



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:00 PM UTC

PDB ID : 3HKC / pdb_00003hkc
Title : Tubulin-ABT751: RB3 stathmin-like domain complex
Authors : Dorleans, A.; Gigant, B.; Ravelli, R.B.G.; Mailliet, P.; Mikol, V.; Knossow, M.
Deposited on : 2009-05-23
Resolution : 3.80 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) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

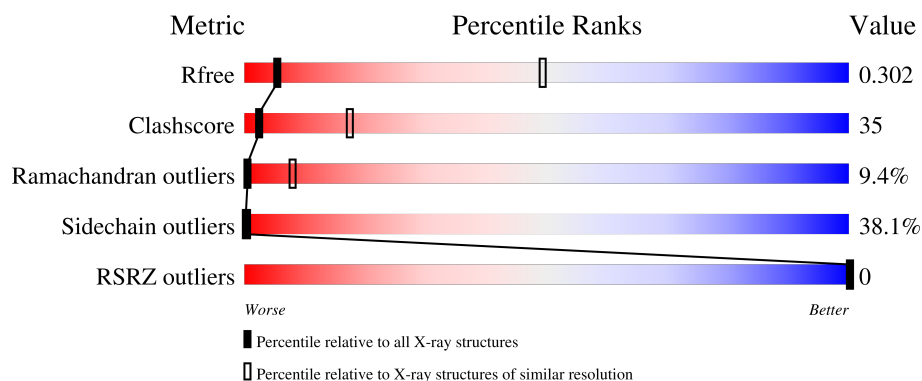
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14145 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
			3300	2097	558	624	21			
1	C	428	Total	C	N	O	S	0	0	0
			3270	2078	553	619	20			

- 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
			3240	2038	546	632	24			
2	D	419	Total	C	N	O	S	0	0	0
			3239	2038	545	632	24			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	0	0
			921	558	175	183	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

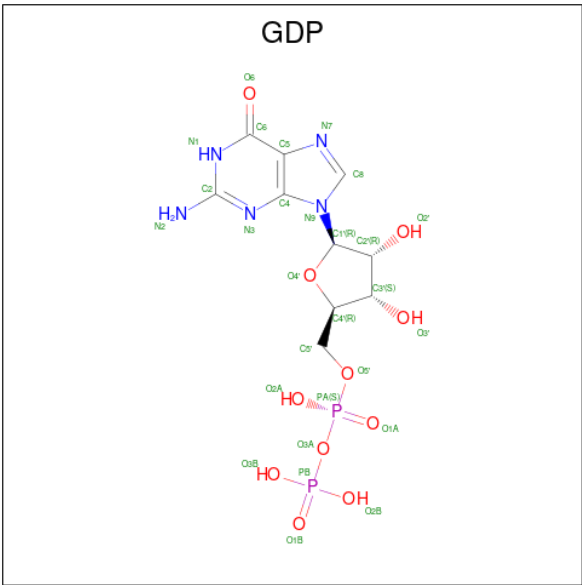


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 5	O 14	P 3	0	0
4	C	1	Total 32	C 10	N 5	O 14	P 3	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

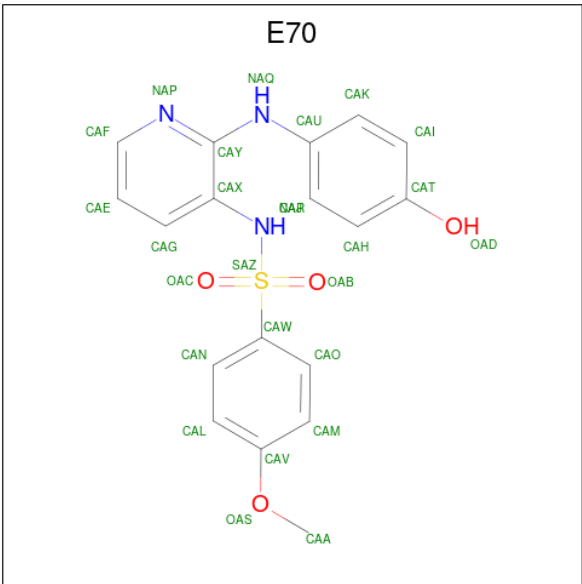
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



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 N-{2-[(4-hydroxyphenyl)amino]pyridin-3-yl}-4-methoxybenzenesulfonamide (CCD ID: E70) (formula: C₁₈H₁₇N₃O₄S).

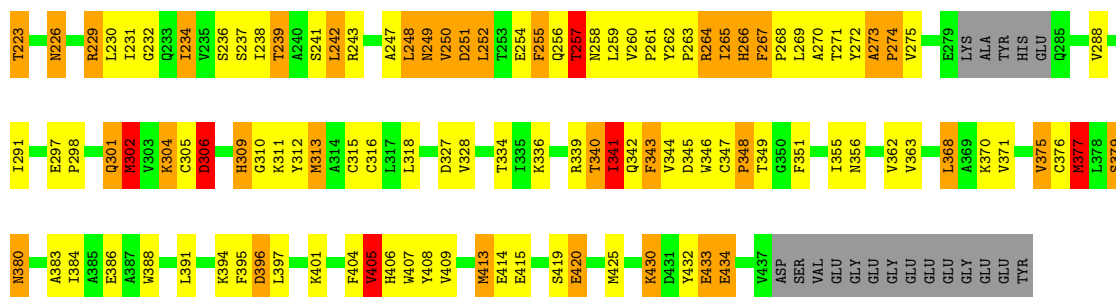


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			26	18	3	4	1		

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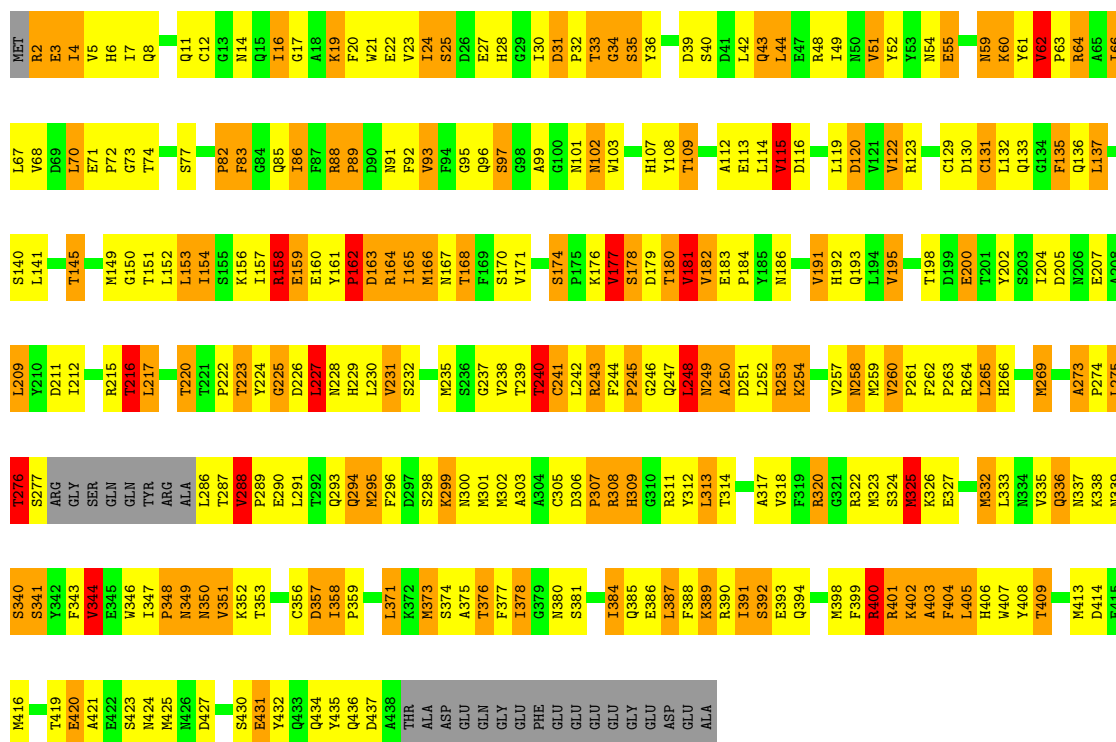
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	S	0	0
			26	18	3	4	1		



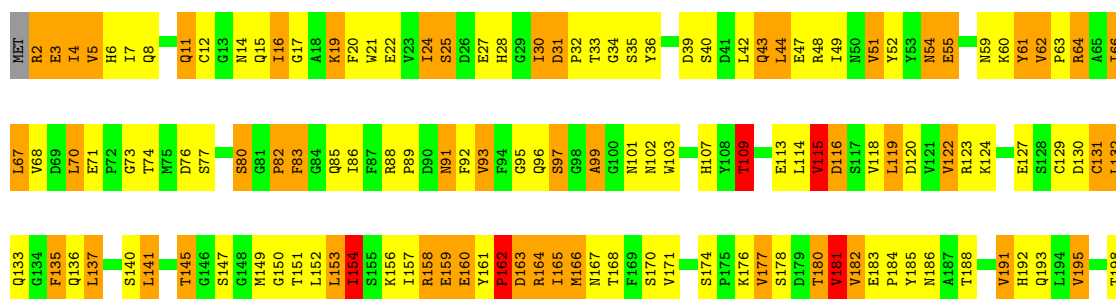
• Molecule 2: Tubulin beta chain

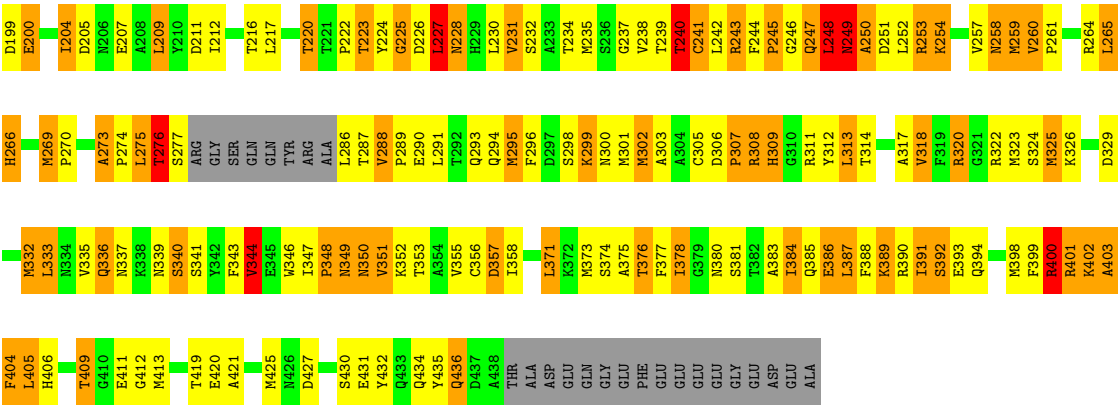
Chain B: 28% 39% 23% 6%



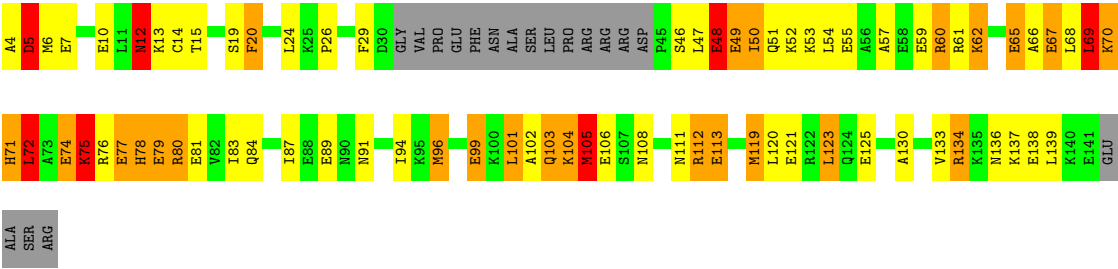
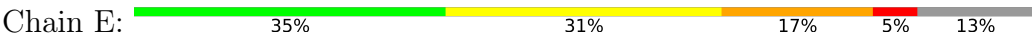
• Molecule 2: Tubulin beta chain

Chain D: 29% 38% 25% 6%





● Molecule 3: Stathmin-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	329.24Å 329.24Å 53.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.80 20.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-3.80) 97.0 (20.00-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.203 , 0.252 0.264 , 0.302	Depositor DCC
R_{free} test set	1674 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	172.4	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.068 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14145	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: E70, GDP, MG, GTP

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	1.00	6/3376 (0.2%)	1.25	18/4588 (0.4%)
1	C	0.87	2/3344 (0.1%)	1.20	12/4552 (0.3%)
2	B	0.91	5/3312 (0.2%)	1.19	13/4498 (0.3%)
2	D	0.89	2/3311 (0.1%)	1.19	12/4495 (0.3%)
3	E	1.04	2/929 (0.2%)	1.36	10/1245 (0.8%)
All	All	0.92	17/14272 (0.1%)	1.22	65/19378 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
2	D	0	2
3	E	0	2
All	All	0	8

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	105	MET	SD-CE	9.57	2.03	1.79
2	D	259	MET	SD-CE	8.36	2.00	1.79
1	C	302	MET	SD-CE	8.06	1.99	1.79
2	B	216	THR	CA-CB	6.53	1.59	1.53
1	A	80	THR	CA-C	6.45	1.58	1.52
1	A	341	ILE	CA-CB	6.42	1.63	1.54
3	E	96	MET	SD-CE	6.15	1.95	1.79
1	A	80	THR	CA-CB	5.61	1.62	1.53
1	A	36	MET	SD-CE	5.57	1.93	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	313	MET	SD-CE	-5.56	1.65	1.79
2	D	154	ILE	CA-CB	5.44	1.62	1.54
1	A	369	ALA	CA-CB	-5.39	1.45	1.53
2	B	437	ASP	CA-C	5.28	1.55	1.52
2	B	177	VAL	CA-CB	5.21	1.61	1.54
2	B	325	MET	SD-CE	5.09	1.92	1.79
1	A	114	ILE	CA-CB	5.07	1.60	1.54
2	B	373	MET	SD-CE	5.07	1.92	1.79

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	104	LYS	N-CA-C	-10.03	98.57	110.41
3	E	78	HIS	N-CA-C	-8.29	102.99	113.43
3	E	51	GLN	N-CA-C	-7.99	102.59	113.30
3	E	46	SER	N-CA-C	7.33	122.07	113.20
1	C	250	VAL	N-CA-C	7.20	122.36	113.00
1	A	376	CYS	N-CA-C	6.94	122.53	114.62
2	D	239	THR	N-CA-C	6.75	118.72	111.36
3	E	6	MET	N-CA-C	6.74	125.15	110.80
2	B	4	ILE	N-CA-C	6.69	118.43	108.46
2	D	220	THR	N-CA-C	6.67	118.24	110.97
3	E	69	LEU	N-CA-C	-6.60	103.28	112.12
1	C	148	GLY	N-CA-C	6.47	120.00	112.50
1	C	102	ASN	N-CA-C	6.36	119.95	108.69
2	B	86	ILE	N-CA-C	6.32	119.91	111.44
1	C	98	ASP	N-CA-C	6.30	118.15	110.41
3	E	96	MET	N-CA-C	-6.27	105.53	113.43
1	A	98	ASP	N-CA-C	6.26	118.11	110.41
1	A	252	LEU	N-CA-C	6.26	118.10	111.28
2	D	160	GLU	N-CA-C	-6.18	104.09	111.69
1	A	24	TYR	N-CA-C	-6.17	104.25	110.97
1	A	266	HIS	CB-CA-C	-6.09	97.43	109.67
1	C	24	TYR	N-CA-C	-6.06	104.58	111.07
3	E	103	GLN	N-CA-C	-6.04	103.65	113.19
1	C	376	CYS	N-CA-C	6.03	121.50	114.62
1	A	102	ASN	N-CA-C	5.93	119.15	109.06
1	A	142	GLY	N-CA-C	-5.93	103.53	112.60
2	B	338	LYS	N-CA-C	-5.88	105.95	113.01
2	D	62	VAL	N-CA-C	5.85	121.53	108.88
1	A	280	LYS	N-CA-C	-5.83	106.21	113.38
2	D	243	ARG	N-CA-C	5.81	117.41	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	220	THR	N-CA-C	5.74	117.40	111.03
1	C	266	HIS	CB-CA-C	-5.70	98.20	109.67
1	A	103	TYR	N-CA-C	-5.65	104.33	111.11
2	B	55	GLU	N-CA-C	5.63	118.14	109.07
3	E	72	LEU	N-CA-C	-5.62	106.26	113.23
2	D	199	ASP	N-CA-C	-5.59	107.00	113.88
1	A	74	VAL	N-CA-C	5.57	116.35	110.72
2	D	4	ILE	N-CA-C	5.53	117.87	108.86
2	B	62	VAL	N-CA-C	5.52	120.81	108.88
1	A	20	CYS	CB-CA-C	5.51	117.96	109.03
2	B	431	GLU	N-CA-C	-5.50	107.22	114.04
2	B	437	ASP	N-CA-C	5.49	116.86	108.12
2	B	288	VAL	N-CA-CB	5.49	118.90	111.21
1	A	139	HIS	N-CA-C	5.45	117.13	108.79
2	B	243	ARG	N-CA-C	5.44	117.85	110.88
1	C	267	PHE	CB-CA-C	5.44	116.34	110.08
2	B	239	THR	N-CA-C	5.40	117.25	111.36
1	C	155	GLU	N-CA-C	-5.40	105.29	111.07
1	A	173	PRO	CA-C-O	-5.39	115.28	121.86
1	C	103	TYR	N-CA-C	-5.36	104.48	111.02
1	A	284	GLU	N-CA-C	-5.32	101.21	109.72
2	D	249	ASN	N-CA-CB	5.30	119.45	110.49
2	D	436	GLN	N-CA-C	-5.28	99.55	110.80
1	A	224	TYR	N-CA-C	-5.25	105.47	111.14
2	D	318	VAL	N-CA-C	5.16	115.47	107.78
2	B	248	LEU	N-CA-C	-5.15	99.83	110.80
3	E	48	GLU	N-CA-C	5.15	120.55	110.56
1	C	343	PHE	N-CA-C	5.15	117.88	109.59
2	B	158	ARG	N-CA-C	-5.13	103.57	110.24
1	A	276	ILE	N-CA-C	5.12	115.11	108.35
2	D	228	ASN	N-CA-C	-5.10	105.80	111.36
2	D	99	ALA	N-CA-C	-5.09	107.02	113.43
1	C	37	PRO	N-CA-C	-5.09	109.39	114.68
1	A	352	LYS	N-CA-C	-5.08	101.68	109.76
1	A	344	VAL	N-CA-C	5.06	115.56	108.89

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	283	HIS	Peptide
1	A	82	THR	Peptide

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Mol	Chain	Res	Type	Group
2	B	162	PRO	Peptide
2	B	248	LEU	Peptide
2	D	162	PRO	Peptide
2	D	248	LEU	Peptide
3	E	5	ASP	Peptide
3	E	50	ILE	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3300	0	3169	196	0
1	C	3270	0	3122	193	0
2	B	3240	0	3056	282	0
2	D	3239	0	3058	282	0
3	E	921	0	814	48	0
4	A	32	0	12	4	0
4	C	32	0	12	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	28	0	12	3	0
6	D	28	0	12	4	0
7	B	26	0	17	5	0
7	D	26	0	17	5	0
All	All	14145	0	13301	967	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 35.

All (967) 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:105:MET:SD	3:E:105:MET:CE	2.03	1.44
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.74	1.16
2:B:165:ILE:HD11	2:B:252:LEU:HG	1.25	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.22	1.15
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.17	1.15
2:D:11:GLN:HG3	2:D:74:THR:CG2	1.77	1.13
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.18	1.12
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.77	1.11
2:B:11:GLN:HG3	2:B:74:THR:CG2	1.80	1.11
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.16	1.11
2:B:99:ALA:HB1	2:B:145:THR:HG22	1.25	1.10
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.28	1.10
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.80	1.09
2:D:99:ALA:HB1	2:D:145:THR:HG22	1.13	1.09
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.28	1.08
2:D:165:ILE:HD11	2:D:252:LEU:HG	1.29	1.07
1:C:90:GLU:O	1:C:121:ARG:HD3	1.57	1.05
2:D:99:ALA:HB1	2:D:145:THR:CG2	1.86	1.04
2:B:11:GLN:HG3	2:B:74:THR:HG21	1.04	1.03
2:D:151:THR:HB	2:D:193:GLN:HG2	1.37	1.03
1:C:273:ALA:CB	1:C:274:PRO:HD3	1.91	1.01
2:D:16:ILE:HG23	2:D:235:MET:HE1	1.42	1.01
2:B:250:ALA:HB1	7:B:700:E70:HAJ	1.44	1.00
2:D:11:GLN:CG	2:D:74:THR:HG21	1.91	0.99
2:B:223:THR:HB	2:B:225:GLY:H	1.27	0.99
1:A:90:GLU:O	1:A:121:ARG:HD3	1.62	0.98
2:D:250:ALA:HB1	7:D:700:E70:HAJ	1.45	0.98
2:D:287:THR:HG22	2:D:290:GLU:HB2	1.46	0.97
2:D:223:THR:HB	2:D:225:GLY:H	1.30	0.96
2:D:251:ASP:HB2	2:D:254:LYS:H	1.31	0.95
1:A:247:ALA:HB1	3:E:19:SER:CB	1.97	0.95
2:B:251:ASP:HB2	2:B:254:LYS:H	1.32	0.95
1:A:206:ASN:HD21	4:A:600:GTP:HN22	1.15	0.94
2:D:11:GLN:HG3	2:D:74:THR:HG21	0.95	0.94
2:B:16:ILE:HG23	2:B:235:MET:HE1	1.47	0.94
1:A:181:VAL:H	2:B:258:ASN:HD21	1.16	0.93
1:A:273:ALA:HB3	1:A:274:PRO:CD	1.99	0.93
1:C:206:ASN:HD21	4:C:600:GTP:HN22	1.08	0.93
2:D:412:GLY:O	3:E:133:VAL:HB	1.69	0.93
2:B:167:ASN:HD22	2:B:252:LEU:HD11	1.34	0.93
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.48	0.93
3:E:57:ALA:HA	3:E:60:ARG:NH1	1.84	0.91
1:C:99:ALA:HB2	1:C:145:THR:CG2	2.01	0.91
2:B:99:ALA:HB1	2:B:145:THR:CG2	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.00	0.91
1:C:167:LEU:HD13	1:C:252:LEU:HD11	1.52	0.91
2:B:11:GLN:CG	2:B:74:THR:HG21	1.99	0.91
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.02	0.90
2:B:54:ASN:ND2	2:B:64:ARG:HD2	1.88	0.90
2:D:135:PHE:HB2	2:D:166:MET:HE1	1.51	0.89
1:A:229:ARG:HG2	1:A:229:ARG:HH11	1.36	0.89
1:A:296:PHE:O	1:A:339:ARG:NH2	2.06	0.89
2:B:192:HIS:HD2	2:B:421:ALA:HA	1.37	0.89
2:B:287:THR:HG22	2:B:290:GLU:HB2	1.54	0.88
2:B:223:THR:HB	2:B:225:GLY:N	1.88	0.88
3:E:57:ALA:HA	3:E:60:ARG:HH12	1.39	0.88
2:B:179:ASP:HB2	1:C:248:LEU:HD21	1.55	0.88
1:C:273:ALA:CB	1:C:375:VAL:H	1.87	0.87
2:D:273:ALA:CB	2:D:274:PRO:CD	2.52	0.87
2:B:273:ALA:CB	2:B:274:PRO:CD	2.53	0.87
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.55	0.86
1:A:273:ALA:CB	1:A:375:VAL:H	1.88	0.86
2:B:401:ARG:NH2	1:C:434:GLU:O	2.09	0.86
1:A:99:ALA:CB	1:A:145:THR:HG22	2.02	0.86
2:B:165:ILE:CD1	2:B:252:LEU:HG	2.06	0.86
2:B:54:ASN:HD22	2:B:64:ARG:HD2	1.38	0.85
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.06	0.85
2:B:306:ASP:O	2:B:308:ARG:N	2.07	0.85
1:A:273:ALA:CB	1:A:274:PRO:CD	2.56	0.83
1:C:199:ASP:HB3	1:C:256:GLN:HE22	1.40	0.83
3:E:48:GLU:HG3	3:E:49:GLU:N	1.92	0.83
1:A:278:ALA:O	1:A:279:GLU:HB3	1.76	0.83
2:B:151:THR:HB	2:B:193:GLN:HG2	1.59	0.83
2:B:245:PRO:HG2	2:B:246:GLY:H	1.44	0.83
2:D:162:PRO:HD2	2:D:163:ASP:HB2	1.60	0.82
2:D:135:PHE:HB2	2:D:166:MET:CE	2.09	0.82
2:D:231:VAL:HG12	2:D:235:MET:HE2	1.63	0.81
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.60	0.81
3:E:76:ARG:O	3:E:78:HIS:N	2.13	0.81
1:C:99:ALA:CB	1:C:145:THR:HG22	2.07	0.81
1:C:229:ARG:HG2	1:C:229:ARG:HH11	1.45	0.81
2:D:145:THR:HG23	6:D:600:GDP:O3B	1.81	0.81
2:D:209:LEU:HD21	2:D:231:VAL:HG22	1.63	0.81
2:B:275:LEU:O	2:B:276:THR:HB	1.80	0.81
2:D:165:ILE:CD1	2:D:252:LEU:HG	2.08	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:VAL:O	1:A:260:VAL:CG2	2.30	0.80
1:A:99:ALA:HB2	1:A:145:THR:CG2	2.07	0.80
2:D:223:THR:HB	2:D:225:GLY:N	1.96	0.80
2:B:251:ASP:C	2:B:253:ARG:H	1.89	0.79
1:C:206:ASN:HD21	4:C:600:GTP:N2	1.80	0.79
2:D:350:ASN:HD22	2:D:350:ASN:H	1.26	0.79
2:B:209:LEU:HD21	2:B:231:VAL:HG22	1.64	0.79
2:B:70:LEU:HA	2:B:95:GLY:HA3	1.64	0.78
2:D:273:ALA:HB1	2:D:274:PRO:HD3	1.64	0.78
2:B:114:LEU:O	2:B:116:ASP:N	2.17	0.78
1:A:181:VAL:H	2:B:258:ASN:ND2	1.82	0.78
1:A:315:CYS:SG	1:A:377:MET:CE	2.72	0.77
1:C:153:LEU:HD13	1:C:157:LEU:HD11	1.66	0.77
2:B:317:ALA:HB3	2:B:353:THR:HG22	1.67	0.77
2:B:385:GLN:HE21	2:B:389:LYS:HD2	1.50	0.76
7:D:700:E70:HAK	7:D:700:E70:NAP	1.98	0.76
1:C:265:ILE:H	1:C:265:ILE:HD12	1.51	0.76
2:D:385:GLN:HE21	2:D:389:LYS:HD2	1.50	0.76
3:E:76:ARG:C	3:E:78:HIS:H	1.93	0.76
2:B:135:PHE:HZ	2:B:161:TYR:CD1	2.03	0.76
2:B:403:ALA:O	2:B:405:LEU:N	2.18	0.76
2:B:291:LEU:HD21	2:B:375:ALA:CB	2.16	0.75
2:D:204:ILE:HD12	2:D:204:ILE:H	1.52	0.75
2:D:36:TYR:OH	2:D:40:SER:O	2.05	0.75
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.67	0.75
2:D:70:LEU:HA	2:D:95:GLY:HA3	1.69	0.75
2:D:275:LEU:O	2:D:276:THR:HB	1.86	0.75
1:C:191:THR:HG23	1:C:425:MET:CE	2.17	0.75
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.68	0.75
2:B:2:ARG:O	2:B:3:GLU:HB2	1.85	0.75
1:A:266:HIS:O	1:A:268:PRO:HD3	1.87	0.75
2:D:306:ASP:O	2:D:308:ARG:N	2.14	0.74
2:D:245:PRO:HG2	2:D:246:GLY:H	1.53	0.74
2:D:114:LEU:O	2:D:116:ASP:N	2.19	0.74
2:D:135:PHE:HZ	2:D:161:TYR:CD1	2.04	0.74
1:A:88:HIS:HB2	1:A:91:GLN:NE2	2.03	0.74
2:B:135:PHE:HB2	2:B:166:MET:HE1	1.70	0.74
1:A:34:GLY:O	1:A:61:HIS:HB2	1.88	0.74
1:C:182:VAL:CG2	1:C:408:TYR:OH	2.36	0.74
2:B:273:ALA:HB1	2:B:274:PRO:HD3	1.67	0.73
1:A:87:PHE:HD2	1:A:87:PHE:N	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:387:LEU:HD23	2:D:388:PHE:N	2.04	0.73
2:B:350:ASN:H	2:B:350:ASN:HD22	1.33	0.73
1:C:266:HIS:O	1:C:268:PRO:HD3	1.88	0.73
1:A:315:CYS:SG	1:A:377:MET:HE2	2.29	0.73
2:D:135:PHE:CZ	2:D:161:TYR:CD1	2.76	0.73
1:A:190:THR:HG23	1:A:191:THR:H	1.54	0.72
2:B:165:ILE:HD11	2:B:252:LEU:CG	2.13	0.72
1:C:181:VAL:H	2:D:258:ASN:HD21	1.34	0.72
2:B:135:PHE:CZ	2:B:161:TYR:CD1	2.77	0.72
2:B:391:ILE:HG13	2:B:392:SER:N	2.05	0.72
2:D:167:ASN:HD22	2:D:252:LEU:HD11	1.54	0.72
2:D:391:ILE:HG13	2:D:392:SER:N	2.03	0.72
2:B:251:ASP:O	2:B:253:ARG:N	2.23	0.72
1:C:90:GLU:O	1:C:121:ARG:CD	2.36	0.72
1:A:249:ASN:HD22	1:A:254:GLU:HG2	1.54	0.71
2:B:135:PHE:HB2	2:B:166:MET:CE	2.20	0.71
2:B:70:LEU:HD12	2:B:145:THR:HB	1.71	0.71
2:D:191:VAL:HG11	2:D:425:MET:HG3	1.72	0.71
1:A:87:PHE:N	1:A:87:PHE:CD2	2.56	0.71
1:C:407:TRP:CG	2:D:257:VAL:HG23	2.25	0.71
2:B:223:THR:CB	2:B:225:GLY:H	2.03	0.71
2:D:192:HIS:HD2	2:D:421:ALA:HA	1.55	0.71
2:D:251:ASP:C	2:D:253:ARG:H	1.97	0.71
2:B:145:THR:HG23	6:B:600:GDP:O3B	1.90	0.71
3:E:48:GLU:O	3:E:50:ILE:N	2.23	0.71
2:D:20:PHE:O	2:D:24:ILE:HG23	1.90	0.71
3:E:10:GLU:HG3	3:E:20:PHE:HB3	1.71	0.71
1:A:270:ALA:HB3	1:A:302:MET:HE2	1.71	0.70
2:D:145:THR:HG23	6:D:600:GDP:PB	2.31	0.70
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.73	0.70
1:A:265:ILE:HD12	1:A:265:ILE:H	1.55	0.70
1:C:341:ILE:HD13	1:C:341:ILE:H	1.55	0.70
1:A:182:VAL:CG2	1:A:408:TYR:OH	2.39	0.70
1:C:20:CYS:HB3	1:C:232:GLY:HA2	1.71	0.70
1:C:79:ARG:HH22	1:C:94:THR:CG2	2.04	0.70
2:D:241:CYS:HB3	2:D:247:GLN:HE21	1.55	0.70
3:E:67:GLU:C	3:E:69:LEU:H	1.98	0.70
2:D:306:ASP:C	2:D:308:ARG:H	2.00	0.70
2:D:317:ALA:HB3	2:D:353:THR:HG22	1.74	0.70
1:C:79:ARG:NH2	1:C:94:THR:HG21	2.07	0.69
2:D:223:THR:CB	2:D:225:GLY:H	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ARG:HH22	1:C:94:THR:HG21	1.56	0.69
2:B:22:GLU:OE1	2:B:82:PRO:HB2	1.93	0.69
1:C:346:TRP:HE3	1:C:346:TRP:O	1.76	0.69
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.73	0.69
2:D:114:LEU:HD23	2:D:149:MET:HE1	1.73	0.69
2:D:164:ARG:NH2	2:D:253:ARG:HH22	1.90	0.69
2:D:307:PRO:CB	2:D:312:TYR:OH	2.41	0.69
1:A:339:ARG:HG3	1:A:340:THR:H	1.57	0.69
2:D:226:ASP:O	2:D:227:LEU:HB3	1.92	0.69
2:D:287:THR:CG2	2:D:290:GLU:HB2	2.22	0.69
2:D:291:LEU:HD21	2:D:375:ALA:CB	2.23	0.69
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.25	0.69
2:D:54:ASN:ND2	2:D:64:ARG:HD2	2.08	0.68
1:A:190:THR:HG23	1:A:191:THR:N	2.08	0.68
1:A:368:LEU:HD12	1:A:368:LEU:H	1.56	0.68
1:C:315:CYS:SG	1:C:377:MET:HE1	2.34	0.68
1:A:246:GLY:O	1:A:247:ALA:O	2.11	0.68
1:A:346:TRP:HE3	1:A:346:TRP:O	1.76	0.68
2:D:298:SER:C	2:D:300:ASN:H	2.01	0.68
2:B:306:ASP:C	2:B:308:ARG:H	2.02	0.68
1:C:34:GLY:O	1:C:61:HIS:HB2	1.93	0.68
2:D:265:LEU:HB3	2:D:432:TYR:CE2	2.28	0.68
1:A:229:ARG:HH11	1:A:229:ARG:CG	2.04	0.68
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.76	0.68
1:A:106:GLY:O	1:A:111:GLY:HA3	1.93	0.68
2:D:238:VAL:HG13	2:D:378:ILE:HD11	1.76	0.68
1:A:273:ALA:HB2	1:A:375:VAL:H	1.57	0.67
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.76	0.67
2:B:241:CYS:HB3	2:B:247:GLN:HE21	1.57	0.67
2:B:54:ASN:HD22	2:B:64:ARG:CD	2.07	0.67
2:B:20:PHE:O	2:B:24:ILE:HG23	1.94	0.67
2:D:158:ARG:O	2:D:159:GLU:HB3	1.93	0.67
2:B:21:TRP:O	2:B:25:SER:HB2	1.94	0.67
1:A:206:ASN:HD21	4:A:600:GTP:N2	1.89	0.67
2:B:167:ASN:ND2	2:B:252:LEU:HD11	2.09	0.67
1:C:315:CYS:SG	1:C:377:MET:CE	2.82	0.67
3:E:133:VAL:HA	3:E:136:ASN:HB3	1.77	0.67
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.60	0.67
2:D:70:LEU:HD11	2:D:149:MET:HE3	1.76	0.67
1:C:190:THR:HG23	1:C:191:THR:H	1.59	0.67
1:A:87:PHE:HD2	1:A:87:PHE:H	1.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ILE:HD12	2:B:204:ILE:H	1.60	0.67
2:D:226:ASP:O	2:D:227:LEU:CB	2.43	0.67
1:A:247:ALA:HA	3:E:12:ASN:OD1	1.94	0.66
1:A:398:MET:HG3	2:B:348:PRO:HD3	1.77	0.66
7:B:700:E70:HAK	7:B:700:E70:NAP	2.10	0.66
2:D:2:ARG:HH12	2:D:133:GLN:HA	1.59	0.66
2:B:336:GLN:HE22	2:B:351:VAL:HG12	1.59	0.66
2:D:99:ALA:CB	2:D:145:THR:CG2	2.71	0.66
1:A:248:LEU:HD22	1:A:249:ASN:ND2	2.11	0.66
2:D:247:GLN:HG3	2:D:248:LEU:H	1.60	0.66
2:D:2:ARG:O	2:D:3:GLU:HB2	1.96	0.66
2:D:247:GLN:CG	2:D:248:LEU:H	2.08	0.66
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.76	0.66
2:D:51:VAL:HG12	2:D:52:TYR:CD1	2.31	0.66
2:B:51:VAL:HG12	2:B:52:TYR:CD1	2.30	0.66
2:D:307:PRO:HB2	2:D:312:TYR:OH	1.96	0.66
1:A:315:CYS:SG	1:A:377:MET:HE1	2.36	0.65
1:A:2:ARG:HA	1:A:2:ARG:NH1	2.12	0.65
2:B:265:LEU:HB3	2:B:432:TYR:CE2	2.32	0.65
1:C:142:GLY:HA3	1:C:183:GLU:HG3	1.77	0.65
3:E:130:ALA:O	3:E:134:ARG:HB3	1.96	0.65
2:B:251:ASP:C	2:B:253:ARG:N	2.50	0.65
1:C:261:PRO:HB2	1:C:262:TYR:CD1	2.32	0.65
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.79	0.64
2:D:205:ASP:OD1	2:D:207:GLU:HB3	1.97	0.64
2:D:336:GLN:HE22	2:D:351:VAL:HG12	1.62	0.64
1:C:206:ASN:ND2	4:C:600:GTP:HN22	1.90	0.64
2:D:403:ALA:O	2:D:405:LEU:N	2.31	0.64
1:C:87:PHE:N	1:C:87:PHE:HD2	1.96	0.64
2:B:296:PHE:HE1	2:B:332:MET:HE1	1.62	0.64
2:B:404:PHE:CE1	1:C:261:PRO:HB3	2.33	0.64
1:C:430:LYS:O	1:C:434:GLU:HB2	1.97	0.63
3:E:70:LYS:O	3:E:70:LYS:HG2	1.97	0.63
1:A:246:GLY:HA2	3:E:14:CYS:SG	2.38	0.63
2:B:403:ALA:C	2:B:405:LEU:H	2.06	0.63
1:C:229:ARG:HH11	1:C:229:ARG:CG	2.10	0.63
1:C:251:ASP:OD1	1:C:252:LEU:N	2.30	0.63
2:B:140:SER:HA	2:B:171:VAL:HG23	1.80	0.63
2:B:238:VAL:HG13	2:B:378:ILE:HD11	1.80	0.63
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.39	0.63
2:B:70:LEU:HD11	2:B:149:MET:HE3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:ASN:HD22	2:D:64:ARG:HD2	1.61	0.63
1:A:264:ARG:NH1	1:A:431:ASP:OD2	2.31	0.63
2:B:245:PRO:HG3	2:B:247:GLN:CD	2.23	0.63
2:B:54:ASN:ND2	2:B:64:ARG:CD	2.62	0.62
2:B:298:SER:C	2:B:300:ASN:H	2.07	0.62
2:D:21:TRP:O	2:D:25:SER:HB2	1.99	0.62
1:C:88:HIS:HB2	1:C:91:GLN:NE2	2.14	0.62
2:B:205:ASP:OD1	2:B:207:GLU:HB3	1.98	0.62
1:C:256:GLN:C	1:C:258:ASN:N	2.55	0.62
1:A:190:THR:CG2	1:A:191:THR:H	2.12	0.62
1:C:87:PHE:N	1:C:87:PHE:CD2	2.65	0.62
1:C:273:ALA:HB2	1:C:375:VAL:H	1.62	0.62
2:D:251:ASP:C	2:D:253:ARG:N	2.55	0.62
2:B:145:THR:HG23	6:B:600:GDP:PB	2.40	0.62
2:B:2:ARG:HH12	2:B:133:GLN:HA	1.64	0.62
2:D:191:VAL:CG1	2:D:425:MET:HG3	2.29	0.62
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.82	0.62
1:A:153:LEU:HD13	1:A:157:LEU:HD11	1.81	0.62
2:B:164:ARG:NH2	2:B:253:ARG:HH22	1.98	0.62
2:B:247:GLN:CG	2:B:248:LEU:H	2.13	0.62
1:A:20:CYS:HB3	1:A:232:GLY:HA2	1.82	0.61
2:D:251:ASP:HB2	2:D:254:LYS:HB2	1.81	0.61
2:D:311:ARG:HD3	2:D:436:GLN:HG2	1.81	0.61
2:B:312:TYR:HE2	2:B:377:PHE:HZ	1.47	0.61
2:B:350:ASN:HD22	2:B:350:ASN:N	1.97	0.61
1:C:405:VAL:CG1	1:C:406:HIS:N	2.62	0.61
2:B:162:PRO:HD2	2:B:163:ASP:HB2	1.81	0.61
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.81	0.61
3:E:76:ARG:O	3:E:79:GLU:N	2.33	0.61
2:D:165:ILE:HD11	2:D:252:LEU:CG	2.18	0.61
1:A:412:GLY:O	3:E:60:ARG:NH1	2.33	0.61
2:D:30:ILE:HD11	2:D:49:ILE:HD11	1.82	0.61
2:B:251:ASP:HB2	2:B:254:LYS:HB2	1.81	0.61
1:C:191:THR:HG23	1:C:425:MET:HE1	1.83	0.60
2:D:288:VAL:HB	2:D:289:PRO:HD3	1.83	0.60
1:A:248:LEU:HD12	1:A:354:GLY:HA3	1.83	0.60
2:B:287:THR:CG2	2:B:290:GLU:HB2	2.28	0.60
3:E:80:ARG:HH21	3:E:84:GLN:HG2	1.65	0.60
1:A:190:THR:O	1:A:192:HIS:N	2.35	0.60
1:A:260:VAL:O	1:A:260:VAL:HG23	2.01	0.60
2:D:70:LEU:HD12	2:D:145:THR:HB	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:245:PRO:HG3	2:D:247:GLN:CD	2.27	0.60
1:C:190:THR:HG23	1:C:191:THR:N	2.15	0.60
2:D:66:ILE:HD13	2:D:122:VAL:HG12	1.83	0.60
2:D:5:VAL:CG2	2:D:135:PHE:HD2	2.14	0.60
1:C:260:VAL:HG23	1:C:260:VAL:O	2.01	0.60
2:D:241:CYS:HB3	2:D:247:GLN:NE2	2.17	0.60
3:E:83:ILE:O	3:E:87:ILE:HD12	2.01	0.60
2:B:30:ILE:HD11	2:B:49:ILE:HD11	1.82	0.60
2:D:158:ARG:O	2:D:159:GLU:CB	2.49	0.60
2:B:226:ASP:O	2:B:227:LEU:CB	2.50	0.60
1:C:190:THR:CG2	1:C:191:THR:H	2.15	0.60
2:B:88:ARG:HG3	2:B:89:PRO:HD2	1.84	0.60
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.82	0.60
2:D:133:GLN:HE21	2:D:252:LEU:HB3	1.66	0.60
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.37	0.59
1:C:368:LEU:H	1:C:368:LEU:HD12	1.67	0.59
2:D:337:ASN:HA	2:D:340:SER:HB3	1.84	0.59
1:A:71:GLU:OE2	4:A:600:GTP:O1G	2.20	0.59
1:C:103:TYR:O	1:C:104:ALA:C	2.41	0.59
2:D:251:ASP:O	2:D:253:ARG:N	2.33	0.59
1:A:12:ALA:O	1:A:13:GLY:C	2.46	0.59
2:D:391:ILE:HG12	2:D:425:MET:HE1	1.84	0.59
2:D:150:GLY:O	2:D:154:ILE:HG23	2.01	0.59
1:C:199:ASP:HB3	1:C:256:GLN:NE2	2.14	0.59
1:A:217:LEU:O	1:A:218:ASP:HB3	2.03	0.58
2:D:204:ILE:HD12	2:D:204:ILE:N	2.17	0.58
1:A:395:PHE:O	1:A:396:ASP:C	2.46	0.58
2:B:88:ARG:HB3	2:B:91:ASN:OD1	2.02	0.58
3:E:101:LEU:O	3:E:103:GLN:N	2.27	0.58
1:A:86:LEU:HB3	1:A:87:PHE:HD2	1.67	0.58
1:A:407:TRP:CG	2:B:257:VAL:HG23	2.38	0.58
2:B:133:GLN:HE21	2:B:252:LEU:HB3	1.69	0.58
2:D:237:GLY:CA	2:D:376:THR:HG21	2.34	0.58
2:D:298:SER:O	2:D:300:ASN:N	2.35	0.58
2:D:308:ARG:HG3	2:D:308:ARG:HH11	1.67	0.58
1:A:2:ARG:HB2	1:A:131:GLY:O	2.03	0.58
1:A:77:GLU:O	1:A:80:THR:HG22	2.03	0.58
1:A:260:VAL:O	1:A:260:VAL:HG22	2.02	0.58
2:B:387:LEU:HD23	2:B:388:PHE:N	2.18	0.58
2:B:357:ASP:OD2	2:B:357:ASP:N	2.35	0.58
2:B:336:GLN:NE2	2:B:351:VAL:CG1	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:435:TYR:O	2:D:436:GLN:HG3	2.02	0.58
1:A:340:THR:O	1:A:340:THR:HG22	2.02	0.58
1:A:430:LYS:O	1:A:434:GLU:HB2	2.04	0.58
2:B:311:ARG:HD3	2:B:436:GLN:HG2	1.86	0.58
2:B:237:GLY:CA	2:B:376:THR:HG21	2.33	0.57
1:C:182:VAL:HG21	1:C:408:TYR:OH	2.03	0.57
1:C:270:ALA:O	1:C:302:MET:HB2	2.03	0.57
1:C:108:TYR:O	1:C:112:LYS:HB2	2.04	0.57
2:B:325:MET:HE3	2:B:326:LYS:H	1.68	0.57
1:C:139:HIS:CG	1:C:150:THR:HG21	2.40	0.57
2:B:3:GLU:HG2	2:B:64:ARG:NH2	2.19	0.57
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.45	0.57
2:D:273:ALA:CB	2:D:375:ALA:H	2.17	0.57
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.85	0.57
2:B:391:ILE:HG12	2:B:425:MET:HE1	1.85	0.57
2:B:179:ASP:CB	1:C:248:LEU:HD21	2.31	0.57
2:B:115:VAL:HG12	2:B:116:ASP:N	2.19	0.57
1:C:105:ARG:NH2	2:D:253:ARG:HH21	2.02	0.57
1:C:313:MET:HG2	1:C:380:ASN:O	2.05	0.57
1:A:105:ARG:HH22	2:B:253:ARG:HH21	1.50	0.57
2:B:407:TRP:CE2	1:C:257:THR:HA	2.40	0.57
1:C:291:ILE:HD12	1:C:375:VAL:HG23	1.87	0.57
2:B:241:CYS:HB3	2:B:247:GLN:NE2	2.19	0.56
1:C:106:GLY:O	1:C:111:GLY:HA3	2.04	0.56
2:D:401:ARG:HG3	2:D:401:ARG:NH1	2.20	0.56
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.40	0.56
1:A:178:SER:OG	2:B:352:LYS:HE3	2.05	0.56
1:C:105:ARG:CZ	2:D:253:ARG:HH21	2.18	0.56
1:C:133:GLN:NE2	1:C:252:LEU:HB2	2.19	0.56
1:A:79:ARG:HH22	1:A:94:THR:CG2	2.18	0.56
1:A:172:TYR:HE2	1:A:391:LEU:HD22	1.70	0.56
1:A:388:TRP:CE3	1:A:388:TRP:HA	2.40	0.56
1:A:420:GLU:O	1:A:420:GLU:HG2	2.05	0.56
1:C:105:ARG:NH1	2:D:253:ARG:HH21	2.02	0.56
2:D:308:ARG:HG3	2:D:308:ARG:NH1	2.20	0.56
2:D:404:PHE:CD1	2:D:404:PHE:N	2.73	0.56
3:E:112:ARG:HG2	3:E:113:GLU:N	2.20	0.56
1:A:133:GLN:OE1	1:A:251:ASP:HB2	2.05	0.56
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.87	0.56
2:B:391:ILE:CG1	2:B:425:MET:HE1	2.35	0.56
2:D:391:ILE:CG1	2:D:425:MET:HE1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:404:PHE:N	2:D:404:PHE:HD1	2.03	0.56
1:A:291:ILE:HD12	1:A:375:VAL:CG2	2.35	0.56
2:B:229:HIS:CE1	2:B:277:SER:HB3	2.40	0.56
2:D:135:PHE:N	2:D:135:PHE:CD1	2.74	0.56
1:C:191:THR:HG23	1:C:425:MET:HE3	1.87	0.56
2:D:312:TYR:HE2	2:D:377:PHE:HZ	1.54	0.56
1:C:71:GLU:OE2	4:C:600:GTP:O1G	2.23	0.56
1:C:183:GLU:HB3	1:C:184:PRO:CD	2.37	0.56
2:B:204:ILE:HD12	2:B:204:ILE:N	2.21	0.55
2:D:3:GLU:HG2	2:D:64:ARG:NH2	2.21	0.55
2:B:102:ASN:O	2:B:102:ASN:OD1	2.24	0.55
2:B:352:LYS:HG3	7:B:700:E70:HAM	1.89	0.55
2:D:401:ARG:HG3	2:D:401:ARG:HH11	1.72	0.55
1:A:3:GLU:HB2	1:A:132:LEU:HA	1.88	0.55
1:A:105:ARG:NH2	2:B:253:ARG:HH21	2.04	0.55
7:D:700:E70:NAP	7:D:700:E70:CAK	2.67	0.55
3:E:74:GLU:C	3:E:76:ARG:H	2.14	0.55
1:A:312:TYR:HE2	1:A:379:SER:CB	2.18	0.55
2:B:435:TYR:O	2:B:436:GLN:HG3	2.06	0.55
2:D:296:PHE:HE1	2:D:332:MET:HE1	1.71	0.55
2:D:320:ARG:HA	2:D:356:CYS:O	2.06	0.55
2:B:8:GLN:HG2	2:B:14:ASN:HA	1.89	0.55
2:B:399:PHE:O	2:B:400:ARG:O	2.24	0.55
1:C:12:ALA:O	1:C:13:GLY:C	2.48	0.55
1:C:105:ARG:HH22	2:D:253:ARG:NH2	2.04	0.55
2:D:136:GLN:HA	2:D:167:ASN:O	2.07	0.55
2:B:171:VAL:HG12	2:B:204:ILE:HB	1.88	0.55
1:C:167:LEU:HD13	1:C:252:LEU:CD1	2.32	0.55
2:D:385:GLN:HE21	2:D:389:LYS:CD	2.20	0.55
1:A:407:TRP:CD2	2:B:257:VAL:HG23	2.42	0.55
2:B:348:PRO:O	2:B:350:ASN:N	2.39	0.55
1:C:105:ARG:NH2	2:D:253:ARG:NH2	2.54	0.55
2:B:337:ASN:HA	2:B:340:SER:HB3	1.89	0.55
2:B:344:VAL:HG22	2:B:346:TRP:NE1	2.22	0.55
1:C:107:HIS:HD2	1:C:108:TYR:CE2	2.25	0.55
2:B:192:HIS:CD2	2:B:421:ALA:HA	2.29	0.54
2:B:247:GLN:HG3	2:B:248:LEU:H	1.72	0.54
2:D:164:ARG:HE	2:D:164:ARG:HA	1.71	0.54
2:B:226:ASP:O	2:B:227:LEU:HB3	2.06	0.54
2:B:253:ARG:O	2:B:254:LYS:C	2.50	0.54
1:C:133:GLN:CD	1:C:252:LEU:HB2	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:VAL:HG21	1:A:408:TYR:OH	2.05	0.54
1:A:311:LYS:HD2	1:A:437:VAL:CB	2.37	0.54
2:D:336:GLN:NE2	2:D:351:VAL:CG1	2.71	0.54
2:B:407:TRP:NE1	1:C:257:THR:HA	2.22	0.54
1:C:273:ALA:CB	1:C:274:PRO:CD	2.65	0.54
2:B:22:GLU:OE1	2:B:82:PRO:CB	2.56	0.54
2:B:36:TYR:OH	2:B:40:SER:O	2.13	0.54
2:B:308:ARG:HG3	2:B:308:ARG:HH11	1.73	0.54
2:B:408:TYR:O	2:B:409:THR:C	2.50	0.54
2:B:167:ASN:HD22	2:B:252:LEU:CD1	2.14	0.54
2:B:308:ARG:HG3	2:B:308:ARG:NH1	2.22	0.54
2:D:5:VAL:HG22	2:D:135:PHE:CD2	2.43	0.54
1:A:346:TRP:O	1:A:346:TRP:CE3	2.60	0.53
1:A:398:MET:HE2	2:B:348:PRO:HD2	1.89	0.53
2:D:88:ARG:O	2:D:91:ASN:HB2	2.08	0.53
2:D:151:THR:O	2:D:154:ILE:HD13	2.08	0.53
1:A:404:PHE:O	1:A:405:VAL:C	2.50	0.53
2:B:414:ASP:HB3	2:B:416:MET:HE3	1.91	0.53
2:D:253:ARG:O	2:D:254:LYS:C	2.49	0.53
2:D:295:MET:CG	2:D:377:PHE:HB2	2.38	0.53
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.89	0.53
2:B:7:ILE:O	2:B:137:LEU:HA	2.07	0.53
1:C:420:GLU:HG2	1:C:420:GLU:O	2.07	0.53
2:D:54:ASN:HD22	2:D:64:ARG:CD	2.21	0.53
3:E:137:LYS:C	3:E:139:LEU:H	2.16	0.53
2:B:70:LEU:CA	2:B:95:GLY:HA3	2.35	0.53
1:C:181:VAL:H	2:D:258:ASN:ND2	2.05	0.53
2:D:8:GLN:HG2	2:D:14:ASN:HA	1.91	0.53
2:D:177:VAL:O	2:D:177:VAL:CG1	2.56	0.53
2:D:350:ASN:HD22	2:D:350:ASN:N	1.97	0.53
1:A:347:CYS:O	1:A:348:PRO:C	2.51	0.53
2:B:385:GLN:HE21	2:B:389:LYS:CD	2.21	0.53
2:D:93:VAL:HG12	2:D:114:LEU:HD11	1.89	0.53
2:D:32:PRO:O	2:D:86:ILE:HD12	2.09	0.53
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.21	0.53
2:D:344:VAL:HG22	2:D:346:TRP:NE1	2.24	0.53
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.43	0.53
1:C:178:SER:OG	2:D:352:LYS:HE3	2.08	0.53
1:C:340:THR:HG22	1:C:340:THR:O	2.09	0.53
2:D:180:THR:C	2:D:182:VAL:H	2.17	0.53
2:D:192:HIS:O	2:D:195:VAL:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ASP:O	1:C:40:LYS:CB	2.57	0.53
1:A:79:ARG:NH2	1:A:94:THR:HG21	2.24	0.53
2:D:181:VAL:HG21	2:D:404:PHE:HE2	1.74	0.53
3:E:19:SER:O	3:E:20:PHE:HB3	2.08	0.53
2:B:70:LEU:C	2:B:95:GLY:HA3	2.34	0.52
1:C:239:THR:HB	1:C:243:ARG:HH11	1.74	0.52
1:C:407:TRP:CD2	2:D:257:VAL:HG23	2.44	0.52
2:D:403:ALA:C	2:D:405:LEU:H	2.18	0.52
2:B:177:VAL:O	2:B:177:VAL:CG1	2.57	0.52
2:D:140:SER:HA	2:D:171:VAL:HG23	1.91	0.52
1:A:68:VAL:HG13	1:A:93:ILE:HB	1.91	0.52
2:B:151:THR:O	2:B:154:ILE:HD13	2.09	0.52
2:B:251:ASP:HB2	2:B:254:LYS:N	2.14	0.52
2:B:400:ARG:C	2:B:402:LYS:H	2.17	0.52
2:D:115:VAL:HG12	2:D:116:ASP:N	2.24	0.52
2:D:309:HIS:H	2:D:309:HIS:CD2	2.27	0.52
1:C:86:LEU:HB3	1:C:87:PHE:HD2	1.74	0.52
2:D:251:ASP:HB2	2:D:254:LYS:N	2.12	0.52
1:A:270:ALA:HB3	1:A:302:MET:CE	2.39	0.52
2:B:99:ALA:CB	2:B:145:THR:CG2	2.83	0.52
1:C:3:GLU:HB2	1:C:132:LEU:HA	1.92	0.52
2:D:88:ARG:HB3	2:D:91:ASN:OD1	2.10	0.52
1:C:384:ILE:CG1	1:C:384:ILE:O	2.58	0.52
1:A:183:GLU:HB3	1:A:184:PRO:CD	2.40	0.52
2:B:191:VAL:HG11	2:B:425:MET:HG3	1.90	0.52
1:C:49:PHE:H	1:C:49:PHE:HD2	1.57	0.52
2:D:225:GLY:O	2:D:228:ASN:N	2.40	0.52
1:C:87:PHE:HD2	1:C:87:PHE:H	1.55	0.52
1:C:128:GLN:O	1:C:128:GLN:HG2	2.09	0.52
2:B:158:ARG:O	2:B:159:GLU:CB	2.57	0.52
2:B:245:PRO:CG	2:B:246:GLY:H	2.10	0.52
2:B:2:ARG:HD2	2:B:131:CYS:SG	2.51	0.51
2:B:404:PHE:N	2:B:404:PHE:CD1	2.77	0.51
2:D:22:GLU:OE1	2:D:82:PRO:HB2	2.11	0.51
2:D:88:ARG:HG3	2:D:89:PRO:HD2	1.92	0.51
1:A:72:PRO:O	1:A:74:VAL:N	2.42	0.51
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.75	0.51
1:A:191:THR:HG23	1:A:425:MET:CE	2.40	0.51
2:D:336:GLN:NE2	2:D:351:VAL:HG12	2.26	0.51
2:B:88:ARG:HH11	2:B:88:ARG:HG2	1.75	0.51
1:C:388:TRP:HA	1:C:388:TRP:CE3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLY:O	1:A:351:PHE:HB2	2.11	0.51
1:C:346:TRP:O	1:C:346:TRP:CE3	2.60	0.51
2:D:103:TRP:HB2	2:D:186:ASN:OD1	2.10	0.51
1:A:190:THR:CG2	1:A:191:THR:N	2.71	0.51
1:A:310:GLY:HA3	1:A:383:ALA:HB2	1.92	0.51
1:C:229:ARG:CG	1:C:229:ARG:NH1	2.72	0.51
2:D:251:ASP:O	2:D:252:LEU:HB3	2.10	0.51
1:A:270:ALA:O	1:A:302:MET:HB2	2.11	0.51
1:A:274:PRO:HG3	1:A:291:ILE:HG21	1.91	0.51
2:B:229:HIS:ND1	2:B:277:SER:HB3	2.26	0.51
2:B:309:HIS:CD2	2:B:309:HIS:H	2.29	0.51
1:C:264:ARG:O	1:C:266:HIS:N	2.43	0.51
2:D:5:VAL:CG2	2:D:135:PHE:CD2	2.93	0.51
2:D:167:ASN:HD22	2:D:252:LEU:CD1	2.23	0.51
2:D:180:THR:C	2:D:182:VAL:N	2.68	0.51
3:E:76:ARG:C	3:E:78:HIS:N	2.63	0.51
1:A:70:LEU:HD22	1:A:110:ILE:HG23	1.93	0.51
1:A:297:GLU:HG3	1:A:299:ALA:H	1.75	0.51
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.92	0.51
1:A:139:HIS:CG	1:A:150:THR:HG21	2.46	0.51
2:B:158:ARG:O	2:B:159:GLU:HB3	2.11	0.51
2:B:401:ARG:NH1	2:B:401:ARG:HG3	2.25	0.51
2:D:24:ILE:O	2:D:28:HIS:HD2	1.94	0.51
1:A:36:MET:O	1:A:36:MET:HG3	2.09	0.50
1:A:223:THR:HB	1:A:226:ASN:H	1.77	0.50
2:B:401:ARG:HG3	2:B:401:ARG:HH11	1.76	0.50
2:B:32:PRO:O	2:B:86:ILE:HD12	2.10	0.50
2:B:306:ASP:C	2:B:308:ARG:N	2.63	0.50
2:B:318:VAL:HG13	2:B:376:THR:HG23	1.93	0.50
2:B:93:VAL:HG12	2:B:114:LEU:HD11	1.93	0.50
3:E:48:GLU:HG3	3:E:49:GLU:H	1.74	0.50
1:C:291:ILE:HD12	1:C:375:VAL:CG2	2.42	0.50
1:C:407:TRP:CE2	2:D:257:VAL:HA	2.46	0.50
2:D:296:PHE:CE1	2:D:332:MET:HE1	2.46	0.50
3:E:65:GLU:C	3:E:67:GLU:H	2.20	0.50
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.46	0.50
1:A:335:ILE:O	1:A:339:ARG:HB3	2.12	0.50
2:B:336:GLN:NE2	2:B:351:VAL:HG11	2.27	0.50
1:C:315:CYS:SG	1:C:377:MET:HE2	2.52	0.50
2:D:384:ILE:HG22	2:D:432:TYR:CE1	2.47	0.50
2:B:296:PHE:CE1	2:B:332:MET:HE1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:205:ASP:HB2	2:B:303:ALA:HA	1.94	0.50
2:B:307:PRO:CB	2:B:312:TYR:OH	2.60	0.50
1:C:72:PRO:O	1:C:74:VAL:N	2.44	0.50
1:C:191:THR:O	1:C:195:LEU:HB3	2.12	0.50
1:C:217:LEU:O	1:C:218:ASP:HB3	2.11	0.50
3:E:69:LEU:C	3:E:71:HIS:H	2.19	0.50
1:A:86:LEU:HB3	1:A:87:PHE:CD2	2.45	0.50
1:C:213:CYS:HA	1:C:217:LEU:HB2	1.92	0.50
2:B:403:ALA:C	2:B:405:LEU:N	2.69	0.50
1:C:32:PRO:C	1:C:34:GLY:H	2.20	0.50
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.30	0.49
2:D:6:HIS:CE1	2:D:8:GLN:HE21	2.30	0.49
2:D:245:PRO:CG	2:D:246:GLY:H	2.15	0.49
1:C:2:ARG:HA	1:C:2:ARG:NH1	2.26	0.49
1:C:241:SER:OG	1:C:242:LEU:HD23	2.11	0.49
2:D:54:ASN:ND2	2:D:64:ARG:CD	2.73	0.49
2:D:347:ILE:CG2	2:D:350:ASN:HB3	2.41	0.49
1:A:273:ALA:HB1	1:A:274:PRO:HD3	1.85	0.49
2:B:180:THR:C	2:B:182:VAL:H	2.21	0.49
2:B:269:MET:HG2	2:B:384:ILE:HG12	1.94	0.49
1:C:191:THR:CG2	1:C:425:MET:CE	2.88	0.49
3:E:67:GLU:C	3:E:69:LEU:N	2.70	0.49
1:A:36:MET:HG2	1:A:61:HIS:NE2	2.27	0.49
2:B:88:ARG:O	2:B:91:ASN:HB2	2.12	0.49
2:D:347:ILE:O	2:D:348:PRO:O	2.30	0.49
2:D:381:SER:O	2:D:384:ILE:HB	2.12	0.49
2:B:135:PHE:CD1	2:B:135:PHE:N	2.80	0.49
1:A:276:ILE:HD11	1:A:280:LYS:HD3	1.95	0.49
1:A:405:VAL:CG1	1:A:406:HIS:N	2.76	0.49
2:B:260:VAL:HG11	2:B:266:HIS:HA	1.95	0.49
2:B:320:ARG:HA	2:B:356:CYS:O	2.12	0.49
2:B:404:PHE:N	2:B:404:PHE:HD1	2.10	0.49
1:C:267:PHE:N	1:C:267:PHE:CD1	2.81	0.49
2:D:183:GLU:N	2:D:184:PRO:HD2	2.28	0.49
2:D:298:SER:C	2:D:300:ASN:N	2.69	0.49
1:A:395:PHE:O	1:A:397:LEU:N	2.45	0.49
1:C:404:PHE:O	1:C:405:VAL:C	2.55	0.49
2:B:274:PRO:C	2:B:275:LEU:HG	2.38	0.49
1:C:21:TRP:CH2	1:C:63:PRO:HB3	2.48	0.49
1:C:265:ILE:HG22	1:C:265:ILE:O	2.12	0.49
2:B:31:ASP:HB3	2:B:32:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LEU:O	1:C:249:ASN:HB2	2.12	0.49
3:E:79:GLU:O	3:E:80:ARG:C	2.56	0.49
2:D:2:ARG:N	2:D:133:GLN:OE1	2.46	0.49
2:D:307:PRO:HB3	2:D:312:TYR:OH	2.13	0.48
1:A:229:ARG:CG	1:A:229:ARG:NH1	2.69	0.48
2:B:240:THR:HG21	2:B:320:ARG:CZ	2.42	0.48
2:D:31:ASP:HB3	2:D:32:PRO:HD2	1.96	0.48
2:D:48:ARG:HB3	2:D:243:ARG:HA	1.95	0.48
1:A:121:ARG:HG3	1:A:121:ARG:HH11	1.78	0.48
2:B:224:TYR:OH	6:B:600:GDP:H2'	2.13	0.48
2:B:242:LEU:HG	7:B:700:E70:HAH	1.96	0.48
1:C:190:THR:CG2	1:C:191:THR:N	2.76	0.48
2:B:181:VAL:HG21	2:B:404:PHE:HE2	1.78	0.48
2:B:295:MET:CG	2:B:377:PHE:HB2	2.44	0.48
1:A:119:LEU:HD22	1:A:156:ARG:HH21	1.79	0.48
1:A:273:ALA:HB2	1:A:375:VAL:O	2.13	0.48
1:C:111:GLY:O	1:C:113:GLU:N	2.47	0.48
1:A:249:ASN:HD22	1:A:249:ASN:N	2.10	0.48
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.96	0.48
2:D:200:GLU:HA	2:D:266:HIS:HB2	1.96	0.48
2:D:357:ASP:OD2	2:D:357:ASP:N	2.46	0.48
2:D:273:ALA:HB2	2:D:375:ALA:N	2.29	0.48
2:B:108:TYR:O	2:B:112:ALA:HB3	2.14	0.48
2:B:406:HIS:HA	2:B:409:THR:HB	1.95	0.48
1:A:66:VAL:HG11	1:A:122:ILE:HG13	1.96	0.48
1:A:249:ASN:ND2	1:A:249:ASN:N	2.61	0.48
2:B:150:GLY:O	2:B:154:ILE:HG23	2.13	0.48
1:C:190:THR:O	1:C:192:HIS:N	2.47	0.48
1:A:280:LYS:O	1:A:282:TYR:N	2.47	0.47
2:B:180:THR:C	2:B:182:VAL:N	2.71	0.47
2:B:380:ASN:C	2:B:380:ASN:HD22	2.21	0.47
2:D:118:VAL:HG11	2:D:153:LEU:HD11	1.96	0.47
2:D:240:THR:HG21	2:D:320:ARG:CZ	2.43	0.47
2:B:70:LEU:CD1	2:B:145:THR:HB	2.43	0.47
1:C:271:THR:HG23	1:C:301:GLN:HA	1.95	0.47
2:B:192:HIS:O	2:B:195:VAL:HG12	2.14	0.47
1:C:273:ALA:HB2	1:C:375:VAL:O	2.13	0.47
1:A:277:SER:O	1:A:280:LYS:HB2	2.15	0.47
1:A:419:SER:O	1:A:423:GLU:HG3	2.13	0.47
2:B:200:GLU:HA	2:B:266:HIS:HB2	1.96	0.47
2:B:245:PRO:CG	2:B:246:GLY:N	2.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:PHE:HD2	2:B:83:PHE:HA	1.64	0.47
1:C:121:ARG:HG3	1:C:121:ARG:NH1	2.29	0.47
2:D:76:ASP:O	2:D:80:SER:HB2	2.15	0.47
3:E:119:MET:HE2	3:E:123:LEU:HD13	1.95	0.47
1:A:231:ILE:O	1:A:232:GLY:C	2.58	0.47
1:A:271:THR:HG23	1:A:301:GLN:HA	1.96	0.47
2:B:177:VAL:O	2:B:177:VAL:HG12	2.15	0.47
2:B:264:ARG:HD3	2:B:431:GLU:OE1	2.14	0.47
2:B:336:GLN:NE2	2:B:351:VAL:HG12	2.25	0.47
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.78	0.47
1:C:309:HIS:ND1	1:C:310:GLY:N	2.62	0.47
1:C:310:GLY:HA3	1:C:383:ALA:HB2	1.97	0.47
2:D:177:VAL:O	2:D:177:VAL:HG12	2.14	0.47
2:D:325:MET:HE3	2:D:326:LYS:H	1.80	0.47
2:D:344:VAL:HG22	2:D:346:TRP:HE1	1.80	0.47
2:D:380:ASN:C	2:D:380:ASN:HD22	2.22	0.47
2:D:399:PHE:O	2:D:400:ARG:O	2.32	0.47
1:A:265:ILE:O	1:A:265:ILE:HG22	2.14	0.47
2:B:120:ASP:HA	2:B:123:ARG:NH1	2.30	0.47
2:B:260:VAL:HA	2:B:261:PRO:HD2	1.68	0.47
1:C:347:CYS:O	1:C:348:PRO:C	2.58	0.47
2:D:51:VAL:CG1	2:D:52:TYR:CD1	2.97	0.47
2:D:107:HIS:O	2:D:152:LEU:HD22	2.15	0.47
2:B:156:LYS:HG2	3:E:76:ARG:CZ	2.45	0.47
1:C:265:ILE:HG21	1:C:313:MET:HE3	1.97	0.47
1:A:181:VAL:N	2:B:258:ASN:HD21	1.97	0.47
2:B:220:THR:O	2:B:222:PRO:HD3	2.14	0.47
2:B:261:PRO:HG2	2:B:262:PHE:H	1.79	0.47
2:B:350:ASN:H	2:B:350:ASN:ND2	2.04	0.47
2:D:157:ILE:HG21	2:D:166:MET:HE3	1.95	0.47
2:D:164:ARG:HH22	2:D:253:ARG:HH22	1.61	0.47
2:D:383:ALA:O	2:D:386:GLU:HB2	2.15	0.47
3:E:72:LEU:HD12	3:E:75:LYS:HZ3	1.80	0.47
2:B:30:ILE:HG22	2:B:31:ASP:O	2.15	0.46
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.50	0.46
2:D:51:VAL:O	2:D:64:ARG:NH2	2.47	0.46
1:A:244:PHE:O	1:A:245:ASP:HB3	2.16	0.46
2:B:287:THR:CG2	2:B:290:GLU:H	2.28	0.46
1:C:231:ILE:O	1:C:232:GLY:C	2.57	0.46
2:D:224:TYR:OH	6:D:600:GDP:H2'	2.15	0.46
1:A:154:MET:O	1:A:158:SER:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.50	0.46
2:B:178:SER:HB2	2:B:183:GLU:OE1	2.14	0.46
1:C:273:ALA:HB2	1:C:375:VAL:N	2.29	0.46
2:D:225:GLY:O	2:D:228:ASN:HB2	2.14	0.46
2:D:348:PRO:O	2:D:350:ASN:N	2.48	0.46
3:E:74:GLU:O	3:E:76:ARG:N	2.48	0.46
1:A:345:ASP:HB3	1:A:346:TRP:CD1	2.50	0.46
2:B:198:THR:OG1	2:B:266:HIS:HE1	1.97	0.46
1:C:77:GLU:O	1:C:80:THR:HG22	2.16	0.46
1:C:112:LYS:HE2	3:E:105:MET:HE3	1.97	0.46
1:C:223:THR:HB	1:C:226:ASN:H	1.80	0.46
2:D:2:ARG:HD2	2:D:131:CYS:SG	2.56	0.46
2:D:273:ALA:HB2	2:D:375:ALA:H	1.80	0.46
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.51	0.46
2:D:30:ILE:HG22	2:D:31:ASP:O	2.16	0.46
2:D:260:VAL:HG11	2:D:266:HIS:HA	1.98	0.46
1:A:190:THR:C	1:A:192:HIS:N	2.72	0.46
1:A:234:ILE:CG1	1:A:272:TYR:HB2	2.46	0.46
1:C:121:ARG:HG3	1:C:121:ARG:HH11	1.81	0.46
2:D:171:VAL:HG12	2:D:204:ILE:HB	1.96	0.46
2:D:261:PRO:HG3	2:D:313:LEU:HG	1.97	0.46
2:D:352:LYS:HG3	7:D:700:E70:HAM	1.96	0.46
3:E:60:ARG:C	3:E:62:LYS:N	2.73	0.46
1:A:344:VAL:O	1:A:346:TRP:N	2.49	0.46
1:C:273:ALA:HB3	1:C:375:VAL:H	1.73	0.46
1:A:249:ASN:H	1:A:254:GLU:CD	2.24	0.46
1:C:188:ILE:HG23	1:C:425:MET:HG3	1.96	0.46
2:D:209:LEU:HD12	2:D:209:LEU:HA	1.79	0.46
3:E:101:LEU:O	3:E:104:LYS:N	2.48	0.46
1:A:252:LEU:O	1:A:255:PHE:HB2	2.16	0.46
2:B:191:VAL:CG1	2:B:425:MET:HG3	2.46	0.46
2:B:136:GLN:HA	2:B:167:ASN:O	2.16	0.45
1:C:86:LEU:HB3	1:C:87:PHE:CD2	2.51	0.45
2:D:242:LEU:HD21	2:D:252:LEU:HB2	1.97	0.45
1:A:267:PHE:CD1	1:A:267:PHE:N	2.85	0.45
1:A:278:ALA:HA	1:A:281:ALA:HB2	1.98	0.45
1:C:70:LEU:HD13	1:C:145:THR:HB	1.97	0.45
1:A:88:HIS:CD2	1:A:90:GLU:OE1	2.69	0.45
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.51	0.45
1:C:264:ARG:O	1:C:266:HIS:CD2	2.69	0.45
1:C:36:MET:C	1:C:38:SER:H	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:ALA:O	1:C:175:PRO:C	2.59	0.45
1:C:344:VAL:O	1:C:346:TRP:N	2.50	0.45
2:D:192:HIS:CD2	2:D:421:ALA:HA	2.44	0.45
2:D:274:PRO:C	2:D:275:LEU:HG	2.41	0.45
2:D:5:VAL:HG21	2:D:135:PHE:HD2	1.80	0.45
1:A:273:ALA:HB3	1:A:375:VAL:H	1.74	0.45
1:A:317:LEU:HD23	1:A:317:LEU:HA	1.80	0.45
1:C:31:GLN:HA	1:C:32:PRO:HD2	1.82	0.45
2:D:20:PHE:CD1	2:D:20:PHE:C	2.94	0.45
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.52	0.45
2:D:224:TYR:O	2:D:228:ASN:ND2	2.50	0.45
2:D:264:ARG:HD3	2:D:431:GLU:OE1	2.17	0.45
2:D:350:ASN:H	2:D:350:ASN:ND2	2.04	0.45
3:E:4:ALA:O	3:E:5:ASP:HB3	2.16	0.45
1:A:83:TYR:O	1:A:84:ARG:C	2.60	0.45
1:A:99:ALA:CB	1:A:145:THR:CG2	2.81	0.45
2:B:273:ALA:HB2	2:B:375:ALA:O	2.17	0.45
1:C:256:GLN:O	1:C:259:LEU:N	2.48	0.45
1:A:103:TYR:O	1:A:104:ALA:C	2.59	0.45
1:A:256:GLN:HA	1:A:260:VAL:HG13	1.98	0.45
2:B:307:PRO:HB2	2:B:312:TYR:OH	2.17	0.45
1:C:190:THR:O	1:C:194:THR:HB	2.17	0.45
2:D:7:ILE:O	2:D:137:LEU:HA	2.17	0.45
2:D:133:GLN:NE2	2:D:252:LEU:HB3	2.30	0.45
2:D:313:LEU:HB2	2:D:380:ASN:O	2.17	0.45
1:A:171:ILE:O	1:A:171:ILE:HG22	2.17	0.44
1:A:191:THR:HG23	1:A:425:MET:HE3	1.97	0.44
7:B:700:E70:NAP	7:B:700:E70:CAK	2.76	0.44
1:C:341:ILE:H	1:C:341:ILE:CD1	2.23	0.44
1:A:105:ARG:HH22	2:B:253:ARG:NH2	2.15	0.44
2:B:62:VAL:HA	2:B:63:PRO:HD2	1.91	0.44
2:B:313:LEU:HD13	2:B:313:LEU:HA	1.80	0.44
1:C:99:ALA:CB	1:C:145:THR:CG2	2.81	0.44
1:C:111:GLY:C	1:C:113:GLU:N	2.76	0.44
1:C:312:TYR:HE2	1:C:379:SER:CB	2.30	0.44
2:D:295:MET:HE3	2:D:295:MET:HB3	1.74	0.44
2:B:19:LYS:HD3	2:B:19:LYS:HA	1.61	0.44
2:B:262:PHE:HA	2:B:263:PRO:HD3	1.85	0.44
2:D:83:PHE:HD2	2:D:83:PHE:HA	1.63	0.44
2:D:141:LEU:HD12	2:D:141:LEU:HA	1.87	0.44
2:B:306:ASP:HA	2:B:307:PRO:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.00	0.44
1:C:202:PHE:CE1	1:C:238:ILE:HG21	2.52	0.44
1:C:223:THR:N	1:C:226:ASN:HB2	2.33	0.44
2:D:306:ASP:C	2:D:308:ARG:N	2.66	0.44
2:D:318:VAL:HG13	2:D:376:THR:HG23	1.98	0.44
2:D:378:ILE:CD1	7:D:700:E70:HAI	2.47	0.44
2:D:406:HIS:HA	2:D:409:THR:HB	2.00	0.44
2:B:351:VAL:CG1	2:B:351:VAL:O	2.66	0.44
2:B:381:SER:O	2:B:384:ILE:HB	2.17	0.44
2:D:180:THR:O	2:D:182:VAL:N	2.51	0.44
2:B:107:HIS:O	2:B:152:LEU:HD22	2.17	0.44
2:B:198:THR:OG1	2:B:266:HIS:CE1	2.70	0.44
2:B:216:THR:O	2:B:217:LEU:HG	2.17	0.44
2:D:152:LEU:O	2:D:153:LEU:C	2.60	0.44
2:D:400:ARG:C	2:D:402:LYS:H	2.25	0.44
2:D:401:ARG:HH11	2:D:401:ARG:CG	2.30	0.44
3:E:112:ARG:CG	3:E:113:GLU:N	2.79	0.44
2:B:174:SER:CB	2:B:207:GLU:HB2	2.47	0.44
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.00	0.44
1:C:395:PHE:O	1:C:396:ASP:C	2.61	0.44
2:D:191:VAL:HG11	2:D:425:MET:CG	2.45	0.44
1:A:273:ALA:HB2	1:A:375:VAL:N	2.28	0.44
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.31	0.44
1:C:172:TYR:HE2	1:C:391:LEU:HD22	1.83	0.44
2:D:6:HIS:HE1	2:D:8:GLN:HE21	1.66	0.44
2:D:19:LYS:HB3	2:D:232:SER:HB3	2.00	0.44
2:D:220:THR:O	2:D:222:PRO:HD3	2.18	0.44
2:D:224:TYR:CD2	6:D:600:GDP:C5	3.06	0.44
2:D:253:ARG:HB2	2:D:253:ARG:HH11	1.83	0.44
1:A:48:SER:O	1:A:243:ARG:O	2.36	0.44
1:A:70:LEU:HD13	1:A:145:THR:HB	1.99	0.44
1:A:191:THR:O	1:A:195:LEU:HB3	2.18	0.44
1:C:405:VAL:HG12	1:C:406:HIS:N	2.33	0.44
2:D:119:LEU:HD11	2:D:156:LYS:HB3	1.99	0.44
2:D:270:PRO:HD2	2:D:302:MET:HB2	2.00	0.44
2:D:276:THR:HG23	2:D:277:SER:N	2.33	0.44
2:B:102:ASN:OD1	2:B:102:ASN:C	2.60	0.43
2:B:427:ASP:O	2:B:430:SER:N	2.51	0.43
2:B:19:LYS:O	2:B:23:VAL:HG23	2.18	0.43
2:B:231:VAL:HG12	2:B:235:MET:HE2	1.99	0.43
1:C:82:THR:O	1:C:83:TYR:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:343:PHE:O	2:D:344:VAL:C	2.61	0.43
1:A:83:TYR:C	1:A:85:GLN:N	2.76	0.43
2:B:24:ILE:O	2:B:28:HIS:HD2	2.01	0.43
1:C:96:LYS:HD3	2:D:131:CYS:HB2	2.01	0.43
2:D:89:PRO:O	2:D:92:PHE:HD1	2.01	0.43
2:D:198:THR:OG1	2:D:266:HIS:CE1	2.71	0.43
2:D:351:VAL:CG1	2:D:351:VAL:O	2.66	0.43
1:A:189:LEU:HD21	1:A:413:MET:HE1	2.01	0.43
2:B:2:ARG:NH1	2:B:133:GLN:HA	2.32	0.43
2:B:347:ILE:CG2	2:B:350:ASN:HB3	2.48	0.43
1:A:341:ILE:HD13	1:A:341:ILE:H	1.82	0.43
2:D:44:LEU:HA	2:D:49:ILE:HB	1.98	0.43
2:D:133:GLN:HE21	2:D:252:LEU:HD23	1.84	0.43
2:D:311:ARG:HE	2:D:344:VAL:HG23	1.83	0.43
1:A:85:GLN:HE21	1:A:85:GLN:HA	1.83	0.43
2:B:51:VAL:CG1	2:B:52:TYR:CD1	3.00	0.43
2:B:339:ASN:O	2:B:341:SER:N	2.51	0.43
1:C:8:HIS:CD2	1:C:17:GLY:HA3	2.53	0.43
1:C:154:MET:O	1:C:158:SER:HB2	2.18	0.43
3:E:65:GLU:C	3:E:67:GLU:N	2.77	0.43
3:E:74:GLU:C	3:E:76:ARG:N	2.76	0.43
2:B:44:LEU:HA	2:B:49:ILE:HB	2.01	0.43
2:B:424:ASN:O	2:B:427:ASP:HB2	2.18	0.43
1:C:50:ASN:HD22	1:C:50:ASN:HA	1.66	0.43
1:C:153:LEU:HD23	1:C:153:LEU:HA	1.92	0.43
2:D:109:THR:OG1	2:D:411:GLU:OE1	2.31	0.43
2:D:188:THR:HG23	2:D:425:MET:SD	2.59	0.43
1:A:50:ASN:HD22	1:A:50:ASN:HA	1.65	0.43
1:A:206:ASN:ND2	4:A:600:GTP:HN22	1.99	0.43
1:A:239:THR:O	1:A:240:ALA:C	2.61	0.43
2:B:2:ARG:N	2:B:133:GLN:OE1	2.52	0.43
1:C:128:GLN:O	1:C:128:GLN:CG	2.66	0.43
1:C:297:GLU:HA	1:C:298:PRO:HD2	1.70	0.43
1:C:405:VAL:HG13	1:C:406:HIS:N	2.33	0.43
2:D:247:GLN:CG	2:D:248:LEU:N	2.77	0.43
2:D:269:MET:HB3	2:D:303:ALA:HB3	1.99	0.43
2:D:308:ARG:HH11	2:D:308:ARG:CG	2.30	0.43
2:D:336:GLN:NE2	2:D:351:VAL:HG11	2.33	0.43
2:D:427:ASP:O	2:D:430:SER:N	2.52	0.43
1:A:6:SER:HB3	1:A:8:HIS:CE1	2.54	0.43
1:A:108:TYR:CE1	1:A:413:MET:HG3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:ASN:ND2	2:B:67:LEU:HD23	2.34	0.43
2:B:48:ARG:HB3	2:B:243:ARG:HA	2.00	0.43
2:B:183:GLU:N	2:B:184:PRO:HD2	2.34	0.43
2:B:298:SER:C	2:B:300:ASN:N	2.76	0.43
1:C:108:TYR:HB3	3:E:108:ASN:OD1	2.18	0.43
1:C:327:ASP:O	1:C:328:VAL:C	2.62	0.43
2:D:151:THR:HA	2:D:154:ILE:HD13	2.00	0.43
1:A:278:ALA:O	1:A:279:GLU:CB	2.57	0.43
2:B:294:GLN:O	2:B:294:GLN:HG3	2.19	0.43
2:B:336:GLN:CD	2:B:351:VAL:HG11	2.44	0.43
2:D:226:ASP:OD1	2:D:226:ASP:N	2.52	0.43
2:D:273:ALA:HB3	2:D:375:ALA:H	1.84	0.43
1:A:375:VAL:HG12	1:A:376:CYS:H	1.84	0.42
2:B:202:TYR:CZ	2:B:238:VAL:HG11	2.54	0.42
2:B:414:ASP:OD2	2:B:416:MET:HE2	2.19	0.42
1:C:81:GLY:O	1:C:82:THR:C	2.61	0.42
1:C:111:GLY:O	1:C:112:LYS:C	2.61	0.42
2:D:384:ILE:CG2	2:D:432:TYR:CE1	3.02	0.42
1:A:223:THR:N	1:A:226:ASN:HB2	2.34	0.42
2:B:59:ASN:O	2:B:60:LYS:O	2.36	0.42
2:B:131:CYS:SG	2:B:131:CYS:O	2.76	0.42
2:D:11:GLN:CG	2:D:74:THR:CG2	2.71	0.42
2:D:123:ARG:HG2	2:D:127:GLU:OE1	2.19	0.42
3:E:75:LYS:HB3	3:E:75:LYS:HE2	1.42	0.42
1:A:244:PHE:CZ	1:A:358:GLN:HG2	2.53	0.42
2:B:225:GLY:O	2:B:228:ASN:HB2	2.19	0.42
2:B:313:LEU:HB2	2:B:380:ASN:O	2.19	0.42
1:C:239:THR:CB	1:C:243:ARG:HH11	2.32	0.42
1:C:262:TYR:O	1:C:263:PRO:C	2.62	0.42
1:A:183:GLU:CB	1:A:184:PRO:HD3	2.45	0.42
2:B:16:ILE:HG22	2:B:17:GLY:N	2.34	0.42
2:B:192:HIS:HD2	2:B:421:ALA:CA	2.20	0.42
1:C:139:HIS:HD2	1:C:146:GLY:O	2.02	0.42
2:D:140:SER:O	2:D:147:SER:HB3	2.19	0.42
1:A:190:THR:O	1:A:191:THR:C	2.62	0.42
1:A:195:LEU:O	1:A:266:HIS:HE1	2.02	0.42
1:A:280:LYS:HA	1:A:283:HIS:CE1	2.54	0.42
2:B:325:MET:C	2:B:327:GLU:N	2.77	0.42
2:B:343:PHE:O	2:B:344:VAL:C	2.62	0.42
2:B:358:ILE:HA	2:B:359:PRO:HD3	1.84	0.42
1:C:82:THR:O	1:C:83:TYR:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:VAL:HA	1:C:261:PRO:HD3	1.75	0.42
1:A:340:THR:O	1:A:340:THR:CG2	2.67	0.42
2:B:153:LEU:O	2:B:157:ILE:HG12	2.19	0.42
2:B:229:HIS:CE1	2:B:276:THR:O	2.73	0.42
1:C:66:VAL:HG11	1:C:122:ILE:HG13	2.01	0.42
2:D:55:GLU:HB3	2:D:61:TYR:HD2	1.83	0.42
2:D:153:LEU:O	2:D:157:ILE:HG12	2.20	0.42
1:A:218:ASP:OD1	1:A:218:ASP:O	2.37	0.42
2:B:259:MET:HE1	2:B:314:THR:O	2.19	0.42
1:C:83:TYR:O	1:C:84:ARG:C	2.62	0.42
2:D:5:VAL:HG13	2:D:132:LEU:HD13	2.00	0.42
1:A:210:TYR:O	1:A:214:ARG:HG3	2.20	0.42
1:C:2:ARG:HB2	1:C:131:GLY:O	2.20	0.42
1:C:79:ARG:HH22	1:C:94:THR:HG22	1.83	0.42
2:D:260:VAL:HA	2:D:261:PRO:HD2	1.75	0.42
1:A:223:THR:H	1:A:226:ASN:HB2	1.84	0.42
1:C:97:GLU:OE2	2:D:164:ARG:NH2	2.50	0.42
1:C:202:PHE:CE2	1:C:268:PRO:HG2	2.55	0.42
2:D:8:GLN:HE22	2:D:21:TRP:CD1	2.38	0.42
1:A:121:ARG:HG3	1:A:121:ARG:NH1	2.34	0.42
2:B:19:LYS:HB3	2:B:232:SER:HB3	2.02	0.42
2:B:103:TRP:HB2	2:B:186:ASN:OD1	2.20	0.42
2:D:245:PRO:CG	2:D:246:GLY:N	2.78	0.42
2:D:325:MET:HE3	2:D:326:LYS:N	2.35	0.42
2:D:339:ASN:HD22	2:D:339:ASN:HA	1.72	0.42
3:E:99:GLU:C	3:E:101:LEU:N	2.78	0.42
1:A:234:ILE:HG13	1:A:272:TYR:HB2	2.01	0.41
2:D:48:ARG:HH22	2:D:249:ASN:HB3	1.84	0.41
1:A:297:GLU:HA	1:A:298:PRO:HD2	1.75	0.41
1:A:408:TYR:C	1:A:410:GLY:N	2.77	0.41
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.67	0.41
2:B:308:ARG:HH11	2:B:308:ARG:CG	2.32	0.41
1:C:312:TYR:HB2	1:C:342:GLN:O	2.21	0.41
1:A:223:THR:O	1:A:227:LEU:HD13	2.19	0.41
1:A:265:ILE:HD12	1:A:265:ILE:N	2.29	0.41
1:A:395:PHE:C	1:A:395:PHE:CD2	2.98	0.41
2:B:180:THR:O	2:B:182:VAL:N	2.53	0.41
2:B:312:TYR:HB2	2:B:343:PHE:CD2	2.55	0.41
2:B:416:MET:O	2:B:420:GLU:HB2	2.19	0.41
1:C:234:ILE:CG1	1:C:272:TYR:HB2	2.50	0.41
2:D:99:ALA:CB	2:D:145:THR:HG21	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.90	0.41
1:A:249:ASN:H	1:A:254:GLU:HG2	1.85	0.41
1:A:287:SER:O	1:A:290:GLU:N	2.53	0.41
1:C:256:GLN:C	1:C:258:ASN:H	2.25	0.41
2:D:234:THR:O	2:D:238:VAL:HG23	2.20	0.41
2:B:209:LEU:HB3	2:B:227:LEU:CD1	2.50	0.41
1:C:262:TYR:HB2	1:C:265:ILE:HD13	2.02	0.41
2:D:259:MET:HE1	2:D:314:THR:O	2.20	0.41
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.72	0.41
2:B:89:PRO:O	2:B:92:PHE:HD1	2.03	0.41
1:A:258:ASN:O	1:A:259:LEU:HD23	2.21	0.41
2:B:247:GLN:CG	2:B:248:LEU:N	2.83	0.41
2:B:298:SER:O	2:B:300:ASN:N	2.53	0.41
2:D:14:ASN:ND2	2:D:67:LEU:HD23	2.36	0.41
1:A:174:ALA:O	1:A:175:PRO:C	2.63	0.41
1:A:384:ILE:O	1:A:384:ILE:CG1	2.69	0.41
2:B:20:PHE:CD1	2:B:20:PHE:C	2.98	0.41
2:B:33:THR:O	2:B:34:GLY:O	2.38	0.41
2:B:48:ARG:HH22	2:B:249:ASN:HB3	1.86	0.41
2:B:167:ASN:O	2:B:168:THR:HG22	2.20	0.41
1:C:108:TYR:HE1	1:C:413:MET:HG3	1.86	0.41
1:C:251:ASP:O	1:C:255:PHE:HB3	2.21	0.41
1:C:260:VAL:O	1:C:260:VAL:CG2	2.67	0.41
1:C:305:CYS:SG	1:C:306:ASP:N	2.94	0.41
2:D:120:ASP:HA	2:D:123:ARG:NH1	2.36	0.41
2:D:132:LEU:HD23	2:D:164:ARG:HG3	2.02	0.41
2:D:204:ILE:N	2:D:204:ILE:CD1	2.82	0.41
2:D:237:GLY:O	2:D:240:THR:OG1	2.39	0.41
2:D:313:LEU:HD13	2:D:313:LEU:HA	1.85	0.41
3:E:67:GLU:HG3	3:E:68:LEU:N	2.36	0.41
1:A:182:VAL:CG2	1:A:182:VAL:O	2.68	0.41
1:A:395:PHE:C	1:A:397:LEU:N	2.79	0.41
2:B:30:ILE:HA	2:B:35:SER:O	2.21	0.41
2:B:350:ASN:N	2:B:350:ASN:ND2	2.67	0.41
1:C:191:THR:CG2	1:C:425:MET:HE3	2.51	0.41
2:D:329:ASP:O	2:D:333:LEU:HB2	2.21	0.41
3:E:60:ARG:C	3:E:62:LYS:H	2.29	0.41
2:B:226:ASP:OD1	2:B:226:ASP:N	2.54	0.40
1:C:256:GLN:O	1:C:257:THR:C	2.64	0.40
2:D:8:GLN:CD	2:D:17:GLY:HA3	2.46	0.40
2:D:15:GLN:HA	2:D:15:GLN:NE2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LEU:HB2	1:A:145:THR:HG21	2.03	0.40
1:A:327:ASP:O	1:A:328:VAL:C	2.63	0.40
2:B:157:ILE:HG21	2:B:166:MET:HE3	2.03	0.40
1:C:108:TYR:CE1	1:C:413:MET:HG3	2.56	0.40
1:C:154:MET:HE3	1:C:154:MET:HB3	1.85	0.40
1:C:208:ALA:O	1:C:212:ILE:HD13	2.21	0.40
2:D:182:VAL:O	2:D:185:TYR:HB2	2.21	0.40
2:D:273:ALA:CB	2:D:375:ALA:N	2.82	0.40
1:A:8:HIS:CD2	1:A:17:GLY:HA3	2.56	0.40
1:A:88:HIS:O	1:A:89:PRO:C	2.64	0.40
1:A:399:TYR:CE2	1:A:402:ARG:NH2	2.89	0.40
2:B:5:VAL:HG21	2:B:135:PHE:HD2	1.86	0.40
2:B:356:CYS:SG	2:B:358:ILE:HG22	2.62	0.40
1:C:40:LYS:O	1:C:41:THR:HB	2.21	0.40
1:C:41:THR:CG2	1:C:61:HIS:HE1	2.35	0.40
3:E:65:GLU:O	3:E:67:GLU:N	2.55	0.40
1:C:182:VAL:CG2	1:C:182:VAL:O	2.68	0.40
1:A:202:PHE:CE2	1:A:268:PRO:HG2	2.57	0.40
2:B:401:ARG:HH11	2:B:401:ARG:CG	2.35	0.40
1:C:187:SER:O	1:C:191:THR:HB	2.22	0.40
2:D:287:THR:CG2	2:D:290:GLU:H	2.34	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	422/451 (94%)	319 (76%)	70 (17%)	33 (8%)	1	11
1	C	422/451 (94%)	316 (75%)	70 (17%)	36 (8%)	0	9
2	B	415/445 (93%)	315 (76%)	58 (14%)	42 (10%)	0	7
2	D	415/445 (93%)	308 (74%)	64 (15%)	43 (10%)	0	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	120/142 (84%)	82 (68%)	24 (20%)	14 (12%)	0	4
All	All	1794/1934 (93%)	1340 (75%)	286 (16%)	168 (9%)	0	8

All (168) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	73	THR
1	A	164	LYS
1	A	191	THR
1	A	247	ALA
1	A	248	LEU
1	A	273	ALA
1	A	341	ILE
1	A	345	ASP
1	A	348	PRO
2	B	3	GLU
2	B	34	GLY
2	B	43	GLN
2	B	60	LYS
2	B	62	VAL
2	B	73	GLY
2	B	97	SER
2	B	115	VAL
2	B	163	ASP
2	B	245	PRO
2	B	273	ALA
2	B	276	THR
2	B	288	VAL
2	B	299	LYS
2	B	348	PRO
2	B	349	ASN
2	B	400	ARG
1	C	40	LYS
1	C	73	THR
1	C	164	LYS
1	C	191	THR
1	C	247	ALA
1	C	265	ILE
1	C	273	ALA
1	C	341	ILE
1	C	345	ASP

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Mol	Chain	Res	Type
1	C	348	PRO
2	D	3	GLU
2	D	43	GLN
2	D	60	LYS
2	D	62	VAL
2	D	73	GLY
2	D	97	SER
2	D	115	VAL
2	D	163	ASP
2	D	181	VAL
2	D	217	LEU
2	D	240	THR
2	D	245	PRO
2	D	273	ALA
2	D	276	THR
2	D	288	VAL
2	D	299	LYS
2	D	344	VAL
2	D	348	PRO
2	D	400	ARG
3	E	5	ASP
3	E	47	LEU
3	E	49	GLU
3	E	77	GLU
3	E	102	ALA
1	A	72	PRO
1	A	83	TYR
1	A	112	LYS
1	A	265	ILE
1	A	279	GLU
1	A	326	LYS
1	A	377	MET
1	A	405	VAL
2	B	35	SER
2	B	82	PRO
2	B	113	GLU
2	B	159	GLU
2	B	181	VAL
2	B	217	LEU
2	B	227	LEU
2	B	240	THR
2	B	250	ALA

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Mol	Chain	Res	Type
2	B	340	SER
2	B	344	VAL
2	B	371	LEU
2	B	404	PHE
1	C	48	SER
1	C	72	PRO
1	C	112	LYS
1	C	162	GLY
1	C	249	ASN
1	C	257	THR
1	C	377	MET
1	C	405	VAL
1	C	432	TYR
2	D	34	GLY
2	D	82	PRO
2	D	113	GLU
2	D	159	GLU
2	D	227	LEU
2	D	307	PRO
2	D	340	SER
2	D	349	ASN
2	D	371	LEU
2	D	403	ALA
2	D	404	PHE
3	E	7	GLU
3	E	20	PHE
3	E	29	PHE
3	E	75	LYS
3	E	105	MET
1	A	32	PRO
1	A	281	ALA
1	A	314	ALA
1	A	366	GLY
1	A	396	ASP
1	A	432	TYR
2	B	109	THR
2	B	162	PRO
2	B	225	GLY
2	B	244	PHE
2	B	307	PRO
2	B	322	ARG
2	B	403	ALA

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Mol	Chain	Res	Type
1	C	18	ASN
1	C	33	ASP
1	C	41	THR
1	C	82	THR
1	C	83	TYR
1	C	264	ARG
1	C	433	GLU
2	D	35	SER
2	D	109	THR
2	D	162	PRO
2	D	244	PHE
2	D	250	ALA
2	D	266	HIS
2	D	322	ARG
2	D	402	LYS
3	E	12	ASN
1	A	18	ASN
1	A	245	ASP
1	A	304	LYS
1	A	351	PHE
2	B	59	ASN
1	C	163	LYS
1	C	304	LYS
2	D	59	ASN
2	D	247	GLN
2	D	248	LEU
3	E	66	ALA
3	E	138	GLU
1	A	175	PRO
2	B	248	LEU
2	B	402	LYS
1	C	32	PRO
1	C	175	PRO
1	C	339	ARG
1	C	351	PHE
1	C	396	ASP
3	E	26	PRO
2	D	225	GLY
1	A	162	GLY
2	B	72	PRO
1	C	34	GLY
1	A	13	GLY

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Mol	Chain	Res	Type
1	A	274	PRO
2	B	89	PRO
1	C	274	PRO
2	D	31	ASP
1	A	306	ASP
1	C	306	ASP

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	347/378 (92%)	222 (64%)	125 (36%)	0	0
1	C	340/378 (90%)	223 (66%)	117 (34%)	0	1
2	B	348/383 (91%)	215 (62%)	133 (38%)	0	0
2	D	348/383 (91%)	208 (60%)	140 (40%)	0	0
3	E	81/126 (64%)	38 (47%)	43 (53%)	0	0
All	All	1464/1648 (89%)	906 (62%)	558 (38%)	0	0

All (558) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	9	VAL
1	A	11	GLN
1	A	15	GLN
1	A	16	ILE
1	A	22	GLU
1	A	23	LEU
1	A	26	LEU
1	A	31	GLN
1	A	36	MET
1	A	48	SER
1	A	50	ASN
1	A	60	LYS

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Mol	Chain	Res	Type
1	A	61	HIS
1	A	62	VAL
1	A	64	ARG
1	A	66	VAL
1	A	68	VAL
1	A	74	VAL
1	A	76	ASP
1	A	78	VAL
1	A	80	THR
1	A	82	THR
1	A	84	ARG
1	A	87	PHE
1	A	88	HIS
1	A	90	GLU
1	A	94	THR
1	A	96	LYS
1	A	105	ARG
1	A	114	ILE
1	A	115	ILE
1	A	116	ASP
1	A	119	LEU
1	A	121	ARG
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	153	LEU
1	A	155	GLU
1	A	158	SER
1	A	163	LYS
1	A	165	SER
1	A	167	LEU
1	A	171	ILE
1	A	176	GLN
1	A	182	VAL
1	A	183	GLU
1	A	187	SER
1	A	191	THR
1	A	193	THR
1	A	194	THR

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Mol	Chain	Res	Type
1	A	195	LEU
1	A	196	GLU
1	A	200	CYS
1	A	206	ASN
1	A	217	LEU
1	A	220	GLU
1	A	223	THR
1	A	226	ASN
1	A	229	ARG
1	A	230	LEU
1	A	234	ILE
1	A	236	SER
1	A	237	SER
1	A	239	THR
1	A	242	LEU
1	A	245	ASP
1	A	248	LEU
1	A	249	ASN
1	A	252	LEU
1	A	253	THR
1	A	256	GLN
1	A	257	THR
1	A	260	VAL
1	A	264	ARG
1	A	269	LEU
1	A	275	VAL
1	A	277	SER
1	A	279	GLU
1	A	284	GLU
1	A	288	VAL
1	A	301	GLN
1	A	302	MET
1	A	304	LYS
1	A	306	ASP
1	A	309	HIS
1	A	311	LYS
1	A	316	CYS
1	A	318	LEU
1	A	326	LYS
1	A	332	ILE
1	A	334	THR
1	A	340	THR

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Mol	Chain	Res	Type
1	A	341	ILE
1	A	343	PHE
1	A	349	THR
1	A	355	ILE
1	A	356	ASN
1	A	361	THR
1	A	362	VAL
1	A	363	VAL
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	382	THR
1	A	386	GLU
1	A	394	LYS
1	A	397	LEU
1	A	401	LYS
1	A	405	VAL
1	A	409	VAL
1	A	413	MET
1	A	414	GLU
1	A	415	GLU
1	A	419	SER
1	A	420	GLU
1	A	433	GLU
1	A	434	GLU
2	B	2	ARG
2	B	4	ILE
2	B	16	ILE
2	B	19	LYS
2	B	24	ILE
2	B	25	SER
2	B	27	GLU
2	B	31	ASP
2	B	33	THR
2	B	39	ASP
2	B	42	LEU
2	B	43	GLN
2	B	44	LEU
2	B	51	VAL

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Mol	Chain	Res	Type
2	B	55	GLU
2	B	61	TYR
2	B	64	ARG
2	B	66	ILE
2	B	68	VAL
2	B	70	LEU
2	B	71	GLU
2	B	77	SER
2	B	83	PHE
2	B	85	GLN
2	B	88	ARG
2	B	93	VAL
2	B	96	GLN
2	B	97	SER
2	B	101	ASN
2	B	102	ASN
2	B	109	THR
2	B	115	VAL
2	B	119	LEU
2	B	120	ASP
2	B	122	VAL
2	B	129	CYS
2	B	130	ASP
2	B	131	CYS
2	B	132	LEU
2	B	135	PHE
2	B	137	LEU
2	B	141	LEU
2	B	145	THR
2	B	153	LEU
2	B	154	ILE
2	B	158	ARG
2	B	160	GLU
2	B	164	ARG
2	B	165	ILE
2	B	166	MET
2	B	168	THR
2	B	170	SER
2	B	174	SER
2	B	176	LYS
2	B	177	VAL
2	B	178	SER

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Mol	Chain	Res	Type
2	B	180	THR
2	B	181	VAL
2	B	182	VAL
2	B	191	VAL
2	B	195	VAL
2	B	200	GLU
2	B	209	LEU
2	B	211	ASP
2	B	212	ILE
2	B	215	ARG
2	B	216	THR
2	B	223	THR
2	B	227	LEU
2	B	230	LEU
2	B	231	VAL
2	B	240	THR
2	B	241	CYS
2	B	248	LEU
2	B	249	ASN
2	B	253	ARG
2	B	254	LYS
2	B	258	ASN
2	B	260	VAL
2	B	265	LEU
2	B	269	MET
2	B	275	LEU
2	B	276	THR
2	B	286	LEU
2	B	293	GLN
2	B	294	GLN
2	B	295	MET
2	B	299	LYS
2	B	301	MET
2	B	302	MET
2	B	305	CYS
2	B	308	ARG
2	B	309	HIS
2	B	313	LEU
2	B	320	ARG
2	B	323	MET
2	B	324	SER
2	B	325	MET

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Mol	Chain	Res	Type
2	B	332	MET
2	B	333	LEU
2	B	335	VAL
2	B	336	GLN
2	B	341	SER
2	B	344	VAL
2	B	349	ASN
2	B	350	ASN
2	B	351	VAL
2	B	357	ASP
2	B	358	ILE
2	B	371	LEU
2	B	373	MET
2	B	374	SER
2	B	376	THR
2	B	378	ILE
2	B	384	ILE
2	B	386	GLU
2	B	387	LEU
2	B	389	LYS
2	B	390	ARG
2	B	391	ILE
2	B	392	SER
2	B	393	GLU
2	B	394	GLN
2	B	398	MET
2	B	400	ARG
2	B	401	ARG
2	B	405	LEU
2	B	409	THR
2	B	413	MET
2	B	419	THR
2	B	420	GLU
2	B	423	SER
2	B	434	GLN
1	C	2	ARG
1	C	9	VAL
1	C	11	GLN
1	C	15	GLN
1	C	16	ILE
1	C	22	GLU
1	C	23	LEU

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Mol	Chain	Res	Type
1	C	26	LEU
1	C	31	GLN
1	C	49	PHE
1	C	50	ASN
1	C	51	THR
1	C	60	LYS
1	C	61	HIS
1	C	62	VAL
1	C	66	VAL
1	C	68	VAL
1	C	74	VAL
1	C	76	ASP
1	C	78	VAL
1	C	79	ARG
1	C	80	THR
1	C	82	THR
1	C	84	ARG
1	C	87	PHE
1	C	88	HIS
1	C	94	THR
1	C	96	LYS
1	C	105	ARG
1	C	114	ILE
1	C	115	ILE
1	C	116	ASP
1	C	119	LEU
1	C	122	ILE
1	C	123	ARG
1	C	124	LYS
1	C	128	GLN
1	C	132	LEU
1	C	140	SER
1	C	141	PHE
1	C	153	LEU
1	C	155	GLU
1	C	158	SER
1	C	163	LYS
1	C	165	SER
1	C	167	LEU
1	C	171	ILE
1	C	182	VAL
1	C	183	GLU

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Mol	Chain	Res	Type
1	C	187	SER
1	C	191	THR
1	C	193	THR
1	C	194	THR
1	C	195	LEU
1	C	196	GLU
1	C	200	CYS
1	C	206	ASN
1	C	217	LEU
1	C	220	GLU
1	C	223	THR
1	C	226	ASN
1	C	229	ARG
1	C	230	LEU
1	C	234	ILE
1	C	236	SER
1	C	237	SER
1	C	239	THR
1	C	242	LEU
1	C	248	LEU
1	C	250	VAL
1	C	251	ASP
1	C	252	LEU
1	C	254	GLU
1	C	255	PHE
1	C	257	THR
1	C	269	LEU
1	C	275	VAL
1	C	288	VAL
1	C	301	GLN
1	C	302	MET
1	C	304	LYS
1	C	306	ASP
1	C	309	HIS
1	C	311	LYS
1	C	316	CYS
1	C	318	LEU
1	C	334	THR
1	C	336	LYS
1	C	340	THR
1	C	341	ILE
1	C	343	PHE

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Mol	Chain	Res	Type
1	C	349	THR
1	C	355	ILE
1	C	356	ASN
1	C	362	VAL
1	C	363	VAL
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	380	ASN
1	C	386	GLU
1	C	394	LYS
1	C	397	LEU
1	C	401	LYS
1	C	405	VAL
1	C	409	VAL
1	C	413	MET
1	C	414	GLU
1	C	415	GLU
1	C	419	SER
1	C	420	GLU
1	C	430	LYS
1	C	433	GLU
1	C	434	GLU
2	D	2	ARG
2	D	4	ILE
2	D	5	VAL
2	D	11	GLN
2	D	16	ILE
2	D	19	LYS
2	D	24	ILE
2	D	25	SER
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	44	LEU
2	D	47	GLU

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Mol	Chain	Res	Type
2	D	51	VAL
2	D	54	ASN
2	D	55	GLU
2	D	61	TYR
2	D	64	ARG
2	D	66	ILE
2	D	67	LEU
2	D	68	VAL
2	D	70	LEU
2	D	71	GLU
2	D	77	SER
2	D	80	SER
2	D	83	PHE
2	D	85	GLN
2	D	91	ASN
2	D	93	VAL
2	D	96	GLN
2	D	97	SER
2	D	101	ASN
2	D	102	ASN
2	D	109	THR
2	D	115	VAL
2	D	116	ASP
2	D	119	LEU
2	D	122	VAL
2	D	124	LYS
2	D	129	CYS
2	D	130	ASP
2	D	131	CYS
2	D	132	LEU
2	D	135	PHE
2	D	137	LEU
2	D	141	LEU
2	D	145	THR
2	D	153	LEU
2	D	154	ILE
2	D	158	ARG
2	D	160	GLU
2	D	164	ARG
2	D	165	ILE
2	D	166	MET
2	D	168	THR

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Mol	Chain	Res	Type
2	D	170	SER
2	D	174	SER
2	D	176	LYS
2	D	177	VAL
2	D	178	SER
2	D	180	THR
2	D	181	VAL
2	D	182	VAL
2	D	191	VAL
2	D	195	VAL
2	D	200	GLU
2	D	204	ILE
2	D	209	LEU
2	D	211	ASP
2	D	212	ILE
2	D	216	THR
2	D	223	THR
2	D	227	LEU
2	D	230	LEU
2	D	231	VAL
2	D	240	THR
2	D	241	CYS
2	D	248	LEU
2	D	249	ASN
2	D	253	ARG
2	D	254	LYS
2	D	258	ASN
2	D	260	VAL
2	D	265	LEU
2	D	269	MET
2	D	275	LEU
2	D	276	THR
2	D	286	LEU
2	D	293	GLN
2	D	294	GLN
2	D	295	MET
2	D	299	LYS
2	D	301	MET
2	D	302	MET
2	D	305	CYS
2	D	308	ARG
2	D	309	HIS

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Mol	Chain	Res	Type
2	D	313	LEU
2	D	320	ARG
2	D	323	MET
2	D	324	SER
2	D	325	MET
2	D	332	MET
2	D	333	LEU
2	D	335	VAL
2	D	336	GLN
2	D	341	SER
2	D	344	VAL
2	D	349	ASN
2	D	350	ASN
2	D	351	VAL
2	D	355	VAL
2	D	357	ASP
2	D	358	ILE
2	D	371	LEU
2	D	373	MET
2	D	374	SER
2	D	376	THR
2	D	378	ILE
2	D	384	ILE
2	D	386	GLU
2	D	387	LEU
2	D	389	LYS
2	D	390	ARG
2	D	391	ILE
2	D	392	SER
2	D	393	GLU
2	D	394	GLN
2	D	398	MET
2	D	400	ARG
2	D	401	ARG
2	D	405	LEU
2	D	409	THR
2	D	413	MET
2	D	419	THR
2	D	420	GLU
2	D	434	GLN
3	E	5	ASP
3	E	12	ASN

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Mol	Chain	Res	Type
3	E	13	LYS
3	E	15	THR
3	E	24	LEU
3	E	48	GLU
3	E	52	LYS
3	E	53	LYS
3	E	54	LEU
3	E	55	GLU
3	E	59	GLU
3	E	60	ARG
3	E	61	ARG
3	E	62	LYS
3	E	65	GLU
3	E	67	GLU
3	E	69	LEU
3	E	70	LYS
3	E	71	HIS
3	E	72	LEU
3	E	74	GLU
3	E	75	LYS
3	E	77	GLU
3	E	79	GLU
3	E	80	ARG
3	E	81	GLU
3	E	89	GLU
3	E	91	ASN
3	E	94	ILE
3	E	96	MET
3	E	99	GLU
3	E	101	LEU
3	E	105	MET
3	E	106	GLU
3	E	111	ASN
3	E	112	ARG
3	E	113	GLU
3	E	119	MET
3	E	120	LEU
3	E	121	GLU
3	E	123	LEU
3	E	125	GLU
3	E	134	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	28	HIS
1	A	50	ASN
1	A	85	GLN
1	A	88	HIS
1	A	91	GLN
1	A	107	HIS
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	329	ASN
1	A	393	HIS
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	15	GLN
2	B	54	ASN
2	B	96	GLN
2	B	133	GLN
2	B	136	GLN
2	B	139	HIS
2	B	192	HIS
2	B	193	GLN
2	B	197	ASN
2	B	206	ASN
2	B	229	HIS
2	B	247	GLN
2	B	258	ASN
2	B	266	HIS
2	B	294	GLN
2	B	336	GLN
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN
2	B	385	GLN
2	B	436	GLN
1	C	50	ASN
1	C	61	HIS
1	C	85	GLN

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Mol	Chain	Res	Type
1	C	107	HIS
1	C	139	HIS
1	C	176	GLN
1	C	206	ASN
1	C	256	GLN
1	C	266	HIS
1	C	406	HIS
2	D	6	HIS
2	D	8	GLN
2	D	14	ASN
2	D	15	GLN
2	D	54	ASN
2	D	96	GLN
2	D	133	GLN
2	D	136	GLN
2	D	192	HIS
2	D	193	GLN
2	D	206	ASN
2	D	247	GLN
2	D	258	ASN
2	D	266	HIS
2	D	294	GLN
2	D	309	HIS
2	D	331	GLN
2	D	336	GLN
2	D	339	ASN
2	D	350	ASN
2	D	380	ASN
2	D	385	GLN
2	D	406	HIS
2	D	436	GLN
3	E	91	ASN
3	E	111	ASN
3	E	129	HIS

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
7	E70	B	700	-	27,28,28	2.62	5 (18%)	39,39,39	1.91	6 (15%)
6	GDP	B	600	-	29,30,30	0.88	1 (3%)	45,47,47	1.89	11 (24%)
7	E70	D	700	-	27,28,28	3.44	7 (25%)	39,39,39	2.04	9 (23%)
6	GDP	D	600	-	29,30,30	0.78	1 (3%)	45,47,47	1.80	12 (26%)
4	GTP	A	600	-	33,34,34	1.14	3 (9%)	50,54,54	1.75	10 (20%)
4	GTP	C	600	-	33,34,34	0.97	3 (9%)	50,54,54	1.89	12 (24%)

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
7	E70	B	700	-	-	7/17/17/17	0/3/3/3
6	GDP	B	600	-	-	6/16/32/32	0/3/3/3
7	E70	D	700	-	-	6/17/17/17	0/3/3/3
6	GDP	D	600	-	-	5/16/32/32	0/3/3/3
4	GTP	A	600	-	-	6/22/38/38	0/3/3/3
4	GTP	C	600	-	-	6/22/38/38	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	700	E70	OAB-SAZ	12.92	1.58	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	700	E70	OAB-SAZ	9.77	1.54	1.43
7	D	700	E70	OAC-SAZ	8.26	1.53	1.43
7	B	700	E70	OAC-SAZ	6.31	1.50	1.43
7	D	700	E70	CAX-NAR	-5.30	1.34	1.42
7	B	700	E70	SAZ-NAR	3.60	1.69	1.63
7	B	700	E70	CAX-NAR	-3.49	1.37	1.42
7	D	700	E70	CAW-SAZ	3.43	1.81	1.76
7	D	700	E70	SAZ-NAR	3.36	1.68	1.63
4	A	600	GTP	PB-O3A	3.35	1.63	1.59
4	A	600	GTP	PB-O3B	3.23	1.63	1.59
7	B	700	E70	CAU-NAQ	-2.98	1.34	1.40
7	D	700	E70	CAU-NAQ	-2.46	1.35	1.40
4	C	600	GTP	O4'-C4'	-2.39	1.39	1.45
4	C	600	GTP	PA-O3A	2.33	1.62	1.59
6	B	600	GDP	C2-N3	2.30	1.38	1.33
7	D	700	E70	CAY-NAP	2.25	1.38	1.35
4	A	600	GTP	O4'-C4'	-2.13	1.40	1.45
6	D	600	GDP	C5-N7	-2.07	1.34	1.39
4	C	600	GTP	C2-N3	2.02	1.38	1.33

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	700	E70	OAC-SAZ-OAB	-8.46	109.25	119.52
7	D	700	E70	OAC-SAZ-OAB	-7.79	110.06	119.52
6	B	600	GDP	C5-C4-N3	-5.57	119.53	128.39
4	C	600	GTP	C2-N3-C4	5.53	121.82	112.30
6	B	600	GDP	C2-N3-C4	5.33	121.49	112.30
6	D	600	GDP	C5-C4-N3	-5.13	120.22	128.39
4	C	600	GTP	C5-C4-N3	-5.08	120.30	128.39
7	B	700	E70	OAB-SAZ-CAW	5.07	114.37	107.98
4	A	600	GTP	C5-C4-N3	-5.06	120.34	128.39
6	D	600	GDP	C2-N3-C4	4.98	120.88	112.30
7	D	700	E70	OAB-SAZ-CAW	4.94	114.21	107.98
4	A	600	GTP	C2-N3-C4	4.69	120.38	112.30
6	B	600	GDP	N9-C4-N3	3.92	133.80	125.95
6	B	600	GDP	O6-C6-C5	-3.77	116.58	126.53
4	A	600	GTP	N9-C4-N3	3.65	133.25	125.95
4	A	600	GTP	C2-N1-C6	-3.64	118.51	125.11
4	C	600	GTP	N9-C8-N7	-3.62	106.69	113.40
4	C	600	GTP	C8-N7-C5	3.49	110.47	104.26
7	D	700	E70	CAW-SAZ-NAR	3.47	111.19	106.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	600	GDP	O6-C6-C5	-3.44	117.46	126.53
6	D	600	GDP	N9-C4-N3	3.39	132.74	125.95
4	A	600	GTP	N9-C8-N7	-3.22	107.44	113.40
7	D	700	E70	CAE-CAF-NAP	-3.13	118.46	123.42
4	A	600	GTP	O6-C6-C5	-3.08	118.40	126.53
4	C	600	GTP	C2-N1-C6	-3.08	119.53	125.11
4	A	600	GTP	C5-C6-N1	2.98	120.85	113.25
4	C	600	GTP	C4-C5-N7	-2.98	105.95	110.67
4	C	600	GTP	C6-C5-N7	2.94	135.63	130.29
4	C	600	GTP	C5-C6-N1	2.91	120.65	113.25
7	D	700	E70	NAQ-CAY-NAP	2.90	121.89	118.38
4	C	600	GTP	N9-C4-N3	2.83	131.61	125.95
6	D	600	GDP	N9-C8-N7	-2.80	108.21	113.40
7	D	700	E70	CAF-NAP-CAY	2.70	122.00	116.74
6	D	600	GDP	C8-N7-C5	2.67	109.02	104.26
6	B	600	GDP	C2-N1-C6	-2.57	120.44	125.11
4	A	600	GTP	C8-N7-C5	2.51	108.73	104.26
4	C	600	GTP	N2-C2-N1	2.50	122.03	116.76
6	B	600	GDP	C5-C6-N1	2.50	119.61	113.25
6	B	600	GDP	C8-N7-C5	2.47	108.66	104.26
6	D	600	GDP	C3'-C2'-C1'	2.45	106.09	101.46
4	A	600	GTP	O3A-PB-O1B	-2.44	103.38	110.70
7	B	700	E70	CAF-NAP-CAY	2.39	121.40	116.74
7	B	700	E70	NAQ-CAY-NAP	2.35	121.23	118.38
6	B	600	GDP	N9-C8-N7	-2.35	109.04	113.40
6	D	600	GDP	N1-C2-N3	-2.33	119.06	123.32
6	B	600	GDP	N1-C2-N3	-2.30	119.11	123.32
7	B	700	E70	CAW-SAZ-NAR	2.28	109.71	106.88
6	B	600	GDP	C2'-C3'-C4'	2.27	106.99	102.61
6	D	600	GDP	O4'-C4'-C3'	2.23	109.57	105.15
4	C	600	GTP	N1-C2-N3	-2.21	119.28	123.32
6	D	600	GDP	O2B-PB-O3A	2.16	111.87	104.64
4	A	600	GTP	O2B-PB-O3A	2.15	113.08	107.27
6	D	600	GDP	C2-N1-C6	-2.10	121.30	125.11
7	B	700	E70	CAX-NAR-SAZ	2.08	130.00	123.34
7	D	700	E70	CAG-CAE-CAF	2.07	121.92	118.92
6	D	600	GDP	C2'-C1'-N9	-2.05	107.54	113.25
4	C	600	GTP	O2G-PG-O3B	2.05	111.51	104.64
7	D	700	E70	CAU-NAQ-CAY	-2.05	124.41	129.43
6	B	600	GDP	O2A-PA-O3A	2.04	112.78	107.27
7	D	700	E70	CAA-OAS-CAV	-2.02	113.17	117.50

There are no chirality outliers.

All (36) torsion outliers are listed below:

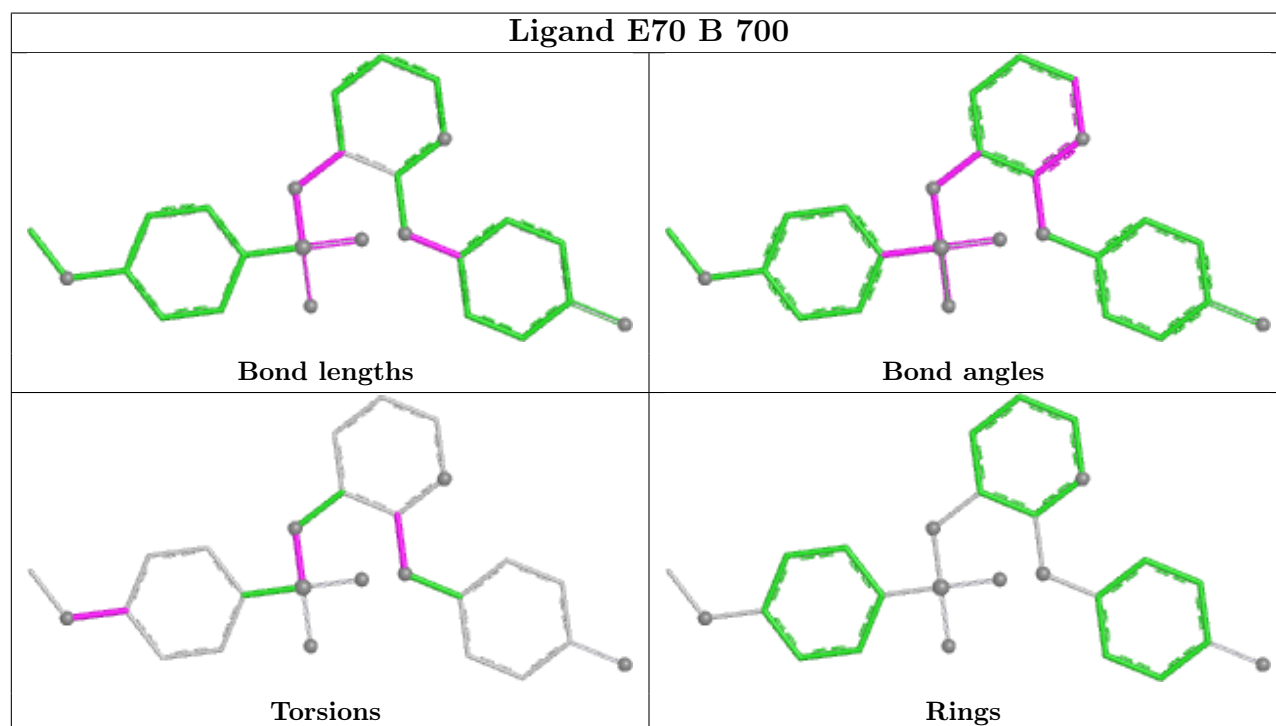
Mol	Chain	Res	Type	Atoms
4	A	600	GTP	C5'-O5'-PA-O3A
4	A	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O1A
6	B	600	GDP	PA-O3A-PB-O2B
6	B	600	GDP	O4'-C4'-C5'-O5'
6	D	600	GDP	PA-O3A-PB-O2B
6	D	600	GDP	O4'-C4'-C5'-O5'
7	B	700	E70	CAX-NAR-SAZ-CAW
7	B	700	E70	CAX-NAR-SAZ-OAC
7	B	700	E70	CAX-CAY-NAQ-CAU
7	D	700	E70	CAX-NAR-SAZ-CAW
7	D	700	E70	CAX-NAR-SAZ-OAC
7	B	700	E70	CAL-CAV-OAS-CAA
7	D	700	E70	CAL-CAV-OAS-CAA
7	B	700	E70	CAM-CAV-OAS-CAA
7	D	700	E70	CAM-CAV-OAS-CAA
7	B	700	E70	CAX-NAR-SAZ-OAB
6	B	600	GDP	C3'-C4'-C5'-O5'
6	D	600	GDP	C3'-C4'-C5'-O5'
7	D	700	E70	CAX-NAR-SAZ-OAB
4	A	600	GTP	PB-O3B-PG-O1G
4	A	600	GTP	C5'-O5'-PA-O2A
4	C	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O2A
6	B	600	GDP	C5'-O5'-PA-O3A
4	C	600	GTP	PB-O3B-PG-O1G
4	A	600	GTP	PG-O3B-PB-O1B
4	C	600	GTP	PG-O3B-PB-O1B
6	B	600	GDP	PA-O3A-PB-O1B
6	D	600	GDP	PA-O3A-PB-O1B
7	B	700	E70	NAP-CAY-NAQ-CAU
6	B	600	GDP	PA-O3A-PB-O3B
6	D	600	GDP	PA-O3A-PB-O3B
7	D	700	E70	CAX-CAY-NAQ-CAU
4	C	600	GTP	PB-O3A-PA-O2A
4	A	600	GTP	PG-O3B-PB-O2B

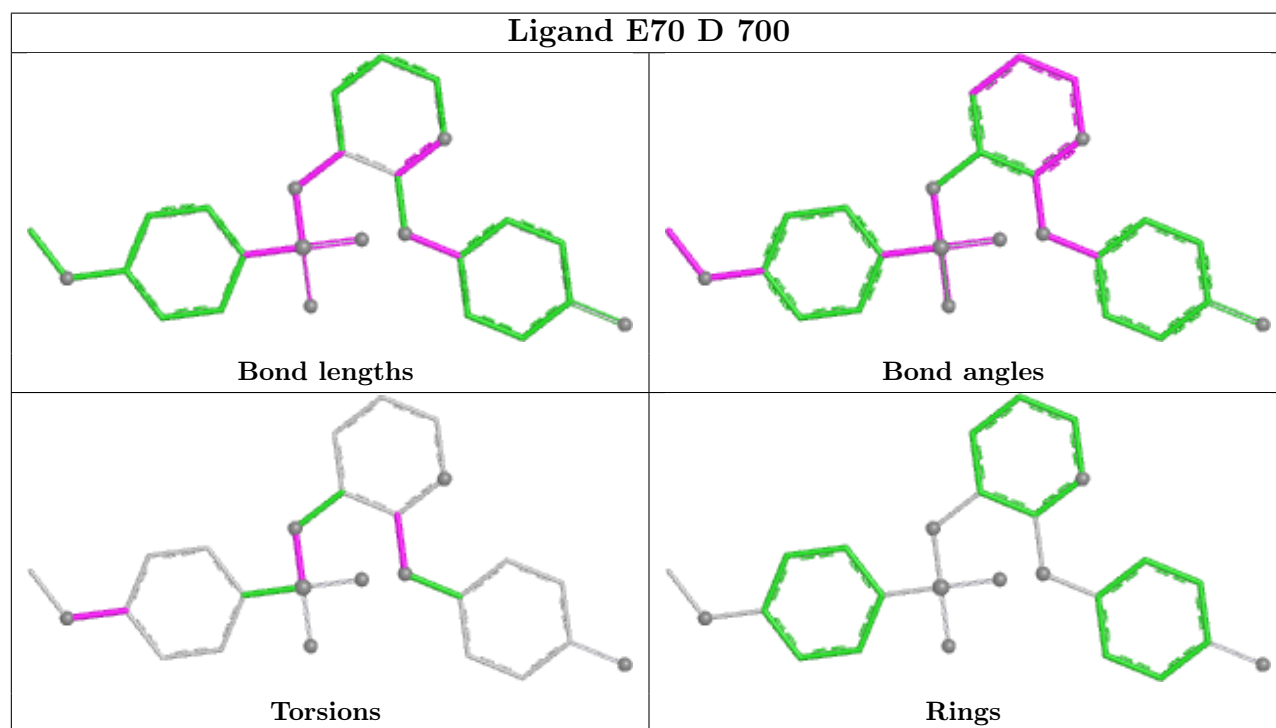
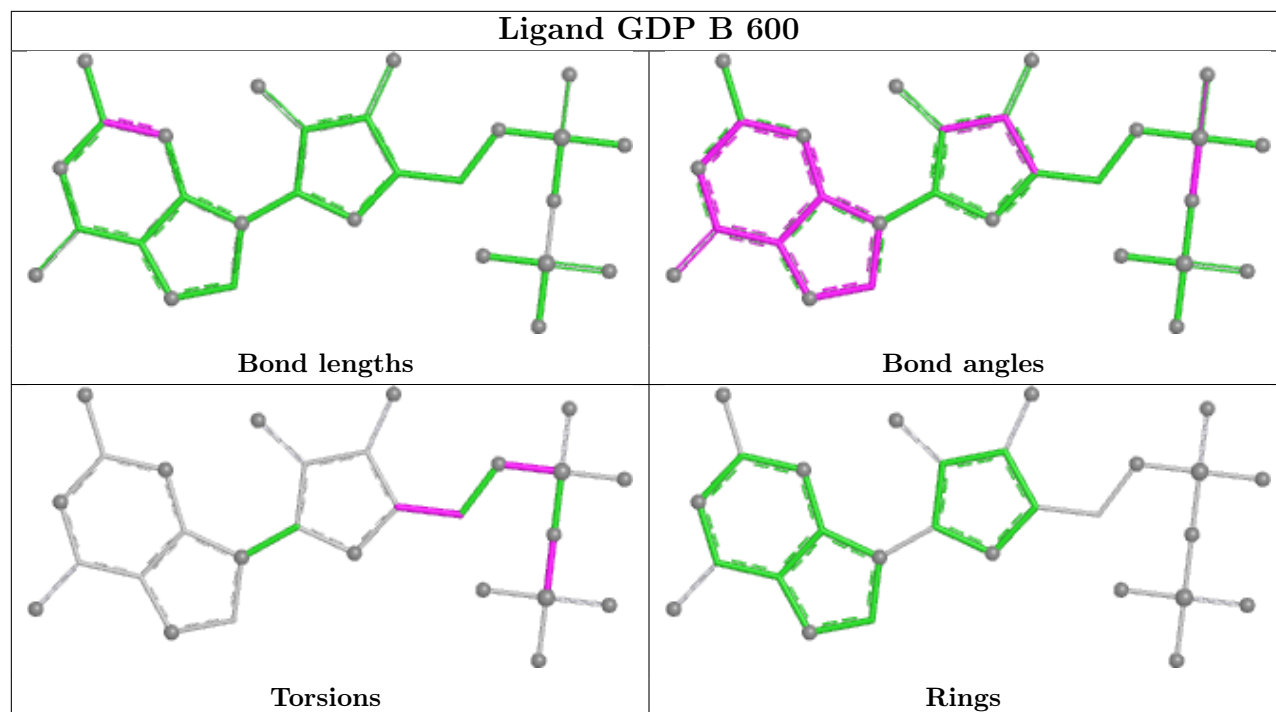
There are no ring outliers.

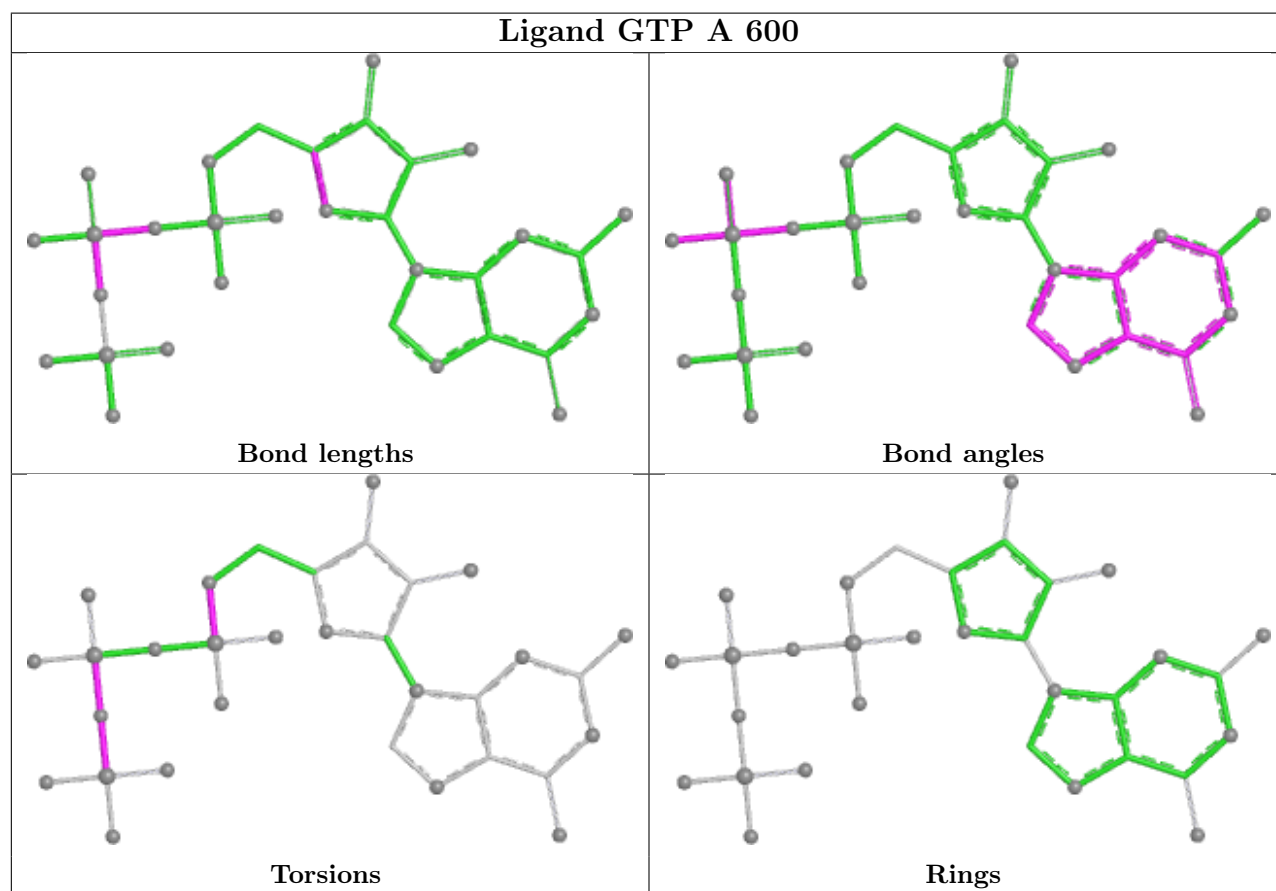
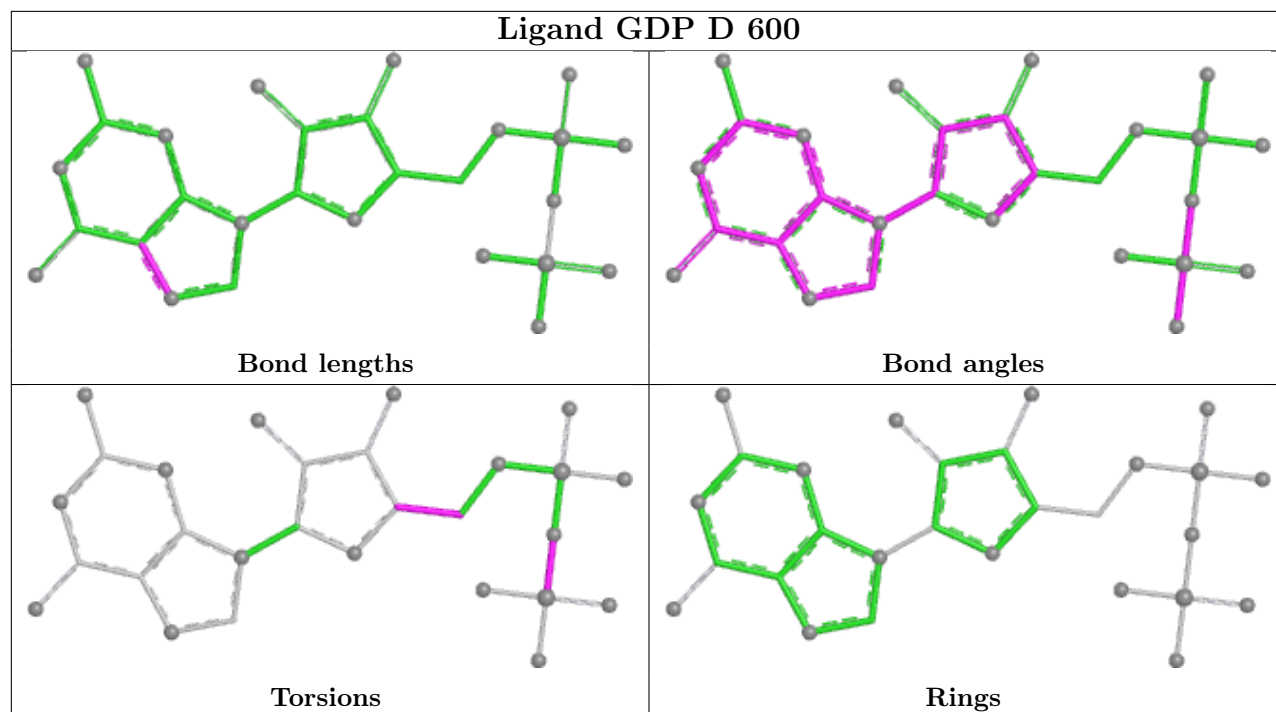
6 monomers are involved in 25 short contacts:

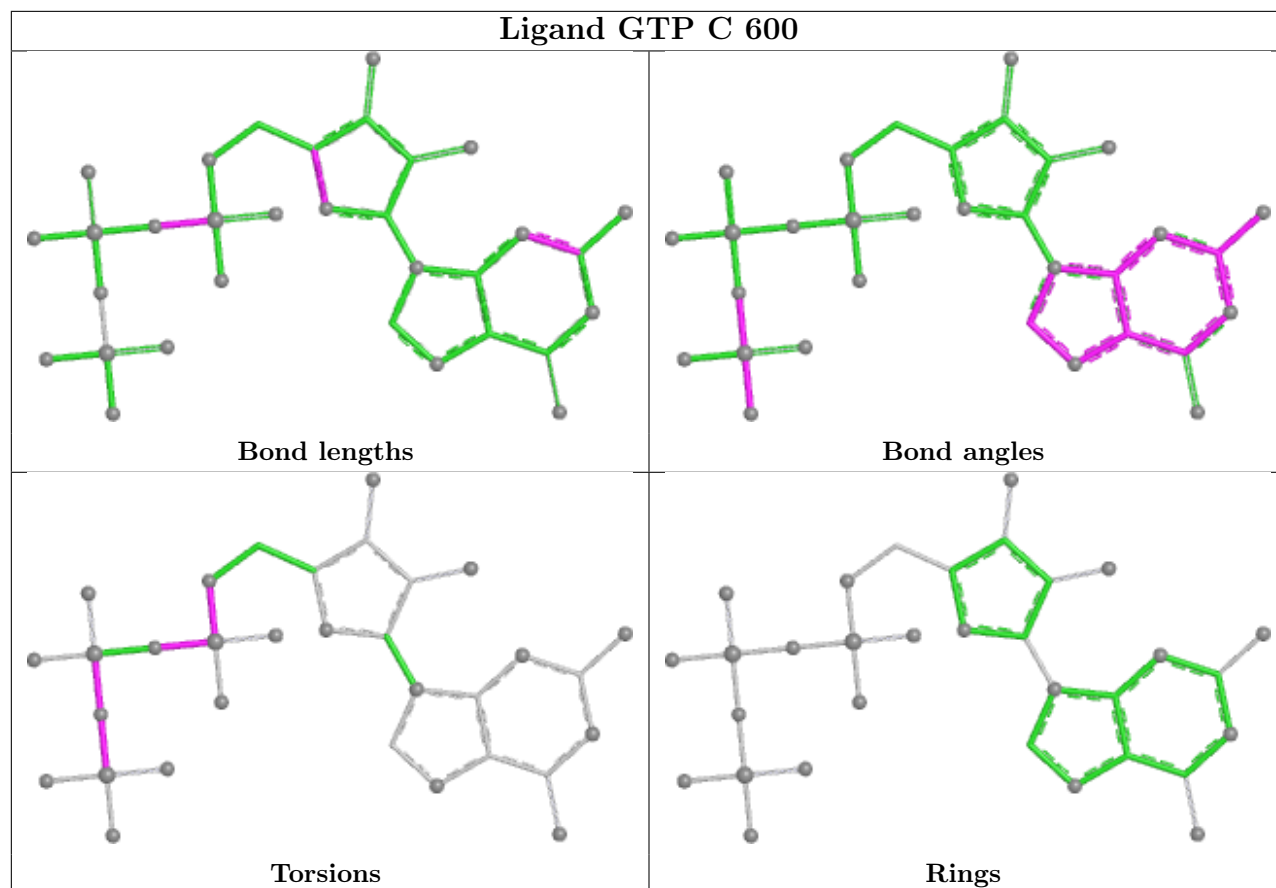
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	700	E70	5	0
6	B	600	GDP	3	0
7	D	700	E70	5	0
6	D	600	GDP	4	0
4	A	600	GTP	4	0
4	C	600	GTP	4	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/451 (94%)	-0.60	0 100 100	46, 51, 52, 57	0
1	C	428/451 (94%)	-0.60	0 100 100	44, 51, 52, 62	0
2	B	419/445 (94%)	-0.61	0 100 100	49, 51, 52, 54	0
2	D	419/445 (94%)	-0.56	0 100 100	48, 51, 52, 54	0
3	E	124/142 (87%)	-0.72	0 100 100	41, 50, 56, 59	0
All	All	1817/1934 (93%)	-0.60	0 100 100	41, 51, 52, 62	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	B	601	1/1	0.80	0.34	47,47,47,47	0
5	MG	C	601	1/1	0.91	0.14	41,41,41,41	0
7	E70	B	700	26/26	0.92	0.07	52,52,57,59	0

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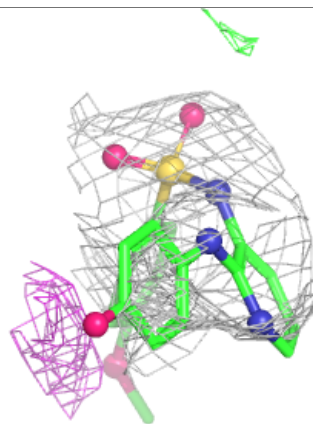
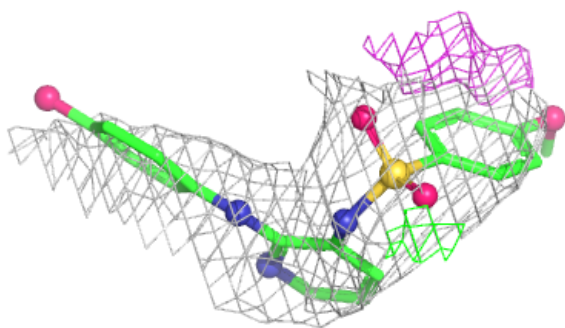
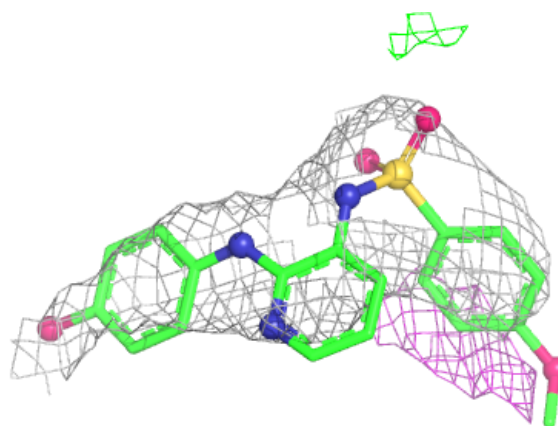
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	E70	D	700	26/26	0.92	0.07	52,53,57,59	0
6	GDP	D	600	28/28	0.93	0.07	48,51,52,52	0
6	GDP	B	600	28/28	0.95	0.08	48,51,52,52	0
4	GTP	C	600	32/32	0.95	0.07	48,49,50,51	0
4	GTP	A	600	32/32	0.96	0.07	47,49,51,51	0
5	MG	A	601	1/1	0.96	0.10	40,40,40,40	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

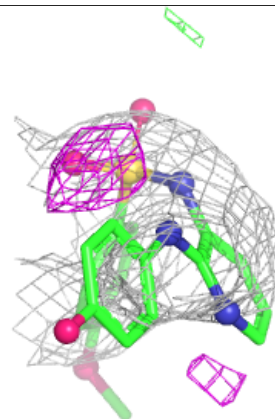
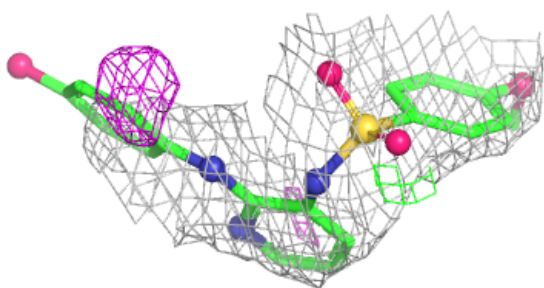
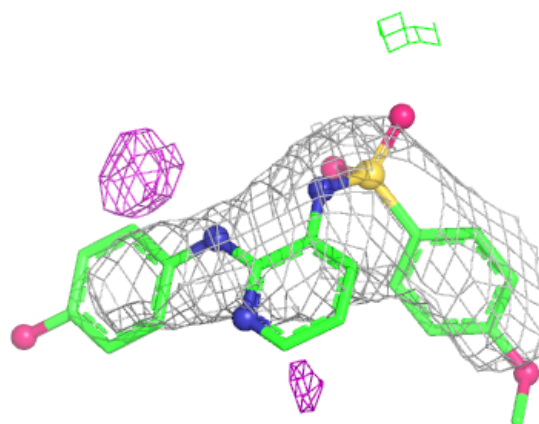
Electron density around E70 B 700:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

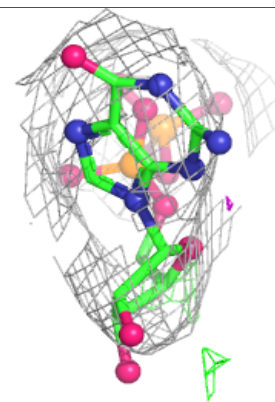
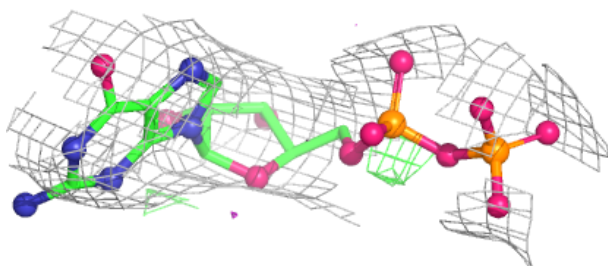
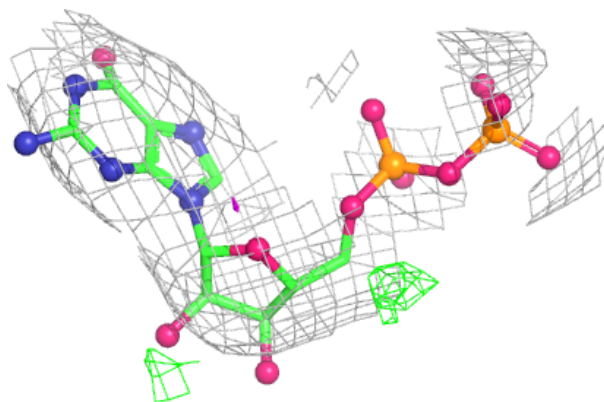


Electron density around E70 D 700:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

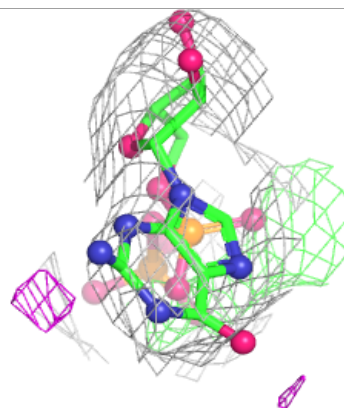
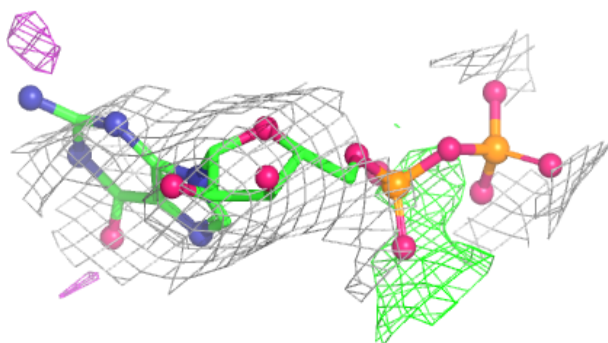
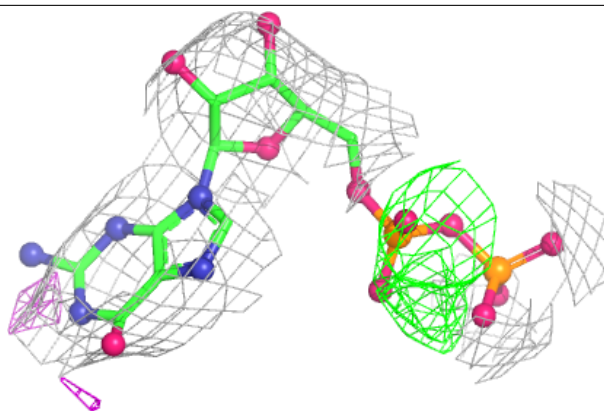
**Electron density around GDP D 600:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

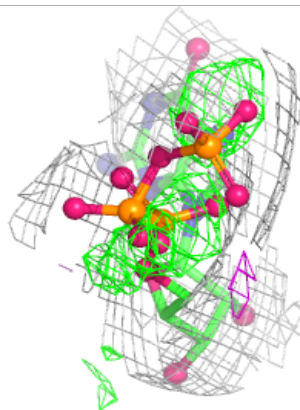
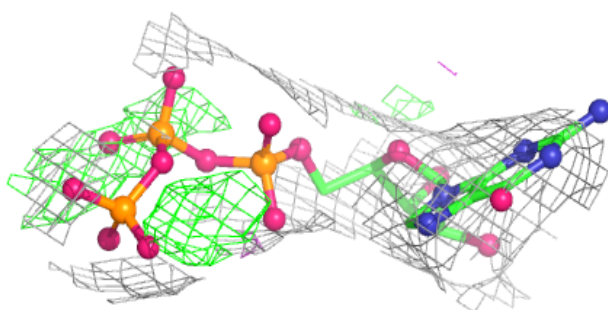
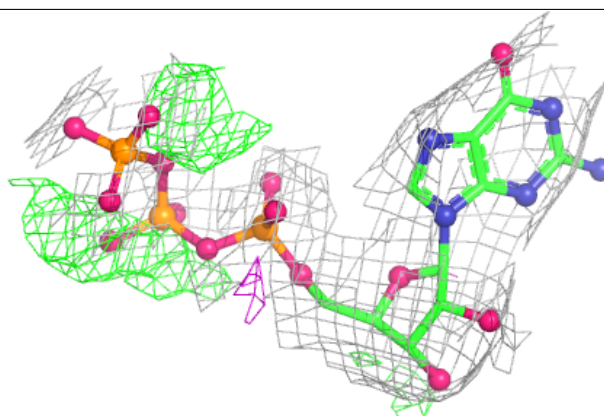


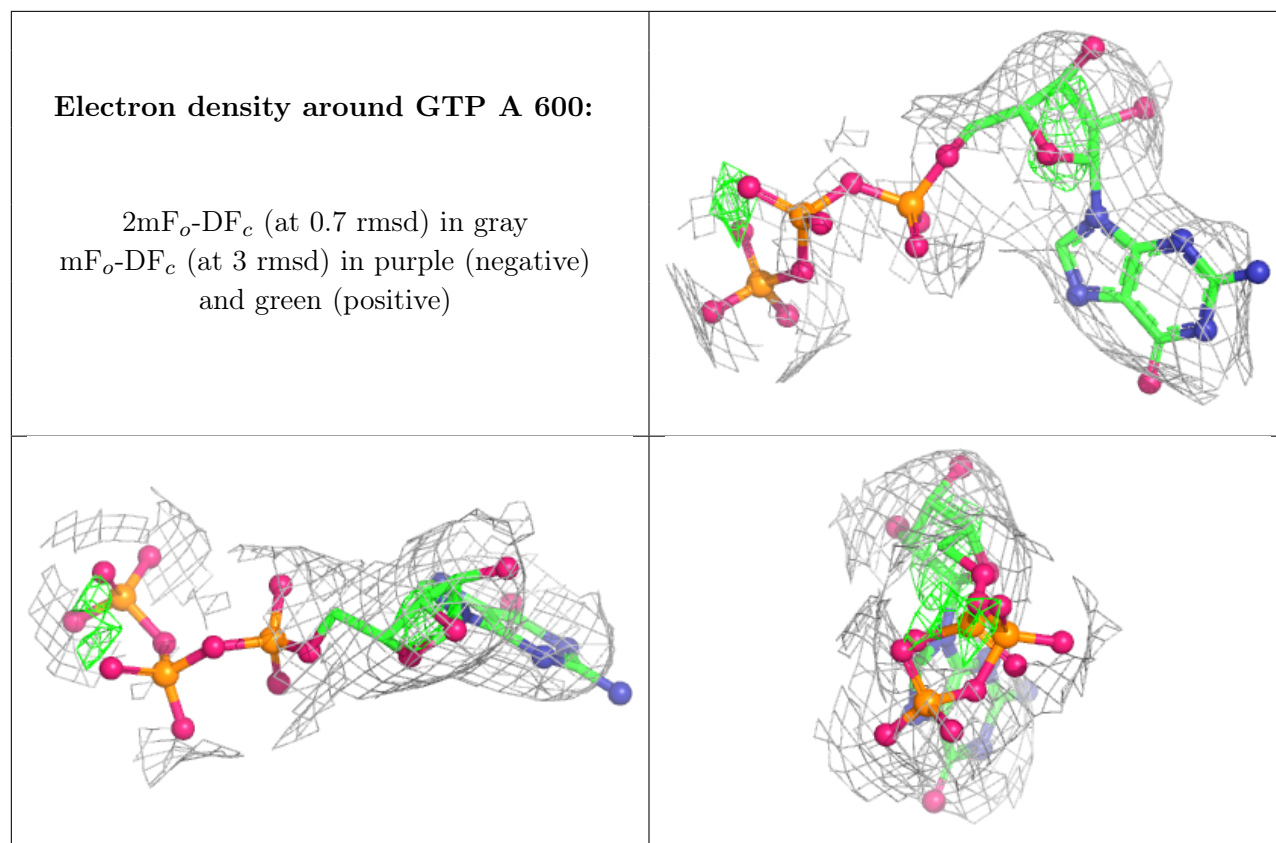
Electron density around GDP B 600:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GTP C 600:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.