341:ILE:HG12	1:C:342:GLN:H	1.43	0.82
2:D:48:ARG:NH1	2:D:245:PRO:HD2	1.93	0.82
2:B:308:ARG:HH11	2:B:308:ARG:HG3	1.42	0.81
2:B:265:LEU:O	2:B:266:HIS:O	1.97	0.81
3:E:85:LYS:O	3:E:89:GLU:HB2	1.81	0.81
2:B:247:GLN:HG2	2:B:248:LEU:H	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.46	0.81
1:C:341:ILE:HG12	1:C:342:GLN:N	1.95	0.81
1:C:105:ARG:NH1	2:D:253:ARG:HH21	1.78	0.81
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.16	0.80
2:D:70:LEU:HA	2:D:95:GLY:HA3	1.63	0.80
2:D:205:ASP:OD1	2:D:207:GLU:HB3	1.81	0.80
1:A:258:ASN:HD21	1:A:352:LYS:HE2	1.45	0.80
1:C:100:ALA:O	1:C:101:ASN:HB2	1.81	0.80
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.08	0.80
1:C:98:ASP:HB3	2:D:251:ASP:OD2	1.81	0.80
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.11	0.79
1:C:316:CYS:O	1:C:377:MET:HA	1.82	0.79
1:A:247:ALA:HB1	3:E:19:SER:CB	2.13	0.79
1:C:229:ARG:HH11	1:C:229:ARG:HG2	1.46	0.79
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.66	0.78
1:A:198:SER:HB3	1:A:265:ILE:HD11	0.88	0.78
2:D:247:GLN:CG	2:D:248:LEU:H	1.97	0.77
1:C:133:GLN:HE21	1:C:252:LEU:HG	1.50	0.77
2:D:36:TYR:OH	2:D:40:SER:O	2.03	0.77
1:A:88:HIS:HB2	1:A:91:GLN:NE2	1.95	0.77
1:C:88:HIS:HB2	1:C:91:GLN:NE2	1.98	0.76
2:B:247:GLN:HG3	2:B:248:LEU:HG	1.68	0.76
2:B:205:ASP:OD1	2:B:207:GLU:HB3	1.87	0.75
1:A:273:ALA:HB3	1:A:274:PRO:CD	2.14	0.75
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.22	0.75
1:C:142:GLY:HA3	1:C:183:GLU:HG3	1.68	0.75
1:C:70:LEU:HD23	1:C:110:ILE:HG23	1.69	0.74
1:A:176:GLN:NE2	1:A:176:GLN:H	1.85	0.74
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.17	0.74
2:B:247:GLN:CG	2:B:248:LEU:H	2.01	0.74
2:B:251:ASP:C	2:B:253:ARG:H	1.90	0.74
2:B:133:GLN:HE21	2:B:252:LEU:HB3	1.51	0.73
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.29	0.73
1:C:101:ASN:HD22	2:D:254:LYS:HG2	1.53	0.73
2:D:265:LEU:O	2:D:266:HIS:O	2.05	0.73
2:B:319:PHE:HB2	2:B:355:VAL:HG12	1.71	0.72
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.30	0.72
1:C:181:VAL:HB	2:D:258:ASN:ND2	2.05	0.72
2:D:247:GLN:HG3	2:D:248:LEU:HG	1.71	0.72
2:B:140:SER:HA	2:B:171:VAL:HG23	1.70	0.72
1:A:270:ALA:O	1:A:302:MET:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASN:HD22	2:B:254:LYS:HG2	1.56	0.71
2:B:164:ARG:HA	2:B:164:ARG:HE	1.56	0.70
1:A:179:THR:O	7:B:700:CN2:H132	1.91	0.70
1:A:278:ALA:O	1:A:279:GLU:CB	2.36	0.70
2:D:251:ASP:C	2:D:253:ARG:H	1.94	0.70
2:D:319:PHE:HB2	2:D:355:VAL:HG12	1.73	0.70
2:B:120:ASP:HB3	2:B:123:ARG:HH12	1.57	0.70
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.72	0.70
2:B:403:ALA:O	2:B:405:LEU:N	2.24	0.69
2:B:316:ALA:HB1	7:B:700:CN2:H21	0.74	0.69
1:A:204:VAL:HG22	1:A:302:MET:HE1	1.73	0.69
2:B:155:SER:HB3	3:E:76:ARG:HH22	1.58	0.69
1:C:70:LEU:HD12	1:C:70:LEU:N	2.08	0.69
2:D:307:PRO:O	2:D:308:ARG:CD	2.41	0.68
2:D:140:SER:HA	2:D:171:VAL:HG23	1.74	0.68
2:B:273:ALA:CB	2:B:274:PRO:CD	2.68	0.68
2:D:307:PRO:O	2:D:308:ARG:HD3	1.93	0.68
2:B:403:ALA:C	2:B:405:LEU:H	1.97	0.68
2:B:337:ASN:HA	2:B:340:SER:HB3	1.74	0.68
2:D:247:GLN:CG	2:D:248:LEU:N	2.56	0.68
1:A:133:GLN:NE2	1:A:252:LEU:HG	2.08	0.68
7:B:700:CN2:C12	7:B:700:CN2:H15	2.22	0.68
2:D:164:ARG:HA	2:D:164:ARG:HE	1.57	0.68
2:D:337:ASN:HA	2:D:340:SER:HB3	1.75	0.68
2:D:133:GLN:HE21	2:D:252:LEU:HB3	1.59	0.68
2:D:54:ASN:HB2	2:D:64:ARG:HD3	1.75	0.68
1:A:176:GLN:HE21	1:A:176:GLN:H	1.43	0.67
1:C:123:ARG:HD3	1:C:161:TYR:OH	1.94	0.67
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.77	0.67
2:D:238:VAL:HG13	2:D:378:ILE:HD11	1.76	0.67
2:D:350:ASN:H	2:D:350:ASN:HD22	1.43	0.67
2:B:54:ASN:HB2	2:B:64:ARG:HD3	1.75	0.67
1:A:99:ALA:HB2	1:A:145:THR:CG2	2.14	0.67
2:D:352:LYS:HG3	7:D:701:CN2:O5	1.94	0.67
1:A:98:ASP:OD1	1:A:99:ALA:N	2.28	0.66
2:B:307:PRO:O	2:B:308:ARG:HD3	1.94	0.66
2:B:59:ASN:O	2:B:60:LYS:O	2.14	0.66
2:D:241:CYS:CB	2:D:248:LEU:HD12	2.24	0.66
1:A:345:ASP:O	3:E:27:PRO:O	2.13	0.66
2:D:241:CYS:HB2	2:D:248:LEU:HD12	1.76	0.66
2:D:289:PRO:O	2:D:293:GLN:HG3	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:ARG:HG3	2:B:308:ARG:NH1	2.11	0.65
2:B:369:ARG:O	2:B:370:GLY:C	2.35	0.65
2:D:369:ARG:O	2:D:370:GLY:C	2.35	0.65
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.77	0.65
2:B:42:LEU:O	2:B:44:LEU:N	2.30	0.65
1:A:100:ALA:O	1:A:101:ASN:CB	2.43	0.65
2:D:42:LEU:O	2:D:44:LEU:N	2.29	0.65
1:C:249:ASN:HB3	1:C:255:PHE:CD2	2.32	0.65
2:B:163:ASP:OD1	2:B:164:ARG:HD2	1.97	0.65
2:D:88:ARG:O	2:D:91:ASN:HB2	1.96	0.65
2:D:308:ARG:NH1	2:D:308:ARG:HG3	2.11	0.64
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.79	0.64
2:B:209:LEU:HB3	2:B:227:LEU:HD11	1.78	0.64
2:B:240:THR:HG21	2:B:320:ARG:CZ	2.27	0.64
1:A:181:VAL:HB	2:B:258:ASN:ND2	2.12	0.64
1:A:29:GLY:O	1:A:36:MET:HB3	1.96	0.64
1:C:208:ALA:O	1:C:212:ILE:HD12	1.98	0.64
1:C:273:ALA:HB2	1:C:375:VAL:N	2.10	0.64
7:D:701:CN2:H43	7:D:701:CN2:H62	1.80	0.64
2:B:247:GLN:CG	2:B:248:LEU:N	2.61	0.64
2:B:307:PRO:O	2:B:308:ARG:CD	2.45	0.64
1:A:348:PRO:HA	3:E:27:PRO:HD3	1.79	0.64
2:D:247:GLN:HG2	2:D:248:LEU:N	2.13	0.64
1:A:412:GLY:O	3:E:60:ARG:NH1	2.31	0.64
1:C:100:ALA:O	1:C:101:ASN:CB	2.46	0.63
2:B:287:THR:CG2	2:B:290:GLU:HG3	2.29	0.63
1:A:229:ARG:CG	1:A:229:ARG:HH11	2.12	0.63
2:D:396:THR:HG22	2:D:400:ARG:HH21	1.64	0.63
2:B:88:ARG:O	2:B:91:ASN:HB2	1.98	0.63
1:C:98:ASP:OD1	1:C:99:ALA:N	2.32	0.63
2:B:120:ASP:HB3	2:B:123:ARG:NH1	2.13	0.63
1:A:248:LEU:HD21	1:A:352:LYS:HB3	1.80	0.63
2:D:59:ASN:O	2:D:60:LYS:O	2.16	0.63
1:C:99:ALA:HB2	1:C:145:THR:CG2	2.14	0.63
2:B:145:THR:HG23	6:B:602:GDP:O3B	1.99	0.62
1:A:273:ALA:HB2	1:A:375:VAL:N	2.09	0.62
1:C:249:ASN:HB3	1:C:255:PHE:HD2	1.64	0.62
1:A:249:ASN:HB3	1:A:255:PHE:CE2	2.34	0.62
2:D:266:HIS:H	2:D:266:HIS:CD2	2.17	0.62
1:A:180:ALA:O	1:A:183:GLU:HB2	2.00	0.62
2:D:401:ARG:HH11	2:D:401:ARG:HG3	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:TYR:OH	6:B:602:GDP:H2'	2.00	0.62
1:A:123:ARG:HD3	1:A:161:TYR:OH	1.99	0.62
1:A:265:ILE:O	1:A:266:HIS:O	2.17	0.62
2:B:266:HIS:H	2:B:266:HIS:CD2	2.16	0.62
2:D:287:THR:CG2	2:D:290:GLU:HG3	2.30	0.62
2:B:350:ASN:HD22	2:B:350:ASN:H	1.48	0.62
3:E:129:HIS:O	3:E:133:VAL:HG23	2.00	0.61
1:A:308:ARG:HA	1:A:340:THR:HG21	1.82	0.61
1:A:398:MET:HG3	2:B:348:PRO:HD3	1.82	0.61
2:B:135:PHE:HB2	2:B:166:MET:CE	2.31	0.61
1:A:11:GLN:HB3	5:A:600:GTP:O2A	2.00	0.61
2:B:263:PRO:O	2:B:265:LEU:N	2.31	0.61
2:B:289:PRO:O	2:B:293:GLN:HG3	2.00	0.61
2:D:287:THR:HG22	2:D:290:GLU:HG3	1.82	0.61
2:B:348:PRO:O	2:B:350:ASN:N	2.33	0.61
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.48	0.61
1:A:246:GLY:HA2	3:E:14:CYS:CB	2.30	0.61
1:C:133:GLN:NE2	1:C:252:LEU:HG	2.14	0.61
2:D:403:ALA:C	2:D:405:LEU:H	2.03	0.61
2:B:266:HIS:HB3	2:B:380:ASN:HD21	1.64	0.61
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.82	0.61
1:A:70:LEU:HD23	1:A:110:ILE:CG2	2.30	0.61
2:B:357:ASP:OD2	2:B:357:ASP:N	2.33	0.61
2:D:205:ASP:OD2	2:D:390:ARG:NH1	2.34	0.60
2:D:126:SER:O	2:D:129:CYS:HB2	2.01	0.60
2:B:401:ARG:HG3	2:B:401:ARG:HH11	1.66	0.60
1:A:206:ASN:HD21	5:A:600:GTP:HN22	1.48	0.60
1:C:206:ASN:HD21	5:C:601:GTP:HN22	1.47	0.60
1:C:176:GLN:H	1:C:176:GLN:NE2	1.98	0.60
2:D:223:THR:HB	2:D:225:GLY:H	1.65	0.60
2:D:158:ARG:O	2:D:159:GLU:CB	2.49	0.60
1:A:66:VAL:HG11	1:A:122:ILE:HG22	1.83	0.60
1:C:229:ARG:HH11	1:C:229:ARG:CG	2.14	0.60
2:B:407:TRP:NE1	1:C:257:THR:HA	2.16	0.60
2:D:158:ARG:O	2:D:159:GLU:HB2	2.00	0.60
2:D:151:THR:HB	2:D:193:GLN:HG2	1.83	0.60
2:B:241:CYS:CB	2:B:248:LEU:HD12	2.32	0.60
1:A:178:SER:HB3	7:B:700:CN2:S1	2.41	0.59
2:B:241:CYS:HB2	2:B:248:LEU:HD12	1.84	0.59
2:D:136:GLN:HA	2:D:167:ASN:O	2.02	0.59
1:C:264:ARG:O	1:C:266:HIS:CD2	2.56	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLN:HA	2:B:167:ASN:O	2.02	0.59
2:B:194:LEU:O	2:B:265:LEU:CD2	2.51	0.59
2:B:158:ARG:O	2:B:159:GLU:HB2	2.01	0.59
1:A:292:THR:O	1:A:295:CYS:HB2	2.02	0.59
2:B:158:ARG:O	2:B:159:GLU:CB	2.50	0.59
1:C:66:VAL:HG11	1:C:122:ILE:HG22	1.85	0.59
2:B:165:ILE:HD11	2:B:252:LEU:HG	1.85	0.59
1:C:115:ILE:CD1	1:C:119:LEU:HD13	2.32	0.59
1:C:168:GLU:HG2	1:C:201:ALA:HB2	1.85	0.59
2:B:396:THR:HG22	2:B:400:ARG:HH21	1.68	0.59
1:C:70:LEU:N	1:C:70:LEU:CD1	2.65	0.58
2:B:352:LYS:HG3	7:B:700:CN2:O5	2.03	0.58
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.85	0.58
2:B:287:THR:HG22	2:B:290:GLU:HG3	1.83	0.58
1:C:265:ILE:CG2	1:C:267:PHE:CZ	2.86	0.58
2:B:287:THR:CG2	2:B:289:PRO:HD2	2.32	0.58
1:C:298:PRO:HA	1:C:301:GLN:NE2	2.19	0.58
1:C:105:ARG:CZ	2:D:253:ARG:HH21	2.15	0.58
2:D:348:PRO:O	2:D:350:ASN:N	2.36	0.58
2:B:223:THR:HB	2:B:225:GLY:H	1.69	0.58
2:D:275:LEU:O	2:D:276:THR:HB	2.03	0.58
1:C:249:ASN:CB	1:C:255:PHE:CD2	2.87	0.57
1:A:298:PRO:HA	1:A:301:GLN:NE2	2.19	0.57
2:B:393:GLU:O	2:B:397:ALA:HB2	2.04	0.57
1:C:301:GLN:HE22	1:C:307:PRO:HD3	1.69	0.57
1:C:313:MET:O	1:C:314:ALA:HB2	2.04	0.57
1:C:308:ARG:HA	1:C:340:THR:HG21	1.85	0.57
1:A:246:GLY:HA2	3:E:14:CYS:HB2	1.85	0.57
2:B:135:PHE:HB2	2:B:166:MET:HE2	1.86	0.57
1:C:346:TRP:CE3	1:C:347:CYS:HB2	2.40	0.57
2:D:145:THR:HG23	6:D:603:GDP:O3B	2.05	0.57
1:C:180:ALA:O	1:C:183:GLU:HB2	2.05	0.57
3:E:57:ALA:HA	3:E:60:ARG:NH1	2.20	0.57
2:D:203:CYS:SG	2:D:267:PHE:HB3	2.44	0.57
2:D:240:THR:HG21	2:D:320:ARG:CZ	2.34	0.57
1:C:265:ILE:HG22	1:C:267:PHE:CZ	2.40	0.57
1:A:187:SER:O	1:A:191:THR:HG22	2.04	0.57
2:B:217:LEU:O	2:B:219:LEU:N	2.36	0.57
1:A:301:GLN:HE22	1:A:307:PRO:HD3	1.67	0.57
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.51	0.57
1:C:8:HIS:CD2	1:C:17:GLY:HA3	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:SER:O	1:C:191:THR:HG22	2.05	0.57
2:D:168:THR:HG1	2:D:201:THR:HG1	1.53	0.57
7:B:700:CN2:H42	7:B:700:CN2:H23	1.84	0.57
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.85	0.57
1:C:69:ASP:C	1:C:70:LEU:HD12	2.25	0.56
2:D:357:ASP:N	2:D:357:ASP:OD2	2.38	0.56
2:D:287:THR:CG2	2:D:289:PRO:HD2	2.31	0.56
1:C:11:GLN:HB3	5:C:601:GTP:O2A	2.04	0.56
1:C:29:GLY:O	1:C:36:MET:HB3	2.05	0.56
2:D:135:PHE:HB2	2:D:166:MET:CE	2.34	0.56
1:A:265:ILE:CG2	1:A:267:PHE:CZ	2.88	0.56
2:B:287:THR:O	2:B:288:VAL:HB	2.05	0.56
2:B:3:GLU:HG2	2:B:64:ARG:NH2	2.20	0.56
2:D:403:ALA:O	2:D:405:LEU:N	2.38	0.56
2:D:164:ARG:HE	2:D:164:ARG:CA	2.14	0.56
2:D:358:ILE:O	2:D:358:ILE:HG23	2.05	0.56
2:D:263:PRO:O	2:D:265:LEU:N	2.31	0.56
2:B:164:ARG:CA	2:B:164:ARG:HE	2.16	0.56
1:A:346:TRP:CE3	1:A:347:CYS:HB2	2.40	0.56
2:B:240:THR:HG21	2:B:320:ARG:NE	2.21	0.56
2:B:216:THR:HG21	2:B:299:LYS:HD3	1.87	0.56
1:A:264:ARG:O	1:A:266:HIS:CD2	2.59	0.56
2:B:342:TYR:CD2	2:B:342:TYR:N	2.74	0.56
1:C:181:VAL:HB	2:D:258:ASN:HD22	1.69	0.56
1:C:256:GLN:C	1:C:258:ASN:N	2.59	0.56
2:D:266:HIS:HB3	2:D:380:ASN:HD21	1.70	0.56
2:B:36:TYR:HH	2:B:40:SER:C	2.07	0.56
2:D:5:VAL:HG22	2:D:135:PHE:CD2	2.41	0.56
1:A:122:ILE:HD11	1:A:157:LEU:HD21	1.88	0.55
2:D:342:TYR:N	2:D:342:TYR:CD2	2.75	0.55
2:B:159:GLU:HB2	3:E:72:LEU:HD23	1.87	0.55
2:D:226:ASP:N	2:D:226:ASP:OD1	2.37	0.55
3:E:99:GLU:HG2	3:E:99:GLU:O	2.06	0.55
2:D:247:GLN:CG	2:D:248:LEU:HG	2.36	0.55
1:A:71:GLU:OE2	5:A:600:GTP:O1G	2.24	0.55
2:B:247:GLN:CG	2:B:248:LEU:HG	2.36	0.55
2:B:120:ASP:CB	2:B:123:ARG:NH1	2.69	0.55
2:D:209:LEU:HB3	2:D:227:LEU:HD11	1.88	0.55
1:A:239:THR:O	1:A:241:SER:N	2.39	0.55
1:C:265:ILE:O	1:C:266:HIS:O	2.24	0.55
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.88	0.55
2:D:177:VAL:HG12	2:D:177:VAL:O	2.07	0.55
1:C:23:LEU:HD23	1:C:236:SER:HB2	1.88	0.55
2:B:126:SER:O	2:B:129:CYS:HB2	2.07	0.55
2:D:2:ARG:HH11	2:D:133:GLN:HA	1.72	0.54
1:A:280:LYS:O	1:A:283:HIS:HB2	2.06	0.54
2:B:251:ASP:HB2	2:B:254:LYS:HD2	1.89	0.54
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.47	0.54
2:B:151:THR:HB	2:B:193:GLN:HG2	1.89	0.54
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.43	0.54
2:D:216:THR:HG21	2:D:299:LYS:HD3	1.90	0.54
2:D:191:VAL:HG11	2:D:425:MET:CE	2.37	0.54
2:B:401:ARG:O	1:C:262:TYR:OH	2.25	0.54
1:A:181:VAL:HB	2:B:258:ASN:HD22	1.71	0.54
2:D:401:ARG:NH1	2:D:401:ARG:HG3	2.23	0.54
1:C:256:GLN:C	1:C:258:ASN:H	2.10	0.54
2:B:2:ARG:O	2:B:3:GLU:HB2	2.07	0.54
2:B:7:ILE:O	2:B:137:LEU:HA	2.08	0.54
1:C:249:ASN:CB	1:C:255:PHE:HD2	2.21	0.54
3:E:67:GLU:C	3:E:69:LEU:H	2.11	0.54
2:D:408:TYR:O	2:D:409:THR:C	2.45	0.54
1:C:271:THR:HG23	1:C:301:GLN:HA	1.90	0.54
1:A:70:LEU:N	1:A:70:LEU:HD12	2.22	0.54
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.43	0.53
2:B:33:THR:O	2:B:34:GLY:O	2.26	0.53
1:A:115:ILE:CD1	1:A:119:LEU:HD13	2.38	0.53
1:C:407:TRP:CD2	2:D:257:VAL:HG23	2.43	0.53
2:D:180:THR:HG21	2:D:182:VAL:HG22	1.89	0.53
1:C:252:LEU:O	1:C:253:THR:C	2.45	0.53
2:D:383:ALA:O	2:D:386:GLU:HB2	2.08	0.53
2:B:291:LEU:HD21	2:B:375:ALA:HB3	1.87	0.53
1:A:133:GLN:HE21	1:A:252:LEU:CG	2.16	0.53
2:D:171:VAL:HA	2:D:204:ILE:O	2.08	0.53
2:B:401:ARG:NH1	2:B:401:ARG:HG3	2.23	0.53
3:E:119:MET:O	3:E:119:MET:HG3	2.08	0.53
2:D:194:LEU:O	2:D:265:LEU:CD2	2.56	0.53
2:D:223:THR:HB	2:D:225:GLY:N	2.23	0.53
2:B:44:LEU:O	2:B:49:ILE:HG22	2.10	0.52
2:D:16:ILE:HG22	2:D:17:GLY:N	2.24	0.52
1:A:263:PRO:O	1:A:265:ILE:N	2.30	0.52
2:D:287:THR:O	2:D:288:VAL:HB	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:LEU:HD21	2:D:375:ALA:HB3	1.87	0.52
2:D:307:PRO:O	2:D:308:ARG:HD2	2.09	0.52
1:A:239:THR:O	1:A:240:ALA:C	2.48	0.52
2:B:11:GLN:HG3	2:B:74:THR:CG2	2.39	0.52
2:B:336:GLN:CD	2:B:351:VAL:HG11	2.28	0.52
2:D:336:GLN:CD	2:D:351:VAL:HG11	2.30	0.52
2:B:29:GLY:O	2:B:36:TYR:HA	2.09	0.52
2:D:2:ARG:O	2:D:3:GLU:HB2	2.09	0.52
1:C:10:GLY:O	1:C:13:GLY:N	2.43	0.52
1:A:313:MET:O	1:A:314:ALA:HB2	2.09	0.52
2:D:273:ALA:CB	2:D:274:PRO:CD	2.67	0.52
1:C:176:GLN:HE21	1:C:176:GLN:H	1.58	0.52
2:D:11:GLN:HG3	2:D:74:THR:CG2	2.40	0.52
2:B:358:ILE:HG23	2:B:358:ILE:O	2.09	0.52
2:D:241:CYS:HB3	2:D:248:LEU:HD12	1.92	0.52
1:C:105:ARG:HD2	1:C:411:GLU:OE1	2.11	0.51
1:C:252:LEU:O	1:C:254:GLU:N	2.43	0.51
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.45	0.51
1:C:270:ALA:O	1:C:302:MET:CG	2.58	0.51
2:B:251:ASP:O	2:B:253:ARG:N	2.41	0.51
2:D:140:SER:O	2:D:147:SER:HB2	2.10	0.51
2:B:225:GLY:O	2:B:227:LEU:N	2.43	0.51
1:A:265:ILE:HG22	1:A:267:PHE:CZ	2.45	0.51
1:C:407:TRP:CG	2:D:257:VAL:HG23	2.45	0.51
2:B:251:ASP:C	2:B:253:ARG:N	2.61	0.51
2:D:36:TYR:HD1	2:D:37:HIS:H	1.58	0.51
1:C:8:HIS:HE1	1:C:21:TRP:HE1	1.59	0.51
1:C:315:CYS:SG	1:C:377:MET:HE2	2.50	0.51
2:D:29:GLY:O	2:D:36:TYR:HA	2.11	0.51
2:D:163:ASP:OD1	2:D:164:ARG:HD2	2.11	0.51
2:B:223:THR:HB	2:B:225:GLY:N	2.25	0.51
3:E:133:VAL:HG12	3:E:136:ASN:HD22	1.75	0.51
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.92	0.51
2:D:44:LEU:O	2:D:49:ILE:HG22	2.11	0.51
1:C:108:TYR:HB3	3:E:108:ASN:OD1	2.10	0.51
2:D:404:PHE:H	2:D:404:PHE:HD1	1.58	0.51
1:A:190:THR:CG2	1:A:191:THR:N	2.73	0.51
2:D:153:LEU:O	2:D:157:ILE:HG12	2.11	0.51
1:A:87:PHE:N	1:A:87:PHE:CD2	2.78	0.51
2:D:205:ASP:OD1	2:D:207:GLU:N	2.43	0.51
1:C:315:CYS:SG	1:C:377:MET:CE	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:GLU:HG2	2:D:64:ARG:NH2	2.25	0.51
2:D:180:THR:CG2	2:D:182:VAL:HG22	2.41	0.51
1:C:239:THR:O	1:C:241:SER:N	2.44	0.51
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.93	0.51
1:C:48:SER:O	1:C:243:ARG:O	2.29	0.50
1:A:208:ALA:O	1:A:212:ILE:HD12	2.11	0.50
2:B:408:TYR:O	2:B:409:THR:C	2.48	0.50
1:C:70:LEU:HD23	1:C:110:ILE:CG2	2.40	0.50
2:B:427:ASP:O	2:B:431:GLU:HG3	2.11	0.50
2:B:178:SER:HB2	2:B:183:GLU:OE1	2.11	0.50
2:D:295:MET:HG2	2:D:295:MET:O	2.11	0.50
1:C:340:THR:O	1:C:340:THR:HG22	2.11	0.50
2:B:191:VAL:HG11	2:B:425:MET:CE	2.41	0.50
2:B:267:PHE:CD1	2:B:267:PHE:N	2.78	0.50
2:B:16:ILE:HG22	2:B:17:GLY:N	2.26	0.50
2:D:241:CYS:HB3	2:D:248:LEU:CD1	2.41	0.50
2:B:154:ILE:HD12	2:B:198:THR:HG22	1.93	0.50
3:E:48:GLU:O	3:E:50:ILE:N	2.44	0.50
2:D:236:SER:O	2:D:240:THR:HG23	2.11	0.50
2:D:320:ARG:NH1	2:D:360:PRO:HG3	2.26	0.50
1:A:87:PHE:N	1:A:87:PHE:HD2	2.10	0.50
2:D:298:ALA:C	2:D:300:ASN:H	2.14	0.50
2:D:2:ARG:NH1	2:D:133:GLN:HA	2.27	0.50
1:C:270:ALA:O	1:C:302:MET:HG2	2.12	0.50
2:D:7:ILE:O	2:D:137:LEU:HA	2.12	0.50
2:B:298:ALA:C	2:B:300:ASN:H	2.15	0.50
2:B:236:SER:O	2:B:240:THR:HG23	2.12	0.50
2:B:320:ARG:NH1	2:B:360:PRO:HG3	2.27	0.50
1:A:229:ARG:CG	1:A:229:ARG:NH1	2.74	0.49
2:D:165:ILE:HD11	2:D:252:LEU:HG	1.93	0.49
2:D:177:VAL:CG1	2:D:177:VAL:O	2.60	0.49
2:B:407:TRP:HE1	1:C:257:THR:HA	1.75	0.49
2:D:267:PHE:N	2:D:267:PHE:CD1	2.80	0.49
2:D:135:PHE:N	2:D:135:PHE:CD1	2.80	0.49
1:C:102:ASN:O	1:C:103:TYR:C	2.51	0.49
2:D:225:GLY:O	2:D:227:LEU:N	2.45	0.49
2:D:135:PHE:HB2	2:D:166:MET:HE1	1.95	0.49
3:E:67:GLU:O	3:E:69:LEU:N	2.35	0.49
1:C:167:LEU:HD11	1:C:256:GLN:NE2	2.27	0.49
1:C:90:GLU:HB3	1:C:121:ARG:HD3	1.94	0.49
2:D:393:GLU:O	2:D:397:ALA:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:PHE:CD1	1:C:267:PHE:N	2.79	0.49
2:D:251:ASP:HB2	2:D:254:LYS:HD2	1.94	0.49
1:A:346:TRP:HE3	1:A:346:TRP:O	1.96	0.49
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.95	0.49
1:A:271:THR:HG23	1:A:301:GLN:HA	1.95	0.49
1:A:102:ASN:O	1:A:103:TYR:C	2.50	0.49
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.95	0.49
1:C:70:LEU:O	1:C:97:GLU:O	2.31	0.49
2:B:198:THR:OG1	2:B:265:LEU:HD22	2.12	0.49
1:C:229:ARG:NH1	1:C:229:ARG:CG	2.76	0.49
2:B:226:ASP:N	2:B:226:ASP:OD1	2.42	0.49
1:A:69:ASP:C	1:A:70:LEU:HD12	2.33	0.49
2:B:241:CYS:HB3	2:B:248:LEU:CD1	2.42	0.49
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.94	0.49
2:B:383:ALA:O	2:B:386:GLU:HB2	2.13	0.49
3:E:57:ALA:HA	3:E:60:ARG:HH12	1.77	0.49
1:A:32:PRO:O	1:A:33:ASP:C	2.51	0.49
1:A:407:TRP:CD2	2:B:257:VAL:HG23	2.47	0.48
2:B:133:GLN:HE21	2:B:252:LEU:CB	2.21	0.48
2:B:275:LEU:O	2:B:276:THR:HB	2.13	0.48
7:D:701:CN2:H15	7:D:701:CN2:C12	2.43	0.48
2:B:240:THR:CG2	2:B:320:ARG:CZ	2.91	0.48
1:C:239:THR:O	1:C:240:ALA:C	2.52	0.48
2:D:295:MET:SD	2:D:377:PHE:HB2	2.54	0.48
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.48	0.48
2:D:241:CYS:CB	2:D:248:LEU:CD1	2.92	0.48
2:D:36:TYR:HH	2:D:40:SER:C	2.08	0.48
2:B:140:SER:O	2:B:147:SER:HB2	2.13	0.48
2:D:240:THR:HG21	2:D:320:ARG:NE	2.28	0.48
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.62	0.48
1:C:191:THR:HA	1:C:194:THR:HG22	1.96	0.48
2:D:180:THR:HG22	2:D:182:VAL:H	1.79	0.48
2:B:264:ARG:O	2:B:266:HIS:CD2	2.67	0.48
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.96	0.48
2:B:400:ARG:HB2	2:B:400:ARG:HE	1.48	0.48
1:A:277:SER:HA	1:A:367:ASP:O	2.14	0.48
2:D:107:HIS:ND1	2:D:152:LEU:HB2	2.29	0.48
1:C:313:MET:O	1:C:314:ALA:CB	2.61	0.48
2:B:177:VAL:O	2:B:177:VAL:HG12	2.14	0.48
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.95	0.47
2:B:150:GLY:O	2:B:154:ILE:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:174:SER:HB2	2:D:207:GLU:HB2	1.96	0.47
2:B:155:SER:HB3	3:E:76:ARG:NH2	2.27	0.47
1:C:87:PHE:CD2	1:C:87:PHE:N	2.82	0.47
1:C:344:VAL:HG13	1:C:344:VAL:O	2.14	0.47
2:B:287:THR:HG22	2:B:290:GLU:H	1.79	0.47
1:C:204:VAL:HG13	1:C:302:MET:HE3	1.96	0.47
3:E:109:LYS:O	3:E:113:GLU:HB2	2.14	0.47
2:B:171:VAL:HA	2:B:204:ILE:O	2.15	0.47
2:B:107:HIS:ND1	2:B:152:LEU:HB2	2.29	0.47
1:C:26:LEU:HD21	1:C:364:PRO:HD3	1.96	0.47
2:B:316:ALA:CB	7:B:700:CN2:H22	2.41	0.47
1:C:198:SER:CB	1:C:265:ILE:CD1	2.66	0.47
2:D:154:ILE:HD12	2:D:198:THR:HG22	1.97	0.47
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.96	0.47
2:D:33:THR:O	2:D:34:GLY:O	2.32	0.47
1:A:395:PHE:CD2	1:A:395:PHE:C	2.87	0.47
2:D:5:VAL:CG2	2:D:135:PHE:CD2	2.97	0.47
1:C:395:PHE:CD2	1:C:395:PHE:C	2.87	0.47
2:D:200:GLU:OE2	2:D:255:LEU:HD12	2.14	0.47
1:A:70:LEU:N	1:A:70:LEU:CD1	2.77	0.47
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.28	0.47
1:C:346:TRP:CZ3	1:C:347:CYS:HB2	2.50	0.47
2:B:11:GLN:HG3	2:B:74:THR:HG22	1.95	0.47
3:E:94:ILE:CG2	3:E:95:LYS:N	2.77	0.47
1:C:71:GLU:HG3	1:C:73:THR:OG1	2.15	0.47
2:B:403:ALA:C	2:B:405:LEU:N	2.65	0.47
2:B:404:PHE:H	2:B:404:PHE:HD1	1.63	0.47
1:A:348:PRO:HD3	3:E:27:PRO:HG3	1.97	0.47
2:D:209:LEU:HD21	2:D:231:VAL:HG22	1.96	0.47
2:D:385:GLN:HE21	2:D:389:LYS:HD2	1.79	0.47
1:C:115:ILE:HD13	1:C:119:LEU:HD13	1.95	0.47
2:D:5:VAL:CG2	2:D:135:PHE:HD2	2.28	0.47
2:D:237:GLY:CA	2:D:376:THR:HG21	2.44	0.46
1:C:313:MET:HG3	1:C:380:ASN:O	2.15	0.46
2:B:295:MET:HG2	2:B:295:MET:O	2.15	0.46
1:C:82:THR:O	1:C:83:TYR:CB	2.63	0.46
1:A:72:PRO:O	1:A:74:VAL:N	2.49	0.46
2:D:259:MET:SD	7:D:701:CN2:H182	2.55	0.46
3:E:26:PRO:HA	3:E:27:PRO:HD2	1.84	0.46
1:C:87:PHE:HD2	1:C:87:PHE:N	2.13	0.46
2:D:112:ALA:HA	2:D:115:VAL:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:48:ARG:NH2	2:B:246:GLY:HA2	2.30	0.46
1:A:341:ILE:CG1	1:A:342:GLN:N	2.71	0.46
2:B:163:ASP:HB3	2:B:164:ARG:H	1.47	0.46
2:B:135:PHE:CD1	2:B:135:PHE:N	2.83	0.46
2:D:320:ARG:HA	2:D:356:CYS:O	2.15	0.46
2:B:185:TYR:CD1	2:B:418:PHE:HE2	2.34	0.46
2:B:112:ALA:HA	2:B:115:VAL:CG2	2.45	0.46
2:B:336:GLN:OE1	2:B:351:VAL:CG1	2.54	0.46
2:D:336:GLN:OE1	2:D:351:VAL:CG1	2.57	0.46
2:D:11:GLN:HG3	2:D:74:THR:HG22	1.95	0.46
2:D:294:GLN:HE21	2:D:294:GLN:HB2	1.63	0.46
2:B:265:LEU:O	2:B:266:HIS:C	2.53	0.46
2:B:237:GLY:CA	2:B:376:THR:HG21	2.44	0.46
2:B:200:GLU:OE2	2:B:255:LEU:HD12	2.15	0.46
1:A:315:CYS:SG	1:A:377:MET:CE	3.04	0.46
2:D:116:ASP:O	2:D:120:ASP:HB2	2.16	0.46
2:D:313:LEU:HA	2:D:313:LEU:HD12	1.87	0.46
2:D:102:ASN:OD1	2:D:105:LYS:HB2	2.15	0.46
2:B:342:TYR:HD2	2:B:342:TYR:N	2.12	0.46
2:B:264:ARG:O	2:B:266:HIS:N	2.49	0.46
2:B:205:ASP:OD2	2:B:390:ARG:NH1	2.49	0.46
2:D:178:SER:HB2	2:D:183:GLU:OE1	2.16	0.46
1:A:267:PHE:CD1	1:A:267:PHE:N	2.83	0.45
2:D:308:ARG:C	2:D:310:GLY:H	2.19	0.45
2:B:102:ASN:OD1	2:B:105:LYS:HB2	2.16	0.45
2:D:308:ARG:NH1	2:D:342:TYR:HE1	2.14	0.45
2:D:250:ALA:CB	7:D:701:CN2:H7	2.46	0.45
2:B:60:LYS:O	2:B:61:TYR:HD2	1.99	0.45
2:D:55:GLU:HG3	2:D:55:GLU:H	1.63	0.45
2:B:89:PRO:O	2:B:92:PHE:HD1	2.00	0.45
1:C:132:LEU:HG	1:C:133:GLN:N	2.31	0.45
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.98	0.45
1:A:168:GLU:HG2	1:A:201:ALA:HB2	1.97	0.45
1:C:263:PRO:O	1:C:265:ILE:N	2.38	0.45
1:C:306:ASP:HA	1:C:307:PRO:HD3	1.57	0.45
2:D:287:THR:HG22	2:D:290:GLU:H	1.81	0.45
2:D:62:VAL:O	2:D:62:VAL:HG22	2.15	0.45
2:D:135:PHE:HB2	2:D:166:MET:HE2	1.97	0.45
2:B:210:TYR:CD1	2:B:210:TYR:C	2.90	0.45
7:B:700:CN2:C12	7:B:700:CN2:C15	2.87	0.45
1:A:306:ASP:HA	1:A:307:PRO:HD3	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:346:TRP:HZ2	1:C:435:VAL:HG13	1.80	0.45
2:D:240:THR:CG2	2:D:320:ARG:CZ	2.95	0.45
1:C:62:VAL:HA	1:C:63:PRO:HD3	1.85	0.45
1:A:71:GLU:HG3	1:A:73:THR:OG1	2.17	0.45
2:D:150:GLY:O	2:D:154:ILE:HG23	2.17	0.45
2:B:205:ASP:OD1	2:B:207:GLU:N	2.49	0.45
2:B:320:ARG:HA	2:B:356:CYS:O	2.16	0.45
1:C:190:THR:CG2	1:C:191:THR:N	2.79	0.45
1:C:82:THR:O	1:C:83:TYR:HB2	2.17	0.45
2:B:20:PHE:O	2:B:24:ILE:HG23	2.17	0.45
2:B:36:TYR:HD1	2:B:37:HIS:H	1.63	0.45
1:C:122:ILE:HD11	1:C:157:LEU:HD21	1.99	0.45
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.47	0.45
1:C:292:THR:O	1:C:295:CYS:HB2	2.17	0.45
2:D:163:ASP:HB3	2:D:164:ARG:H	1.46	0.45
1:A:315:CYS:SG	1:A:377:MET:HE2	2.57	0.45
2:B:241:CYS:CB	2:B:248:LEU:CD1	2.95	0.45
2:D:225:GLY:O	2:D:228:ASN:N	2.49	0.45
2:B:191:VAL:HG11	2:B:425:MET:HE3	1.98	0.45
2:B:385:GLN:HE21	2:B:389:LYS:HD2	1.82	0.44
1:A:265:ILE:O	1:A:265:ILE:HG23	2.18	0.44
2:D:265:LEU:O	2:D:266:HIS:C	2.55	0.44
2:D:403:ALA:C	2:D:405:LEU:N	2.71	0.44
3:E:16:SER:OG	3:E:16:SER:O	2.34	0.44
1:A:82:THR:O	1:A:83:TYR:CB	2.65	0.44
1:A:344:VAL:O	1:A:344:VAL:HG13	2.16	0.44
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.52	0.44
1:C:318:LEU:HB2	1:C:376:CYS:HB3	1.99	0.44
2:D:273:ALA:HB2	2:D:375:ALA:HB3	1.98	0.44
2:D:401:ARG:O	2:D:402:LYS:C	2.55	0.44
1:C:266:HIS:H	1:C:266:HIS:CD2	2.35	0.44
2:B:308:ARG:NH1	2:B:342:TYR:HE1	2.15	0.44
2:B:247:GLN:HG2	2:B:248:LEU:N	2.19	0.44
2:B:241:CYS:HB3	2:B:248:LEU:HD12	1.99	0.44
2:B:70:LEU:CA	2:B:95:GLY:HA3	2.38	0.44
1:A:164:LYS:H	1:A:164:LYS:HG2	1.62	0.44
2:D:359:PRO:HA	2:D:360:PRO:HD3	1.82	0.44
1:A:10:GLY:O	1:A:13:GLY:N	2.50	0.44
2:D:343:PHE:O	2:D:344:VAL:C	2.55	0.44
2:B:386:GLU:O	2:B:390:ARG:HG2	2.18	0.44
2:D:209:LEU:HD21	2:D:231:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:SER:O	1:C:155:GLU:HG2	2.17	0.44
1:C:51:THR:HG21	1:C:242:LEU:O	2.17	0.44
1:C:256:GLN:O	1:C:258:ASN:N	2.51	0.44
1:A:48:SER:O	1:A:243:ARG:O	2.35	0.44
2:B:135:PHE:HB2	2:B:166:MET:HE1	1.98	0.44
1:C:244:PHE:N	1:C:245:ASP:HA	2.32	0.44
1:C:80:THR:HG22	1:C:81:GLY:N	2.33	0.44
2:B:16:ILE:CG2	2:B:17:GLY:N	2.80	0.43
2:D:431:GLU:O	2:D:434:GLN:HB2	2.17	0.43
2:B:103:TRP:O	2:B:104:ALA:C	2.56	0.43
2:D:251:ASP:C	2:D:253:ARG:N	2.64	0.43
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.88	0.43
1:C:298:PRO:HA	1:C:301:GLN:HE21	1.82	0.43
1:C:98:ASP:CB	2:D:251:ASP:OD2	2.58	0.43
1:A:273:ALA:HB1	1:A:274:PRO:CD	2.26	0.43
2:D:378:ILE:HD12	7:D:701:CN2:C4	2.48	0.43
1:C:71:GLU:O	1:C:71:GLU:HG2	2.17	0.43
1:C:31:GLN:O	1:C:32:PRO:C	2.56	0.43
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.88	0.43
1:A:153:LEU:HD22	1:A:157:LEU:HG	2.00	0.43
1:C:251:ASP:O	1:C:251:ASP:OD1	2.36	0.43
1:C:205:ASP:HB2	1:C:303:VAL:HA	1.99	0.43
1:A:36:MET:HA	1:A:37:PRO:HD3	1.87	0.43
1:A:171:ILE:O	1:A:171:ILE:HG22	2.19	0.43
2:D:111:GLY:HA2	2:D:149:MET:CE	2.49	0.43
2:B:217:LEU:C	2:B:219:LEU:H	2.22	0.43
1:C:174:ALA:HA	1:C:175:PRO:HD2	1.66	0.43
2:D:319:PHE:CD1	2:D:319:PHE:N	2.87	0.43
1:A:36:MET:H	1:A:36:MET:HG3	1.45	0.43
1:A:122:ILE:CD1	1:A:157:LEU:HD21	2.49	0.43
1:C:153:LEU:HD22	1:C:157:LEU:HG	2.01	0.43
1:A:313:MET:O	1:A:314:ALA:CB	2.67	0.43
1:A:391:LEU:HA	1:A:391:LEU:HD12	1.87	0.43
2:B:312:TYR:CD2	2:B:381:SER:HB2	2.54	0.43
2:B:245:PRO:HB2	2:B:246:GLY:H	1.44	0.43
1:A:246:GLY:O	1:A:247:ALA:O	2.37	0.43
2:B:156:LYS:CG	3:E:76:ARG:HE	2.32	0.43
1:C:347:CYS:HA	1:C:348:PRO:HD2	1.88	0.43
1:C:163:LYS:H	1:C:163:LYS:HG3	1.48	0.43
1:C:260:VAL:HG23	1:C:260:VAL:O	2.18	0.43
1:C:210:TYR:CE1	1:C:214:ARG:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:245:PRO:HB2	2:D:246:GLY:H	1.37	0.43
2:D:342:TYR:HD2	2:D:342:TYR:N	2.15	0.43
3:E:67:GLU:C	3:E:69:LEU:N	2.72	0.43
2:D:16:ILE:CG2	2:D:17:GLY:N	2.81	0.43
2:B:270:PRO:O	2:B:302:MET:HB2	2.18	0.43
1:A:278:ALA:HA	1:A:281:ALA:HB2	2.01	0.42
1:C:141:PHE:HA	1:C:141:PHE:HD2	1.72	0.42
3:E:15:THR:CG2	3:E:16:SER:N	2.82	0.42
1:C:31:GLN:HA	1:C:32:PRO:HD2	1.89	0.42
1:C:54:SER:O	1:C:56:THR:N	2.52	0.42
1:C:6:SER:O	1:C:65:ALA:HA	2.19	0.42
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.01	0.42
2:B:101:ASN:HB2	1:C:254:GLU:OE2	2.18	0.42
1:A:347:CYS:HA	1:A:348:PRO:HD2	1.83	0.42
1:A:62:VAL:HA	1:A:63:PRO:HD3	1.84	0.42
2:D:118:VAL:O	2:D:122:VAL:HG13	2.19	0.42
1:C:97:GLU:OE2	2:D:164:ARG:NH1	2.50	0.42
2:B:264:ARG:C	2:B:266:HIS:H	2.22	0.42
2:B:308:ARG:C	2:B:310:GLY:H	2.22	0.42
1:C:277:SER:HA	1:C:367:ASP:O	2.19	0.42
2:B:208:ALA:HB2	2:B:304:ALA:N	2.34	0.42
1:C:258:ASN:HA	1:C:258:ASN:HD22	1.56	0.42
1:A:105:ARG:HD2	1:A:411:GLU:OE1	2.18	0.42
1:A:132:LEU:HG	1:A:133:GLN:N	2.34	0.42
1:A:340:THR:O	1:A:340:THR:HG22	2.20	0.42
1:C:36:MET:HG3	1:C:36:MET:H	1.44	0.42
2:B:177:VAL:O	2:B:177:VAL:CG1	2.67	0.42
2:B:149:MET:O	2:B:152:LEU:HB3	2.19	0.42
2:B:431:GLU:O	2:B:434:GLN:HB2	2.20	0.42
1:A:207:GLU:HG2	1:A:304:LYS:NZ	2.35	0.42
1:C:164:LYS:H	1:C:164:LYS:HG2	1.69	0.42
1:A:191:THR:HA	1:A:194:THR:HG22	2.00	0.42
2:B:231:VAL:HG12	2:B:235:MET:HE2	2.02	0.42
2:D:6:HIS:HD2	2:D:136:GLN:HG3	1.83	0.42
1:A:276:ILE:HD11	1:A:280:LYS:HD2	2.01	0.42
1:A:146:GLY:O	1:A:150:THR:OG1	2.30	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.42
2:D:83:PHE:HD2	2:D:83:PHE:HA	1.77	0.42
2:B:55:GLU:H	2:B:55:GLU:HG3	1.60	0.42
1:C:68:VAL:HG11	1:C:118:VAL:HG21	2.01	0.42
2:D:269:MET:HA	2:D:270:PRO:HD3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:THR:O	1:A:83:TYR:HB2	2.20	0.42
1:A:174:ALA:CB	1:A:207:GLU:HB2	2.49	0.42
2:D:89:PRO:O	2:D:92:PHE:HD1	2.03	0.42
1:C:230:LEU:O	1:C:230:LEU:HD12	2.20	0.42
1:A:145:THR:HG23	5:A:600:GTP:O2B	2.20	0.42
2:D:255:LEU:HD23	7:D:701:CN2:C22	2.50	0.42
1:C:152:LEU:HA	1:C:155:GLU:HG3	2.01	0.42
1:A:306:ASP:O	1:A:309:HIS:HB3	2.20	0.42
1:A:205:ASP:HB2	1:A:303:VAL:HA	2.02	0.42
1:C:143:GLY:O	1:C:147:SER:OG	2.33	0.42
1:C:392:ASP:OD1	1:C:429:GLU:OE1	2.38	0.42
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.55	0.42
2:D:298:ALA:O	2:D:300:ASN:N	2.52	0.41
2:D:427:ASP:O	2:D:431:GLU:HG3	2.20	0.41
1:A:163:LYS:HG3	1:A:163:LYS:H	1.49	0.41
1:C:84:ARG:HE	1:C:84:ARG:HB3	1.65	0.41
2:D:164:ARG:NH2	2:D:253:ARG:HH22	2.18	0.41
2:B:183:GLU:N	2:B:184:PRO:HD2	2.35	0.41
2:D:248:LEU:HB2	2:D:249:ASN:H	1.46	0.41
1:C:190:THR:O	1:C:194:THR:HB	2.20	0.41
2:B:74:THR:O	2:B:77:SER:HB2	2.21	0.41
1:C:47:ASP:O	1:C:49:PHE:N	2.53	0.41
2:B:256:ALA:O	2:B:260:VAL:HG22	2.20	0.41
2:D:93:VAL:HG12	2:D:114:LEU:HD11	2.01	0.41
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.55	0.41
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.39	0.41
1:C:407:TRP:CE2	2:D:257:VAL:HA	2.55	0.41
2:B:404:PHE:CE1	1:C:261:PRO:HB3	2.55	0.41
2:B:67:LEU:HD12	2:B:92:PHE:CE2	2.55	0.41
2:B:153:LEU:O	2:B:157:ILE:HG12	2.19	0.41
1:C:291:ILE:HD12	1:C:375:VAL:HG23	2.03	0.41
1:A:298:PRO:HA	1:A:301:GLN:HE21	1.84	0.41
1:A:141:PHE:HD2	1:A:141:PHE:HA	1.76	0.41
1:A:358:GLU:HG3	1:A:358:GLU:O	2.21	0.41
1:C:154:MET:HE3	1:C:154:MET:HB3	1.92	0.41
2:B:21:TRP:CH2	2:B:63:PRO:HB3	2.56	0.41
2:D:208:ALA:HB2	2:D:304:ALA:N	2.35	0.41
1:A:54:SER:O	1:A:56:THR:N	2.54	0.41
2:D:141:LEU:HD12	2:D:141:LEU:HA	1.81	0.41
1:A:252:LEU:HA	1:A:252:LEU:HD23	1.75	0.41
1:A:398:MET:HG3	2:B:348:PRO:CD	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:ASN:O	2:D:62:VAL:O	2.39	0.41
2:D:251:ASP:O	2:D:253:ARG:N	2.49	0.41
2:D:264:ARG:O	2:D:266:HIS:CD2	2.74	0.41
2:B:156:LYS:HG2	3:E:76:ARG:HE	1.85	0.41
1:C:171:ILE:HG23	1:C:206:ASN:ND2	2.35	0.41
1:C:122:ILE:CD1	1:C:157:LEU:HD21	2.51	0.41
1:A:198:SER:O	1:A:265:ILE:HG13	2.21	0.41
2:D:270:PRO:HA	2:D:377:PHE:O	2.21	0.41
1:A:31:GLN:O	1:A:32:PRO:C	2.60	0.41
1:A:188:ILE:HD12	1:A:425:MET:HG3	2.03	0.41
3:E:123:LEU:O	3:E:127:ASP:HB2	2.21	0.41
2:D:289:PRO:O	2:D:293:GLN:CG	2.68	0.40
2:B:359:PRO:HA	2:B:360:PRO:HD3	1.83	0.40
1:C:8:HIS:CE1	1:C:21:TRP:HE1	2.39	0.40
1:A:252:LEU:O	1:A:255:PHE:HB2	2.21	0.40
2:B:36:TYR:OH	2:B:40:SER:C	2.55	0.40
1:C:214:ARG:HH11	1:C:214:ARG:HD3	1.77	0.40
2:D:71:GLU:O	2:D:71:GLU:HG2	2.22	0.40
2:B:371:LEU:H	2:B:371:LEU:HD13	1.87	0.40
1:A:291:ILE:HD12	1:A:375:VAL:CG2	2.51	0.40
2:B:262:PHE:O	2:B:266:HIS:CD2	2.75	0.40
2:D:198:THR:OG1	2:D:265:LEU:HD22	2.20	0.40
2:B:308:ARG:HD2	2:B:308:ARG:HA	1.87	0.40
2:D:224:TYR:O	2:D:228:ASN:ND2	2.54	0.40
2:D:358:ILE:O	2:D:358:ILE:CG2	2.68	0.40
2:D:102:ASN:OD1	2:D:102:ASN:O	2.39	0.40
1:C:141:PHE:HB2	1:C:171:ILE:O	2.22	0.40
1:C:115:ILE:HG13	1:C:152:LEU:CD2	2.51	0.40
2:D:99:ALA:HB1	2:D:145:THR:HG21	2.03	0.40
2:D:191:VAL:HG11	2:D:425:MET:HE3	2.03	0.40
1:A:115:ILE:HD13	1:A:119:LEU:HD13	2.03	0.40
2:B:11:GLN:HG3	2:B:74:THR:HG21	2.03	0.40
2:D:404:PHE:N	2:D:404:PHE:CD1	2.89	0.40
2:D:298:ALA:C	2:D:300:ASN:N	2.74	0.40
1:C:344:VAL:O	1:C:344:VAL:CG1	2.70	0.40
2:B:270:PRO:HA	2:B:377:PHE:O	2.20	0.40
1:A:251:ASP:HB3	1:A:254:GLU:HB2	2.03	0.40
2:D:76:ASP:N	2:D:76:ASP:OD1	2.54	0.40
1:C:274:PRO:HG3	1:C:291:ILE:HG21	2.02	0.40
2:D:133:GLN:HE21	2:D:252:LEU:CB	2.31	0.40
2:D:239:THR:O	2:D:240:THR:C	2.59	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ASP:CB	1:C:303:VAL:HA	2.51	0.40
2:B:260:VAL:HG23	2:B:260:VAL:O	2.22	0.40
1:C:317:LEU:HD23	1:C:317:LEU:HA	1.93	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%)	327 (77%)	53 (12%)	43 (10%)	1 11
1	C	415/451 (92%)	316 (76%)	59 (14%)	40 (10%)	1 12
2	B	415/445 (93%)	310 (75%)	58 (14%)	47 (11%)	0 9
2	D	415/445 (93%)	311 (75%)	56 (14%)	48 (12%)	0 9
3	E	120/142 (84%)	91 (76%)	21 (18%)	8 (7%)	1 21
All	All	1788/1934 (92%)	1355 (76%)	247 (14%)	186 (10%)	1 11

All (186) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	62	VAL
1	A	73	THR
1	A	178	SER
1	A	240	ALA
1	A	247	ALA
1	A	248	LEU
1	A	265	ILE
1	A	266	HIS
1	A	273	ALA
1	A	314	ALA

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Mol	Chain	Res	Type
1	A	345	ASP
1	A	348	PRO
1	A	349	THR
1	A	350	GLY
2	B	3	GLU
2	B	11	GLN
2	B	43	GLN
2	B	60	LYS
2	B	62	VAL
2	B	115	VAL
2	B	159	GLU
2	B	217	LEU
2	B	218	LYS
2	B	220	THR
2	B	245	PRO
2	B	264	ARG
2	B	265	LEU
2	B	266	HIS
2	B	273	ALA
2	B	288	VAL
2	B	348	PRO
2	B	371	LEU
2	B	400	ARG
2	B	404	PHE
1	C	11	GLN
1	C	55	GLU
1	C	62	VAL
1	C	73	THR
1	C	178	SER
1	C	240	ALA
1	C	253	THR
1	C	265	ILE
1	C	266	HIS
1	C	273	ALA
1	C	314	ALA
1	C	345	ASP
1	C	348	PRO
1	C	377	MET
2	D	3	GLU
2	D	11	GLN
2	D	42	LEU
2	D	43	GLN

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Mol	Chain	Res	Type
2	D	60	LYS
2	D	62	VAL
2	D	115	VAL
2	D	159	GLU
2	D	217	LEU
2	D	218	LYS
2	D	220	THR
2	D	264	ARG
2	D	265	LEU
2	D	266	HIS
2	D	273	ALA
2	D	276	THR
2	D	288	VAL
2	D	348	PRO
2	D	371	LEU
2	D	404	PHE
3	E	5	ASP
1	A	55	GLU
1	A	72	PRO
1	A	83	TYR
1	A	101	ASN
1	A	112	LYS
1	A	164	LYS
1	A	264	ARG
1	A	279	GLU
1	A	283	HIS
1	A	357	TYR
1	A	377	MET
2	B	34	GLY
2	B	42	LEU
2	B	73	GLY
2	B	82	PRO
2	B	163	ASP
2	B	225	GLY
2	B	226	ASP
2	B	227	LEU
2	B	249	ASN
2	B	276	THR
2	B	299	LYS
2	B	308	ARG
2	B	349	ASN
2	B	370	GLY

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Mol	Chain	Res	Type
2	B	402	LYS
2	B	403	ALA
1	C	72	PRO
1	C	83	TYR
1	C	144	GLY
1	C	164	LYS
1	C	246	GLY
1	C	305	CYS
1	C	350	GLY
1	C	357	TYR
1	C	403	ALA
2	D	34	GLY
2	D	73	GLY
2	D	82	PRO
2	D	109	THR
2	D	163	ASP
2	D	225	GLY
2	D	227	LEU
2	D	245	PRO
2	D	249	ASN
2	D	299	LYS
2	D	308	ARG
2	D	349	ASN
2	D	370	GLY
2	D	400	ARG
2	D	402	LYS
2	D	403	ALA
3	E	7	GLU
3	E	49	GLU
3	E	50	ILE
1	A	32	PRO
1	A	34	GLY
1	A	175	PRO
1	A	305	CYS
1	A	403	ALA
2	B	39	ASP
2	B	47	GLU
2	B	109	THR
2	B	244	PHE
2	B	246	GLY
2	B	252	LEU
2	B	340	SER

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Mol	Chain	Res	Type
1	C	59	GLY
1	C	112	LYS
1	C	175	PRO
1	C	257	THR
1	C	264	ARG
1	C	349	THR
2	D	226	ASP
2	D	244	PHE
2	D	340	SER
3	E	68	LEU
3	E	140	LYS
1	A	59	GLY
1	A	60	LYS
1	A	103	TYR
1	C	32	PRO
1	C	48	SER
1	C	101	ASN
1	C	109	THR
1	C	248	LEU
2	D	47	GLU
2	D	99	ALA
2	D	246	GLY
2	D	252	LEU
2	D	344	VAL
1	A	4	CYS
1	A	48	SER
1	A	109	THR
1	A	144	GLY
1	A	245	ASP
2	B	99	ALA
2	B	146	GLY
1	C	34	GLY
2	D	37	HIS
2	D	39	ASP
2	D	146	GLY
3	E	95	LYS
1	A	241	SER
2	B	250	ALA
2	B	344	VAL
1	C	4	CYS
1	C	241	SER
2	D	240	THR

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Mol	Chain	Res	Type
3	E	12	ASN
1	A	10	GLY
1	C	162	GLY
1	A	246	GLY
1	C	274	PRO
1	C	10	GLY
1	A	274	PRO

5.3.2 Protein sidechains

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%)	235 (68%)	111 (32%)	0	2
1	C	336/378 (89%)	229 (68%)	107 (32%)	0	3
2	B	348/381 (91%)	240 (69%)	108 (31%)	0	3
2	D	348/381 (91%)	241 (69%)	107 (31%)	0	3
3	E	78/126 (62%)	46 (59%)	32 (41%)	0	1
All	All	1456/1644 (89%)	991 (68%)	465 (32%)	0	3

All (465) 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	16	ILE
1	A	22	GLU
1	A	27	GLU
1	A	36	MET
1	A	50	ASN
1	A	62	VAL
1	A	68	VAL
1	A	73	THR
1	A	74	VAL

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Mol	Chain	Res	Type
1	A	79	ARG
1	A	80	THR
1	A	82	THR
1	A	85	GLN
1	A	87	PHE
1	A	88	HIS
1	A	90	GLU
1	A	91	GLN
1	A	94	THR
1	A	96	LYS
1	A	101	ASN
1	A	105	ARG
1	A	112	LYS
1	A	114	ILE
1	A	115	ILE
1	A	116	ASP
1	A	120	ASP
1	A	122	ILE
1	A	123	ARG
1	A	124	LYS
1	A	128	GLN
1	A	140	SER
1	A	141	PHE
1	A	145	THR
1	A	147	SER
1	A	153	LEU
1	A	163	LYS
1	A	164	LYS
1	A	165	SER
1	A	176	GLN
1	A	178	SER
1	A	182	VAL
1	A	183	GLU
1	A	187	SER
1	A	193	THR
1	A	194	THR
1	A	195	LEU
1	A	198	SER
1	A	199	ASP
1	A	200	CYS
1	A	206	ASN
1	A	210	TYR

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Mol	Chain	Res	Type
1	A	211	ASP
1	A	212	ILE
1	A	220	GLU
1	A	223	THR
1	A	224	TYR
1	A	225	THR
1	A	226	ASN
1	A	227	LEU
1	A	230	LEU
1	A	234	ILE
1	A	236	SER
1	A	241	SER
1	A	242	LEU
1	A	245	ASP
1	A	248	LEU
1	A	253	THR
1	A	254	GLU
1	A	255	PHE
1	A	256	GLN
1	A	257	THR
1	A	258	ASN
1	A	265	ILE
1	A	271	THR
1	A	279	GLU
1	A	283	HIS
1	A	287	SER
1	A	288	VAL
1	A	295	CYS
1	A	306	ASP
1	A	313	MET
1	A	315	CYS
1	A	316	CYS
1	A	329	ASN
1	A	340	THR
1	A	341	ILE
1	A	343	PHE
1	A	344	VAL
1	A	349	THR
1	A	355	ILE
1	A	356	ASN
1	A	358	GLU
1	A	362	VAL

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Mol	Chain	Res	Type
1	A	363	VAL
1	A	367	ASP
1	A	368	LEU
1	A	370	LYS
1	A	371	VAL
1	A	377	MET
1	A	379	SER
1	A	384	ILE
1	A	394	LYS
1	A	397	LEU
1	A	401	LYS
1	A	405	VAL
1	A	414	GLU
1	A	415	GLU
1	A	430	LYS
2	B	2	ARG
2	B	4	ILE
2	B	5	VAL
2	B	11	GLN
2	B	16	ILE
2	B	23	VAL
2	B	26	ASP
2	B	31	ASP
2	B	33	THR
2	B	36	TYR
2	B	39	ASP
2	B	40	SER
2	B	42	LEU
2	B	43	GLN
2	B	49	ILE
2	B	55	GLU
2	B	61	TYR
2	B	62	VAL
2	B	71	GLU
2	B	77	SER
2	B	80	SER
2	B	83	PHE
2	B	91	ASN
2	B	101	ASN
2	B	102	ASN
2	B	109	THR
2	B	120	ASP

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Mol	Chain	Res	Type
2	B	122	VAL
2	B	130	ASP
2	B	137	LEU
2	B	138	THR
2	B	141	LEU
2	B	147	SER
2	B	151	THR
2	B	154	ILE
2	B	155	SER
2	B	156	LYS
2	B	158	ARG
2	B	164	ARG
2	B	166	MET
2	B	170	SER
2	B	171	VAL
2	B	174	SER
2	B	176	LYS
2	B	177	VAL
2	B	179	ASP
2	B	181	VAL
2	B	190	SER
2	B	193	GLN
2	B	195	VAL
2	B	197	ASN
2	B	198	THR
2	B	200	GLU
2	B	209	LEU
2	B	212	ILE
2	B	216	THR
2	B	217	LEU
2	B	223	THR
2	B	224	TYR
2	B	226	ASP
2	B	230	LEU
2	B	241	CYS
2	B	242	LEU
2	B	243	ARG
2	B	244	PHE
2	B	248	LEU
2	B	251	ASP
2	B	253	ARG
2	B	257	VAL

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Mol	Chain	Res	Type
2	B	258	ASN
2	B	265	LEU
2	B	269	MET
2	B	275	LEU
2	B	276	THR
2	B	287	THR
2	B	292	THR
2	B	294	GLN
2	B	295	MET
2	B	300	ASN
2	B	302	MET
2	B	308	ARG
2	B	313	LEU
2	B	318	VAL
2	B	320	ARG
2	B	323	MET
2	B	325	MET
2	B	336	GLN
2	B	341	SER
2	B	345	GLU
2	B	350	ASN
2	B	357	ASP
2	B	358	ILE
2	B	371	LEU
2	B	374	SER
2	B	376	THR
2	B	380	ASN
2	B	384	ILE
2	B	390	ARG
2	B	400	ARG
2	B	401	ARG
2	B	402	LYS
2	B	405	LEU
2	B	415	GLU
2	B	416	MET
2	B	419	THR
2	B	423	SER
2	B	425	MET
2	B	430	SER
1	C	2	ARG
1	C	4	CYS
1	C	9	VAL

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Mol	Chain	Res	Type
1	C	16	ILE
1	C	20	CYS
1	C	22	GLU
1	C	27	GLU
1	C	36	MET
1	C	50	ASN
1	C	51	THR
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	82	THR
1	C	85	GLN
1	C	87	PHE
1	C	88	HIS
1	C	90	GLU
1	C	91	GLN
1	C	94	THR
1	C	97	GLU
1	C	101	ASN
1	C	105	ARG
1	C	110	ILE
1	C	112	LYS
1	C	114	ILE
1	C	115	ILE
1	C	116	ASP
1	C	120	ASP
1	C	122	ILE
1	C	123	ARG
1	C	124	LYS
1	C	128	GLN
1	C	140	SER
1	C	141	PHE
1	C	145	THR
1	C	147	SER
1	C	153	LEU
1	C	155	GLU
1	C	163	LYS
1	C	165	SER
1	C	176	GLN

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Mol	Chain	Res	Type
1	C	178	SER
1	C	182	VAL
1	C	183	GLU
1	C	187	SER
1	C	193	THR
1	C	194	THR
1	C	195	LEU
1	C	198	SER
1	C	199	ASP
1	C	200	CYS
1	C	206	ASN
1	C	211	ASP
1	C	212	ILE
1	C	220	GLU
1	C	223	THR
1	C	225	THR
1	C	226	ASN
1	C	227	LEU
1	C	230	LEU
1	C	234	ILE
1	C	241	SER
1	C	242	LEU
1	C	250	VAL
1	C	251	ASP
1	C	256	GLN
1	C	257	THR
1	C	258	ASN
1	C	265	ILE
1	C	271	THR
1	C	287	SER
1	C	288	VAL
1	C	306	ASP
1	C	313	MET
1	C	315	CYS
1	C	316	CYS
1	C	329	ASN
1	C	340	THR
1	C	341	ILE
1	C	343	PHE
1	C	344	VAL
1	C	349	THR
1	C	355	ILE

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Mol	Chain	Res	Type
1	C	356	ASN
1	C	358	GLU
1	C	362	VAL
1	C	363	VAL
1	C	367	ASP
1	C	368	LEU
1	C	370	LYS
1	C	371	VAL
1	C	377	MET
1	C	379	SER
1	C	381	THR
1	C	384	ILE
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	430	LYS
2	D	2	ARG
2	D	4	ILE
2	D	5	VAL
2	D	11	GLN
2	D	12	CYS
2	D	16	ILE
2	D	23	VAL
2	D	26	ASP
2	D	31	ASP
2	D	33	THR
2	D	36	TYR
2	D	39	ASP
2	D	40	SER
2	D	42	LEU
2	D	43	GLN
2	D	49	ILE
2	D	55	GLU
2	D	61	TYR
2	D	62	VAL
2	D	71	GLU
2	D	76	ASP
2	D	77	SER

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Mol	Chain	Res	Type
2	D	80	SER
2	D	83	PHE
2	D	91	ASN
2	D	101	ASN
2	D	102	ASN
2	D	109	THR
2	D	120	ASP
2	D	122	VAL
2	D	130	ASP
2	D	137	LEU
2	D	138	THR
2	D	141	LEU
2	D	147	SER
2	D	151	THR
2	D	154	ILE
2	D	155	SER
2	D	156	LYS
2	D	158	ARG
2	D	164	ARG
2	D	166	MET
2	D	170	SER
2	D	171	VAL
2	D	174	SER
2	D	176	LYS
2	D	177	VAL
2	D	179	ASP
2	D	181	VAL
2	D	190	SER
2	D	193	GLN
2	D	195	VAL
2	D	197	ASN
2	D	198	THR
2	D	200	GLU
2	D	209	LEU
2	D	216	THR
2	D	223	THR
2	D	224	TYR
2	D	226	ASP
2	D	230	LEU
2	D	241	CYS
2	D	242	LEU
2	D	243	ARG

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Mol	Chain	Res	Type
2	D	244	PHE
2	D	251	ASP
2	D	253	ARG
2	D	257	VAL
2	D	258	ASN
2	D	265	LEU
2	D	269	MET
2	D	275	LEU
2	D	276	THR
2	D	286	LEU
2	D	287	THR
2	D	292	THR
2	D	294	GLN
2	D	295	MET
2	D	300	ASN
2	D	302	MET
2	D	308	ARG
2	D	313	LEU
2	D	318	VAL
2	D	320	ARG
2	D	323	MET
2	D	325	MET
2	D	336	GLN
2	D	341	SER
2	D	345	GLU
2	D	350	ASN
2	D	357	ASP
2	D	358	ILE
2	D	371	LEU
2	D	374	SER
2	D	376	THR
2	D	380	ASN
2	D	384	ILE
2	D	400	ARG
2	D	401	ARG
2	D	402	LYS
2	D	405	LEU
2	D	415	GLU
2	D	416	MET
2	D	419	THR
2	D	423	SER
2	D	425	MET

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Mol	Chain	Res	Type
2	D	430	SER
3	E	6	MET
3	E	10	GLU
3	E	11	LEU
3	E	13	LYS
3	E	14	CYS
3	E	16	SER
3	E	24	LEU
3	E	28	SER
3	E	51	GLN
3	E	59	GLU
3	E	64	GLN
3	E	69	LEU
3	E	70	LYS
3	E	76	ARG
3	E	87	ILE
3	E	89	GLU
3	E	94	ILE
3	E	96	MET
3	E	98	LYS
3	E	99	GLU
3	E	101	LEU
3	E	105	MET
3	E	107	SER
3	E	113	GLU
3	E	115	HIS
3	E	119	MET
3	E	120	LEU
3	E	122	ARG
3	E	123	LEU
3	E	126	LYS
3	E	129	HIS
3	E	133	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	88	HIS
1	A	91	GLN
1	A	101	ASN
1	A	107	HIS

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Mol	Chain	Res	Type
1	A	133	GLN
1	A	139	HIS
1	A	176	GLN
1	A	206	ASN
1	A	249	ASN
1	A	258	ASN
1	A	266	HIS
1	A	301	GLN
1	A	329	ASN
1	A	372	GLN
1	A	380	ASN
2	B	6	HIS
2	B	43	GLN
2	B	54	ASN
2	B	136	GLN
2	B	139	HIS
2	B	294	GLN
2	B	300	ASN
2	B	331	GLN
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN
2	B	385	GLN
1	C	88	HIS
1	C	91	GLN
1	C	101	ASN
1	C	107	HIS
1	C	133	GLN
1	C	139	HIS
1	C	176	GLN
1	C	206	ASN
1	C	256	GLN
1	C	258	ASN
1	C	266	HIS
1	C	301	GLN
1	C	329	ASN
1	C	372	GLN
2	D	6	HIS
2	D	43	GLN
2	D	54	ASN
2	D	136	GLN
2	D	139	HIS

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Mol	Chain	Res	Type
2	D	294	GLN
2	D	300	ASN
2	D	339	ASN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
3	E	136	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	$\#\|Z\| > 2$
5	GTP	A	600	4	25,34,34	0.96	2 (8%)	34,54,54	1.77	7 (20%)
6	GDP	B	602	4	23,30,30	0.99	2 (8%)	30,47,47	1.92	6 (20%)
7	CN2	B	700	-	30,32,32	3.37	7 (23%)	28,45,45	2.81	15 (53%)
5	GTP	C	601	4	25,34,34	1.10	3 (12%)	34,54,54	2.05	11 (32%)
6	GDP	D	603	-	23,30,30	0.98	1 (4%)	30,47,47	1.71	5 (16%)
7	CN2	D	701	-	30,32,32	3.15	7 (23%)	28,45,45	3.21	10 (35%)

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
5	GTP	A	600	4	-	0/18/38/38	0/3/3/3
6	GDP	B	602	4	-	0/12/32/32	0/3/3/3
7	CN2	B	700	-	-	0/10/27/27	0/3/3/3
5	GTP	C	601	4	-	0/18/38/38	0/3/3/3
6	GDP	D	603	-	-	0/12/32/32	0/3/3/3
7	CN2	D	701	-	-	0/10/27/27	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	CN2	C20-C21	-11.02	1.23	1.40
7	D	701	CN2	C20-C21	-9.84	1.24	1.40
7	B	700	CN2	C19-C17	-8.90	1.23	1.39
7	D	701	CN2	C19-C17	-7.85	1.25	1.39
7	B	700	CN2	C19-C20	-6.72	1.20	1.40
7	D	701	CN2	C19-C20	-5.46	1.24	1.40
5	C	601	GTP	O4'-C4'	-2.26	1.39	1.45
7	B	700	CN2	C11-N1	-2.25	1.43	1.46
7	D	701	CN2	C11-N1	-2.17	1.43	1.46
5	A	600	GTP	O4'-C4'	-2.02	1.40	1.45
6	B	602	GDP	O4'-C4'	-2.01	1.40	1.45
5	C	601	GTP	C2-N1	2.07	1.39	1.35
7	B	700	CN2	C22-C8	2.43	1.44	1.40
5	A	600	GTP	C6-N1	2.58	1.37	1.33
7	D	701	CN2	C22-C8	2.62	1.45	1.40
6	D	603	GDP	C6-N1	2.69	1.38	1.33
6	B	602	GDP	C6-N1	2.73	1.38	1.33
5	C	601	GTP	C6-N1	3.55	1.39	1.33
7	B	700	CN2	O6-C17	4.92	1.45	1.37
7	D	701	CN2	O6-C17	5.38	1.45	1.37
7	B	700	CN2	C15-C16	6.71	1.52	1.39
7	D	701	CN2	C15-C16	7.42	1.54	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	701	CN2	C10-C11-N1	-8.72	94.02	109.96
7	D	701	CN2	C13-C12-N1	-6.42	104.82	115.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	602	GDP	C2'-C1'-N9	-6.05	105.05	114.29
6	D	603	GDP	N3-C2-N1	-5.27	119.42	127.44
5	C	601	GTP	N3-C2-N1	-5.25	119.45	127.44
7	B	700	CN2	C10-C11-N1	-5.19	100.47	109.96
6	B	602	GDP	N3-C2-N1	-5.03	119.78	127.44
5	A	600	GTP	PB-O3B-PG	-4.78	116.66	132.67
7	D	701	CN2	O3-C5-C7	-4.54	116.45	124.21
7	D	701	CN2	C10-C9-C8	-4.27	103.39	113.62
5	A	600	GTP	N3-C2-N1	-3.77	121.69	127.44
5	C	601	GTP	PB-O3B-PG	-3.72	120.21	132.67
7	B	700	CN2	C21-C22-C8	-3.66	116.67	120.63
5	C	601	GTP	O3'-C3'-C4'	-3.33	101.07	111.05
5	C	601	GTP	C1'-N9-C4	-3.27	122.01	126.94
7	B	700	CN2	C12-C13-S1	-3.16	98.77	111.92
6	D	603	GDP	C5-C6-N1	-3.02	119.46	123.59
7	D	701	CN2	C21-C22-C8	-2.97	117.42	120.63
5	C	601	GTP	PA-O3A-PB	-2.96	124.40	132.73
7	B	700	CN2	C10-C9-C8	-2.95	106.56	113.62
7	B	700	CN2	O3-C5-C7	-2.89	119.28	124.21
6	D	603	GDP	C4-C5-N7	-2.77	106.93	109.48
7	B	700	CN2	C9-C8-C22	-2.69	116.68	119.24
5	A	600	GTP	C5-C6-N1	-2.66	119.96	123.59
5	A	600	GTP	O3'-C3'-C4'	-2.65	103.10	111.05
6	B	602	GDP	C5-C6-N1	-2.60	120.03	123.59
5	C	601	GTP	C5-C6-N1	-2.57	120.07	123.59
5	A	600	GTP	PA-O3A-PB	-2.33	126.19	132.73
6	B	602	GDP	PA-O3A-PB	-2.28	125.02	132.67
7	B	700	CN2	C13-C12-N1	-2.15	111.87	115.43
5	C	601	GTP	C6-C5-C4	-2.01	118.50	120.90
7	B	700	CN2	C9-C8-C7	2.00	123.47	119.10
6	B	602	GDP	C2'-C3'-C4'	2.09	106.91	102.61
7	B	700	CN2	O4-C12-N1	2.17	126.70	123.01
5	C	601	GTP	C4'-O4'-C1'	2.26	112.20	109.72
7	B	700	CN2	C18-O6-C17	2.27	120.98	117.54
5	A	600	GTP	N2-C2-N1	2.36	121.11	117.20
7	B	700	CN2	C4-O2-C3	2.38	121.08	114.82
7	B	700	CN2	C21-C22-C1	2.62	124.88	121.05
5	C	601	GTP	N2-C2-N1	2.64	121.57	117.20
7	D	701	CN2	O4-C12-N1	2.76	127.69	123.01
6	B	602	GDP	C6-N1-C2	2.77	119.78	115.94
6	D	603	GDP	C6-N1-C2	3.00	120.10	115.94
5	A	600	GTP	C2'-C1'-N9	3.00	118.88	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	700	CN2	O3-C5-C3	3.02	120.72	115.26
5	C	601	GTP	C6-N1-C2	3.04	120.16	115.94
7	D	701	CN2	O3-C5-C3	3.32	121.25	115.26
7	D	701	CN2	O4-C12-C13	3.36	127.48	121.47
7	D	701	CN2	C4-O2-C3	3.37	123.69	114.82
6	D	603	GDP	C4'-O4'-C1'	3.40	113.46	109.72
7	B	700	CN2	C6-O3-C5	3.56	122.95	117.54
5	C	601	GTP	C2'-C1'-N9	4.64	121.39	114.29
7	D	701	CN2	C20-C19-C17	7.91	142.63	130.90
7	B	700	CN2	C20-C19-C17	9.61	145.16	130.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	GTP	4	0
6	B	602	GDP	2	0
7	B	700	CN2	12	0
5	C	601	GTP	2	0
6	D	603	GDP	1	0
7	D	701	CN2	8	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.