



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:59 PM UTC

PDB ID : 1SA0 / pdb_00001sa0
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

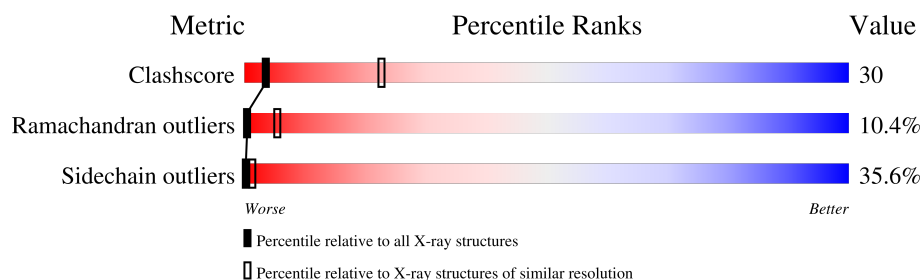
1 Overall quality at a glance

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	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	451	
1	C	451	
2	B	445	
2	D	445	
3	E	142	

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	-
7	CN2	D	701	-	-	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			

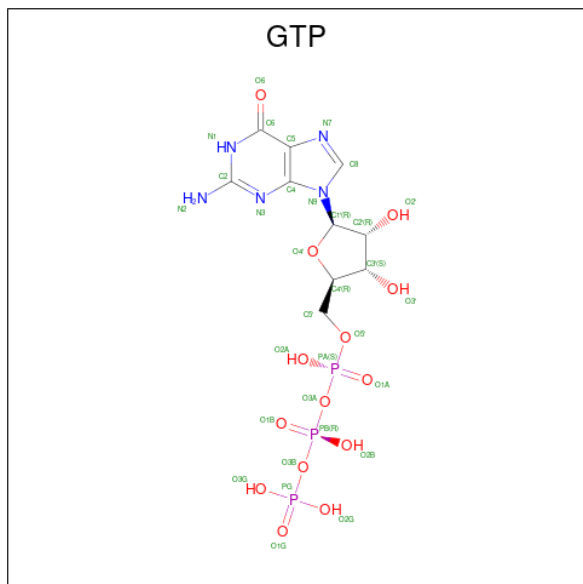
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

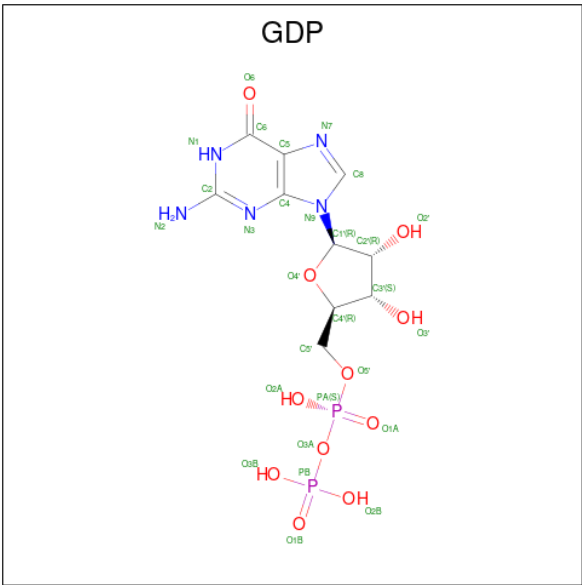
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0

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



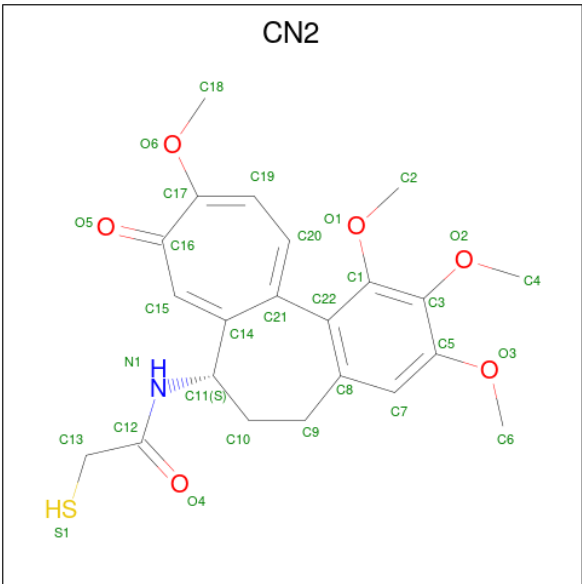
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O P 32 10 5 14 3	0	0
5	C	1	Total C N O P 32 10 5 14 3	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: 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 (CCD ID: CN2) (formula: C₂₂H₂₅NO₆S).



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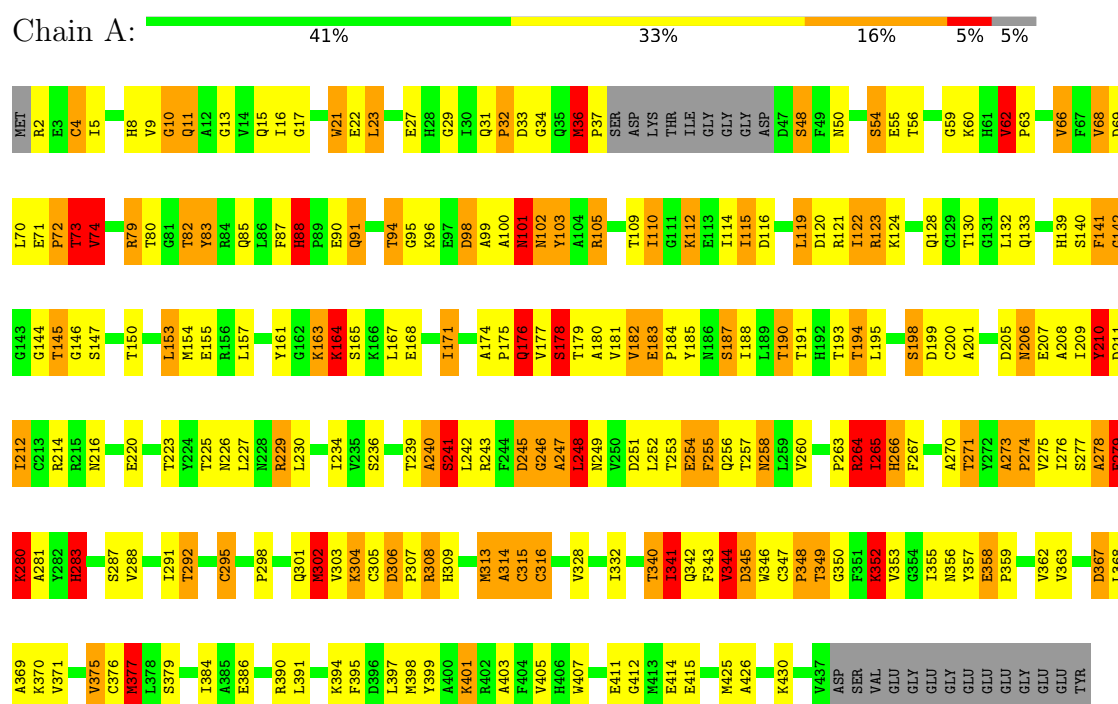
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	S	0	0
			30	22	1	6	1		

3 Residue-property plots

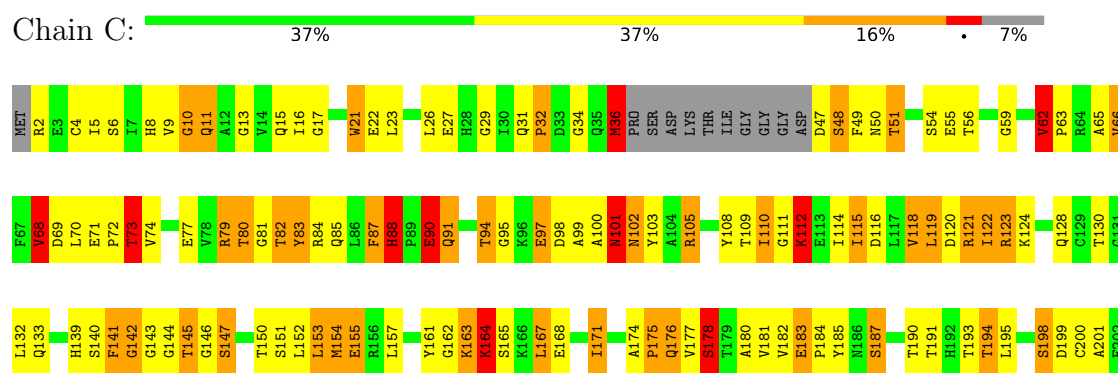
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

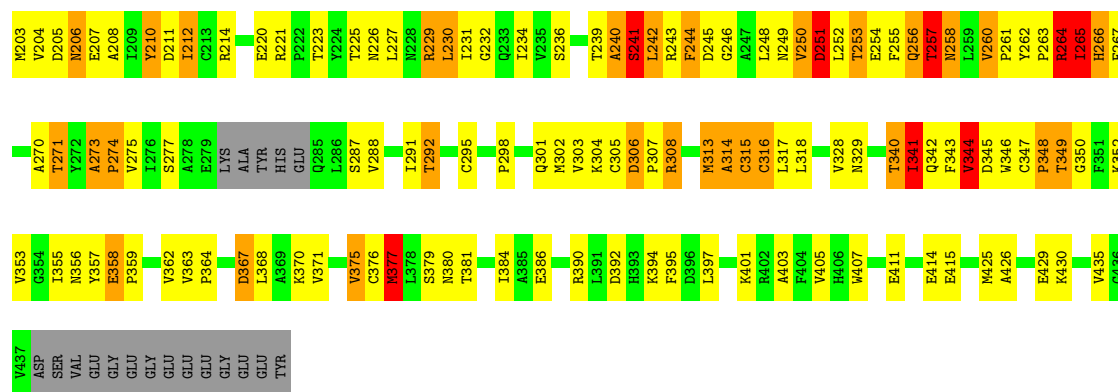
Note EDS was not executed.

• Molecule 1: Tubulin alpha chain

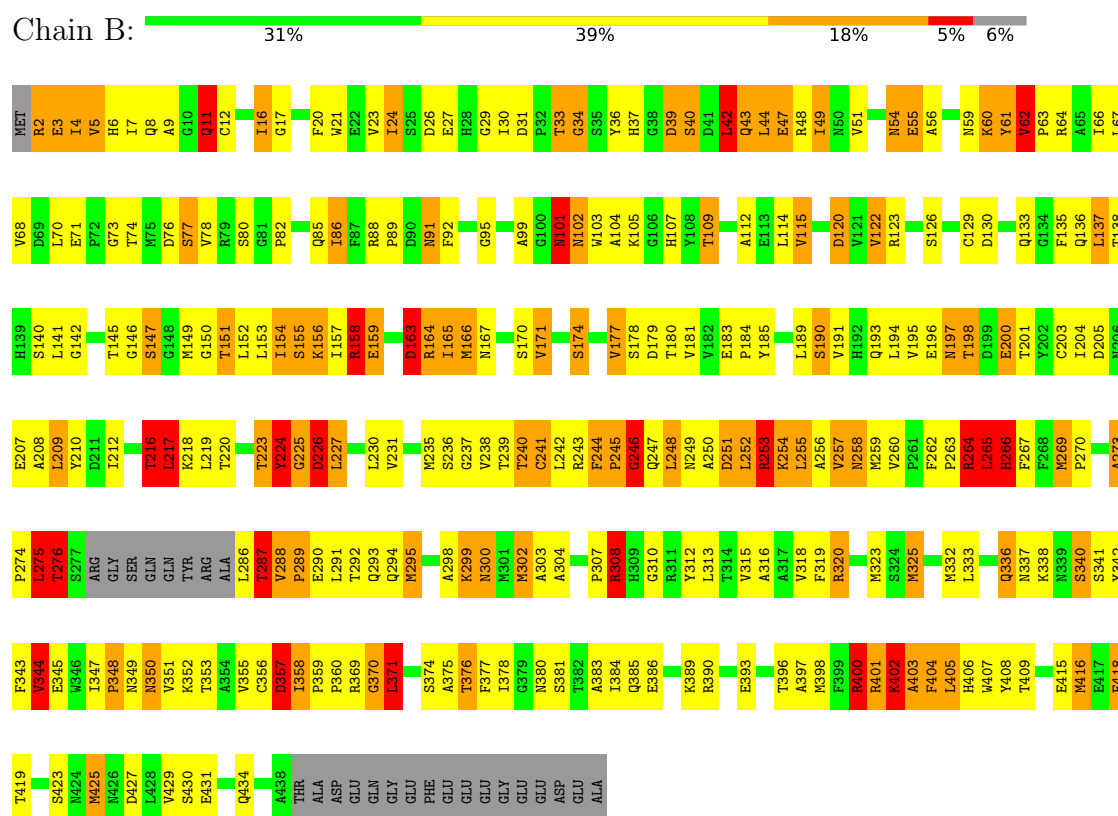


• Molecule 1: Tubulin alpha chain

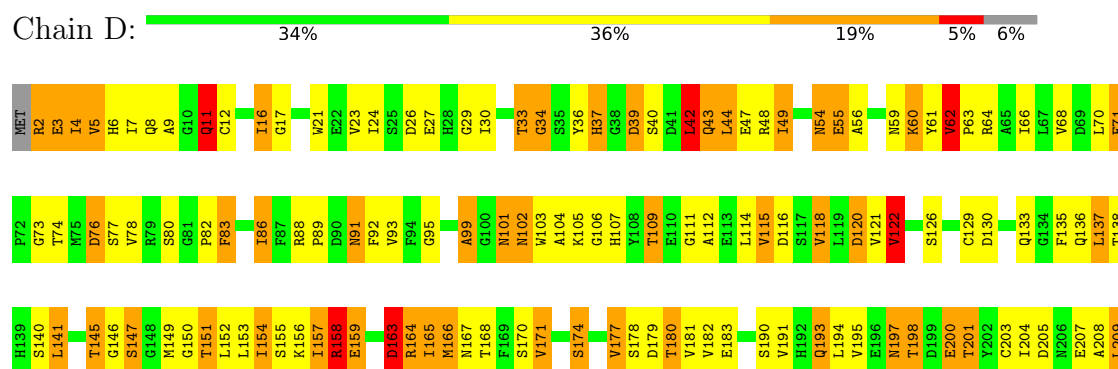


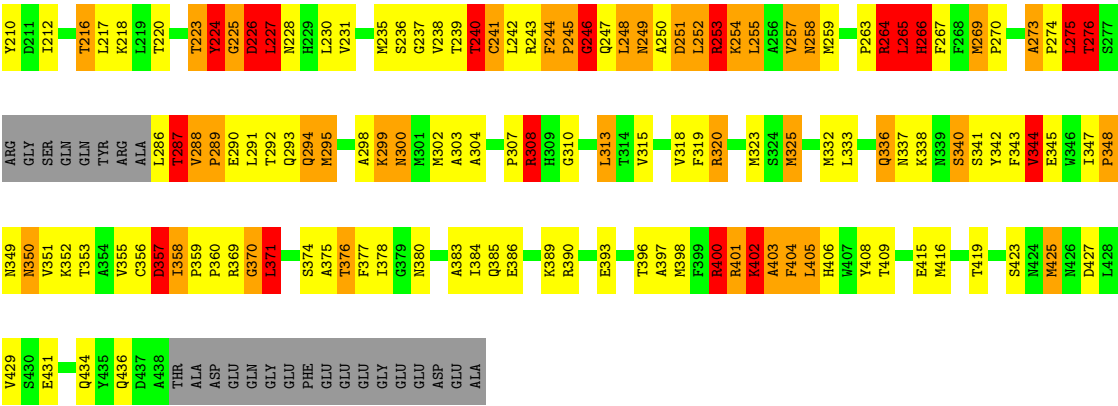


• Molecule 2: Tubulin beta chain

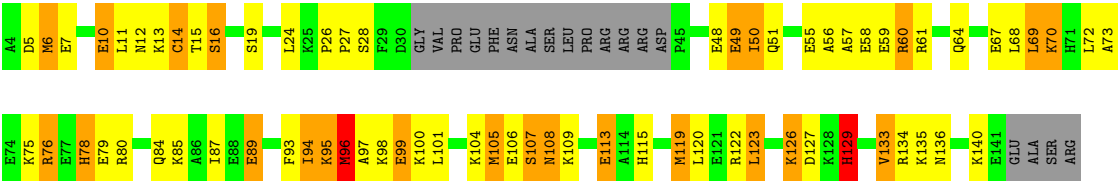
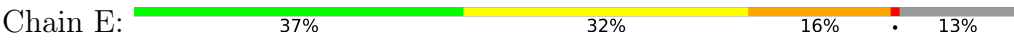


• Molecule 2: Tubulin beta chain





● Molecule 3: Stathmin 4



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CN2, GTP, GDP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.89	3/3368 (0.1%)	1.30	30/4581 (0.7%)
1	C	0.84	5/3292 (0.2%)	1.30	28/4479 (0.6%)
2	B	0.82	4/3308 (0.1%)	1.31	35/4494 (0.8%)
2	D	0.79	1/3309 (0.0%)	1.31	33/4494 (0.7%)
3	E	0.96	2/915 (0.2%)	1.57	24/1230 (2.0%)
All	All	0.84	15/14192 (0.1%)	1.32	150/19278 (0.8%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	96	MET	SD-CE	8.90	2.01	1.79
1	A	36	MET	SD-CE	7.79	1.99	1.79
3	E	105	MET	SD-CE	7.78	1.99	1.79
1	C	341	ILE	CA-CB	6.45	1.61	1.54
1	C	250	VAL	CA-CB	6.24	1.61	1.54
1	C	203	MET	SD-CE	6.03	1.94	1.79
2	B	325	MET	SD-CE	5.89	1.94	1.79
1	A	341	ILE	CA-CB	5.77	1.60	1.54
2	B	216	THR	CA-CB	5.70	1.59	1.53
1	C	36	MET	SD-CE	5.23	1.92	1.79
1	C	250	VAL	CA-C	5.16	1.58	1.52
1	A	302	MET	SD-CE	-5.13	1.66	1.79
2	B	276	THR	CA-CB	5.03	1.61	1.53
2	B	416	MET	SD-CE	5.01	1.92	1.79
2	D	145	THR	CA-CB	5.01	1.61	1.53

All (150) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	244	PHE	N-CA-C	12.50	129.26	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	51	GLN	N-CA-C	-9.19	101.77	113.72
1	C	142	GLY	N-CA-C	-8.93	98.77	112.89
1	A	142	GLY	N-CA-C	-8.86	98.89	112.89
3	E	93	PHE	N-CA-C	-8.85	102.40	113.55
1	C	344	VAL	N-CA-C	8.81	121.48	107.73
1	A	344	VAL	N-CA-C	8.50	120.98	107.73
3	E	56	ALA	N-CA-C	-8.47	103.46	113.88
2	D	253	ARG	N-CA-C	-8.38	102.64	113.12
1	C	251	ASP	N-CA-C	8.35	123.00	111.74
3	E	100	LYS	N-CA-C	-8.27	103.32	113.41
2	B	244	PHE	N-CA-C	8.27	128.09	109.81
3	E	78	HIS	N-CA-C	-8.19	102.74	114.12
2	D	436	GLN	N-CA-C	-8.16	100.37	110.65
2	D	244	PHE	N-CA-C	8.06	127.61	109.81
2	D	86	ILE	N-CA-C	8.05	118.83	110.62
2	B	158	ARG	N-CA-C	-8.04	98.37	110.28
3	E	126	LYS	N-CA-C	-7.97	100.64	111.55
1	C	210	TYR	N-CA-C	-7.93	102.64	111.28
3	E	107	SER	N-CA-C	-7.86	102.03	111.69
2	B	287	THR	N-CA-C	7.83	120.91	111.82
3	E	106	GLU	N-CA-C	-7.82	104.63	114.56
2	B	86	ILE	N-CA-C	7.72	118.50	110.62
3	E	98	LYS	N-CA-C	-7.60	103.62	113.12
2	D	224	TYR	N-CA-C	-7.51	103.38	112.54
1	A	62	VAL	N-CA-C	7.47	125.01	108.88
1	A	280	LYS	N-CA-C	-7.46	103.91	113.16
2	B	338	LYS	N-CA-C	-7.46	104.06	113.01
2	B	224	TYR	N-CA-C	-7.34	103.59	112.54
2	D	158	ARG	N-CA-C	-7.32	99.61	110.23
1	A	210	TYR	N-CA-C	-7.32	103.30	111.28
1	C	359	PRO	N-CA-C	7.28	117.46	110.47
2	D	287	THR	N-CA-C	7.25	120.22	111.82
3	E	79	GLU	N-CA-C	-7.24	103.41	112.90
1	C	62	VAL	N-CA-C	7.19	124.40	108.88
2	D	4	ILE	N-CA-C	7.19	118.83	108.48
2	D	275	LEU	N-CA-C	7.12	119.58	108.96
1	A	5	ILE	N-CA-C	7.11	118.28	108.89
2	B	308	ARG	N-CA-C	-7.00	95.88	110.80
2	D	101	ASN	N-CA-C	-6.97	104.08	112.58
3	E	96	MET	N-CA-C	-6.96	106.69	114.62
1	A	21	TRP	N-CA-C	-6.95	104.28	112.89
2	B	44	LEU	N-CA-C	6.78	119.51	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	275	LEU	N-CA-C	6.74	119.00	108.96
2	B	266	HIS	CB-CA-C	6.73	123.81	110.42
2	B	253	ARG	N-CA-C	-6.69	103.15	112.45
2	B	4	ILE	N-CA-C	6.64	118.04	108.48
1	C	5	ILE	N-CA-C	6.60	117.60	108.89
1	A	359	PRO	N-CA-C	6.54	116.75	110.47
2	D	308	ARG	N-CA-C	-6.54	96.88	110.80
2	D	9	ALA	N-CA-C	6.53	120.14	109.24
3	E	134	ARG	N-CA-C	-6.52	96.91	110.80
1	C	308	ARG	N-CA-C	-6.51	105.30	113.18
2	D	122	VAL	N-CA-C	-6.41	104.24	110.72
1	C	250	VAL	N-CA-C	6.39	117.29	109.30
2	B	54	ASN	N-CA-C	-6.34	100.45	109.96
2	D	44	LEU	N-CA-C	6.31	120.08	112.38
2	D	54	ASN	N-CA-C	-6.29	99.75	109.76
2	D	165	ILE	N-CA-C	6.24	118.64	108.97
1	C	358	GLU	CA-C-N	6.22	124.20	119.66
1	C	358	GLU	C-N-CA	6.22	124.20	119.66
2	D	338	LYS	N-CA-C	-6.17	105.60	113.01
2	D	289	PRO	N-CA-C	-6.16	104.58	113.75
1	A	95	GLY	N-CA-C	6.15	127.76	113.18
1	C	264	ARG	CA-C-N	6.14	133.03	121.97
1	C	264	ARG	C-N-CA	6.14	133.03	121.97
2	B	264	ARG	CA-C-N	6.14	133.27	121.54
2	B	264	ARG	C-N-CA	6.14	133.27	121.54
2	B	289	PRO	N-CA-C	-6.13	104.61	113.75
1	A	308	ARG	N-CA-C	-6.12	105.67	113.01
1	C	88	HIS	N-CA-C	-6.11	102.39	110.40
1	A	426	ALA	N-CA-C	-6.10	104.72	111.36
3	E	10	GLU	N-CA-C	6.07	119.88	107.69
1	A	98	ASP	N-CA-C	6.05	118.52	110.53
2	D	254	LYS	N-CA-C	-6.04	104.69	111.28
1	C	95	GLY	N-CA-C	6.00	127.40	113.18
1	C	21	TRP	N-CA-C	-5.97	105.48	112.89
1	A	352	LYS	N-CA-C	-5.96	99.43	108.67
2	D	180	THR	N-CA-C	5.95	119.18	109.24
1	A	292	THR	N-CA-C	-5.95	104.71	111.07
2	D	197	ASN	N-CA-C	5.95	119.85	112.59
3	E	6	MET	N-CA-C	5.94	120.83	112.93
3	E	70	LYS	N-CA-C	-5.93	105.31	112.54
1	A	68	VAL	CB-CA-C	-5.91	100.94	110.28
2	D	121	VAL	N-CA-C	-5.88	107.08	112.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	358	GLU	CA-C-N	5.86	123.94	119.66
1	A	358	GLU	C-N-CA	5.86	123.94	119.66
2	B	120	ASP	CB-CA-C	5.84	120.92	110.81
1	C	102	ASN	N-CA-C	5.84	117.90	107.80
2	D	264	ARG	CA-C-N	5.83	132.67	121.54
2	D	264	ARG	C-N-CA	5.83	132.67	121.54
1	C	185	TYR	N-CA-C	-5.83	104.62	110.97
2	D	266	HIS	CB-CA-C	5.82	122.01	110.42
1	C	352	LYS	N-CA-C	-5.82	99.33	108.63
1	A	102	ASN	N-CA-C	5.80	117.84	107.80
2	B	9	ALA	N-CA-C	5.80	118.92	109.24
2	D	357	ASP	N-CA-C	5.74	119.27	112.72
1	A	376	CYS	N-CA-C	5.72	120.79	113.18
1	A	264	ARG	CA-C-N	5.71	132.25	121.97
1	A	264	ARG	C-N-CA	5.71	132.25	121.97
1	C	118	VAL	N-CA-C	-5.71	105.54	110.74
3	E	104	LYS	N-CA-C	-5.70	107.32	114.56
3	E	135	LYS	N-CA-C	-5.69	106.32	113.20
3	E	60	ARG	N-CA-C	-5.67	107.01	114.04
2	B	246	GLY	N-CA-C	-5.64	99.81	113.18
1	C	68	VAL	CB-CA-C	-5.64	101.37	110.28
2	D	118	VAL	N-CA-C	-5.62	106.23	111.45
1	A	265	ILE	N-CA-C	5.60	120.99	109.34
2	B	197	ASN	N-CA-C	5.58	119.62	112.26
1	A	278	ALA	N-CA-C	-5.57	103.14	110.43
1	A	176	GLN	N-CA-C	5.55	117.19	111.03
2	B	122	VAL	N-CA-C	-5.53	104.17	111.09
1	A	185	TYR	N-CA-C	-5.52	104.95	110.97
3	E	84	GLN	N-CA-C	5.49	118.10	111.40
2	B	101	ASN	N-CA-C	-5.47	105.23	112.24
3	E	80	ARG	N-CA-C	-5.47	105.40	111.36
1	C	260	VAL	N-CA-C	5.47	113.89	107.77
1	A	216	ASN	N-CA-C	5.47	119.62	112.13
2	B	196	GLU	N-CA-C	5.46	118.40	111.69
2	D	157	ILE	N-CA-C	-5.41	105.57	110.82
1	C	265	ILE	N-CA-C	5.40	120.57	109.34
1	A	88	HIS	N-CA-C	-5.40	103.38	110.39
3	E	129	HIS	N-CA-C	-5.37	106.78	113.55
1	C	359	PRO	O-C-N	5.36	123.78	121.31
2	D	246	GLY	N-CA-C	-5.36	100.49	113.18
1	C	426	ALA	N-CA-C	-5.35	105.53	111.36
3	E	73	ALA	N-CA-C	-5.34	106.60	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	120	ASP	N-CA-C	5.33	118.90	112.93
3	E	108	ASN	N-CA-C	5.31	116.93	111.03
2	D	163	ASP	N-CA-CB	-5.31	101.52	110.49
2	B	56	ALA	N-CA-C	5.28	117.49	109.63
2	B	180	THR	N-CA-C	5.23	117.97	109.24
2	B	163	ASP	N-CA-CB	-5.22	101.67	110.49
1	C	90	GLU	CB-CA-C	-5.18	102.04	110.85
2	B	371	LEU	N-CA-C	5.15	121.78	110.80
2	D	371	LEU	N-CA-C	5.15	121.78	110.80
2	B	357	ASP	N-CA-C	5.15	118.87	112.59
1	A	23	LEU	N-CA-C	-5.14	105.75	112.23
2	D	56	ALA	N-CA-C	5.14	117.29	109.63
1	A	74	VAL	N-CA-C	5.13	115.34	110.42
2	B	418	PHE	N-CA-C	-5.12	105.15	111.40
1	A	260	VAL	N-CA-C	5.12	113.50	107.77
2	B	165	ILE	N-CA-C	5.12	116.91	108.97
2	B	120	ASP	CA-CB-CG	5.11	117.71	112.60
2	B	142	GLY	N-CA-C	-5.11	104.82	112.89
3	E	75	LYS	N-CA-C	-5.05	105.67	111.07
1	C	292	THR	N-CA-C	-5.04	105.86	111.36
2	B	51	VAL	N-CA-C	5.04	116.37	110.62
2	D	227	LEU	N-CA-C	-5.04	100.07	110.80
2	B	254	LYS	N-CA-C	-5.02	105.80	111.28

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	162	0
1	C	3220	0	3074	188	0
2	B	3236	0	3058	226	0
2	D	3237	0	3060	229	0
3	E	907	0	781	33	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
7	D	30	0	23	9	0
All	All	14074	0	13222	808	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 30.

All (808) 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:CE	3:E:96:MET:SD	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
1:A:79:ARG:NH2	1:A:94:THR:HG21	1.68	1.09
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H43	7:B:700:CN2:H62	1.48	0.92
1:C:273:ALA:CB	1:C:375:VAL:H	1.82	0.92
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.50	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
1:A:273:ALA:CB	1:A:274:PRO:CD	2.52	0.86
2:B:316:ALA:CB	7:B:700:CN2:C2	2.38	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:HD12	2:D:265:LEU:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HD23	1:A:110:ILE:HG23	1.59	0.82
2:D:191:VAL:HG11	2:D:425:MET:HE3	1.60	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:HG3	2:B:308:ARG:HH11	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
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.46	0.81
2:B:247:GLN:HG2	2:B:248:LEU:H	1.44	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
1:C:341:ILE:HG12	1:C:342:GLN:N	1.95	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
2:B:251:ASP:C	2:B:253:ARG:H	1.90	0.79
1:A:247:ALA:HB1	3:E:19:SER:CB	2.13	0.79
1:C:229:ARG:HG2	1:C:229:ARG:HH11	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:B:191:VAL:HG11	2:B:425:MET:HE3	1.65	0.78
1:A:209:ILE:HD11	1:A:302:MET:HE3	1.64	0.78
2:D:231:VAL:HG12	2:D:235:MET:HE2	1.66	0.77
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:D:251:ASP:C	2:D:253:ARG:H	1.94	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:A:176:GLN:H	1:A:176:GLN:NE2	1.85	0.74
1:C:70:LEU:HD23	1:C:110:ILE:HG23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:403:ALA:C	2:B:405:LEU:H	1.97	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
1:C:181:VAL:HB	2:D:258:ASN:ND2	2.05	0.72
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.30	0.72
1:A:270:ALA:O	1:A:302:MET:HG3	1.89	0.72
2:B:140:SER:HA	2:B:171:VAL:HG23	1.70	0.72
2:D:247:GLN:HG3	2:D:248:LEU:HG	1.71	0.72
1:A:101:ASN:HD22	2:B:254:LYS:HG2	1.56	0.71
2:B:164:ARG:HE	2:B:164:ARG:HA	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:B:369:ARG:O	2:B:370:GLY:C	2.35	0.70
2:D:369:ARG:O	2:D:370:GLY:C	2.35	0.70
2:B:120:ASP:HB3	2:B:123:ARG:HH12	1.57	0.70
2:D:319:PHE:HB2	2:D:355:VAL:HG12	1.73	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
2:B:155:SER:HB3	3:E:76:ARG:HH22	1.58	0.69
1:C:70:LEU:N	1:C:70:LEU:HD12	2.08	0.69
2:D:140:SER:HA	2:D:171:VAL:HG23	1.74	0.68
2:D:307:PRO:O	2:D:308:ARG:CD	2.41	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:337:ASN:HA	2:B:340:SER:HB3	1.74	0.68
1:A:133:GLN:NE2	1:A:252:LEU:HG	2.08	0.68
2:B:231:VAL:HG12	2:B:235:MET:HE2	1.74	0.68
2:D:247:GLN:CG	2:D:248:LEU:N	2.56	0.68
7:B:700:CN2:C12	7:B:700:CN2:H15	2.22	0.68
2:D:54:ASN:HB2	2:D:64:ARG:HD3	1.75	0.68
2:D:133:GLN:HE21	2:D:252:LEU:HB3	1.59	0.68
2:D:164:ARG:HE	2:D:164:ARG:HA	1.57	0.68
2:D:337:ASN:HA	2:D:340:SER:HB3	1.75	0.68
1:A:176:GLN:H	1:A:176:GLN:HE21	1.43	0.67
1:C:123:ARG:HD3	1:C:161:TYR:OH	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.77	0.67
2:B:54:ASN:HB2	2:B:64:ARG:HD3	1.75	0.67
2:D:238:VAL:HG13	2:D:378:ILE:HD11	1.76	0.67
2:D:350:ASN:HD22	2:D:350:ASN:H	1.43	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:403:ALA:C	2:D:405:LEU:H	2.03	0.66
2:D:289:PRO:O	2:D:293:GLN:HG3	1.96	0.66
2:B:308:ARG:HG3	2:B:308:ARG:NH1	2.11	0.65
2:B:42:LEU:O	2:B:44:LEU:N	2.30	0.65
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.77	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
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:D:308:ARG:HG3	2:D:308:ARG:NH1	2.11	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
2:B:247:GLN:CG	2:B:248:LEU:N	2.61	0.64
1:C:273:ALA:HB2	1:C:375:VAL:N	2.10	0.64
7:D:701:CN2:H62	7:D:701:CN2:H43	1.80	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
1:A:412:GLY:O	3:E:60:ARG:NH1	2.31	0.64
2:D:247:GLN:HG2	2:D:248:LEU:N	2.13	0.64
2:B:287:THR:CG2	2:B:290:GLU:HG3	2.29	0.63
1:C:100:ALA:O	1:C:101:ASN:CB	2.46	0.63
1:A:229:ARG:HH11	1:A:229:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:120:ASP:HB3	2:B:123:ARG:NH1	2.13	0.63
1:C:98:ASP:OD1	1:C:99:ALA:N	2.32	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:180:ALA:O	1:A:183:GLU:HB2	2.00	0.62
1:A:249:ASN:HB3	1:A:255:PHE:CE2	2.34	0.62
2:D:266:HIS:CD2	2:D:266:HIS:H	2.17	0.62
2:D:401:ARG:HG3	2:D:401:ARG:HH11	1.63	0.62
1:A:123:ARG:HD3	1:A:161:TYR:OH	1.99	0.62
2:B:224:TYR:OH	6:B:602:GDP:H2'	2.00	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:H	2:B:350:ASN:HD22	1.48	0.62
2:B:36:TYR:HH	2:B:40:SER:C	2.05	0.62
1:A:308:ARG:HA	1:A:340:THR:HG21	1.82	0.61
3:E:129:HIS:O	3:E:133:VAL:HG23	2.00	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: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
2:D:287:THR:HG22	2:D:290:GLU:HG3	1.82	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: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:B:401:ARG:HG3	2:B:401:ARG:HH11	1.66	0.60
2:D:126:SER:O	2:D:129:CYS:HB2	2.01	0.60
2:D:205:ASP:OD2	2:D:390:ARG:NH1	2.34	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:69:ASP:C	1:C:70:LEU:HD12	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:GLN:H	1:C:176:GLN:NE2	1.98	0.60
2:D:158:ARG:O	2:D:159:GLU:CB	2.49	0.60
2:D:223:THR:HB	2:D:225:GLY:H	1.65	0.60
1:A:66:VAL:HG11	1:A:122:ILE:HG22	1.83	0.60
2:D:36:TYR:HH	2:D:40:SER:C	2.08	0.60
2:B:407:TRP:NE1	1:C:257:THR:HA	2.16	0.60
1:C:229:ARG:HH11	1:C:229:ARG:CG	2.14	0.60
2:D:151:THR:HB	2:D:193:GLN:HG2	1.83	0.60
2:D:158:ARG:O	2:D:159:GLU:HB2	2.00	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
2:B:136:GLN:HA	2:B:167:ASN:O	2.02	0.59
1:C:264:ARG:O	1:C:266:HIS:CD2	2.56	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:HB2	2.01	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: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
2:B:396:THR:HG22	2:B:400:ARG:HH21	1.68	0.59
1:C:168:GLU:HG2	1:C:201:ALA:HB2	1.85	0.59
1:C:256:GLN:C	1:C:258:ASN:H	2.10	0.58
1:C:70:LEU:N	1:C:70:LEU:CD1	2.65	0.58
2:D:408:TYR:O	2:D:409:THR:C	2.45	0.58
3:E:67:GLU:C	3:E:69:LEU:H	2.11	0.58
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.85	0.58
2:B:352:LYS:HG3	7:B:700:CN2:O5	2.03	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
1:C:252:LEU:O	1:C:253:THR:C	2.45	0.58
2:D:275:LEU:O	2:D:276:THR:HB	2.03	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ASN:CB	1:C:255:PHE:CD2	2.87	0.57
2:B:251:ASP:C	2:B:253:ARG:N	2.61	0.57
1:C:256:GLN:C	1:C:258:ASN:N	2.59	0.57
1:C:301:GLN:HE22	1:C:307:PRO:HD3	1.69	0.57
1:C:308:ARG:HA	1:C:340:THR:HG21	1.85	0.57
1:C:313:MET:O	1:C:314:ALA:HB2	2.04	0.57
1:A:246:GLY:HA2	3:E:14:CYS:HB2	1.85	0.57
2:B:336:GLN:CD	2:B:351:VAL:HG11	2.28	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
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
3:E:57:ALA:HA	3:E:60:ARG:NH1	2.20	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:C:265:ILE:HG22	1:C:267:PHE:CZ	2.40	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
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
2:D:357:ASP:OD2	2:D:357:ASP:N	2.38	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
2:D:287:THR:CG2	2:D:289:PRO:HD2	2.31	0.56
2:D:336:GLN:CD	2:D:351:VAL:HG11	2.30	0.56
1:A:239:THR:O	1:A:240:ALA:C	2.48	0.56
1:A:265:ILE:CG2	1:A:267:PHE:CZ	2.88	0.56
2:B:3:GLU:HG2	2:B:64:ARG:NH2	2.20	0.56
2:B:287:THR:O	2:B:288:VAL:HB	2.05	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:HG23	2:D:358:ILE:O	2.05	0.56
1:A:346:TRP:CE3	1:A:347:CYS:HB2	2.40	0.56
2:B:135:PHE:HB2	2:B:166:MET:HE2	1.88	0.56
2:B:164:ARG:HE	2:B:164:ARG:CA	2.16	0.56
2:B:216:THR:HG21	2:B:299:LYS:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:240:THR:HG21	2:B:320:ARG:NE	2.21	0.56
2:D:263:PRO:O	2:D:265:LEU:N	2.31	0.56
1:A:264:ARG:O	1:A:266:HIS:CD2	2.59	0.56
2:B:342:TYR:N	2:B:342:TYR:CD2	2.74	0.56
1:C:181:VAL:HB	2:D:258:ASN:HD22	1.69	0.56
2:D:5:VAL:HG22	2:D:135:PHE:CD2	2.41	0.56
2:D:266:HIS:HB3	2:D:380:ASN:HD21	1.70	0.56
1:A:122:ILE:HD11	1:A:157:LEU:HD21	1.88	0.55
2:B:159:GLU:HB2	3:E:72:LEU:HD23	1.87	0.55
2:D:226:ASP:OD1	2:D:226:ASP:N	2.37	0.55
2:D:342:TYR:CD2	2:D:342:TYR:N	2.75	0.55
3:E:96:MET:HE2	3:E:97:ALA:HB2	1.88	0.55
3:E:99:GLU:O	3:E:99:GLU:HG2	2.06	0.55
2:B:408:TYR:O	2:B:409:THR:C	2.48	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:120:ASP:CB	2:B:123:ARG:NH1	2.69	0.55
2:B:247:GLN:CG	2:B:248:LEU:HG	2.36	0.55
1:A:239:THR:O	1:A:241:SER:N	2.39	0.55
2:D:209:LEU:HB3	2:D:227:LEU:HD11	1.88	0.55
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.41	0.55
1:C:265:ILE:O	1:C:266:HIS:O	2.24	0.55
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
1:A:280:LYS:O	1:A:283:HIS:HB2	2.06	0.54
2:B:298:ALA:C	2:B:300:ASN:H	2.15	0.54
2:D:2:ARG:HH11	2:D:133:GLN:HA	1.72	0.54
2:B:151:THR:HB	2:B:193:GLN:HG2	1.89	0.54
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.47	0.54
2:B:251:ASP:HB2	2:B:254:LYS:HD2	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: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
1:C:102:ASN:O	1:C:103:TYR:C	2.51	0.54
2:D:298:ALA:C	2:D:300:ASN:H	2.14	0.54
2:D:401:ARG:HG3	2:D:401:ARG:NH1	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ASN:CB	1:C:255:PHE:HD2	2.21	0.54
1:A:102:ASN:O	1:A:103:TYR:C	2.50	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:A:32:PRO:O	1:A:33:ASP:C	2.51	0.53
1:A:69:ASP:C	1:A:70:LEU:HD12	2.33	0.53
1:A:115:ILE:CD1	1:A:119:LEU:HD13	2.38	0.53
2:B:33:THR:O	2:B:34:GLY:O	2.26	0.53
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.43	0.53
1:C:407:TRP:CD2	2:D:257:VAL:HG23	2.43	0.53
1:C:239:THR:O	1:C:240:ALA:C	2.52	0.53
2:D:180:THR:HG21	2:D:182:VAL:HG22	1.89	0.53
2:D:383:ALA:O	2:D:386:GLU:HB2	2.08	0.53
1:A:133:GLN:HE21	1:A:252:LEU:CG	2.16	0.53
2:B:291:LEU:HD21	2:B:375:ALA:HB3	1.87	0.53
2:B:401:ARG:HG3	2:B:401:ARG:NH1	2.23	0.53
2:D:171:VAL:HA	2:D:204:ILE:O	2.08	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
2:D:135:PHE:HB2	2:D:166:MET:HE2	1.90	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
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:395:PHE:C	1:A:395:PHE:CD2	2.87	0.52
2:B:11:GLN:HG3	2:B:74:THR:CG2	2.39	0.52
1:C:395:PHE:C	1:C:395:PHE:CD2	2.87	0.52
2:B:29:GLY:O	2:B:36:TYR:HA	2.09	0.52
1:C:10:GLY:O	1:C:13:GLY:N	2.43	0.52
2:D:2:ARG:O	2:D:3:GLU:HB2	2.09	0.52
2:B:358:ILE:HG23	2:B:358:ILE:O	2.09	0.52
1:C:176:GLN:H	1:C:176:GLN:HE21	1.58	0.52
2:D:11:GLN:HG3	2:D:74:THR:CG2	2.40	0.52
2:D:273:ALA:CB	2:D:274:PRO:CD	2.67	0.52
1:A:313:MET:O	1:A:314:ALA:HB2	2.09	0.52
2:D:241:CYS:HB3	2:D:248:LEU:HD12	1.92	0.52
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.45	0.51
1:C:105:ARG:HD2	1:C:411:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:LEU:O	1:C:254:GLU:N	2.43	0.51
1:C:270:ALA:O	1:C:302:MET:CG	2.58	0.51
2:B:225:GLY:O	2:B:227:LEU:N	2.43	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
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:265:LEU:O	2:B:266:HIS:C	2.53	0.51
2:B:403:ALA:C	2:B:405:LEU:N	2.65	0.51
1:C:8:HIS:HE1	1:C:21:TRP:HE1	1.59	0.51
2:D:36:TYR:HD1	2:D:37:HIS:H	1.58	0.51
2:D:29:GLY:O	2:D:36:TYR:HA	2.11	0.51
2:B:223:THR:HB	2:B:225:GLY:N	2.25	0.51
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.92	0.51
2:D:163:ASP:OD1	2:D:164:ARG:HD2	2.11	0.51
3:E:133:VAL:HG12	3:E:136:ASN:HD22	1.75	0.51
1:C:108:TYR:HB3	3:E:108:ASN:OD1	2.10	0.51
2:D:44:LEU:O	2:D:49:ILE:HG22	2.11	0.51
2:D:404:PHE:HD1	2:D:404:PHE:H	1.58	0.51
1:A:87:PHE:N	1:A:87:PHE:CD2	2.78	0.51
1:A:190:THR:CG2	1:A:191:THR:N	2.73	0.51
1:C:221:ARG:CB	2:D:325:MET:HE2	2.41	0.51
2:D:153:LEU:O	2:D:157:ILE:HG12	2.11	0.51
1:C:239:THR:O	1:C:241:SER:N	2.44	0.51
1:C:315:CYS:SG	1:C:377:MET:CE	2.99	0.51
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
2:D:205:ASP:OD1	2:D:207:GLU:N	2.43	0.51
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.93	0.51
1:A:208:ALA:O	1:A:212:ILE:HD12	2.11	0.50
1:C:48:SER:O	1:C:243:ARG:O	2.29	0.50
2:B:178:SER:HB2	2:B:183:GLU:OE1	2.11	0.50
2:B:427:ASP:O	2:B:431:GLU:HG3	2.11	0.50
1:C:70:LEU:HD23	1:C:110:ILE:CG2	2.40	0.50
2:D:295:MET:O	2:D:295:MET:HG2	2.11	0.50
1:C:340:THR:HG22	1:C:340:THR:O	2.11	0.50
2:B:267:PHE:N	2:B:267:PHE:CD1	2.78	0.50
2:D:308:ARG:C	2:D:310:GLY:H	2.19	0.50
2:B:154:ILE:HD12	2:B:198:THR:HG22	1.93	0.50
2:D:241:CYS:HB3	2:D:248:LEU:CD1	2.41	0.50
3:E:48:GLU:O	3:E:50:ILE:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PHE:N	1:A:87:PHE:HD2	2.10	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:146:GLY:O	1:A:150:THR:OG1	2.30	0.50
1:C:270:ALA:O	1:C:302:MET:HG2	2.12	0.50
2:D:2:ARG:NH1	2:D:133:GLN:HA	2.27	0.50
2:D:7:ILE:O	2:D:137:LEU:HA	2.12	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:O	2:D:177:VAL:CG1	2.60	0.49
2:B:407:TRP:HE1	1:C:257:THR:HA	1.75	0.49
2:D:135:PHE:N	2:D:135:PHE:CD1	2.80	0.49
2:D:267:PHE:CD1	2:D:267:PHE:N	2.80	0.49
2:B:210:TYR:CD1	2:B:210:TYR:C	2.90	0.49
2:D:225:GLY:O	2:D:227:LEU:N	2.45	0.49
3:E:67:GLU:O	3:E:69:LEU:N	2.35	0.49
1:C:315:CYS:SG	1:C:377:MET:HE1	2.52	0.49
2:D:403:ALA:C	2:D:405:LEU:N	2.71	0.49
1:C:90:GLU:HB3	1:C:121:ARG:HD3	1.94	0.49
1:C:167:LEU:HD11	1:C:256:GLN:NE2	2.27	0.49
2:D:265:LEU:O	2:D:266:HIS:C	2.55	0.49
2:D:393:GLU:O	2:D:397:ALA:HB2	2.12	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:346:TRP:HE3	1:A:346:TRP:O	1.96	0.49
1:C:267:PHE:N	1:C:267:PHE:CD1	2.79	0.49
2:D:251:ASP:HB2	2:D:254:LYS:HD2	1.94	0.49
2:D:269:MET:HE1	2:D:307:PRO:HD3	1.94	0.49
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.95	0.49
2:B:16:ILE:HG22	2:B:17:GLY:N	2.26	0.49
2:D:401:ARG:O	2:D:402:LYS:C	2.55	0.49
2:B:198:THR:OG1	2:B:265:LEU:HD22	2.12	0.49
2:B:226:ASP:OD1	2:B:226:ASP:N	2.42	0.49
1:C:70:LEU:O	1:C:97:GLU:O	2.31	0.49
1:C:229:ARG:CG	1:C:229:ARG:NH1	2.76	0.49
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.94	0.49
2:B:241:CYS:HB3	2:B:248:LEU:CD1	2.42	0.49
2:B:383:ALA:O	2:B:386:GLU:HB2	2.13	0.49
2:D:343:PHE:O	2:D:344:VAL:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:57:ALA:HA	3:E:60:ARG:HH12	1.77	0.49
1:A:407:TRP:CD2	2:B:257:VAL:HG23	2.47	0.48
2:B:103:TRP:O	2:B:104:ALA:C	2.56	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
1:A:210:TYR:CE1	1:A:214:ARG:HD2	2.48	0.48
2:B:240:THR:CG2	2:B:320:ARG:CZ	2.91	0.48
2:D:295:MET:SD	2:D:377:PHE:HB2	2.54	0.48
7:D:701:CN2:C12	7:D:701:CN2:H15	2.43	0.48
1:A:8:HIS:HE1	1:A:21:TRP:HE1	1.62	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
2:D:241:CYS:CB	2:D:248:LEU:CD1	2.92	0.48
1:C:31:GLN:O	1:C:32:PRO:C	2.56	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:217:LEU:C	2:B:219:LEU:H	2.22	0.48
2:B:264:ARG:O	2:B:266:HIS:CD2	2.67	0.48
1:A:277:SER:HA	1:A:367:ASP:O	2.14	0.48
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.96	0.48
2:B:400:ARG:HE	2:B:400:ARG:HB2	1.48	0.48
2:D:107:HIS:ND1	2:D:152:LEU:HB2	2.29	0.48
2:B:177:VAL:HG12	2:B:177:VAL:O	2.14	0.48
1:C:313:MET:O	1:C:314:ALA:CB	2.61	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
2:B:155:SER:HB3	3:E:76:ARG:NH2	2.27	0.47
1:C:87:PHE:N	1:C:87:PHE:CD2	2.82	0.47
1:C:344:VAL:HG13	1:C:344:VAL:O	2.14	0.47
2:D:174:SER:HB2	2:D:207:GLU:HB2	1.96	0.47
2:B:287:THR:HG22	2:B:290:GLU:H	1.79	0.47
3:E:109:LYS:O	3:E:113:GLU:HB2	2.14	0.47
2:B:107:HIS:ND1	2:B:152:LEU:HB2	2.29	0.47
2:B:171:VAL:HA	2:B:204:ILE:O	2.15	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:33:THR:O	2:D:34:GLY:O	2.32	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:B:264:ARG:C	2:B:266:HIS:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:ARG:C	2:B:310:GLY:H	2.22	0.47
2:D:5:VAL:CG2	2:D:135:PHE:CD2	2.97	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
2:B:11:GLN:HG3	2:B:74:THR:HG22	1.95	0.47
1:C:71:GLU:HG3	1:C:73:THR:OG1	2.15	0.47
1:C:346:TRP:CZ3	1:C:347:CYS:HB2	2.50	0.47
2:D:200:GLU:OE2	2:D:255:LEU:HD12	2.14	0.47
3:E:94:ILE:CG2	3:E:95:LYS:N	2.77	0.47
2:B:404:PHE:HD1	2:B:404:PHE:H	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:B:295:MET:O	2:B:295:MET:HG2	2.15	0.46
1:C:313:MET:HG3	1:C:380:ASN:O	2.15	0.46
2:D:191:VAL:HG11	2:D:425:MET:CE	2.37	0.46
2:D:237:GLY:CA	2:D:376:THR:HG21	2.44	0.46
1:A:72:PRO:O	1:A:74:VAL:N	2.49	0.46
1:C:82:THR:O	1:C:83:TYR:CB	2.63	0.46
1:C:87:PHE:N	1:C:87:PHE:HD2	2.13	0.46
2:D:112:ALA:HA	2:D:115:VAL:CG2	2.45	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:A:341:ILE:CG1	1:A:342:GLN:N	2.71	0.46
2:B:48:ARG:NH2	2:B:246:GLY:HA2	2.30	0.46
2:B:112:ALA:HA	2:B:115:VAL:CG2	2.45	0.46
2:B:135:PHE:CD1	2:B:135:PHE:N	2.83	0.46
2:B:163:ASP:HB3	2:B:164:ARG:H	1.47	0.46
2:B:185:TYR:CD1	2:B:418:PHE:HE2	2.34	0.46
2:D:320:ARG:HA	2:D:356:CYS:O	2.15	0.46
2:B:336:GLN:OE1	2:B:351:VAL:CG1	2.54	0.46
2:D:11:GLN:HG3	2:D:74:THR:HG22	1.95	0.46
2:D:336:GLN:OE1	2:D:351:VAL:CG1	2.57	0.46
2:D:294:GLN:HE21	2:D:294:GLN:HB2	1.63	0.46
2:B:200:GLU:OE2	2:B:255:LEU:HD12	2.15	0.46
2:B:237:GLY:CA	2:B:376:THR:HG21	2.44	0.46
1:A:315:CYS:SG	1:A:377:MET:CE	3.04	0.46
1:C:204:VAL:HG13	1:C:302:MET:HE3	1.97	0.46
2:D:102:ASN:OD1	2:D:105:LYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:116:ASP:O	2:D:120:ASP:HB2	2.16	0.46
2:D:251:ASP:C	2:D:253:ARG:N	2.64	0.46
2:D:313:LEU:HD12	2:D:313:LEU:HA	1.87	0.46
2:B:342:TYR:N	2:B:342:TYR:HD2	2.12	0.46
2:B:205:ASP:OD2	2:B:390:ARG:NH1	2.49	0.46
2:B:264:ARG:O	2:B:266:HIS:N	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:B:135:PHE:HB2	2:B:166:MET:HE1	1.96	0.45
2:B:269:MET:HE1	2:B:307:PRO:HD3	1.97	0.45
3:E:67:GLU:C	3:E:69:LEU:N	2.72	0.45
2:B:102:ASN:OD1	2:B:105:LYS:HB2	2.16	0.45
1:A:31:GLN:O	1:A:32:PRO:C	2.60	0.45
2:B:60:LYS:O	2:B:61:TYR:HD2	1.99	0.45
2:B:89:PRO:O	2:B:92:PHE:HD1	2.00	0.45
2:D:55:GLU:H	2:D:55:GLU:HG3	1.63	0.45
2:D:250:ALA:CB	7:D:701:CN2:H7	2.46	0.45
2:D:308:ARG:NH1	2:D:342:TYR:HE1	2.14	0.45
1:A:168:GLU:HG2	1:A:201:ALA:HB2	1.97	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
2:B:36:TYR:OH	2:B:40:SER:C	2.55	0.45
2:B:259:MET:HE2	2:B:378:ILE:HG22	1.99	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:62:VAL:O	2:D:62:VAL:HG22	2.15	0.45
2:D:287:THR:HG22	2:D:290:GLU:H	1.81	0.45
1:A:306:ASP:HA	1:A:307:PRO:HD3	1.63	0.45
7:B:700:CN2:C12	7:B:700:CN2:C15	2.87	0.45
1:C:62:VAL:HA	1:C:63:PRO:HD3	1.85	0.45
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:A:71:GLU:HG3	1:A:73:THR:OG1	2.17	0.45
2:B:20:PHE:O	2:B:24: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
2:B:401:ARG:O	2:B:402:LYS:C	2.59	0.45
1:C:82:THR:O	1:C:83:TYR:HB2	2.17	0.45
1:C:190:THR:CG2	1:C:191:THR:N	2.79	0.45
2:D:150:GLY:O	2:D:154:ILE:HG23	2.17	0.45
2:B:36:TYR:HD1	2:B:37:HIS:H	1.63	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:239:THR:O	2:D:240:THR:C	2.59	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:B:343:PHE:O	2:B:344:VAL:C	2.59	0.45
2:D:163:ASP:HB3	2:D:164:ARG:H	1.46	0.45
2:D:225:GLY:O	2:D:228:ASN:N	2.49	0.45
2:D:298:ALA:C	2:D:300:ASN:N	2.74	0.45
2:B:385:GLN:HE21	2:B:389:LYS:HD2	1.82	0.44
2:D:103:TRP:O	2:D:104:ALA:C	2.59	0.44
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.52	0.44
1:A:265:ILE:O	1:A:265:ILE:HG23	2.18	0.44
1:A:344:VAL:O	1:A:344:VAL:HG13	2.16	0.44
2:B:44:LEU:O	2:B:47:GLU:C	2.60	0.44
3:E:16:SER:O	3:E:16:SER:OG	2.34	0.44
1:A:82:THR:O	1:A:83:TYR:CB	2.65	0.44
1:C:318:LEU:HB2	1:C:376:CYS:HB3	1.99	0.44
2:B:262:PHE:O	2:B:263:PRO:C	2.61	0.44
2:D:273:ALA:HB2	2:D:375:ALA:HB3	1.98	0.44
1:A:163:LYS:O	1:A:164:LYS:C	2.60	0.44
2:B:241:CYS:HB3	2:B:248:LEU:HD12	1.99	0.44
2:B:247:GLN:HG2	2:B:248:LEU:N	2.19	0.44
2:B:308:ARG:NH1	2:B:342:TYR:HE1	2.15	0.44
1:C:266:HIS:CD2	1:C:266:HIS:H	2.35	0.44
1:A:10:GLY:O	1:A:13:GLY:N	2.50	0.44
1:A:164:LYS:H	1:A:164:LYS:HG2	1.62	0.44
2:B:70:LEU:CA	2:B:95:GLY:HA3	2.38	0.44
2:D:264:ARG:C	2:D:266:HIS:H	2.25	0.44
2:D:359:PRO:HA	2:D:360:PRO:HD3	1.82	0.44
2:B:386:GLU:O	2:B:390:ARG:HG2	2.18	0.44
1:C:51:THR:HG21	1:C:242:LEU:O	2.17	0.44
1:C:151:SER:O	1:C:155:GLU:HG2	2.17	0.44
2:D:209:LEU:HD21	2:D:231:VAL:CG2	2.48	0.44
1:A:48:SER:O	1:A:243:ARG:O	2.35	0.44
1:C:256:GLN:O	1:C:258:ASN:N	2.51	0.44
1:C:80:THR:HG22	1:C:81:GLY:N	2.33	0.44
1:C:244:PHE:N	1:C:245:ASP:HA	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:273:ALA:HB1	1:A:274:PRO:CD	2.26	0.43
1:C:98:ASP:CB	2:D:251:ASP:OD2	2.58	0.43
2:D:378:ILE:HD12	7:D:701:CN2:C4	2.48	0.43
1:A:153:LEU:HD22	1:A:157:LEU:HG	2.00	0.43
1:C:205:ASP:HB2	1:C:303:VAL:HA	1.99	0.43
1:C:251:ASP:OD1	1:C:251:ASP:O	2.36	0.43
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.88	0.43
2:D:210:TYR:CD1	2:D:210:TYR:C	2.97	0.43
2:B:190:SER:O	2:B:191:VAL:C	2.62	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:B:298:ALA:C	2:B:300:ASN:N	2.75	0.43
2:D:36:TYR:OH	2:D:40:SER:C	2.60	0.43
2:D:111:GLY:HA2	2:D:149:MET:CE	2.49	0.43
1:A:191:THR:HG23	1:A:425:MET:HE3	2.01	0.43
1:C:71:GLU:O	1:C:71:GLU:HG2	2.17	0.43
1:C:174:ALA:HA	1:C:175:PRO:HD2	1.66	0.43
3:E:48:GLU:O	3:E:49:GLU:C	2.62	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:A:313:MET:O	1:A:314:ALA:CB	2.67	0.43
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.87	0.43
2:B:239:THR:O	2:B:240:THR:C	2.62	0.43
2:B:312:TYR:CD2	2:B:381:SER:HB2	2.54	0.43
1:C:153:LEU:HD22	1:C:157:LEU:HG	2.01	0.43
2:D:319:PHE:CD1	2:D:319:PHE:N	2.87	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
2:B:245:PRO:HB2	2:B:246:GLY:H	1.44	0.43
1:C:163:LYS:H	1:C:163:LYS:HG3	1.48	0.43
1:C:210:TYR:CE1	1:C:214:ARG:HD2	2.54	0.43
1:C:260:VAL:HG23	1:C:260:VAL:O	2.18	0.43
1:C:347:CYS:HA	1:C:348:PRO:HD2	1.88	0.43
2:B:270:PRO:O	2:B:302:MET:HB2	2.18	0.43
1:C:154:MET:HB3	1:C:154:MET:HE3	1.68	0.43
1:C:315:CYS:SG	1:C:377:MET:HE2	2.59	0.43
2:D:245:PRO:HB2	2:D:246:GLY:H	1.37	0.43
2:D:342:TYR:N	2:D:342:TYR:HD2	2.15	0.43
1:A:278:ALA:HA	1:A:281:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:SER:O	1:C:65:ALA:HA	2.19	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:141:PHE:HD2	1:C:141:PHE:HA	1.72	0.42
2:D:259:MET:HE2	2:D:378:ILE:HG22	2.01	0.42
3:E:15:THR:CG2	3:E:16:SER:N	2.82	0.42
1:A:62:VAL:HA	1:A:63:PRO:HD3	1.84	0.42
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.01	0.42
1:A:347:CYS:HA	1:A:348:PRO:HD2	1.83	0.42
2:B:101:ASN:HB2	1:C:254:GLU:OE2	2.18	0.42
2:B:191:VAL:HG11	2:B:425:MET:CE	2.41	0.42
2:D:118:VAL:O	2:D:122:VAL:HG13	2.19	0.42
2:B:208:ALA:HB2	2:B:304:ALA:N	2.34	0.42
1:C:97:GLU:OE2	2:D:164:ARG:NH1	2.50	0.42
1:C:277:SER:HA	1:C:367:ASP:O	2.19	0.42
1:A:105:ARG:HD2	1:A:411:GLU:OE1	2.18	0.42
1:C:178:SER:HB3	7:D:701:CN2:HS1	1.80	0.42
1:C:258:ASN:HD22	1:C:258:ASN:HA	1.56	0.42
1:A:340:THR:O	1:A:340:THR:HG22	2.20	0.42
2:B:149:MET:O	2:B:152:LEU:HB3	2.19	0.42
2:B:177:VAL:O	2:B:177:VAL:CG1	2.67	0.42
1:C:36:MET:H	1:C:36:MET:HG3	1.44	0.42
1:A:207:GLU:HG2	1:A:304:LYS:NZ	2.35	0.42
2:B:431:GLU:O	2:B:434:GLN:HB2	2.20	0.42
1:C:163:LYS:O	1:C:164:LYS:C	2.62	0.42
1:C:164:LYS:H	1:C:164:LYS:HG2	1.69	0.42
1:C:191:THR:HG23	1:C:425:MET:HE3	2.02	0.42
2:D:291:LEU:C	2:D:291:LEU:HD23	2.45	0.42
1:A:191:THR:HA	1:A:194:THR:HG22	2.00	0.42
1:A:276:ILE:HD11	1:A:280:LYS:HD2	2.01	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:6:HIS:HD2	2:D:136:GLN:HG3	1.83	0.42
2:D:83:PHE:HD2	2:D:83:PHE:HA	1.77	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.42
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:B:264:ARG:C	2:B:266:HIS:CD2	2.98	0.42
1:C:230:LEU:HD12	1:C:230:LEU:O	2.20	0.42
2:D:89:PRO:O	2:D:92:PHE:HD1	2.03	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:145:THR:HG23	5:A:600:GTP:O2B	2.20	0.42
1:A:205:ASP:HB2	1:A:303:VAL:HA	2.02	0.42
1:A:306:ASP:O	1:A:309:HIS:HB3	2.20	0.42
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.55	0.42
1:C:143:GLY:O	1:C:147:SER:OG	2.33	0.42
1:C:152:LEU:HA	1:C:155:GLU:HG3	2.01	0.42
1:C:392:ASP:OD1	1:C:429:GLU:OE1	2.38	0.42
2:D:255:LEU:HD23	7:D:701:CN2:C22	2.50	0.42
2:D:308:ARG:C	2:D:310:GLY:N	2.77	0.42
1:A:163:LYS:H	1:A:163:LYS:HG3	1.49	0.41
1:C:84:ARG:HE	1:C:84:ARG:HB3	1.65	0.41
2:D:149:MET:HE3	2:D:149:MET:HB2	1.96	0.41
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
2:B:183:GLU:N	2:B:184:PRO:HD2	2.35	0.41
2:D:164:ARG:NH2	2:D:253:ARG:HH22	2.18	0.41
1:A:132:LEU:HG	1:A:133:GLN:N	2.34	0.41
2:B:74:THR:O	2:B:77:SER:HB2	2.21	0.41
2:B:114:LEU:O	2:B:115:VAL:C	2.63	0.41
2:B:256:ALA:O	2:B:260:VAL:HG22	2.20	0.41
1:C:47:ASP:O	1:C:49:PHE:N	2.53	0.41
1:C:190:THR:O	1:C:194:THR:HB	2.20	0.41
2:D:248:LEU:HB2	2:D:249:ASN:H	1.46	0.41
2:D:93:VAL:HG12	2:D:114:LEU:HD11	2.01	0.41
1:A:8:HIS:CE1	1:A:21:TRP:HE1	2.39	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
2:B:404:PHE:CE1	1:C:261:PRO:HB3	2.55	0.41
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.55	0.41
1:C:407:TRP:CE2	2:D:257:VAL:HA	2.55	0.41
2:D:135:PHE:HB2	2:D:166:MET:HE1	2.02	0.41
1:A:141:PHE:HD2	1:A:141:PHE:HA	1.76	0.41
1:A:298:PRO:HA	1:A:301:GLN:HE21	1.84	0.41
1:C:146:GLY:O	1:C:150:THR:OG1	2.36	0.41
1:C:231:ILE:O	1:C:232:GLY:C	2.64	0.41
1:C:291:ILE:HD12	1:C:375:VAL:HG23	2.03	0.41
1:A:54:SER:O	1:A:56:THR:N	2.54	0.41
2:B:21:TRP:CH2	2:B:63:PRO:HB3	2.56	0.41
2:D:141:LEU:HA	2:D:141:LEU:HD12	1.81	0.41
2:D:208:ALA:HB2	2:D:304:ALA:N	2.35	0.41
1:A:252:LEU:HD23	1:A:252:LEU:HA	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:MET:HG3	2:B:348:PRO:CD	2.48	0.41
2:D:54:ASN:O	2:D:62:VAL:O	2.39	0.41
2:D:114:LEU:O	2:D:115:VAL:C	2.64	0.41
1:A:399:TYR:C	1:A:401:LYS:H	2.29	0.41
2:B:156:LYS:HG2	3:E:76:ARG:HE	1.85	0.41
1:C:122:ILE:CD1	1:C:157:LEU:HD21	2.51	0.41
1:C:171:ILE:HG23	1:C:206:ASN:ND2	2.35	0.41
2:D:89:PRO:C	2:D:91:ASN:H	2.29	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
1:A:188:ILE:HD12	1:A:425:MET:HG3	2.03	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
3:E:123:LEU:O	3:E:127:ASP:HB2	2.21	0.41
1:A:182:VAL:O	1:A:183:GLU:C	2.64	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:C:111:GLY:O	1:C:112:LYS:C	2.64	0.40
2:D:289:PRO:O	2:D:293:GLN:CG	2.68	0.40
1:A:252:LEU:O	1:A:255:PHE:HB2	2.21	0.40
2:B:371:LEU:H	2:B:371:LEU:HD13	1.87	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
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:B:308:ARG:HA	2:B:308:ARG:HD2	1.87	0.40
2:D:102:ASN:OD1	2:D:102:ASN:O	2.39	0.40
2:D:198:THR:OG1	2:D:265:LEU:HD22	2.20	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
1:A:115:ILE:HD13	1:A:119:LEU:HD13	2.03	0.40
1:A:251:ASP:HB3	1:A:254:GLU:HB2	2.03	0.40
2:B:11:GLN:HG3	2:B:74:THR:HG21	2.03	0.40
2:B:270:PRO:HA	2:B:377:PHE:O	2.20	0.40
1:C:115:ILE:HG13	1:C:152:LEU:CD2	2.51	0.40
1:C:141:PHE:HB2	1:C:171:ILE:O	2.22	0.40
1:C:344:VAL:O	1:C:344:VAL:CG1	2.70	0.40
2:D:76:ASP:OD1	2:D:76:ASP:N	2.54	0.40
2:D:99:ALA:HB1	2:D:145:THR:HG21	2.03	0.40
2:D:404:PHE:CD1	2:D:404:PHE:N	2.89	0.40
2:B:260:VAL:HG23	2:B:260:VAL:O	2.22	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
1:C:274:PRO:HG3	1:C:291:ILE:HG21	2.02	0.40
1:C:317:LEU:HD23	1:C:317:LEU:HA	1.93	0.40
2:D:133:GLN:HE21	2:D:252:LEU:CB	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	0	5
1	C	415/451 (92%)	316 (76%)	59 (14%)	40 (10%)	0	6
2	B	415/445 (93%)	310 (75%)	58 (14%)	47 (11%)	0	4
2	D	415/445 (93%)	311 (75%)	56 (14%)	48 (12%)	0	4
3	E	120/142 (84%)	91 (76%)	21 (18%)	8 (7%)	1	11
All	All	1788/1934 (92%)	1355 (76%)	247 (14%)	186 (10%)	0	5

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

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Mol	Chain	Res	Type
1	A	314	ALA
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

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Mol	Chain	Res	Type
2	D	43	GLN
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

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Mol	Chain	Res	Type
2	B	370	GLY
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

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Mol	Chain	Res	Type
2	B	340	SER
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

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Mol	Chain	Res	Type
2	D	240	THR
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%)	218 (63%)	128 (37%)	0	1
1	C	336/378 (89%)	217 (65%)	119 (35%)	0	1
2	B	348/381 (91%)	228 (66%)	120 (34%)	0	2
2	D	348/381 (91%)	231 (66%)	117 (34%)	0	2
3	E	78/126 (62%)	44 (56%)	34 (44%)	0	0
All	All	1456/1644 (89%)	938 (64%)	518 (36%)	0	1

All (518) 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	15	GLN
1	A	16	ILE
1	A	22	GLU
1	A	27	GLU
1	A	36	MET
1	A	50	ASN
1	A	54	SER
1	A	62	VAL

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Mol	Chain	Res	Type
1	A	66	VAL
1	A	68	VAL
1	A	73	THR
1	A	74	VAL
1	A	79	ARG
1	A	80	THR
1	A	82	THR
1	A	85	GLN
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	110	ILE
1	A	112	LYS
1	A	114	ILE
1	A	115	ILE
1	A	116	ASP
1	A	119	LEU
1	A	120	ASP
1	A	121	ARG
1	A	122	ILE
1	A	123	ARG
1	A	124	LYS
1	A	128	GLN
1	A	130	THR
1	A	140	SER
1	A	141	PHE
1	A	145	THR
1	A	147	SER
1	A	153	LEU
1	A	154	MET
1	A	155	GLU
1	A	163	LYS
1	A	164	LYS
1	A	165	SER
1	A	167	LEU
1	A	171	ILE
1	A	176	GLN
1	A	177	VAL

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Mol	Chain	Res	Type
1	A	178	SER
1	A	182	VAL
1	A	183	GLU
1	A	187	SER
1	A	190	THR
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
1	A	211	ASP
1	A	212	ILE
1	A	220	GLU
1	A	223	THR
1	A	225	THR
1	A	226	ASN
1	A	227	LEU
1	A	229	ARG
1	A	230	LEU
1	A	234	ILE
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	275	VAL
1	A	279	GLU
1	A	280	LYS
1	A	283	HIS
1	A	287	SER
1	A	288	VAL
1	A	295	CYS

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Mol	Chain	Res	Type
1	A	302	MET
1	A	304	LYS
1	A	306	ASP
1	A	313	MET
1	A	315	CYS
1	A	316	CYS
1	A	332	ILE
1	A	340	THR
1	A	341	ILE
1	A	343	PHE
1	A	344	VAL
1	A	349	THR
1	A	352	LYS
1	A	355	ILE
1	A	356	ASN
1	A	358	GLU
1	A	362	VAL
1	A	363	VAL
1	A	367	ASP
1	A	368	LEU
1	A	370	LYS
1	A	371	VAL
1	A	375	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	24	ILE
2	B	26	ASP
2	B	27	GLU

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Mol	Chain	Res	Type
2	B	30	ILE
2	B	31	ASP
2	B	33	THR
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	66	ILE
2	B	68	VAL
2	B	71	GLU
2	B	76	ASP
2	B	77	SER
2	B	78	VAL
2	B	80	SER
2	B	85	GLN
2	B	86	ILE
2	B	91	ASN
2	B	101	ASN
2	B	102	ASN
2	B	109	THR
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	177	VAL
2	B	179	ASP

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Mol	Chain	Res	Type
2	B	181	VAL
2	B	189	LEU
2	B	190	SER
2	B	195	VAL
2	B	197	ASN
2	B	198	THR
2	B	200	GLU
2	B	201	THR
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	240	THR
2	B	241	CYS
2	B	242	LEU
2	B	243	ARG
2	B	248	LEU
2	B	251	ASP
2	B	253	ARG
2	B	255	LEU
2	B	257	VAL
2	B	258	ASN
2	B	265	LEU
2	B	269	MET
2	B	275	LEU
2	B	276	THR
2	B	286	LEU
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	315	VAL
2	B	318	VAL
2	B	320	ARG

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Mol	Chain	Res	Type
2	B	323	MET
2	B	325	MET
2	B	333	LEU
2	B	336	GLN
2	B	341	SER
2	B	344	VAL
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	384	ILE
2	B	398	MET
2	B	400	ARG
2	B	401	ARG
2	B	402	LYS
2	B	405	LEU
2	B	406	HIS
2	B	415	GLU
2	B	416	MET
2	B	419	THR
2	B	423	SER
2	B	425	MET
2	B	429	VAL
2	B	430	SER
1	C	2	ARG
1	C	9	VAL
1	C	15	GLN
1	C	16	ILE
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	66	VAL
1	C	68	VAL
1	C	73	THR
1	C	74	VAL
1	C	77	GLU

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Mol	Chain	Res	Type
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	119	LEU
1	C	120	ASP
1	C	121	ARG
1	C	122	ILE
1	C	123	ARG
1	C	124	LYS
1	C	128	GLN
1	C	130	THR
1	C	140	SER
1	C	141	PHE
1	C	145	THR
1	C	147	SER
1	C	153	LEU
1	C	154	MET
1	C	155	GLU
1	C	163	LYS
1	C	164	LYS
1	C	165	SER
1	C	167	LEU
1	C	171	ILE
1	C	176	GLN
1	C	177	VAL
1	C	178	SER
1	C	182	VAL
1	C	183	GLU

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Mol	Chain	Res	Type
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	229	ARG
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	275	VAL
1	C	287	SER
1	C	288	VAL
1	C	304	LYS
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	375	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	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	16	ILE
2	D	23	VAL
2	D	24	ILE
2	D	26	ASP
2	D	27	GLU
2	D	30	ILE
2	D	33	THR
2	D	39	ASP
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	66	ILE
2	D	68	VAL
2	D	71	GLU
2	D	76	ASP

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Mol	Chain	Res	Type
2	D	77	SER
2	D	78	VAL
2	D	80	SER
2	D	83	PHE
2	D	86	ILE
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	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	201	THR
2	D	209	LEU
2	D	212	ILE
2	D	216	THR
2	D	223	THR
2	D	224	TYR
2	D	226	ASP

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Mol	Chain	Res	Type
2	D	230	LEU
2	D	240	THR
2	D	241	CYS
2	D	242	LEU
2	D	243	ARG
2	D	248	LEU
2	D	251	ASP
2	D	253	ARG
2	D	255	LEU
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	315	VAL
2	D	318	VAL
2	D	320	ARG
2	D	323	MET
2	D	325	MET
2	D	333	LEU
2	D	336	GLN
2	D	341	SER
2	D	344	VAL
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	384	ILE
2	D	398	MET

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Mol	Chain	Res	Type
2	D	400	ARG
2	D	401	ARG
2	D	402	LYS
2	D	405	LEU
2	D	406	HIS
2	D	415	GLU
2	D	416	MET
2	D	419	THR
2	D	423	SER
2	D	425	MET
2	D	429	VAL
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	55	GLU
3	E	58	GLU
3	E	59	GLU
3	E	61	ARG
3	E	64	GLN
3	E	69	LEU
3	E	70	LYS
3	E	76	ARG
3	E	78	HIS
3	E	87	ILE
3	E	89	GLU
3	E	94	ILE
3	E	96	MET
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

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Mol	Chain	Res	Type
3	E	126	LYS
3	E	129	HIS
3	E	133	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) 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
1	A	133	GLN
1	A	139	HIS
1	A	176	GLN
1	A	197	HIS
1	A	206	ASN
1	A	249	ASN
1	A	258	ASN
1	A	266	HIS
1	A	283	HIS
1	A	301	GLN
1	A	372	GLN
1	A	380	ASN
2	B	6	HIS
2	B	14	ASN
2	B	43	GLN
2	B	54	ASN
2	B	136	GLN
2	B	139	HIS
2	B	266	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
2	B	433	GLN
1	C	88	HIS
1	C	91	GLN
1	C	101	ASN

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Mol	Chain	Res	Type
1	C	102	ASN
1	C	107	HIS
1	C	133	GLN
1	C	139	HIS
1	C	176	GLN
1	C	197	HIS
1	C	206	ASN
1	C	233	GLN
1	C	258	ASN
1	C	266	HIS
1	C	301	GLN
1	C	372	GLN
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	43	GLN
2	D	54	ASN
2	D	136	GLN
2	D	139	HIS
2	D	197	ASN
2	D	294	GLN
2	D	300	ASN
2	D	331	GLN
2	D	339	ASN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
3	E	18	GLN
3	E	71	HIS
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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
6	GDP	B	602	4	29,30,30	0.92	1 (3%)	45,47,47	1.86	11 (24%)
5	GTP	C	601	4	33,34,34	1.22	4 (12%)	50,54,54	1.73	12 (24%)
7	CN2	B	700	-	32,32,32	2.85	6 (18%)	44,45,45	4.50	24 (54%)
5	GTP	A	600	4	33,34,34	1.34	4 (12%)	50,54,54	1.72	11 (22%)
6	GDP	D	603	-	29,30,30	1.05	3 (10%)	45,47,47	1.87	12 (26%)
7	CN2	D	701	-	32,32,32	2.61	7 (21%)	44,45,45	4.46	22 (50%)

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
6	GDP	B	602	4	-	4/16/32/32	0/3/3/3
5	GTP	C	601	4	-	5/22/38/38	0/3/3/3
7	CN2	B	700	-	-	4/12/27/27	0/3/3/3
5	GTP	A	600	4	-	5/22/38/38	0/3/3/3
6	GDP	D	603	-	-	3/16/32/32	0/3/3/3
7	CN2	D	701	-	-	4/12/27/27	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	CN2	C20-C21	-8.34	1.23	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	701	CN2	C20-C21	-7.28	1.24	1.37
7	B	700	CN2	C19-C20	-7.24	1.20	1.41
7	B	700	CN2	C21-C14	-6.50	1.34	1.43
7	D	701	CN2	C21-C14	-6.12	1.34	1.43
7	B	700	CN2	C19-C17	-6.02	1.23	1.39
7	D	701	CN2	C19-C20	-5.94	1.24	1.41
7	D	701	CN2	C19-C17	-5.29	1.25	1.39
7	D	701	CN2	O6-C17	4.87	1.45	1.36
7	B	700	CN2	O6-C17	4.50	1.45	1.36
5	A	600	GTP	PB-O3A	4.27	1.64	1.59
5	A	600	GTP	PB-O3B	3.56	1.63	1.59
5	C	601	GTP	PB-O3B	3.35	1.63	1.59
7	D	701	CN2	C15-C16	3.30	1.54	1.44
6	D	603	GDP	PA-O3A	3.21	1.63	1.59
5	A	600	GTP	PA-O3A	2.93	1.62	1.59
7	B	700	CN2	C15-C16	2.85	1.52	1.44
5	C	601	GTP	PB-O3A	2.80	1.62	1.59
5	C	601	GTP	PA-O3A	2.64	1.62	1.59
5	C	601	GTP	O4'-C4'	-2.34	1.39	1.45
6	D	603	GDP	C2-N3	2.17	1.38	1.33
5	A	600	GTP	O4'-C4'	-2.09	1.40	1.45
6	B	602	GDP	O4'-C4'	-2.08	1.40	1.45
7	D	701	CN2	C15-C14	2.06	1.40	1.36
6	D	603	GDP	C5-N7	-2.01	1.35	1.39

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	701	CN2	O6-C17-C16	14.80	123.20	109.60
7	B	700	CN2	O6-C17-C16	13.93	122.40	109.60
7	B	700	CN2	C19-C17-C16	-11.99	109.25	128.57
7	B	700	CN2	C20-C21-C14	-11.59	112.91	124.67
7	D	701	CN2	C19-C17-C16	-11.10	110.68	128.57
7	B	700	CN2	C19-C20-C21	8.80	148.34	131.06
7	D	701	CN2	C10-C11-N1	-8.59	94.02	109.76
7	D	701	CN2	C13-C12-N1	-8.52	104.82	115.33
7	D	701	CN2	C20-C21-C14	-8.22	116.34	124.67
7	D	701	CN2	C19-C20-C21	7.85	146.47	131.06
7	B	700	CN2	C20-C19-C17	7.13	145.16	130.27
7	B	700	CN2	C22-C21-C14	6.22	123.71	118.62
7	B	700	CN2	C14-C11-N1	-6.02	109.56	114.31
7	D	701	CN2	C20-C19-C17	5.92	142.63	130.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	701	CN2	C11-C14-C15	5.77	122.14	117.06
6	D	603	GDP	C5-C4-N3	-5.55	119.56	128.39
6	D	603	GDP	C2-N3-C4	5.27	121.38	112.30
7	B	700	CN2	C10-C11-N1	-5.07	100.47	109.76
6	B	602	GDP	C5-C4-N3	-4.89	120.60	128.39
5	A	600	GTP	C5-C4-N3	-4.87	120.63	128.39
6	B	602	GDP	C2-N3-C4	4.84	120.63	112.30
5	C	601	GTP	C2-N3-C4	4.70	120.39	112.30
7	D	701	CN2	C10-C9-C8	-4.63	103.39	113.48
7	D	701	CN2	O3-C5-C7	-4.43	116.45	124.08
5	C	601	GTP	C5-C4-N3	-4.37	121.43	128.39
5	A	600	GTP	C2-N3-C4	4.25	119.62	112.30
7	B	700	CN2	O6-C17-C19	4.18	128.35	122.29
7	D	701	CN2	C15-C14-C21	-4.11	124.05	127.56
7	B	700	CN2	C15-C14-C21	-3.98	124.16	127.56
7	B	700	CN2	C10-C11-C14	3.97	115.71	110.71
7	B	700	CN2	O5-C16-C17	-3.93	114.33	119.06
7	B	700	CN2	C22-C21-C20	3.92	123.32	116.95
7	B	700	CN2	C6-O3-C5	3.71	122.95	117.51
7	D	701	CN2	C22-C21-C20	3.60	122.79	116.95
7	D	701	CN2	O4-C12-C13	3.57	127.48	121.44
7	D	701	CN2	O3-C5-C3	3.56	121.25	115.14
5	A	600	GTP	C2-N1-C6	-3.56	118.65	125.11
5	C	601	GTP	O3'-C3'-C4'	-3.49	101.07	111.08
6	D	603	GDP	N9-C4-N3	3.40	132.76	125.95
7	B	700	CN2	C1-C22-C21	3.37	124.88	121.33
6	B	602	GDP	N9-C4-N3	3.31	132.58	125.95
7	D	701	CN2	C4-O2-C3	3.29	123.69	114.74
6	B	602	GDP	N9-C8-N7	-3.27	107.33	113.40
7	B	700	CN2	O3-C5-C3	3.26	120.72	115.14
7	B	700	CN2	C11-C14-C15	3.25	119.92	117.06
7	B	700	CN2	C10-C9-C8	-3.18	106.56	113.48
7	B	700	CN2	C8-C22-C21	-3.18	116.67	120.20
6	D	603	GDP	C8-N7-C5	3.14	109.85	104.26
5	C	601	GTP	O6-C6-C5	-3.04	118.52	126.53
6	D	603	GDP	N9-C8-N7	-2.97	107.89	113.40
6	B	602	GDP	C2'-C1'-N9	-2.94	105.05	113.25
6	B	602	GDP	C2-N1-C6	-2.94	119.78	125.11
5	A	600	GTP	N9-C4-N3	2.93	131.82	125.95
5	C	601	GTP	C2'-C1'-N9	2.92	121.39	113.25
5	C	601	GTP	N9-C4-N3	2.87	131.70	125.95
5	A	600	GTP	O6-C6-C5	-2.86	118.97	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	602	GDP	O6-C6-C5	-2.86	118.97	126.53
7	D	701	CN2	O5-C16-C17	-2.82	115.67	119.06
7	D	701	CN2	C10-C11-C14	2.81	114.25	110.71
7	B	700	CN2	C13-C12-N1	-2.80	111.87	115.33
7	D	701	CN2	O4-C12-N1	2.80	127.69	122.95
6	B	602	GDP	C8-N7-C5	2.80	109.24	104.26
7	B	700	CN2	O3-C5-C7	-2.78	119.28	124.08
5	C	601	GTP	N9-C8-N7	-2.78	108.24	113.40
5	A	600	GTP	O3'-C3'-C4'	-2.78	103.10	111.08
6	D	603	GDP	C2-N1-C6	-2.76	120.10	125.11
7	D	701	CN2	C11-N1-C12	2.76	128.60	121.68
7	D	701	CN2	C22-C21-C14	2.74	120.87	118.62
5	C	601	GTP	C2-N1-C6	-2.73	120.16	125.11
5	C	601	GTP	C5-C6-N1	2.68	120.07	113.25
6	B	602	GDP	C5-C6-N1	2.66	120.03	113.25
7	D	701	CN2	O6-C17-C19	2.64	126.11	122.29
5	A	600	GTP	C5-C6-N1	2.63	119.96	113.25
7	D	701	CN2	C8-C22-C21	-2.51	117.42	120.20
5	A	600	GTP	N9-C8-N7	-2.46	108.85	113.40
6	D	603	GDP	C5-C6-N1	2.44	119.46	113.25
6	D	603	GDP	O6-C6-C5	-2.40	120.20	126.53
6	D	603	GDP	C4-C5-N7	-2.36	106.93	110.67
7	B	700	CN2	C4-O2-C3	2.33	121.08	114.74
5	C	601	GTP	C8-N7-C5	2.31	108.37	104.26
6	D	603	GDP	O3B-PB-O3A	2.28	112.29	104.64
5	C	601	GTP	N2-C2-N1	2.28	121.57	116.76
6	D	603	GDP	O2B-PB-O3A	2.25	112.17	104.64
6	B	602	GDP	C2'-C3'-C4'	2.22	106.91	102.61
7	B	700	CN2	O4-C12-N1	2.21	126.70	122.95
5	A	600	GTP	C8-N7-C5	2.20	108.18	104.26
6	D	603	GDP	N1-C2-N3	-2.13	119.42	123.32
5	C	601	GTP	N1-C2-N3	-2.11	119.45	123.32
6	B	602	GDP	O2B-PB-O3A	2.10	111.68	104.64
7	B	700	CN2	C18-O6-C17	2.07	120.98	116.96
5	A	600	GTP	N2-C2-N1	2.06	121.11	116.76
5	A	600	GTP	C2'-C1'-N9	2.02	118.88	113.25

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	600	GTP	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
5	A	600	GTP	C5'-O5'-PA-O1A
5	C	601	GTP	C5'-O5'-PA-O3A
5	C	601	GTP	C5'-O5'-PA-O1A
6	B	602	GDP	PA-O3A-PB-O2B
6	B	602	GDP	O4'-C4'-C5'-O5'
6	B	602	GDP	C3'-C4'-C5'-O5'
7	B	700	CN2	C19-C17-O6-C18
7	B	700	CN2	C16-C17-O6-C18
7	D	701	CN2	C19-C17-O6-C18
7	D	701	CN2	C16-C17-O6-C18
6	D	603	GDP	O4'-C4'-C5'-O5'
7	B	700	CN2	C7-C5-O3-C6
7	D	701	CN2	C7-C5-O3-C6
6	D	603	GDP	C3'-C4'-C5'-O5'
7	B	700	CN2	C3-C5-O3-C6
7	D	701	CN2	C3-C5-O3-C6
6	D	603	GDP	PA-O3A-PB-O1B
5	A	600	GTP	PG-O3B-PB-O1B
5	A	600	GTP	C5'-O5'-PA-O2A
5	C	601	GTP	C5'-O5'-PA-O2A
5	A	600	GTP	PG-O3B-PB-O2B
5	C	601	GTP	PG-O3B-PB-O1B
6	B	602	GDP	PA-O3A-PB-O1B
5	C	601	GTP	PG-O3B-PB-O2B

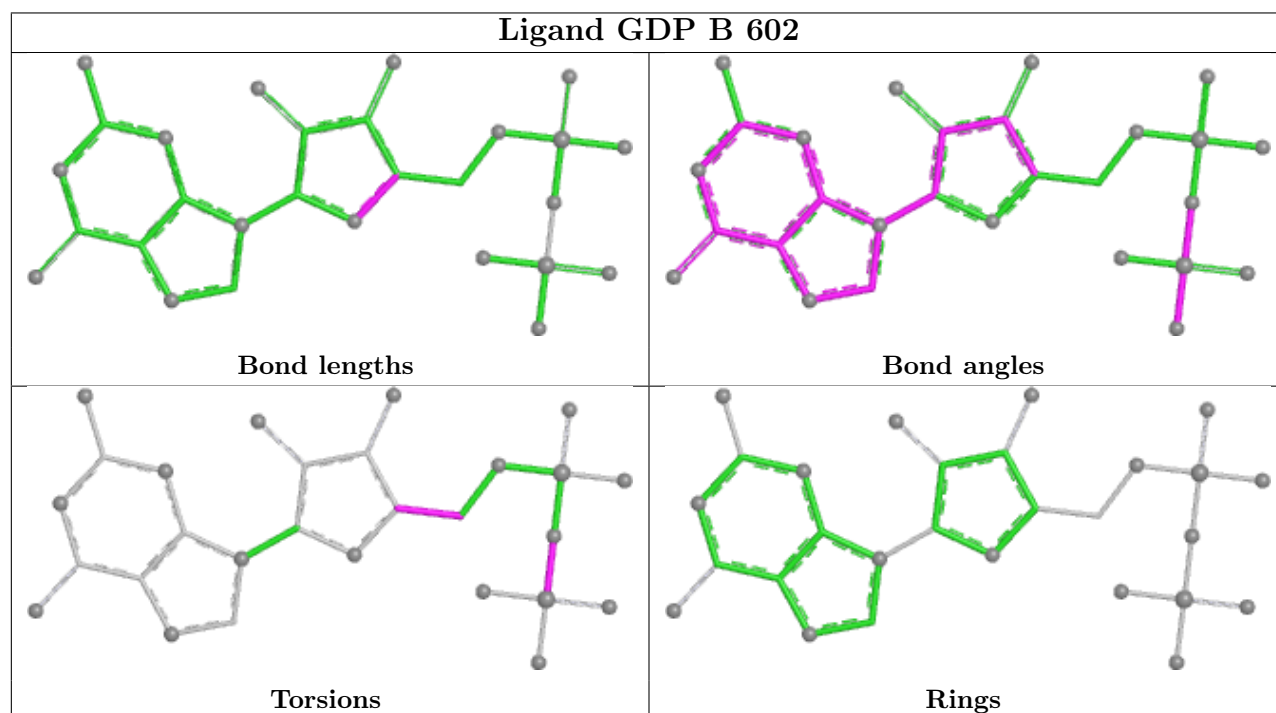
There are no ring outliers.

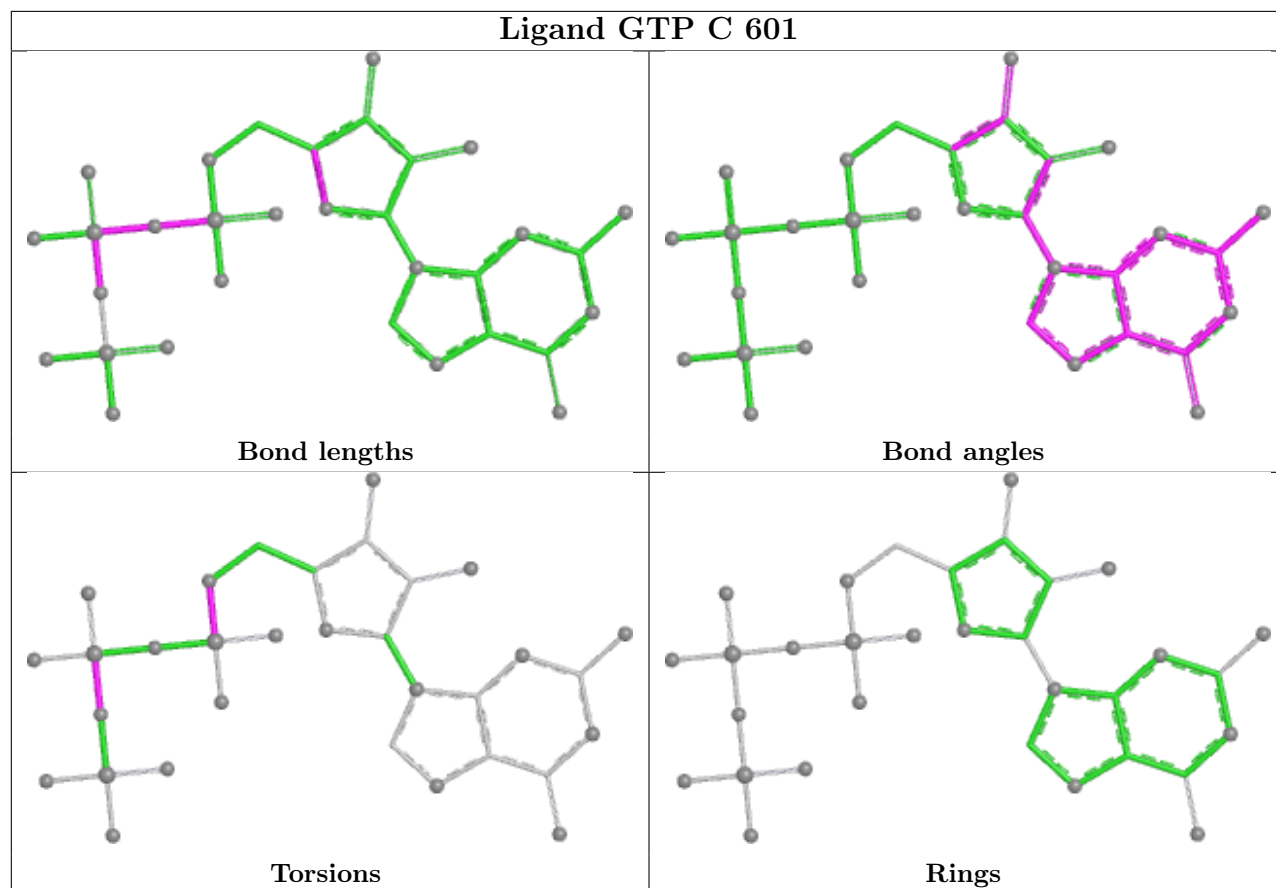
6 monomers are involved in 30 short contacts:

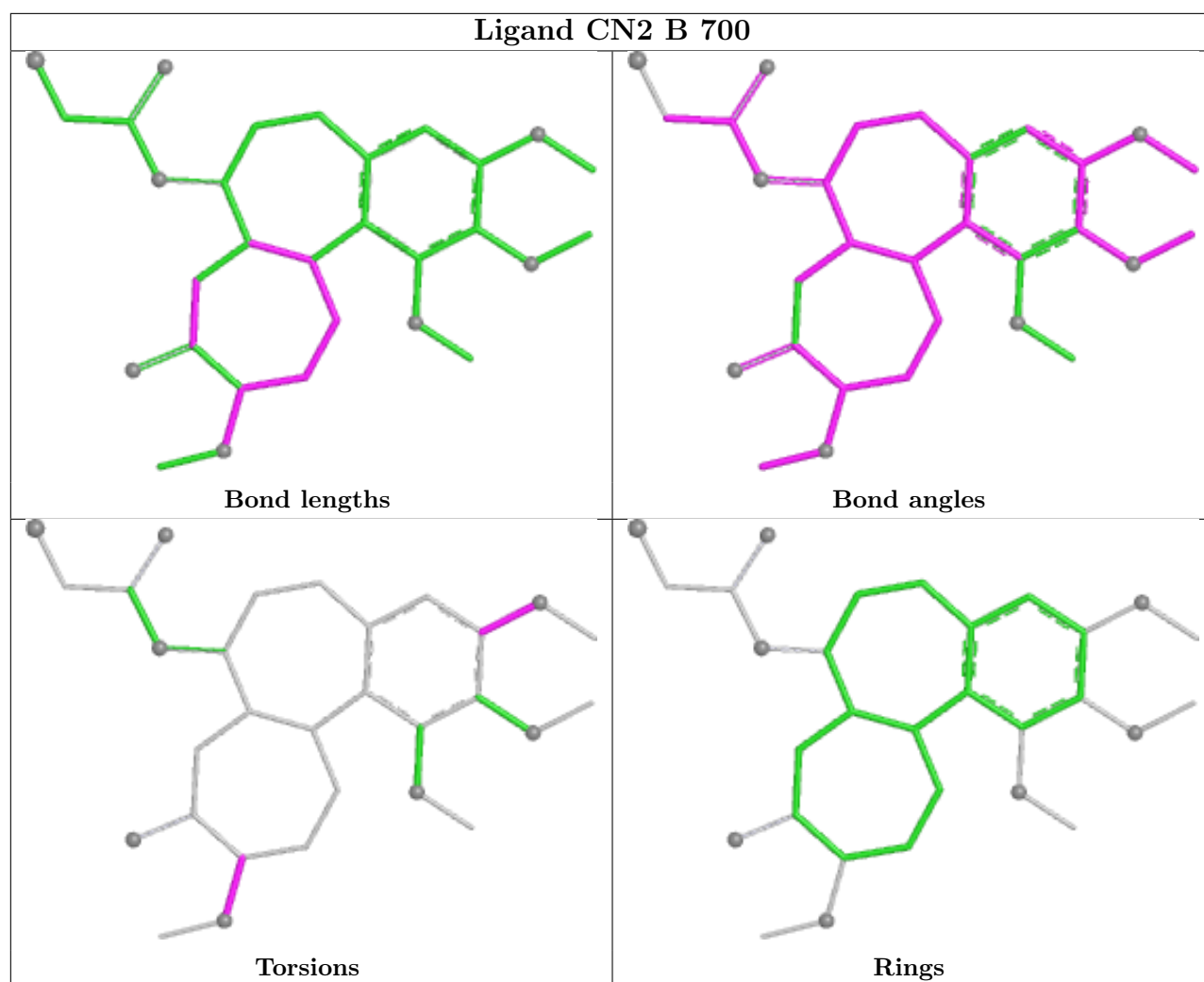
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	602	GDP	2	0
5	C	601	GTP	2	0
7	B	700	CN2	12	0
5	A	600	GTP	4	0
6	D	603	GDP	1	0
7	D	701	CN2	9	0

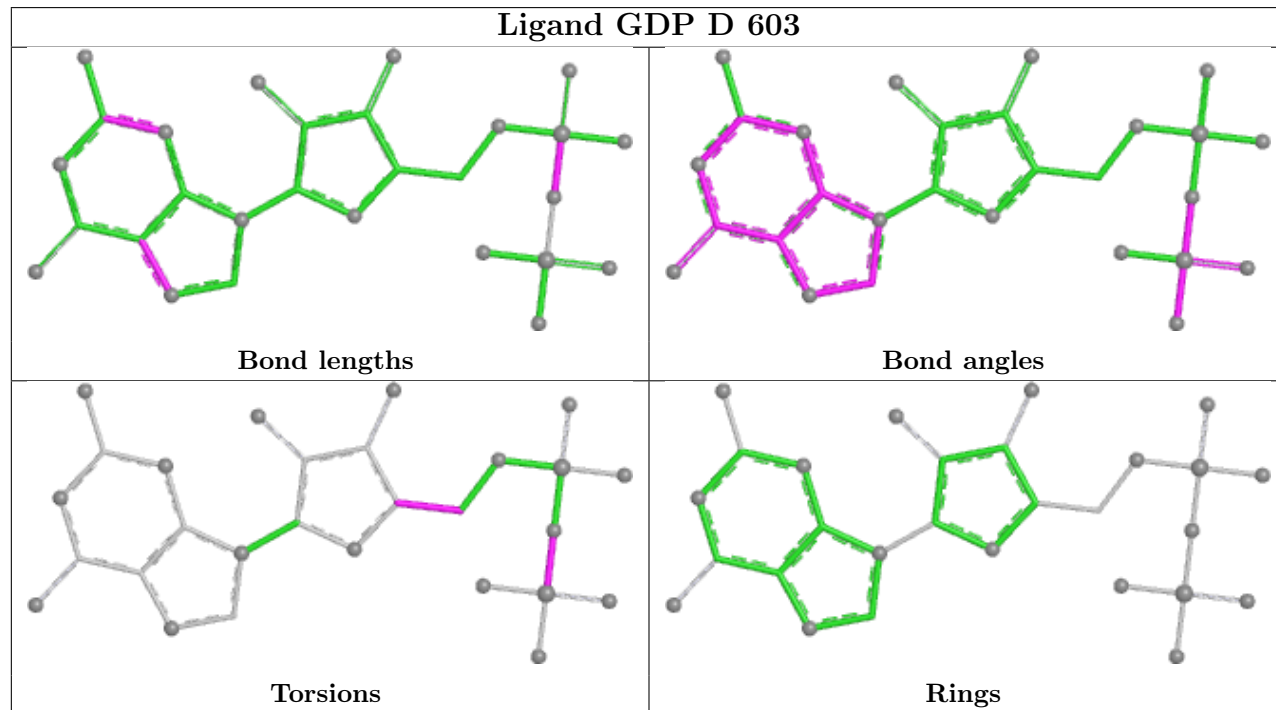
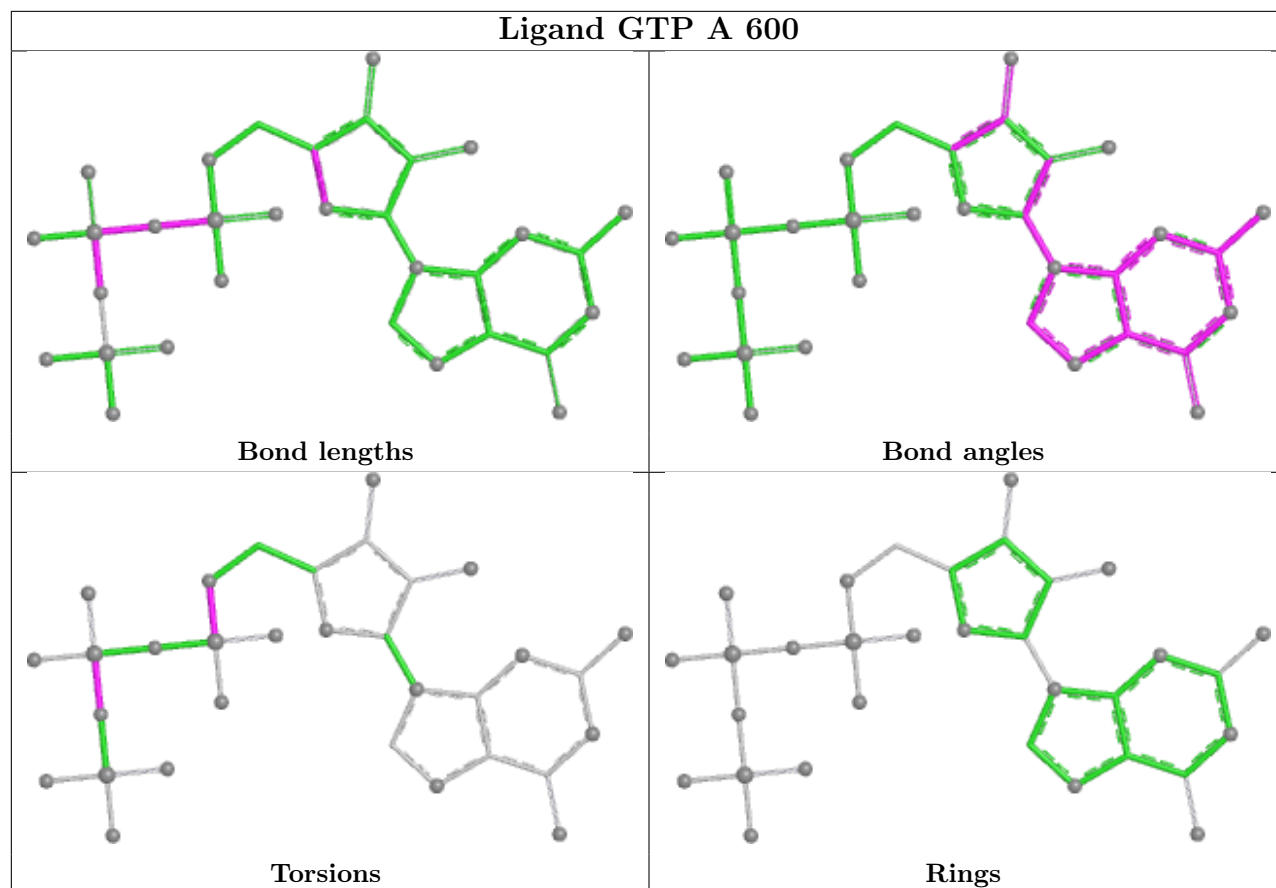
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

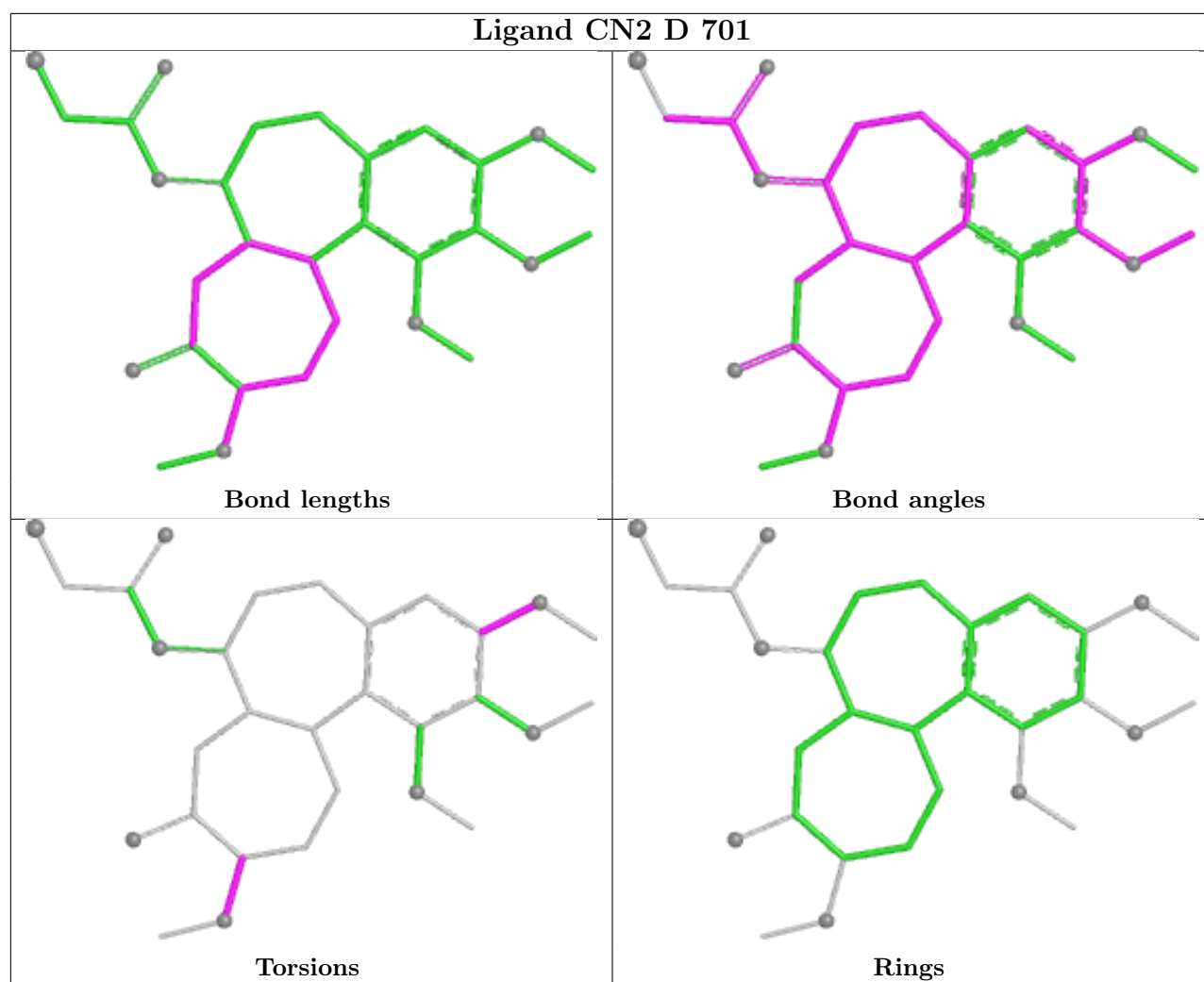
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.