



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 05:38 am BST

PDB ID : 3HKE
Title : Tubulin-T138067: 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 : 3.60 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

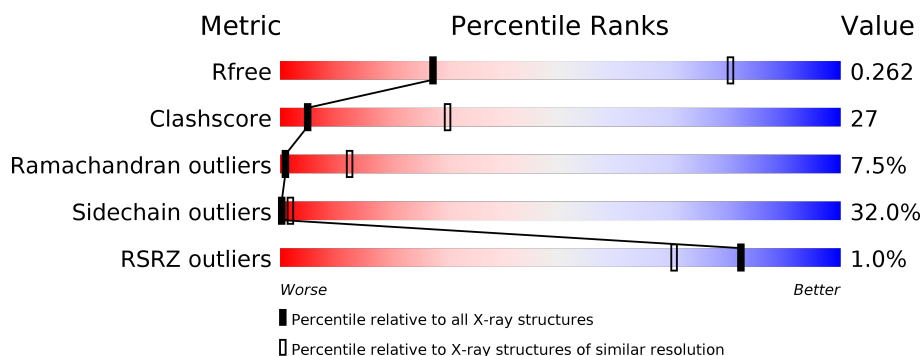
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div> <div></div> <div>41% 38% 13% • 5%</div> </div>
1	C	451	<div> <div>2%</div> <div>46% 33% 15% • 5%</div> </div>
2	B	445	<div> <div>%</div> <div>37% 39% 17% • 6%</div> </div>
2	D	445	<div> <div>%</div> <div>39% 38% 17% • •</div> </div>
3	E	142	<div> <div>%</div> <div>37% 37% 12% • 13%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14244 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
			3297	2095	559	622	21			
1	C	428	Total	C	N	O	S	0	0	0
			3269	2075	553	621	20			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	420	Total	C	N	O	S	0	0	0
			3248	2043	547	633	25			
2	D	427	Total	C	N	O	S	0	0	0
			3296	2071	557	644	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
			917	555	174	183	5			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

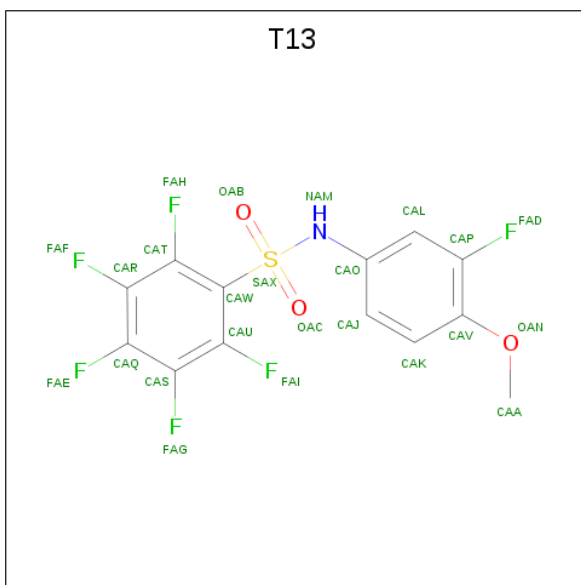


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

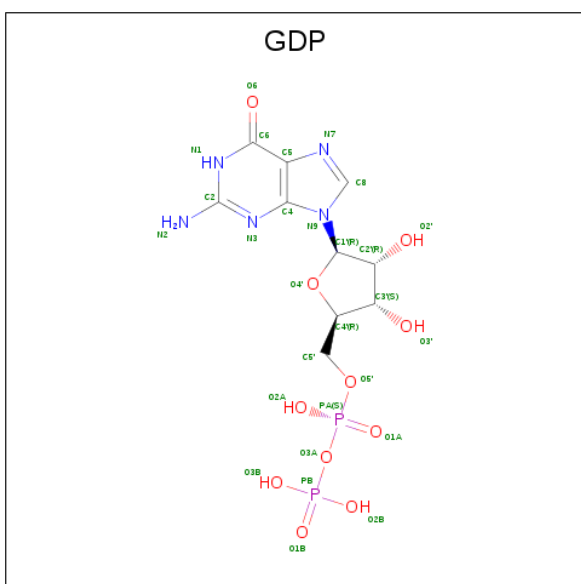
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is 2,3,4,5,6-pentafluoro-N-(3-fluoro-4-methoxyphenyl)benzenesulfonamide (three-letter code: T13) (formula: C₁₃H₇F₆NO₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	B	1	Total 23	C 13	F 5	N 1	O 3	S 1	9	0
6	B	1	Total 24	C 13	F 6	N 1	O 3	S 1	0	0
6	D	1	Total 23	C 13	F 5	N 1	O 3	S 1	9	0
6	D	1	Total 24	C 13	F 6	N 1	O 3	S 1	0	0

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).

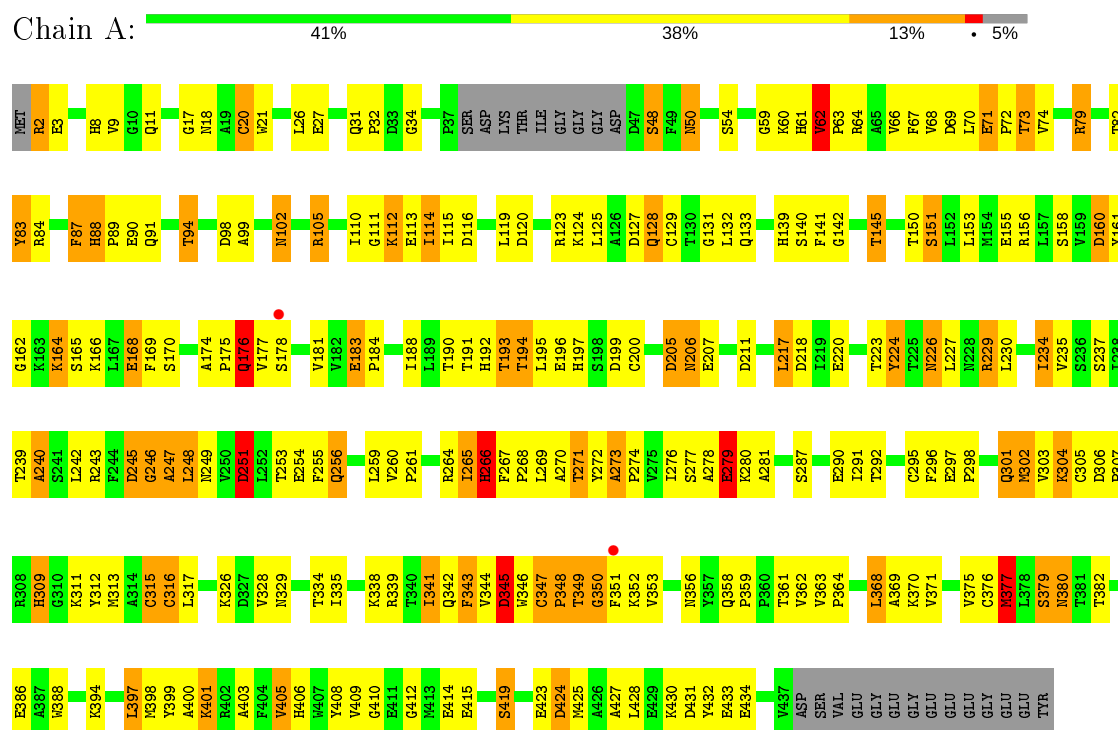


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
7	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

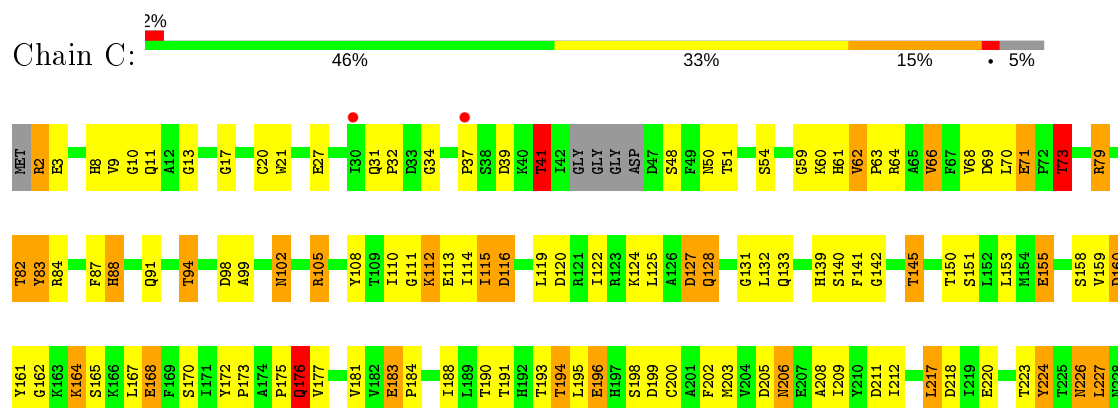
3 Residue-property plots [i](#)

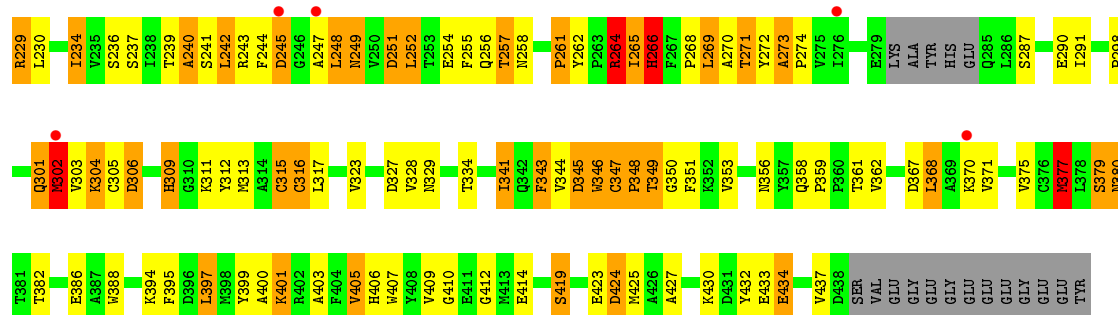
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tubulin alpha chain

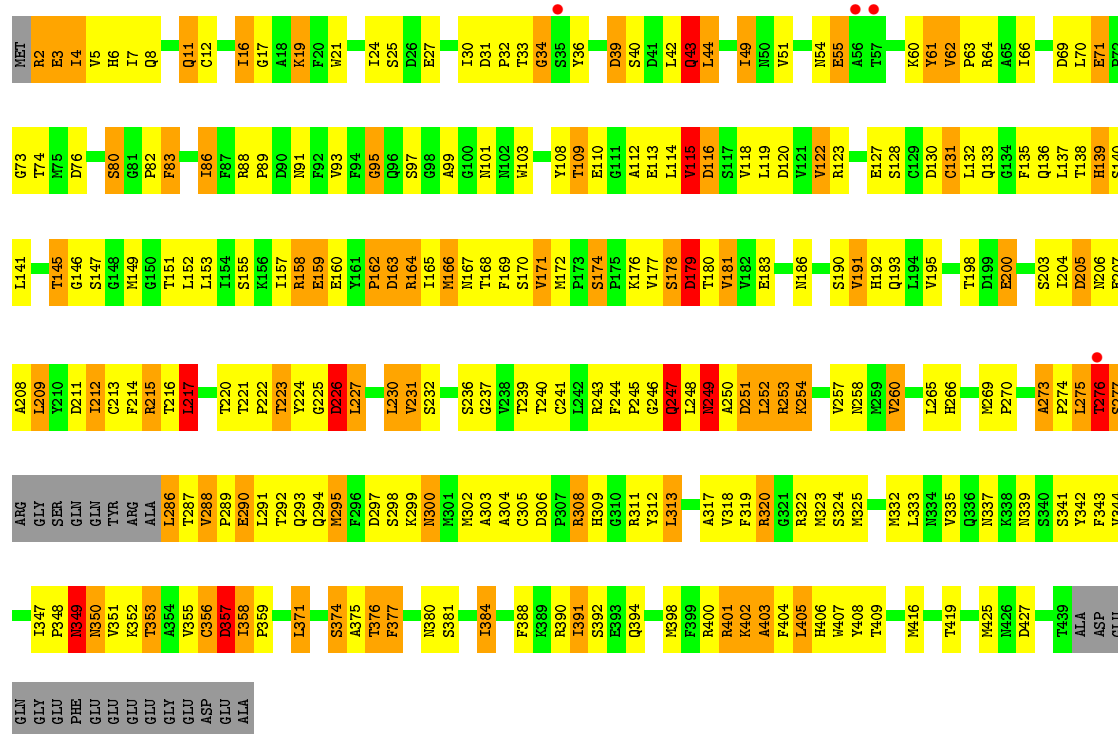


• Molecule 1: Tubulin alpha chain

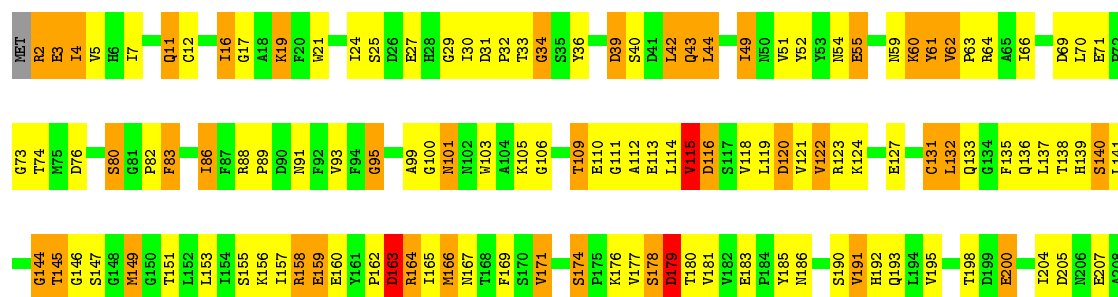


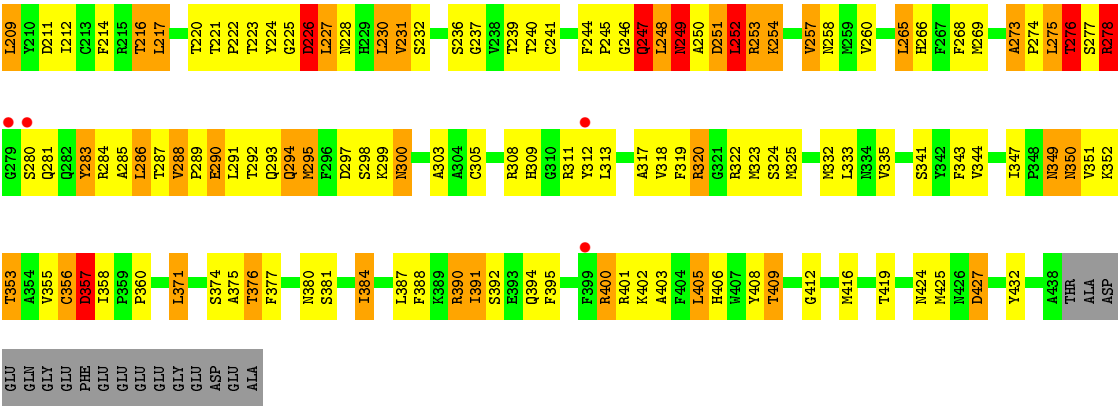


• Molecule 2: Tubulin beta chain



• Molecule 2: Tubulin beta chain





• Molecule 3: Stathmin-4



SER
ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	326.71 Å 326.71 Å 54.12 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.60 48.29 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-3.60) 98.6 (48.29-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.57 Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.207 , 0.253 0.226 , 0.262	Depositor DCC
R_{free} test set	1953 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	133.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 132.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.116 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14244	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, GTP, MG, T13

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.69	0/3374	0.94	14/4588 (0.3%)
1	C	0.59	1/3342 (0.0%)	0.89	12/4550 (0.3%)
2	B	0.62	0/3320	0.91	14/4508 (0.3%)
2	D	0.57	0/3370	0.87	15/4577 (0.3%)
3	E	0.65	0/925	0.82	1/1241 (0.1%)
All	All	0.62	1/14331 (0.0%)	0.90	56/19464 (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	1
1	C	0	1
2	B	0	2
2	D	0	2
3	E	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	302	MET	SD-CE	5.27	2.07	1.77

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	241	CYS	CA-CB-SG	-10.22	95.61	114.00
1	A	424	ASP	CB-CG-OD2	7.49	125.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	397	LEU	CA-CB-CG	7.08	131.57	115.30
1	C	397	LEU	CA-CB-CG	7.05	131.51	115.30
1	C	120	ASP	CB-CG-OD2	6.98	124.58	118.30
1	C	211	ASP	CB-CG-OD2	6.97	124.57	118.30
2	D	252	LEU	CA-CB-CG	6.90	131.16	115.30
2	B	116	ASP	CB-CG-OD2	6.87	124.49	118.30
2	D	427	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	266	HIS	CB-CA-C	-6.67	97.07	110.40
2	B	427	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	269	LEU	CA-CB-CG	6.55	130.36	115.30
2	D	69	ASP	CB-CG-OD2	6.53	124.18	118.30
1	C	116	ASP	CB-CG-OD2	6.43	124.08	118.30
1	A	251	ASP	CB-CG-OD2	6.41	124.07	118.30
2	D	241	CYS	CA-CB-SG	-6.37	102.54	114.00
1	C	269	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	120	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	160	ASP	CB-CG-OD2	6.27	123.94	118.30
2	D	297	ASP	CB-CG-OD2	6.16	123.84	118.30
2	D	179	ASP	CB-CG-OD2	6.09	123.79	118.30
1	A	69	ASP	CB-CG-OD2	6.08	123.77	118.30
2	B	249	ASN	N-CA-C	6.08	127.41	111.00
2	D	116	ASP	CB-CG-OD2	6.06	123.75	118.30
2	D	357	ASP	CB-CG-OD2	6.05	123.75	118.30
2	B	69	ASP	CB-CG-OD2	5.99	123.69	118.30
2	B	39	ASP	CB-CG-OD2	5.97	123.68	118.30
1	C	160	ASP	CB-CG-OD2	5.92	123.63	118.30
2	B	252	LEU	CA-CB-CG	5.91	128.89	115.30
2	B	179	ASP	CB-CG-OD2	5.86	123.57	118.30
2	D	163	ASP	CB-CG-OD2	5.78	123.50	118.30
2	B	357	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	211	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	20	CYS	CA-CB-SG	5.68	124.22	114.00
1	C	424	ASP	CB-CG-OD2	5.60	123.34	118.30
2	B	205	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	205	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	116	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	345	ASP	CB-CG-OD2	5.52	123.27	118.30
1	C	127	ASP	CB-CG-OD2	5.51	123.26	118.30
2	B	130	ASP	CB-CG-OD2	5.47	123.23	118.30
2	B	297	ASP	CB-CG-OD2	5.43	123.19	118.30
1	C	69	ASP	CB-CG-OD2	5.40	123.16	118.30
2	D	39	ASP	CB-CG-OD2	5.39	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	249	ASN	N-CA-C	5.34	125.42	111.00
1	C	266	HIS	CB-CA-C	-5.31	99.78	110.40
2	D	226	ASP	CB-CG-OD2	5.25	123.03	118.30
1	A	199	ASP	CB-CG-OD2	5.22	123.00	118.30
2	B	120	ASP	CB-CG-OD2	5.17	122.95	118.30
2	D	120	ASP	CB-CG-OD2	5.14	122.93	118.30
2	B	306	ASP	CB-CG-OD2	5.13	122.91	118.30
2	D	211	ASP	CB-CG-OD2	5.12	122.91	118.30
3	E	5	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	367	ASP	CB-CG-OD2	5.02	122.82	118.30
2	D	144	GLY	N-CA-C	5.01	125.63	113.10
1	C	306	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	HIS	Peptide
2	B	162	PRO	Peptide
2	B	247	GLN	Peptide
1	C	266	HIS	Peptide
2	D	162	PRO	Peptide
2	D	247	GLN	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	3297	0	3167	173	0
1	C	3269	0	3118	161	0
2	B	3248	0	3064	213	0
2	D	3296	0	3100	199	0
3	E	917	0	803	41	0
4	A	32	0	12	4	0
4	C	32	0	12	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	B	47	0	14	6	0
6	D	47	0	14	6	0
7	B	28	0	12	5	0
7	D	28	0	12	4	0
All	All	14244	0	13328	756	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 27.

All (756) 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	2.04	1.45
1:C:302:MET:SD	1:C:302:MET:CE	2.07	1.41
2:D:273:ALA:HB3	2:D:274:PRO:HD3	1.17	1.15
1:A:99:ALA:HB2	1:A:145:THR:HG22	1.26	1.14
1:C:273:ALA:HB3	1:C:274:PRO:HD3	1.30	1.12
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.18	1.12
2:B:151:THR:HB	2:B:193:GLN:HG2	1.29	1.10
1:C:99:ALA:HB2	1:C:145:THR:HG22	1.26	1.09
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.29	1.09
1:C:99:ALA:CB	1:C:145:THR:HG22	1.83	1.08
1:C:79:ARG:HH22	1:C:94:THR:HG21	1.15	1.07
1:A:99:ALA:CB	1:A:145:THR:HG22	1.84	1.06
1:A:79:ARG:HH22	1:A:94:THR:HG21	1.16	1.06
2:D:273:ALA:CB	2:D:274:PRO:HD3	1.86	1.05
2:D:251:ASP:HB2	2:D:254:LYS:HD3	1.33	1.05
2:B:273:ALA:CB	2:B:274:PRO:HD3	1.86	1.04
2:B:251:ASP:HB2	2:B:254:LYS:HD3	1.37	1.03
2:D:151:THR:HB	2:D:193:GLN:HG2	1.38	1.02
2:B:287:THR:HG22	2:B:290:GLU:HB2	1.41	1.01
1:C:73:THR:HG21	2:D:248:LEU:HD21	1.40	1.01
1:A:273:ALA:CB	1:A:274:PRO:HD3	1.90	1.01
1:C:8:HIS:CD2	1:C:17:GLY:HA3	1.96	1.01
2:D:287:THR:HG22	2:D:290:GLU:HB2	1.39	1.00
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.42	1.00
1:A:8:HIS:CD2	1:A:17:GLY:HA3	1.97	0.98
1:A:88:HIS:HB2	1:A:91:GLN:HE21	1.22	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ALA:O	1:C:302:MET:HB2	1.63	0.98
3:E:48:GLU:HG3	3:E:49:GLU:H	1.25	0.97
1:A:270:ALA:O	1:A:302:MET:HB2	1.64	0.97
2:D:276:THR:CG2	2:D:277:SER:H	1.78	0.96
1:A:346:TRP:O	1:A:346:TRP:HE3	1.49	0.94
1:C:88:HIS:HB2	1:C:91:GLN:HE21	1.33	0.93
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.50	0.93
1:A:278:ALA:O	1:A:279:GLU:HB3	1.66	0.92
2:B:223:THR:HB	2:B:225:GLY:H	1.31	0.92
2:D:273:ALA:HB3	2:D:274:PRO:CD	2.00	0.92
2:B:276:THR:CG2	2:B:277:SER:H	1.83	0.91
1:C:273:ALA:CB	1:C:274:PRO:HD3	2.00	0.91
1:A:181:VAL:H	2:B:258:ASN:HD21	1.19	0.91
1:C:248:LEU:HD13	1:C:249:ASN:OD1	1.71	0.91
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.00	0.90
2:D:140:SER:HA	2:D:171:VAL:HG23	1.54	0.89
2:B:2:ARG:HD2	2:B:131:CYS:SG	2.13	0.89
2:D:223:THR:HB	2:D:225:GLY:H	1.38	0.89
2:B:275:LEU:O	2:B:276:THR:HB	1.72	0.88
1:C:70:LEU:HD13	1:C:145:THR:HB	1.55	0.87
1:C:79:ARG:HH22	1:C:94:THR:CG2	1.88	0.87
2:D:247:GLN:HB2	6:D:1241:T13:OAC	1.75	0.86
1:A:273:ALA:HB3	1:A:274:PRO:CD	2.05	0.86
1:A:70:LEU:HD13	1:A:145:THR:HB	1.56	0.86
1:C:79:ARG:NH2	1:C:94:THR:HG21	1.90	0.86
1:A:206:ASN:HD21	4:A:600:GTP:HN22	1.23	0.86
2:B:158:ARG:HH11	2:B:158:ARG:HG3	1.41	0.85
1:C:346:TRP:O	1:C:346:TRP:HE3	1.58	0.85
2:B:276:THR:HG23	2:B:277:SER:H	1.40	0.85
2:D:350:ASN:H	2:D:350:ASN:HD22	1.21	0.84
1:A:79:ARG:HH22	1:A:94:THR:CG2	1.90	0.84
2:D:247:GLN:CB	6:D:1241:T13:OAC	2.27	0.83
2:B:140:SER:HA	2:B:171:VAL:HG23	1.57	0.83
1:A:176:GLN:HE21	1:A:176:GLN:H	1.26	0.83
1:A:79:ARG:NH2	1:A:94:THR:HG21	1.92	0.82
1:C:316:CYS:O	1:C:377:MET:HA	1.80	0.81
1:A:271:THR:HG23	1:A:301:GLN:HA	1.63	0.80
1:A:142:GLY:HA3	1:A:183:GLU:HG3	1.63	0.80
1:A:273:ALA:CB	1:A:375:VAL:H	1.94	0.80
2:D:275:LEU:O	2:D:276:THR:HB	1.79	0.80
1:C:206:ASN:HD21	4:C:600:GTP:HN22	1.27	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:ARG:O	2:D:127:GLU:HB2	1.82	0.79
1:A:346:TRP:CE3	1:A:346:TRP:O	2.34	0.79
1:C:271:THR:HG23	1:C:301:GLN:HA	1.65	0.78
1:A:229:ARG:HH11	1:A:229:ARG:HG3	1.48	0.78
1:A:264:ARG:NH2	1:A:424:ASP:OD1	2.16	0.77
1:C:273:ALA:CB	1:C:375:VAL:H	1.97	0.77
1:C:264:ARG:NH2	1:C:424:ASP:OD1	2.18	0.77
2:B:237:GLY:HA3	2:B:376:THR:HG21	1.65	0.77
2:D:276:THR:HG23	2:D:277:SER:H	1.48	0.77
3:E:48:GLU:HG3	3:E:49:GLU:N	2.00	0.76
2:B:213:CYS:O	2:B:217:LEU:HB3	1.85	0.76
1:A:368:LEU:HD12	1:A:368:LEU:H	1.51	0.76
2:D:11:GLN:HG2	2:D:74:THR:HG21	1.68	0.75
1:C:181:VAL:H	2:D:258:ASN:HD21	1.35	0.75
1:C:142:GLY:HA3	1:C:183:GLU:HG3	1.66	0.75
1:A:176:GLN:H	1:A:176:GLN:NE2	1.84	0.75
2:B:291:LEU:HD21	2:B:375:ALA:CB	2.17	0.74
2:D:276:THR:CG2	2:D:277:SER:N	2.47	0.74
2:D:276:THR:HG22	2:D:277:SER:H	1.51	0.74
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.13	0.74
2:D:273:ALA:CB	2:D:274:PRO:CD	2.62	0.74
1:A:347:CYS:O	1:A:348:PRO:O	2.05	0.74
1:A:112:LYS:HE3	3:E:58:GLU:HG3	1.69	0.74
2:D:3:GLU:HG3	2:D:64:ARG:NH2	2.03	0.74
2:B:11:GLN:HG2	2:B:74:THR:HG21	1.69	0.74
2:B:388:PHE:HD2	2:B:425:MET:HE2	1.52	0.74
2:D:2:ARG:HD2	2:D:131:CYS:SG	2.27	0.74
1:A:70:LEU:CD1	1:A:145:THR:HB	2.18	0.73
2:D:200:GLU:HA	2:D:266:HIS:HB2	1.69	0.73
2:B:401:ARG:NH2	1:C:434:GLU:O	2.21	0.73
2:D:277:SER:HB3	2:D:278:ARG:NE	2.04	0.72
3:E:14:CYS:SG	3:E:15:THR:N	2.62	0.72
2:B:166:MET:HB3	2:B:198:THR:HA	1.71	0.72
2:D:158:ARG:HH11	2:D:158:ARG:HG3	1.53	0.72
2:D:388:PHE:HD2	2:D:425:MET:HE2	1.54	0.72
2:B:159:GLU:HB2	3:E:72:LEU:HD23	1.71	0.72
2:B:291:LEU:HD21	2:B:375:ALA:HB2	1.71	0.72
2:D:291:LEU:HD21	2:D:375:ALA:CB	2.19	0.72
1:C:273:ALA:HB3	1:C:375:VAL:H	1.54	0.72
2:D:251:ASP:HB2	2:D:254:LYS:CD	2.16	0.72
2:B:165:ILE:HD11	2:B:252:LEU:CD1	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:H	2:B:258:ASN:ND2	1.86	0.71
1:C:346:TRP:O	1:C:346:TRP:CE3	2.43	0.71
2:B:350:ASN:HD22	2:B:350:ASN:H	1.36	0.71
2:D:179:ASP:N	2:D:179:ASP:OD1	2.22	0.71
1:C:206:ASN:HD21	4:C:600:GTP:N2	1.89	0.71
1:A:316:CYS:O	1:A:377:MET:HA	1.90	0.71
1:C:167:LEU:HD13	1:C:252:LEU:HD11	1.73	0.70
2:D:237:GLY:HA3	2:D:376:THR:HG21	1.73	0.70
3:E:12:ASN:HD22	3:E:12:ASN:C	1.94	0.70
2:B:153:LEU:O	2:B:157:ILE:HG12	1.91	0.70
1:A:206:ASN:HD21	4:A:600:GTP:N2	1.89	0.70
1:C:229:ARG:HH11	1:C:229:ARG:HG3	1.56	0.70
1:C:70:LEU:CD1	1:C:145:THR:HB	2.21	0.70
1:C:266:HIS:O	1:C:268:PRO:HD3	1.91	0.70
2:D:164:ARG:NH2	2:D:253:ARG:HH22	1.88	0.69
3:E:12:ASN:ND2	3:E:12:ASN:C	2.46	0.69
2:B:158:ARG:NH1	2:B:158:ARG:HG3	2.08	0.68
2:D:276:THR:HG23	2:D:277:SER:N	2.08	0.68
1:A:217:LEU:O	1:A:218:ASP:CB	2.40	0.68
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.26	0.68
1:A:70:LEU:HD13	1:A:145:THR:CB	2.22	0.68
2:B:114:LEU:O	2:B:116:ASP:N	2.26	0.68
2:B:164:ARG:NH2	2:B:253:ARG:HH22	1.90	0.68
2:B:178:SER:HB2	2:B:183:GLU:OE1	1.94	0.68
2:B:223:THR:HB	2:B:225:GLY:N	2.06	0.68
2:B:352:LYS:HG3	6:B:700:T13:FAD	1.82	0.68
2:D:153:LEU:O	2:D:157:ILE:HG12	1.94	0.68
2:D:158:ARG:O	2:D:159:GLU:HB3	1.93	0.67
1:A:273:ALA:HB3	1:A:375:VAL:H	1.59	0.67
2:B:200:GLU:HA	2:B:266:HIS:HB2	1.77	0.67
2:D:223:THR:CB	2:D:225:GLY:H	2.08	0.67
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.77	0.66
1:C:313:MET:HG2	1:C:380:ASN:O	1.95	0.66
1:C:70:LEU:HD13	1:C:145:THR:CB	2.23	0.66
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.34	0.66
2:D:247:GLN:N	2:D:248:LEU:HA	2.09	0.66
2:B:247:GLN:O	6:B:1241:T13:CAW	2.42	0.66
2:B:276:THR:CG2	2:B:277:SER:N	2.56	0.66
1:A:181:VAL:HB	2:B:258:ASN:HD22	1.61	0.66
2:D:165:ILE:HD11	2:D:252:LEU:HG	1.78	0.66
1:A:278:ALA:O	1:A:279:GLU:CB	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:LEU:HD21	2:D:375:ALA:HB2	1.77	0.66
2:B:123:ARG:O	2:B:127:GLU:HB2	1.96	0.66
2:B:276:THR:HG23	2:B:277:SER:N	2.11	0.66
2:D:158:ARG:HG3	2:D:158:ARG:NH1	2.10	0.65
2:B:179:ASP:OD1	2:B:179:ASP:N	2.29	0.65
1:C:99:ALA:HB3	1:C:145:THR:HG22	1.76	0.65
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.79	0.65
2:D:166:MET:HB3	2:D:198:THR:HA	1.78	0.65
2:B:398:MET:HE2	1:C:348:PRO:HD2	1.77	0.65
1:C:176:GLN:NE2	1:C:176:GLN:H	1.95	0.64
2:D:138:THR:HG22	2:D:169:PHE:HB2	1.78	0.64
3:E:12:ASN:HD22	3:E:13:LYS:N	1.95	0.64
2:B:103:TRP:HB2	2:B:186:ASN:OD1	1.98	0.64
2:B:223:THR:CB	2:B:225:GLY:H	2.08	0.64
1:C:217:LEU:O	1:C:218:ASP:CB	2.44	0.64
1:C:347:CYS:O	1:C:348:PRO:O	2.16	0.64
1:A:313:MET:HG2	1:A:380:ASN:O	1.97	0.64
1:A:306:ASP:O	1:A:309:HIS:HB3	1.97	0.64
2:D:114:LEU:O	2:D:116:ASP:N	2.30	0.63
1:C:105:ARG:NH1	2:D:253:ARG:HH21	1.96	0.63
2:D:99:ALA:HB1	2:D:145:THR:HG22	1.79	0.63
1:C:176:GLN:HE21	1:C:176:GLN:H	1.47	0.63
1:C:181:VAL:H	2:D:258:ASN:ND2	1.96	0.63
1:C:256:GLN:C	1:C:258:ASN:H	2.03	0.62
2:B:145:THR:HG22	7:B:600:GDP:O3B	1.99	0.62
3:E:109:LYS:O	3:E:113:GLU:HB2	1.98	0.62
2:D:277:SER:HB3	2:D:278:ARG:HE	1.64	0.62
1:A:139:HIS:HE1	1:A:168:GLU:HG3	1.64	0.62
2:D:178:SER:HB2	2:D:183:GLU:OE1	1.99	0.62
2:B:32:PRO:O	2:B:86:ILE:HD12	1.99	0.62
2:B:133:GLN:HE21	2:B:252:LEU:HB3	1.65	0.62
2:B:99:ALA:HB1	2:B:145:THR:HG22	1.82	0.62
1:C:205:ASP:HB3	1:C:303:VAL:HA	1.82	0.62
2:D:347:ILE:HG22	2:D:350:ASN:CB	2.26	0.62
1:A:270:ALA:HB3	1:A:302:MET:HE3	1.80	0.61
2:B:273:ALA:CB	2:B:274:PRO:CD	2.61	0.61
1:C:306:ASP:O	1:C:309:HIS:HB3	2.00	0.61
1:C:8:HIS:NE2	1:C:17:GLY:HA3	2.14	0.61
2:B:2:ARG:O	2:B:3:GLU:CB	2.48	0.61
2:D:158:ARG:O	2:D:159:GLU:CB	2.47	0.61
2:D:44:LEU:HA	2:D:49:ILE:HB	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:LEU:HD21	2:B:231:VAL:HG22	1.82	0.61
2:D:223:THR:HB	2:D:225:GLY:N	2.10	0.61
2:B:401:ARG:O	1:C:262:TYR:OH	2.17	0.61
2:B:247:GLN:HB3	6:B:1241:T13:OAC	2.01	0.61
1:A:88:HIS:HB2	1:A:91:GLN:NE2	2.06	0.61
2:B:12:CYS:SG	2:B:171:VAL:HG21	2.39	0.61
1:A:99:ALA:HB3	1:A:145:THR:HG22	1.76	0.60
1:A:223:THR:HB	1:A:226:ASN:H	1.64	0.60
2:B:247:GLN:N	2:B:248:LEU:HA	2.16	0.60
2:B:350:ASN:N	2:B:350:ASN:HD22	1.99	0.60
2:B:118:VAL:O	2:B:122:VAL:HG13	2.00	0.60
2:B:33:THR:O	2:B:34:GLY:O	2.18	0.60
2:B:70:LEU:C	2:B:95:GLY:HA3	2.21	0.60
2:B:332:MET:HG3	2:B:353:THR:HG21	1.82	0.60
1:C:105:ARG:HH12	2:D:253:ARG:HH21	1.50	0.60
2:B:165:ILE:HD11	2:B:252:LEU:HG	1.83	0.60
2:B:287:THR:CG2	2:B:290:GLU:HB2	2.26	0.60
1:A:87:PHE:N	1:A:87:PHE:CD2	2.69	0.60
3:E:127:ASP:C	3:E:129:HIS:H	2.04	0.60
2:D:292:THR:HA	2:D:295:MET:HE3	1.84	0.59
2:D:350:ASN:HD22	2:D:350:ASN:N	1.92	0.59
2:D:118:VAL:O	2:D:122:VAL:HG13	2.02	0.59
1:C:102:ASN:OD1	1:C:105:ARG:HB2	2.03	0.59
1:A:3:GLU:HG2	1:A:129:CYS:SG	2.42	0.59
1:A:3:GLU:HB2	1:A:132:LEU:HA	1.85	0.59
3:E:48:GLU:CG	3:E:49:GLU:H	2.05	0.59
1:A:205:ASP:HB3	1:A:303:VAL:HA	1.84	0.59
1:A:276:ILE:HD11	1:A:280:LYS:HD2	1.84	0.59
2:B:384:ILE:HG23	2:B:388:PHE:HE1	1.68	0.59
1:A:266:HIS:O	1:A:268:PRO:HD3	2.02	0.58
2:D:191:VAL:HG11	2:D:425:MET:CE	2.32	0.58
2:B:30:ILE:HD11	2:B:49:ILE:HD11	1.85	0.58
2:B:44:LEU:HA	2:B:49:ILE:HB	1.86	0.58
2:D:350:ASN:ND2	2:D:350:ASN:H	1.98	0.58
2:B:19:LYS:HG3	2:B:232:SER:CB	2.33	0.58
2:B:406:HIS:HA	2:B:409:THR:HB	1.85	0.58
2:D:287:THR:CG2	2:D:290:GLU:HB2	2.26	0.58
2:D:2:ARG:HH12	2:D:133:GLN:HA	1.68	0.58
1:C:111:GLY:O	1:C:113:GLU:N	2.36	0.58
2:D:19:LYS:HG3	2:D:232:SER:CB	2.34	0.58
2:D:291:LEU:HD21	2:D:375:ALA:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:ASP:C	2:D:253:ARG:H	2.07	0.58
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.38	0.58
2:D:205:ASP:OD1	2:D:207:GLU:HB3	2.04	0.57
1:C:176:GLN:HG2	1:C:177:VAL:H	1.69	0.57
1:A:176:GLN:HG2	1:A:177:VAL:H	1.69	0.57
2:B:55:GLU:HB3	2:B:61:TYR:HD2	1.69	0.57
1:C:167:LEU:HD13	1:C:252:LEU:CD1	2.34	0.57
2:D:191:VAL:HG11	2:D:425:MET:HE2	1.87	0.57
2:D:112:ALA:HA	2:D:115:VAL:HB	1.86	0.57
1:A:217:LEU:O	1:A:218:ASP:HB2	2.05	0.57
2:B:211:ASP:HB3	2:B:215:ARG:HH12	1.69	0.57
1:A:8:HIS:CD2	1:A:17:GLY:CA	2.82	0.57
2:D:136:GLN:HA	2:D:167:ASN:O	2.04	0.57
2:D:165:ILE:HD11	2:D:252:LEU:CD1	2.34	0.57
2:D:317:ALA:HB3	2:D:353:THR:HG22	1.87	0.57
2:D:55:GLU:HB3	2:D:61:TYR:HD2	1.69	0.57
1:A:71:GLU:HG3	1:A:73:THR:OG1	2.04	0.57
2:B:2:ARG:O	2:B:3:GLU:HB2	2.04	0.57
1:A:191:THR:O	1:A:195:LEU:HB2	2.05	0.57
3:E:67:GLU:C	3:E:69:LEU:H	2.07	0.57
2:B:270:PRO:HD2	2:B:302:MET:HB2	1.87	0.56
2:D:391:ILE:HG13	2:D:392:SER:N	2.19	0.56
2:B:292:THR:HA	2:B:295:MET:HE3	1.87	0.56
2:D:406:HIS:HA	2:D:409:THR:HB	1.88	0.56
2:D:2:ARG:O	2:D:3:GLU:CB	2.53	0.56
1:A:2:ARG:HB2	1:A:131:GLY:O	2.06	0.56
2:B:70:LEU:HD21	2:B:149:MET:CE	2.36	0.56
2:D:36:TYR:OH	2:D:40:SER:O	2.19	0.56
1:A:277:SER:O	1:A:280:LYS:HB2	2.06	0.56
1:A:260:VAL:CG2	1:A:260:VAL:O	2.53	0.56
2:B:36:TYR:OH	2:B:40:SER:O	2.23	0.56
1:C:191:THR:O	1:C:195:LEU:HB2	2.05	0.56
1:C:206:ASN:ND2	4:C:600:GTP:HN22	2.01	0.56
2:B:398:MET:CE	1:C:348:PRO:HD2	2.35	0.55
2:D:209:LEU:HD21	2:D:231:VAL:HG22	1.88	0.55
2:B:251:ASP:C	2:B:253:ARG:H	2.08	0.55
1:C:181:VAL:HB	2:D:258:ASN:HD22	1.71	0.55
2:B:291:LEU:HD21	2:B:375:ALA:HB3	1.88	0.55
1:A:190:THR:HG23	1:A:191:THR:N	2.22	0.55
1:C:125:LEU:HD23	1:C:128:GLN:NE2	2.22	0.55
1:C:2:ARG:HB2	1:C:131:GLY:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:CYS:SG	1:C:377:MET:CE	2.95	0.55
2:D:114:LEU:HD23	2:D:149:MET:HE1	1.88	0.55
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.89	0.55
2:B:357:ASP:OD2	2:B:357:ASP:N	2.40	0.55
1:C:8:HIS:HD2	1:C:17:GLY:HA3	1.66	0.55
2:D:247:GLN:HB3	6:D:1241:T13:OAB	2.07	0.55
2:D:33:THR:O	2:D:34:GLY:O	2.25	0.55
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.89	0.55
2:B:287:THR:HG23	2:B:289:PRO:HD2	1.89	0.55
2:B:3:GLU:HG3	2:B:64:ARG:NH2	2.21	0.55
2:B:88:ARG:HB3	2:B:91:ASN:OD1	2.06	0.55
2:D:177:VAL:HG12	2:D:177:VAL:O	2.06	0.55
2:B:251:ASP:HB2	2:B:254:LYS:CD	2.24	0.55
2:B:347:ILE:HG22	2:B:350:ASN:CB	2.31	0.55
1:C:328:VAL:HG11	1:C:353:VAL:HG11	1.88	0.55
2:D:4:ILE:HG22	2:D:133:GLN:OE1	2.07	0.54
2:D:332:MET:HG3	2:D:353:THR:HG21	1.89	0.54
2:B:4:ILE:HG22	2:B:133:GLN:OE1	2.06	0.54
1:C:261:PRO:HD2	1:C:262:TYR:H	1.70	0.54
2:D:283:TYR:C	2:D:285:ALA:H	2.10	0.54
2:D:55:GLU:HB3	2:D:61:TYR:CD2	2.43	0.54
1:A:206:ASN:ND2	4:A:600:GTP:HN22	1.98	0.54
1:C:244:PHE:O	1:C:245:ASP:HB3	2.07	0.54
1:C:66:VAL:HG11	1:C:122:ILE:HG12	1.89	0.54
2:B:312:TYR:HB2	2:B:343:PHE:HD2	1.73	0.54
2:D:225:GLY:O	2:D:227:LEU:N	2.40	0.54
2:D:88:ARG:HG3	2:D:89:PRO:HD2	1.90	0.54
2:B:158:ARG:O	2:B:159:GLU:HB3	2.08	0.54
1:C:234:ILE:HG13	1:C:272:TYR:HB2	1.90	0.54
1:C:368:LEU:H	1:C:368:LEU:HD12	1.72	0.54
1:A:335:ILE:O	1:A:339:ARG:HB2	2.08	0.54
2:B:55:GLU:HB3	2:B:61:TYR:CD2	2.43	0.54
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.90	0.54
1:C:315:CYS:SG	1:C:377:MET:HE1	2.48	0.54
1:C:430:LYS:O	1:C:434:GLU:HB2	2.08	0.54
2:D:277:SER:HB3	2:D:278:ARG:CZ	2.38	0.54
1:C:190:THR:O	1:C:194:THR:HB	2.07	0.53
2:D:381:SER:O	2:D:384:ILE:HB	2.08	0.53
1:A:190:THR:O	1:A:194:THR:HB	2.08	0.53
2:B:276:THR:HG22	2:B:277:SER:H	1.72	0.53
2:B:384:ILE:HG23	2:B:388:PHE:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ALA:CB	1:A:207:GLU:HB2	2.39	0.53
2:B:88:ARG:HG3	2:B:89:PRO:HD2	1.89	0.53
1:C:419:SER:O	1:C:423:GLU:HG2	2.08	0.53
2:D:30:ILE:HD11	2:D:49:ILE:HD11	1.91	0.53
1:A:181:VAL:HB	2:B:258:ASN:ND2	2.23	0.53
2:B:145:THR:HG23	7:B:600:GDP:PB	2.48	0.53
2:B:172:MET:CE	2:B:203:SER:HB3	2.38	0.53
2:B:224:TYR:OH	7:B:600:GDP:H2'	2.08	0.53
2:D:135:PHE:N	2:D:135:PHE:CD1	2.77	0.53
1:C:175:PRO:HB3	2:D:349:ASN:ND2	2.23	0.53
2:D:24:ILE:HG13	2:D:25:SER:N	2.24	0.53
1:A:273:ALA:HB2	1:A:375:VAL:H	1.70	0.53
2:D:247:GLN:HB3	6:D:1241:T13:SAX	2.49	0.53
2:D:287:THR:HG23	2:D:289:PRO:HD2	1.90	0.53
3:E:119:MET:C	3:E:121:GLU:H	2.12	0.53
1:A:247:ALA:HB1	3:E:19:SER:CB	2.39	0.53
2:B:320:ARG:HA	2:B:356:CYS:O	2.08	0.53
1:A:133:GLN:OE1	1:A:251:ASP:CB	2.57	0.52
2:D:5:VAL:CG2	2:D:135:PHE:CD2	2.92	0.52
2:D:224:TYR:OH	7:D:600:GDP:H2'	2.09	0.52
1:A:169:PHE:CE2	1:A:235:VAL:HG22	2.44	0.52
2:B:115:VAL:CG1	2:B:116:ASP:N	2.71	0.52
1:C:70:LEU:HD12	1:C:70:LEU:N	2.24	0.52
2:D:177:VAL:CG1	2:D:177:VAL:O	2.57	0.52
2:B:146:GLY:N	7:B:600:GDP:O1B	2.36	0.52
1:C:264:ARG:O	1:C:266:HIS:HD2	1.91	0.52
2:D:412:GLY:O	3:E:133:VAL:HB	2.09	0.52
3:E:76:ARG:O	3:E:79:GLU:N	2.43	0.52
1:A:183:GLU:HB3	1:A:184:PRO:HD3	1.91	0.52
1:A:419:SER:O	1:A:423:GLU:HG2	2.08	0.52
2:B:165:ILE:HD11	2:B:252:LEU:CG	2.40	0.52
1:C:256:GLN:C	1:C:258:ASN:N	2.60	0.52
2:D:70:LEU:HD12	2:D:145:THR:HB	1.90	0.52
1:C:205:ASP:CB	1:C:303:VAL:HA	2.40	0.52
1:C:317:LEU:HD23	1:C:377:MET:HB2	1.92	0.52
1:A:260:VAL:O	1:A:260:VAL:HG22	2.09	0.52
1:C:54:SER:HB3	1:C:64:ARG:HE	1.75	0.52
1:C:71:GLU:HG3	1:C:73:THR:OG1	2.10	0.52
2:D:237:GLY:CA	2:D:376:THR:HG21	2.40	0.52
1:C:188:ILE:HG23	1:C:425:MET:HG3	1.91	0.52
2:B:388:PHE:CD2	2:B:425:MET:HE2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:GLY:O	1:C:13:GLY:N	2.43	0.52
1:C:34:GLY:O	1:C:61:HIS:HB2	2.10	0.52
2:D:136:GLN:HB3	2:D:167:ASN:HB3	1.91	0.52
1:C:251:ASP:OD1	1:C:252:LEU:N	2.43	0.51
1:C:88:HIS:HB2	1:C:91:GLN:NE2	2.13	0.51
1:A:8:HIS:HD2	1:A:17:GLY:HA3	1.62	0.51
1:A:229:ARG:CG	1:A:229:ARG:HH11	2.20	0.51
1:A:270:ALA:HB3	1:A:302:MET:CE	2.39	0.51
1:C:256:GLN:O	1:C:258:ASN:N	2.43	0.51
1:A:151:SER:OG	1:A:193:THR:HB	2.10	0.51
1:C:8:HIS:CD2	1:C:17:GLY:CA	2.84	0.51
1:A:8:HIS:NE2	1:A:17:GLY:HA3	2.25	0.51
2:B:205:ASP:HB2	2:B:303:ALA:HA	1.92	0.51
1:C:27:GLU:OE2	1:C:243:ARG:NH2	2.43	0.51
2:D:163:ASP:HB3	2:D:164:ARG:HG2	1.93	0.51
2:D:402:LYS:HB3	2:D:405:LEU:HD22	1.92	0.51
2:D:388:PHE:CD2	2:D:425:MET:HE2	2.42	0.51
1:A:175:PRO:HB3	2:B:349:ASN:ND2	2.25	0.51
1:A:317:LEU:HD23	1:A:377:MET:HB2	1.93	0.51
2:B:251:ASP:O	2:B:252:LEU:HB3	2.09	0.51
1:C:217:LEU:O	1:C:218:ASP:HB2	2.10	0.51
1:C:405:VAL:CG1	1:C:406:HIS:N	2.73	0.51
3:E:80:ARG:O	3:E:84:GLN:HB2	2.10	0.51
2:B:165:ILE:HD11	2:B:252:LEU:HD12	1.92	0.51
2:B:403:ALA:C	2:B:405:LEU:H	2.13	0.51
1:C:183:GLU:HB3	1:C:184:PRO:HD3	1.92	0.51
1:A:412:GLY:O	3:E:60:ARG:NH1	2.44	0.50
2:B:21:TRP:CH2	2:B:63:PRO:HB2	2.47	0.50
2:B:2:ARG:HH12	2:B:133:GLN:HA	1.76	0.50
1:C:252:LEU:O	1:C:256:GLN:HG2	2.11	0.50
1:A:344:VAL:O	1:A:344:VAL:HG13	2.11	0.50
1:A:70:LEU:HD13	1:A:145:THR:CG2	2.41	0.50
1:A:87:PHE:H	1:A:87:PHE:HD2	1.59	0.50
2:D:88:ARG:HB3	2:D:91:ASN:OD1	2.12	0.50
2:B:158:ARG:O	2:B:159:GLU:CB	2.58	0.50
2:D:165:ILE:HD11	2:D:252:LEU:CG	2.40	0.50
3:E:78:HIS:CD2	3:E:78:HIS:C	2.84	0.50
2:B:145:THR:CG2	7:B:600:GDP:O3B	2.60	0.50
1:C:108:TYR:O	1:C:112:LYS:HB2	2.11	0.50
2:D:32:PRO:O	2:D:86:ILE:HD12	2.11	0.50
1:A:205:ASP:CB	1:A:303:VAL:HA	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:408:TYR:O	2:B:409:THR:C	2.50	0.50
2:D:103:TRP:HB2	2:D:186:ASN:OD1	2.11	0.50
2:B:16:ILE:HG22	2:B:17:GLY:N	2.26	0.50
3:E:123:LEU:O	3:E:127:ASP:HB2	2.12	0.50
2:B:4:ILE:HG23	2:B:51:VAL:HG13	1.94	0.49
2:D:2:ARG:NH1	2:D:133:GLN:HA	2.26	0.49
1:A:34:GLY:O	1:A:61:HIS:HB2	2.12	0.49
2:B:163:ASP:HB3	2:B:164:ARG:HG2	1.93	0.49
1:C:161:TYR:HB3	1:C:164:LYS:HG3	1.94	0.49
2:D:133:GLN:HE21	2:D:252:LEU:HB3	1.77	0.49
2:D:16:ILE:HG22	2:D:17:GLY:N	2.28	0.49
2:D:19:LYS:HG3	2:D:232:SER:HB2	1.94	0.49
1:C:344:VAL:O	1:C:346:TRP:N	2.46	0.49
2:B:247:GLN:O	6:B:1241:T13:CAU	2.61	0.49
1:C:264:ARG:O	1:C:266:HIS:CD2	2.65	0.49
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.48	0.49
1:A:190:THR:CG2	1:A:191:THR:N	2.76	0.49
1:A:32:PRO:HB3	1:A:83:TYR:HD2	1.76	0.49
1:C:159:VAL:HG13	3:E:94:ILE:HG23	1.95	0.49
2:D:99:ALA:CB	2:D:145:THR:HG22	2.43	0.49
1:A:70:LEU:N	1:A:70:LEU:HD12	2.28	0.49
2:B:136:GLN:HA	2:B:167:ASN:O	2.13	0.49
2:B:174:SER:HB2	2:B:207:GLU:HB2	1.95	0.49
1:C:265:ILE:HG22	1:C:265:ILE:O	2.11	0.49
2:D:226:ASP:N	2:D:226:ASP:OD1	2.43	0.49
1:A:405:VAL:O	1:A:409:VAL:HG23	2.13	0.49
2:B:112:ALA:HA	2:B:115:VAL:HB	1.94	0.49
2:B:381:SER:O	2:B:384:ILE:HB	2.12	0.49
2:B:269:MET:HG2	2:B:384:ILE:HG12	1.95	0.49
1:C:223:THR:N	1:C:226:ASN:HB2	2.28	0.48
2:D:141:LEU:HA	2:D:141:LEU:HD12	1.69	0.48
2:D:2:ARG:NH2	2:D:133:GLN:HG3	2.28	0.48
1:A:312:TYR:HE2	1:A:379:SER:HB2	1.78	0.48
2:B:19:LYS:HG3	2:B:232:SER:HB2	1.95	0.48
1:C:112:LYS:O	1:C:115:ILE:HG22	2.13	0.48
2:D:115:VAL:CG1	2:D:116:ASP:N	2.76	0.48
1:A:234:ILE:HG13	1:A:272:TYR:HB2	1.95	0.48
2:B:237:GLY:CA	2:B:376:THR:HG21	2.38	0.48
1:C:287:SER:O	1:C:291:ILE:HG12	2.13	0.48
2:B:7:ILE:O	2:B:137:LEU:HA	2.13	0.48
2:B:32:PRO:HA	2:B:83:PHE:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.49	0.48
1:A:223:THR:N	1:A:226:ASN:HB2	2.28	0.48
2:B:391:ILE:HG13	2:B:392:SER:N	2.28	0.48
1:C:73:THR:HG21	2:D:248:LEU:CD2	2.29	0.48
1:A:265:ILE:O	1:A:265:ILE:HG22	2.13	0.48
2:B:225:GLY:O	2:B:227:LEU:N	2.46	0.48
1:A:317:LEU:CD2	1:A:377:MET:HE3	2.43	0.48
1:C:145:THR:HG23	4:C:600:GTP:O2B	2.14	0.48
1:A:405:VAL:CG1	1:A:406:HIS:N	2.77	0.48
2:B:141:LEU:HA	2:B:147:SER:HB3	1.94	0.48
2:B:99:ALA:CB	2:B:145:THR:HG22	2.44	0.48
2:B:147:SER:HB2	2:B:190:SER:OG	2.14	0.48
1:C:155:GLU:HB2	3:E:101:LEU:HD11	1.95	0.48
1:C:202:PHE:HE2	1:C:268:PRO:HG2	1.79	0.48
1:C:291:ILE:HB	1:C:375:VAL:HG23	1.94	0.48
1:A:256:GLN:HA	1:A:260:VAL:HG13	1.95	0.48
1:A:273:ALA:CB	1:A:274:PRO:CD	2.62	0.48
2:B:181:VAL:O	2:B:398:MET:HE1	2.14	0.48
2:B:16:ILE:HD11	2:B:231:VAL:HG11	1.95	0.48
2:B:317:ALA:HB3	2:B:353:THR:HG22	1.95	0.48
2:D:247:GLN:CB	6:D:1241:T13:SAX	3.01	0.48
1:C:208:ALA:O	1:C:212:ILE:HD13	2.14	0.48
2:D:212:ILE:CG2	2:D:230:LEU:HD21	2.43	0.48
1:A:296:PHE:HB2	1:A:339:ARG:HH12	1.79	0.47
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.95	0.47
1:C:223:THR:HB	1:C:226:ASN:H	1.79	0.47
2:D:269:MET:HG2	2:D:384:ILE:HG12	1.96	0.47
1:A:296:PHE:HB3	1:A:339:ARG:HH22	1.78	0.47
2:B:177:VAL:O	2:B:177:VAL:HG12	2.14	0.47
1:C:139:HIS:CG	1:C:150:THR:HG21	2.49	0.47
1:C:133:GLN:NE2	1:C:252:LEU:HD23	2.29	0.47
1:A:145:THR:HG23	4:A:600:GTP:O2B	2.14	0.47
1:A:119:LEU:HD22	1:A:156:ARG:NH2	2.29	0.47
1:A:399:TYR:C	1:A:401:LYS:H	2.18	0.47
1:A:239:THR:O	1:A:240:ALA:C	2.52	0.47
3:E:67:GLU:O	3:E:71:HIS:HB2	2.14	0.47
2:B:174:SER:O	2:B:178:SER:HB3	2.14	0.47
1:C:343:PHE:CD1	1:C:349:THR:HG22	2.50	0.47
1:C:399:TYR:C	1:C:401:LYS:H	2.17	0.47
2:D:145:THR:HG22	7:D:600:GDP:O3B	2.14	0.47
2:B:115:VAL:HG13	2:B:116:ASP:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:MET:HB3	1:C:302:MET:CE	2.43	0.47
1:C:273:ALA:HB2	1:C:375:VAL:H	1.78	0.47
2:D:4:ILE:HG23	2:D:51:VAL:HG13	1.97	0.47
3:E:15:THR:HG23	3:E:16:SER:N	2.30	0.47
1:A:102:ASN:OD1	1:A:105:ARG:HB2	2.15	0.47
1:C:3:GLU:HB2	1:C:132:LEU:HA	1.96	0.47
3:E:48:GLU:CG	3:E:49:GLU:N	2.67	0.47
1:A:111:GLY:O	1:A:113:GLU:N	2.48	0.47
2:B:350:ASN:ND2	2:B:350:ASN:H	2.08	0.47
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.50	0.47
1:A:249:ASN:HD22	1:A:254:GLU:HG2	1.80	0.47
1:A:388:TRP:CE3	1:A:388:TRP:HA	2.50	0.47
1:A:32:PRO:HB3	1:A:83:TYR:CD2	2.49	0.47
2:B:2:ARG:NH1	2:B:133:GLN:HA	2.29	0.47
1:C:234:ILE:CG1	1:C:272:TYR:HB2	2.44	0.47
1:C:41:THR:HG21	1:C:61:HIS:CE1	2.50	0.47
2:D:200:GLU:HB3	2:D:268:PHE:CE1	2.50	0.47
2:D:286:LEU:H	2:D:286:LEU:HG	1.43	0.47
1:A:88:HIS:O	1:A:89:PRO:C	2.52	0.47
1:C:167:LEU:CD1	1:C:252:LEU:CD1	2.93	0.47
1:C:87:PHE:N	1:C:87:PHE:CD2	2.82	0.47
2:B:70:LEU:HD12	2:B:145:THR:HB	1.97	0.46
1:C:407:TRP:CE2	2:D:257:VAL:HA	2.51	0.46
2:D:2:ARG:O	2:D:3:GLU:HB2	2.15	0.46
2:B:21:TRP:CZ3	2:B:63:PRO:CB	2.99	0.46
1:A:166:LYS:HD2	1:A:197:HIS:O	2.16	0.46
1:A:346:TRP:CE3	1:A:346:TRP:C	2.89	0.46
1:A:350:GLY:O	1:A:351:PHE:HB2	2.16	0.46
2:B:205:ASP:OD1	2:B:207:GLU:HB3	2.14	0.46
2:D:70:LEU:C	2:D:95:GLY:HA3	2.35	0.46
2:B:138:THR:O	2:B:139:HIS:HB3	2.16	0.46
2:B:16:ILE:CG2	2:B:17:GLY:N	2.78	0.46
1:C:273:ALA:HB2	1:C:375:VAL:HB	1.96	0.46
2:D:76:ASP:O	2:D:80:SER:HB2	2.15	0.46
1:A:217:LEU:HD12	1:A:277:SER:HB3	1.96	0.46
2:B:226:ASP:N	2:B:226:ASP:OD1	2.48	0.46
1:A:328:VAL:HG11	1:A:353:VAL:HG11	1.96	0.46
2:B:212:ILE:CG2	2:B:230:LEU:HD21	2.45	0.46
3:E:125:GLU:C	3:E:127:ASP:H	2.18	0.46
1:A:346:TRP:C	1:A:346:TRP:HE3	2.17	0.46
2:B:135:PHE:CD1	2:B:135:PHE:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:MET:O	2:B:152:LEU:HB3	2.16	0.46
2:B:177:VAL:O	2:B:177:VAL:CG1	2.63	0.46
2:B:24:ILE:HG13	2:B:25:SER:N	2.30	0.46
2:B:251:ASP:C	2:B:253:ARG:N	2.70	0.46
1:A:344:VAL:O	1:A:346:TRP:N	2.49	0.46
1:A:430:LYS:O	1:A:431:ASP:C	2.54	0.46
2:B:76:ASP:O	2:B:80:SER:HB2	2.16	0.46
1:C:427:ALA:O	1:C:430:LYS:HB3	2.15	0.46
2:D:312:TYR:HB2	2:D:343:PHE:HD2	1.80	0.46
2:D:83:PHE:HD2	2:D:83:PHE:HA	1.70	0.46
1:A:54:SER:HB3	1:A:64:ARG:HE	1.81	0.45
2:D:32:PRO:HA	2:D:83:PHE:CE2	2.50	0.45
1:A:265:ILE:HD12	1:A:265:ILE:H	1.81	0.45
2:B:54:ASN:HB2	2:B:64:ARG:HD3	1.98	0.45
2:D:251:ASP:HB3	2:D:254:LYS:H	1.82	0.45
2:D:408:TYR:O	2:D:409:THR:C	2.55	0.45
1:A:273:ALA:HB1	1:A:274:PRO:HD3	1.90	0.45
1:A:139:HIS:CG	1:A:150:THR:HG21	2.52	0.45
2:B:151:THR:CB	2:B:193:GLN:HG2	2.21	0.45
2:B:404:PHE:CE1	1:C:261:PRO:HB3	2.51	0.45
2:B:40:SER:CB	2:B:43:GLN:NE2	2.80	0.45
1:C:202:PHE:CE2	1:C:268:PRO:HG2	2.52	0.45
2:D:66:ILE:HG12	2:D:121:VAL:HG12	1.96	0.45
2:D:5:VAL:HG21	2:D:135:PHE:CD2	2.51	0.45
2:B:108:TYR:O	2:B:112:ALA:HB3	2.17	0.45
2:B:8:GLN:CD	2:B:17:GLY:HA3	2.37	0.45
1:C:236:SER:O	1:C:240:ALA:HB2	2.17	0.45
2:D:106:GLY:O	2:D:111:GLY:HA3	2.17	0.45
2:D:145:THR:HG23	7:D:600:GDP:PB	2.57	0.45
2:B:220:THR:O	2:B:222:PRO:HD3	2.17	0.45
2:D:115:VAL:HG13	2:D:116:ASP:N	2.31	0.45
2:D:7:ILE:O	2:D:137:LEU:HA	2.16	0.45
2:D:101:ASN:HA	2:D:144:GLY:H	1.82	0.45
2:D:174:SER:O	2:D:178:SER:HB3	2.16	0.45
1:A:246:GLY:O	1:A:247:ALA:O	2.34	0.45
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.99	0.45
3:E:101:LEU:O	3:E:105:MET:HB2	2.17	0.45
1:A:368:LEU:N	1:A:368:LEU:HD12	2.28	0.45
2:B:298:SER:C	2:B:300:ASN:H	2.20	0.45
1:C:32:PRO:HB3	1:C:83:TYR:HD2	1.82	0.45
2:D:55:GLU:H	2:D:55:GLU:HG3	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:54:ASN:HB2	2:D:64:ARG:HD3	1.98	0.45
2:D:209:LEU:HD12	2:D:209:LEU:HA	1.90	0.44
1:C:298:PRO:O	1:C:301:GLN:HB2	2.18	0.44
2:D:251:ASP:C	2:D:253:ARG:N	2.70	0.44
1:A:125:LEU:HD23	1:A:128:GLN:NE2	2.31	0.44
1:A:375:VAL:HG12	1:A:376:CYS:N	2.32	0.44
1:C:206:ASN:HD22	1:C:206:ASN:HA	1.55	0.44
2:B:137:LEU:HB3	2:B:168:THR:HG22	2.00	0.44
2:B:398:MET:HE3	1:C:348:PRO:CD	2.47	0.44
2:D:51:VAL:HG12	2:D:52:TYR:CD1	2.53	0.44
2:D:11:GLN:CG	2:D:74:THR:HG21	2.44	0.44
1:A:259:LEU:HA	1:A:259:LEU:HD23	1.75	0.44
1:C:261:PRO:CD	1:C:262:TYR:H	2.30	0.44
1:C:388:TRP:CE3	1:C:388:TRP:HA	2.53	0.44
2:D:147:SER:HB2	2:D:190:SER:OG	2.17	0.44
1:A:119:LEU:HD22	1:A:156:ARG:HH21	1.82	0.44
1:A:8:HIS:CE1	1:A:67:PHE:HE1	2.36	0.44
2:D:424:ASN:O	2:D:427:ASP:HB2	2.18	0.44
3:E:82:VAL:O	3:E:83:ILE:C	2.56	0.44
1:C:410:GLY:C	1:C:412:GLY:H	2.20	0.44
2:D:132:LEU:HD23	2:D:164:ARG:HD3	1.99	0.44
2:D:357:ASP:OD2	2:D:357:ASP:N	2.44	0.44
2:D:384:ILE:HG23	2:D:388:PHE:HE1	1.82	0.44
2:B:398:MET:CE	1:C:348:PRO:CD	2.95	0.44
2:D:265:LEU:HB3	2:D:432:TYR:CE2	2.52	0.44
3:E:134:ARG:C	3:E:136:ASN:H	2.20	0.44
2:B:288:VAL:HB	2:B:289:PRO:HD3	2.00	0.44
3:E:55:GLU:HA	3:E:58:GLU:HB2	1.99	0.44
1:C:399:TYR:C	1:C:401:LYS:N	2.72	0.43
3:E:15:THR:HG23	3:E:16:SER:H	1.83	0.43
1:A:2:ARG:HB3	1:A:3:GLU:OE1	2.19	0.43
2:B:239:THR:O	2:B:240:THR:C	2.55	0.43
2:B:319:PHE:HB2	2:B:355:VAL:HG12	1.99	0.43
2:B:358:ILE:HA	2:B:359:PRO:HD3	1.81	0.43
1:C:248:LEU:HD22	1:C:249:ASN:H	1.82	0.43
2:D:158:ARG:HH11	2:D:158:ARG:CG	2.27	0.43
2:D:274:PRO:HB3	2:D:286:LEU:HD22	1.99	0.43
1:A:2:ARG:HA	1:A:2:ARG:NH1	2.33	0.43
2:B:374:SER:OG	2:B:375:ALA:N	2.51	0.43
2:D:132:LEU:HD23	2:D:164:ARG:HG3	2.00	0.43
3:E:125:GLU:C	3:E:127:ASP:N	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLN:HB3	2:B:167:ASN:HB3	2.00	0.43
1:A:8:HIS:ND1	1:A:67:PHE:CE1	2.87	0.43
2:B:191:VAL:HG11	2:B:425:MET:CE	2.49	0.43
2:B:171:VAL:HA	2:B:204:ILE:O	2.18	0.43
1:A:398:MET:HG3	2:B:348:PRO:HD3	2.00	0.43
1:C:172:TYR:HA	1:C:173:PRO:HD3	1.86	0.43
1:C:405:VAL:O	1:C:409:VAL:HG23	2.17	0.43
3:E:108:ASN:O	3:E:111:ASN:HB2	2.19	0.43
3:E:76:ARG:HA	3:E:76:ARG:HD3	1.61	0.43
2:B:212:ILE:HG21	2:B:230:LEU:HD21	2.01	0.43
2:B:312:TYR:HB2	2:B:343:PHE:CD2	2.53	0.43
2:B:402:LYS:HB3	2:B:405:LEU:HD22	2.01	0.43
1:C:315:CYS:HG	1:C:351:PHE:HE2	1.66	0.43
2:D:298:SER:C	2:D:300:ASN:H	2.21	0.43
2:B:5:VAL:CG2	2:B:135:PHE:CD2	3.01	0.43
2:D:16:ILE:CG2	2:D:17:GLY:N	2.82	0.43
1:A:223:THR:HG22	1:A:224:TYR:N	2.34	0.43
1:A:375:VAL:HG12	1:A:376:CYS:H	1.84	0.43
1:A:264:ARG:NH1	1:A:428:LEU:HA	2.34	0.43
1:A:133:GLN:OE1	1:A:251:ASP:HB3	2.19	0.43
2:B:337:ASN:C	2:B:339:ASN:H	2.21	0.43
2:B:403:ALA:O	2:B:405:LEU:N	2.52	0.43
1:C:32:PRO:C	1:C:34:GLY:H	2.22	0.43
2:D:30:ILE:HG22	2:D:31:ASP:O	2.19	0.43
2:D:320:ARG:HA	2:D:356:CYS:O	2.19	0.43
2:D:388:PHE:HD2	2:D:425:MET:CE	2.29	0.43
3:E:4:ALA:O	3:E:5:ASP:CB	2.66	0.43
1:A:292:THR:O	1:A:295:CYS:HB2	2.18	0.43
2:B:208:ALA:HB2	2:B:304:ALA:N	2.34	0.43
1:C:190:THR:HG23	1:C:191:THR:N	2.34	0.43
1:A:223:THR:HG22	1:A:224:TYR:H	1.84	0.42
1:A:251:ASP:OD2	1:A:251:ASP:N	2.52	0.42
6:B:700:T13:OAB	6:B:700:T13:FAI	2.27	0.42
1:C:255:PHE:O	1:C:258:ASN:HB2	2.19	0.42
1:C:32:PRO:HB3	1:C:83:TYR:CD2	2.54	0.42
3:E:4:ALA:O	3:E:5:ASP:HB3	2.19	0.42
1:A:70:LEU:CD1	1:A:145:THR:CB	2.91	0.42
2:D:174:SER:HB2	2:D:207:GLU:HB2	2.01	0.42
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.53	0.42
1:C:196:GLU:H	1:C:196:GLU:HG3	1.63	0.42
2:D:205:ASP:HB2	2:D:303:ALA:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:VAL:HG11	1:C:328:VAL:HG23	2.01	0.42
1:C:358:GLN:HA	1:C:359:PRO:HD3	1.90	0.42
1:A:298:PRO:O	1:A:301:GLN:HB2	2.19	0.42
2:D:319:PHE:HB2	2:D:355:VAL:HG12	2.01	0.42
1:A:424:ASP:O	1:A:427:ALA:HB3	2.19	0.42
2:B:287:THR:CG2	2:B:290:GLU:H	2.32	0.42
2:B:407:TRP:CE2	1:C:257:THR:HA	2.55	0.42
1:C:395:PHE:CD2	1:C:395:PHE:C	2.93	0.42
2:D:212:ILE:O	2:D:216:THR:O	2.36	0.42
2:D:239:THR:O	2:D:240:THR:C	2.58	0.42
1:A:306:ASP:HA	1:A:307:PRO:HD3	1.91	0.42
2:B:191:VAL:HG11	2:B:425:MET:HG3	2.02	0.42
1:C:312:TYR:HE2	1:C:379:SER:HB2	1.85	0.42
2:D:212:ILE:HG21	2:D:230:LEU:HD21	2.02	0.42
2:D:42:LEU:O	2:D:44:LEU:N	2.53	0.42
1:A:399:TYR:C	1:A:401:LYS:N	2.73	0.42
2:B:223:THR:C	2:B:225:GLY:N	2.72	0.42
2:B:260:VAL:HG11	2:B:266:HIS:HB3	2.01	0.42
2:B:30:ILE:HG22	2:B:31:ASP:O	2.20	0.42
2:D:223:THR:C	2:D:225:GLY:N	2.73	0.42
1:C:199:ASP:HB3	1:C:256:GLN:HE22	1.84	0.42
2:D:317:ALA:HB3	2:D:353:THR:CG2	2.48	0.42
1:A:343:PHE:CD1	1:A:349:THR:HG22	2.55	0.41
1:A:363:VAL:CG1	1:A:364:PRO:HD2	2.50	0.41
1:A:273:ALA:HB2	1:A:375:VAL:HB	2.02	0.41
1:A:71:GLU:HA	1:A:72:PRO:HD3	1.89	0.41
2:B:71:GLU:O	2:B:71:GLU:HG2	2.19	0.41
1:C:139:HIS:HE1	1:C:168:GLU:HG3	1.85	0.41
2:D:292:THR:HG22	2:D:335:VAL:HG21	2.01	0.41
2:D:384:ILE:HD13	2:D:384:ILE:HA	1.89	0.41
3:E:99:GLU:HG2	3:E:99:GLU:O	2.19	0.41
1:A:174:ALA:HB1	1:A:207:GLU:HB2	2.01	0.41
1:A:62:VAL:O	1:A:62:VAL:HG22	2.20	0.41
2:B:247:GLN:HB3	6:B:1241:T13:SAX	2.61	0.41
1:C:224:TYR:HD2	1:C:224:TYR:HA	1.73	0.41
1:C:264:ARG:O	1:C:265:ILE:C	2.58	0.41
2:D:287:THR:O	2:D:288:VAL:HB	2.20	0.41
2:D:70:LEU:HA	2:D:95:GLY:HA3	2.02	0.41
1:A:408:TYR:C	1:A:410:GLY:N	2.73	0.41
2:B:40:SER:HB2	2:B:43:GLN:NE2	2.35	0.41
1:C:70:LEU:HD12	1:C:70:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:185:TYR:HD2	2:D:395:PHE:CE1	2.38	0.41
2:D:288:VAL:HB	2:D:289:PRO:HD3	2.02	0.41
2:D:312:TYR:HB2	2:D:343:PHE:CD2	2.55	0.41
3:E:119:MET:C	3:E:121:GLU:N	2.73	0.41
1:A:358:GLN:HA	1:A:359:PRO:HD3	1.91	0.41
2:B:292:THR:HG22	2:B:335:VAL:HG21	2.03	0.41
2:D:220:THR:O	2:D:222:PRO:HD3	2.19	0.41
2:B:217:LEU:CD2	2:B:276:THR:OG1	2.69	0.41
2:B:295:MET:HE3	2:B:295:MET:HB3	1.93	0.41
2:B:308:ARG:O	2:B:342:TYR:HE1	2.03	0.41
2:B:313:LEU:HD12	2:B:313:LEU:HA	1.69	0.41
2:B:11:GLN:CG	2:B:74:THR:HG21	2.45	0.41
1:C:111:GLY:O	1:C:112:LYS:C	2.58	0.41
2:B:407:TRP:CZ2	1:C:257:THR:HA	2.54	0.41
2:B:248:LEU:HD22	2:B:249:ASN:HB3	2.01	0.41
2:B:83:PHE:HA	2:B:83:PHE:HD2	1.62	0.41
1:C:269:LEU:HD21	1:C:301:GLN:HG2	2.03	0.41
2:D:287:THR:CG2	2:D:290:GLU:H	2.33	0.41
2:D:352:LYS:HG3	6:D:700:T13:FAD	2.10	0.41
1:A:338:LYS:C	1:A:339:ARG:HG2	2.40	0.41
1:C:82:THR:O	1:C:83:TYR:CB	2.68	0.41
2:D:384:ILE:HG23	2:D:388:PHE:CE1	2.56	0.41
2:D:4:ILE:O	2:D:4:ILE:HG12	2.20	0.41
1:A:267:PHE:N	1:A:267:PHE:CD1	2.89	0.41
1:A:291:ILE:HB	1:A:375:VAL:HG23	2.02	0.41
2:B:110:GLU:HG2	2:B:110:GLU:H	1.65	0.41
2:B:209:LEU:HA	2:B:209:LEU:HD12	1.87	0.41
2:B:404:PHE:CD1	2:B:404:PHE:N	2.89	0.41
2:B:70:LEU:HD21	2:B:149:MET:HE3	2.02	0.41
2:D:59:ASN:O	2:D:60:LYS:O	2.38	0.41
1:C:346:TRP:CE3	1:C:346:TRP:C	2.93	0.41
2:D:225:GLY:O	2:D:228:ASN:N	2.53	0.41
3:E:127:ASP:C	3:E:129:HIS:N	2.74	0.41
1:A:234:ILE:CG1	1:A:272:TYR:HB2	2.51	0.41
1:A:315:CYS:SG	1:A:377:MET:CE	3.09	0.41
2:B:191:VAL:HG11	2:B:425:MET:HE2	2.03	0.41
2:B:4:ILE:O	2:B:4:ILE:HG12	2.21	0.41
2:D:320:ARG:HG2	2:D:360:PRO:HD3	2.03	0.41
1:A:190:THR:O	1:A:192:HIS:N	2.54	0.41
1:A:217:LEU:O	1:A:218:ASP:HB3	2.21	0.41
1:A:50:ASN:HD22	1:A:50:ASN:HA	1.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:ILE:CG2	2:B:350:ASN:HB3	2.37	0.41
2:D:100:GLY:HA3	2:D:105:LYS:HD2	2.03	0.41
2:D:70:LEU:HD21	2:D:149:MET:CE	2.51	0.41
1:A:174:ALA:HB2	1:A:207:GLU:HB2	2.02	0.40
2:D:223:THR:C	2:D:225:GLY:H	2.24	0.40
2:D:294:GLN:HE21	2:D:294:GLN:HB2	1.65	0.40
1:A:114:ILE:HA	1:A:114:ILE:HD12	1.97	0.40
1:A:287:SER:O	1:A:291:ILE:HG12	2.21	0.40
1:A:264:ARG:HD3	1:A:431:ASP:OD2	2.21	0.40
2:B:215:ARG:CZ	2:B:215:ARG:HB3	2.51	0.40
2:B:269:MET:HA	2:B:270:PRO:HD3	1.87	0.40
2:B:6:HIS:HE1	2:B:8:GLN:HE21	1.69	0.40
1:C:407:TRP:CD2	2:D:257:VAL:HG23	2.56	0.40
3:E:105:MET:HB3	3:E:105:MET:CE	2.50	0.40
1:A:164:LYS:H	1:A:164:LYS:HG2	1.69	0.40
1:A:297:GLU:HA	1:A:298:PRO:HD2	1.87	0.40
2:B:128:SER:O	2:B:128:SER:OG	2.29	0.40
2:B:164:ARG:HH22	2:B:253:ARG:HH22	1.64	0.40
2:B:287:THR:O	2:B:288:VAL:HB	2.22	0.40
1:C:240:ALA:O	1:C:242:LEU:N	2.54	0.40
2:D:171:VAL:HA	2:D:204:ILE:O	2.21	0.40
2:D:387:LEU:O	2:D:390:ARG:HG3	2.21	0.40
2:D:146:GLY:N	7:D:600:GDP:O1B	2.41	0.40
2:B:6:HIS:CE1	2:B:8:GLN:HE21	2.39	0.40
1:C:209:ILE:HG22	1:C:227:LEU:HG	2.03	0.40
2:D:216:THR:O	2:D:217:LEU:CB	2.69	0.40
1:A:111:GLY:O	1:A:112:LYS:C	2.60	0.40
1:A:260:VAL:HA	1:A:261:PRO:HD3	1.83	0.40
1:A:26:LEU:HD21	1:A:364:PRO:HD3	2.03	0.40
2:B:223:THR:C	2:B:225:GLY:H	2.23	0.40
2:B:295:MET:HG3	2:B:377:PHE:HB3	2.04	0.40
1:C:377:MET:CG	1:C:377:MET:O	2.70	0.40
2:D:29:GLY:O	2:D:30:ILE:HG13	2.21	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%)	337 (80%)	56 (13%)	30 (7%)	1	14
1	C	422/451 (94%)	332 (79%)	58 (14%)	32 (8%)	1	12
2	B	416/445 (94%)	324 (78%)	60 (14%)	32 (8%)	1	12
2	D	425/445 (96%)	339 (80%)	56 (13%)	30 (7%)	1	14
3	E	120/142 (84%)	81 (68%)	27 (22%)	12 (10%)	0	8
All	All	1806/1934 (93%)	1413 (78%)	257 (14%)	136 (8%)	1	12

All (136) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	62	VAL
1	A	112	LYS
1	A	247	ALA
1	A	265	ILE
1	A	273	ALA
1	A	345	ASP
1	A	348	PRO
1	A	350	GLY
1	A	403	ALA
2	B	3	GLU
2	B	34	GLY
2	B	43	GLN
2	B	115	VAL
2	B	163	ASP
2	B	250	ALA
2	B	273	ALA
2	B	276	THR
2	B	288	VAL
2	B	324	SER
2	B	400	ARG

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Mol	Chain	Res	Type
2	B	403	ALA
1	C	62	VAL
1	C	73	THR
1	C	112	LYS
1	C	240	ALA
1	C	241	SER
1	C	247	ALA
1	C	264	ARG
1	C	265	ILE
1	C	345	ASP
1	C	348	PRO
1	C	350	GLY
1	C	437	VAL
2	D	3	GLU
2	D	34	GLY
2	D	43	GLN
2	D	115	VAL
2	D	163	ASP
2	D	217	LEU
2	D	273	ALA
2	D	276	THR
2	D	284	ARG
2	D	288	VAL
2	D	400	ARG
2	D	403	ALA
3	E	5	ASP
1	A	73	THR
1	A	83	TYR
1	A	162	GLY
1	A	240	ALA
1	A	245	ASP
1	A	248	LEU
1	A	304	LYS
1	A	341	ILE
1	A	377	MET
1	A	400	ALA
2	B	60	LYS
2	B	73	GLY
2	B	217	LEU
2	B	227	LEU
2	B	244	PHE
2	B	245	PRO

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Mol	Chain	Res	Type
2	B	299	LYS
2	B	322	ARG
2	B	371	LEU
1	C	11	GLN
1	C	41	THR
1	C	48	SER
1	C	83	TYR
1	C	162	GLY
1	C	249	ASN
1	C	257	THR
1	C	377	MET
1	C	403	ALA
2	D	60	LYS
2	D	73	GLY
2	D	227	LEU
2	D	244	PHE
2	D	245	PRO
2	D	278	ARG
2	D	324	SER
2	D	371	LEU
3	E	28	SER
3	E	120	LEU
1	A	48	SER
1	A	59	GLY
1	A	164	LYS
1	A	279	GLU
1	A	281	ALA
1	A	309	HIS
2	B	97	SER
2	B	109	THR
1	C	59	GLY
1	C	164	LYS
1	C	273	ALA
1	C	304	LYS
1	C	309	HIS
2	D	109	THR
2	D	246	GLY
2	D	249	ASN
2	D	250	ALA
2	D	299	LYS
2	D	322	ARG
3	E	26	PRO

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Mol	Chain	Res	Type
3	E	47	LEU
3	E	68	LEU
3	E	128	LYS
3	E	139	LEU
1	A	176	GLN
1	A	342	GLN
2	B	82	PRO
2	B	349	ASN
1	C	39	ASP
1	C	341	ILE
1	C	400	ALA
2	D	82	PRO
2	D	159	GLU
3	E	48	GLU
3	E	64	GLN
2	B	62	VAL
2	B	159	GLU
1	C	176	GLN
3	E	7	GLU
3	E	12	ASN
1	A	18	ASN
2	B	226	ASP
2	B	402	LYS
1	C	245	ASP
2	D	62	VAL
1	C	261	PRO
2	D	95	GLY
1	A	246	GLY
2	B	95	GLY
2	B	162	PRO
2	B	246	GLY

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/378 (92%)	242 (70%)	104 (30%)	0	2
1	C	340/378 (90%)	236 (69%)	104 (31%)	0	2
2	B	349/383 (91%)	240 (69%)	109 (31%)	0	2
2	D	352/383 (92%)	237 (67%)	115 (33%)	0	2
3	E	80/126 (64%)	43 (54%)	37 (46%)	0	0
All	All	1467/1648 (89%)	998 (68%)	469 (32%)	0	2

All (469) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	9	VAL
1	A	20	CYS
1	A	31	GLN
1	A	48	SER
1	A	50	ASN
1	A	60	LYS
1	A	62	VAL
1	A	66	VAL
1	A	68	VAL
1	A	71	GLU
1	A	74	VAL
1	A	79	ARG
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	98	ASP
1	A	102	ASN
1	A	105	ARG
1	A	110	ILE
1	A	114	ILE
1	A	115	ILE
1	A	123	ARG
1	A	124	LYS
1	A	127	ASP

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Mol	Chain	Res	Type
1	A	128	GLN
1	A	140	SER
1	A	141	PHE
1	A	145	THR
1	A	151	SER
1	A	153	LEU
1	A	155	GLU
1	A	158	SER
1	A	160	ASP
1	A	165	SER
1	A	168	GLU
1	A	170	SER
1	A	176	GLN
1	A	178	SER
1	A	183	GLU
1	A	193	THR
1	A	194	THR
1	A	196	GLU
1	A	200	CYS
1	A	206	ASN
1	A	217	LEU
1	A	220	GLU
1	A	224	TYR
1	A	226	ASN
1	A	227	LEU
1	A	229	ARG
1	A	230	LEU
1	A	234	ILE
1	A	237	SER
1	A	242	LEU
1	A	245	ASP
1	A	248	LEU
1	A	251	ASP
1	A	253	THR
1	A	255	PHE
1	A	256	GLN
1	A	271	THR
1	A	279	GLU
1	A	290	GLU
1	A	301	GLN
1	A	302	MET
1	A	304	LYS

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Mol	Chain	Res	Type
1	A	305	CYS
1	A	311	LYS
1	A	315	CYS
1	A	316	CYS
1	A	326	LYS
1	A	329	ASN
1	A	334	THR
1	A	341	ILE
1	A	343	PHE
1	A	345	ASP
1	A	347	CYS
1	A	349	THR
1	A	352	LYS
1	A	356	ASN
1	A	361	THR
1	A	362	VAL
1	A	368	LEU
1	A	370	LYS
1	A	371	VAL
1	A	377	MET
1	A	379	SER
1	A	380	ASN
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	414	GLU
1	A	415	GLU
1	A	419	SER
1	A	432	TYR
1	A	433	GLU
1	A	434	GLU
2	B	2	ARG
2	B	4	ILE
2	B	11	GLN
2	B	16	ILE
2	B	19	LYS
2	B	27	GLU
2	B	39	ASP
2	B	42	LEU

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Mol	Chain	Res	Type
2	B	43	GLN
2	B	44	LEU
2	B	49	ILE
2	B	55	GLU
2	B	61	TYR
2	B	62	VAL
2	B	71	GLU
2	B	80	SER
2	B	83	PHE
2	B	86	ILE
2	B	93	VAL
2	B	101	ASN
2	B	109	THR
2	B	113	GLU
2	B	115	VAL
2	B	119	LEU
2	B	122	VAL
2	B	131	CYS
2	B	132	LEU
2	B	139	HIS
2	B	145	THR
2	B	155	SER
2	B	158	ARG
2	B	160	GLU
2	B	164	ARG
2	B	166	MET
2	B	170	SER
2	B	171	VAL
2	B	174	SER
2	B	176	LYS
2	B	178	SER
2	B	179	ASP
2	B	180	THR
2	B	181	VAL
2	B	191	VAL
2	B	192	HIS
2	B	195	VAL
2	B	200	GLU
2	B	206	ASN
2	B	209	LEU
2	B	212	ILE
2	B	214	PHE

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Mol	Chain	Res	Type
2	B	215	ARG
2	B	216	THR
2	B	217	LEU
2	B	221	THR
2	B	223	THR
2	B	226	ASP
2	B	230	LEU
2	B	231	VAL
2	B	236	SER
2	B	243	ARG
2	B	247	GLN
2	B	249	ASN
2	B	251	ASP
2	B	253	ARG
2	B	254	LYS
2	B	257	VAL
2	B	260	VAL
2	B	265	LEU
2	B	275	LEU
2	B	276	THR
2	B	277	SER
2	B	286	LEU
2	B	290	GLU
2	B	293	GLN
2	B	294	GLN
2	B	295	MET
2	B	300	ASN
2	B	305	CYS
2	B	308	ARG
2	B	309	HIS
2	B	311	ARG
2	B	313	LEU
2	B	318	VAL
2	B	320	ARG
2	B	323	MET
2	B	325	MET
2	B	333	LEU
2	B	341	SER
2	B	344	VAL
2	B	349	ASN
2	B	350	ASN
2	B	351	VAL

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Mol	Chain	Res	Type
2	B	353	THR
2	B	356	CYS
2	B	357	ASP
2	B	358	ILE
2	B	371	LEU
2	B	374	SER
2	B	376	THR
2	B	377	PHE
2	B	380	ASN
2	B	384	ILE
2	B	390	ARG
2	B	391	ILE
2	B	394	GLN
2	B	401	ARG
2	B	405	LEU
2	B	416	MET
2	B	419	THR
1	C	2	ARG
1	C	9	VAL
1	C	20	CYS
1	C	31	GLN
1	C	37	PRO
1	C	41	THR
1	C	50	ASN
1	C	51	THR
1	C	60	LYS
1	C	62	VAL
1	C	66	VAL
1	C	68	VAL
1	C	71	GLU
1	C	73	THR
1	C	79	ARG
1	C	82	THR
1	C	84	ARG
1	C	88	HIS
1	C	94	THR
1	C	98	ASP
1	C	102	ASN
1	C	105	ARG
1	C	110	ILE
1	C	114	ILE
1	C	115	ILE

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Mol	Chain	Res	Type
1	C	116	ASP
1	C	119	LEU
1	C	124	LYS
1	C	127	ASP
1	C	128	GLN
1	C	140	SER
1	C	141	PHE
1	C	145	THR
1	C	151	SER
1	C	153	LEU
1	C	155	GLU
1	C	158	SER
1	C	160	ASP
1	C	165	SER
1	C	168	GLU
1	C	170	SER
1	C	176	GLN
1	C	183	GLU
1	C	193	THR
1	C	194	THR
1	C	196	GLU
1	C	198	SER
1	C	200	CYS
1	C	203	MET
1	C	206	ASN
1	C	217	LEU
1	C	220	GLU
1	C	224	TYR
1	C	226	ASN
1	C	227	LEU
1	C	229	ARG
1	C	230	LEU
1	C	234	ILE
1	C	237	SER
1	C	239	THR
1	C	242	LEU
1	C	248	LEU
1	C	251	ASP
1	C	252	LEU
1	C	254	GLU
1	C	264	ARG
1	C	271	THR

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Mol	Chain	Res	Type
1	C	290	GLU
1	C	301	GLN
1	C	302	MET
1	C	304	LYS
1	C	305	CYS
1	C	311	LYS
1	C	315	CYS
1	C	316	CYS
1	C	327	ASP
1	C	329	ASN
1	C	334	THR
1	C	341	ILE
1	C	343	PHE
1	C	345	ASP
1	C	346	TRP
1	C	347	CYS
1	C	349	THR
1	C	356	ASN
1	C	361	THR
1	C	362	VAL
1	C	368	LEU
1	C	370	LYS
1	C	371	VAL
1	C	377	MET
1	C	379	SER
1	C	380	ASN
1	C	382	THR
1	C	386	GLU
1	C	394	LYS
1	C	397	LEU
1	C	401	LYS
1	C	405	VAL
1	C	414	GLU
1	C	419	SER
1	C	432	TYR
1	C	433	GLU
1	C	434	GLU
2	D	2	ARG
2	D	4	ILE
2	D	11	GLN
2	D	16	ILE
2	D	19	LYS

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Mol	Chain	Res	Type
2	D	27	GLU
2	D	39	ASP
2	D	42	LEU
2	D	43	GLN
2	D	44	LEU
2	D	49	ILE
2	D	55	GLU
2	D	61	TYR
2	D	62	VAL
2	D	71	GLU
2	D	80	SER
2	D	83	PHE
2	D	86	ILE
2	D	93	VAL
2	D	101	ASN
2	D	109	THR
2	D	110	GLU
2	D	113	GLU
2	D	115	VAL
2	D	119	LEU
2	D	120	ASP
2	D	122	VAL
2	D	124	LYS
2	D	131	CYS
2	D	132	LEU
2	D	139	HIS
2	D	140	SER
2	D	145	THR
2	D	149	MET
2	D	155	SER
2	D	156	LYS
2	D	158	ARG
2	D	160	GLU
2	D	164	ARG
2	D	166	MET
2	D	171	VAL
2	D	174	SER
2	D	176	LYS
2	D	178	SER
2	D	179	ASP
2	D	180	THR
2	D	181	VAL

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Mol	Chain	Res	Type
2	D	191	VAL
2	D	192	HIS
2	D	195	VAL
2	D	200	GLU
2	D	209	LEU
2	D	214	PHE
2	D	216	THR
2	D	221	THR
2	D	226	ASP
2	D	230	LEU
2	D	231	VAL
2	D	236	SER
2	D	247	GLN
2	D	248	LEU
2	D	249	ASN
2	D	251	ASP
2	D	252	LEU
2	D	253	ARG
2	D	254	LYS
2	D	257	VAL
2	D	260	VAL
2	D	265	LEU
2	D	275	LEU
2	D	276	THR
2	D	278	ARG
2	D	280	SER
2	D	281	GLN
2	D	283	TYR
2	D	286	LEU
2	D	290	GLU
2	D	293	GLN
2	D	294	GLN
2	D	295	MET
2	D	300	ASN
2	D	305	CYS
2	D	308	ARG
2	D	309	HIS
2	D	311	ARG
2	D	313	LEU
2	D	318	VAL
2	D	320	ARG
2	D	323	MET

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Mol	Chain	Res	Type
2	D	325	MET
2	D	333	LEU
2	D	341	SER
2	D	344	VAL
2	D	349	ASN
2	D	350	ASN
2	D	351	VAL
2	D	353	THR
2	D	356	CYS
2	D	357	ASP
2	D	358	ILE
2	D	371	LEU
2	D	374	SER
2	D	376	THR
2	D	377	PHE
2	D	380	ASN
2	D	384	ILE
2	D	390	ARG
2	D	391	ILE
2	D	394	GLN
2	D	400	ARG
2	D	401	ARG
2	D	405	LEU
2	D	409	THR
2	D	416	MET
2	D	419	THR
3	E	6	MET
3	E	11	LEU
3	E	12	ASN
3	E	22	VAL
3	E	28	SER
3	E	52	LYS
3	E	53	LYS
3	E	58	GLU
3	E	59	GLU
3	E	62	LYS
3	E	65	GLU
3	E	69	LEU
3	E	71	HIS
3	E	72	LEU
3	E	74	GLU
3	E	76	ARG

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Mol	Chain	Res	Type
3	E	77	GLU
3	E	78	HIS
3	E	80	ARG
3	E	91	ASN
3	E	96	MET
3	E	98	LYS
3	E	99	GLU
3	E	101	LEU
3	E	105	MET
3	E	106	GLU
3	E	107	SER
3	E	109	LYS
3	E	112	ARG
3	E	113	GLU
3	E	115	HIS
3	E	120	LEU
3	E	122	ARG
3	E	123	LEU
3	E	124	GLN
3	E	126	LYS
3	E	127	ASP

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

Mol	Chain	Res	Type
1	A	28	HIS
1	A	50	ASN
1	A	91	GLN
1	A	139	HIS
1	A	176	GLN
1	A	206	ASN
1	A	216	ASN
1	A	249	ASN
1	A	258	ASN
1	A	266	HIS
1	A	329	ASN
1	A	356	ASN
2	B	6	HIS
2	B	8	GLN
2	B	14	ASN
2	B	43	GLN
2	B	136	GLN

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Mol	Chain	Res	Type
2	B	139	HIS
2	B	192	HIS
2	B	193	GLN
2	B	258	ASN
2	B	266	HIS
2	B	331	GLN
2	B	339	ASN
2	B	349	ASN
2	B	350	ASN
2	B	380	ASN
2	B	436	GLN
1	C	50	ASN
1	C	61	HIS
1	C	91	GLN
1	C	139	HIS
1	C	176	GLN
1	C	197	HIS
1	C	206	ASN
1	C	256	GLN
1	C	266	HIS
1	C	301	GLN
1	C	329	ASN
2	D	6	HIS
2	D	43	GLN
2	D	139	HIS
2	D	193	GLN
2	D	206	ASN
2	D	258	ASN
2	D	266	HIS
2	D	349	ASN
2	D	350	ASN
2	D	380	ASN
2	D	394	GLN
2	D	436	GLN
3	E	12	ASN
3	E	64	GLN
3	E	78	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	T13	B	1241	2	24,24,25	2.38	4 (16%)	34,36,38	2.13	9 (26%)
7	GDP	B	600	-	24,30,30	1.10	1 (4%)	31,47,47	1.72	8 (25%)
7	GDP	D	600	-	24,30,30	1.02	1 (4%)	31,47,47	1.89	7 (22%)
6	T13	D	700	-	25,25,25	2.53	4 (16%)	36,38,38	2.56	10 (27%)
6	T13	B	700	-	25,25,25	2.62	5 (20%)	36,38,38	2.23	8 (22%)
4	GTP	A	600	-	26,34,34	1.04	2 (7%)	33,54,54	1.77	8 (24%)
4	GTP	C	600	-	26,34,34	1.09	3 (11%)	33,54,54	2.00	10 (30%)
6	T13	D	1241	2	24,24,25	2.36	4 (16%)	34,36,38	1.83	8 (23%)

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	T13	B	1241	2	-	4/13/13/13	0/2/2/2
7	GDP	B	600	-	-	6/12/32/32	0/3/3/3
7	GDP	D	600	-	-	5/12/32/32	0/3/3/3
6	T13	D	700	-	-	7/13/13/13	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	T13	B	700	-	-	5/13/13/13	0/2/2/2
4	GTP	A	600	-	-	5/18/38/38	0/3/3/3
4	GTP	C	600	-	-	6/18/38/38	0/3/3/3
6	T13	D	1241	2	-	3/13/13/13	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	700	T13	OAC-SAX	8.67	1.53	1.43
6	D	1241	T13	CAO-NAM	-7.17	1.31	1.43
6	B	1241	T13	CAO-NAM	-7.03	1.31	1.43
6	D	700	T13	OAC-SAX	6.34	1.50	1.43
6	D	700	T13	OAB-SAX	6.33	1.50	1.43
6	B	700	T13	CAO-NAM	-6.30	1.32	1.43
6	B	1241	T13	OAC-SAX	5.94	1.50	1.43
6	D	700	T13	CAW-SAX	-5.78	1.70	1.79
6	D	1241	T13	OAC-SAX	5.58	1.49	1.43
6	B	700	T13	OAB-SAX	5.53	1.49	1.43
6	B	1241	T13	OAB-SAX	5.53	1.49	1.43
6	D	1241	T13	OAB-SAX	5.51	1.49	1.43
6	D	700	T13	CAO-NAM	-5.27	1.34	1.43
7	B	600	GDP	C6-N1	3.28	1.38	1.33
7	D	600	GDP	C6-N1	3.27	1.38	1.33
4	C	600	GTP	C6-N1	3.16	1.38	1.33
6	B	700	T13	CAW-SAX	-3.02	1.74	1.79
6	D	1241	T13	CAW-SAX	-2.96	1.74	1.79
4	A	600	GTP	C6-N1	2.58	1.37	1.33
4	C	600	GTP	C2-N1	2.11	1.39	1.35
4	A	600	GTP	O4'-C4'	-2.08	1.40	1.45
6	B	700	T13	CAQ-CAR	2.06	1.41	1.37
6	B	1241	T13	CAQ-CAR	2.01	1.41	1.37
4	C	600	GTP	O4'-C4'	-2.00	1.40	1.45

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	700	T13	CAA-OAN-CAV	-7.88	105.64	117.53
6	D	700	T13	CAU-CAW-CAT	7.28	121.77	116.67
6	D	700	T13	OAC-SAX-OAB	-6.68	111.33	119.55
6	B	1241	T13	OAC-SAX-OAB	-6.54	111.51	119.55
6	B	700	T13	CAA-OAN-CAV	-5.95	108.55	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	700	T13	OAC-SAX-OAB	-5.88	112.33	119.55
7	D	600	GDP	N3-C2-N1	-5.61	119.73	127.22
6	B	700	T13	CAU-CAW-CAT	5.61	120.60	116.67
6	B	1241	T13	CAA-OAN-CAV	-5.48	109.26	117.53
6	D	1241	T13	CAA-OAN-CAV	-5.44	109.32	117.53
4	C	600	GTP	N3-C2-N1	-5.39	120.03	127.22
6	B	700	T13	CAW-SAX-NAM	5.26	112.61	106.68
7	B	600	GDP	N3-C2-N1	-4.94	120.63	127.22
7	D	600	GDP	C2-N3-C4	4.86	120.91	115.36
6	D	700	T13	CAW-SAX-NAM	4.44	111.69	106.68
4	C	600	GTP	C2-N3-C4	4.38	120.36	115.36
4	A	600	GTP	N3-C2-N1	-4.31	121.47	127.22
6	B	1241	T13	OAB-SAX-CAW	4.28	115.11	108.74
4	C	600	GTP	PB-O3B-PG	-4.19	118.43	132.83
4	A	600	GTP	PB-O3B-PG	-4.12	118.69	132.83
4	A	600	GTP	C2-N3-C4	4.12	120.06	115.36
6	D	1241	T13	CAU-CAW-CAT	3.88	119.39	116.67
6	D	1241	T13	OAC-SAX-OAB	-3.75	114.94	119.55
7	B	600	GDP	C2-N3-C4	3.71	119.60	115.36
7	B	600	GDP	C5-C6-N1	-3.53	118.60	123.43
7	D	600	GDP	C5-C6-N1	-3.22	119.02	123.43
4	C	600	GTP	N2-C2-N1	3.19	122.21	117.25
4	C	600	GTP	PA-O3A-PB	-3.10	122.17	132.83
6	B	1241	T13	CAL-CAP-CAV	-2.92	118.52	122.81
6	D	1241	T13	CAL-CAP-CAV	-2.90	118.56	122.81
6	B	1241	T13	CAU-CAW-CAT	2.83	118.65	116.67
6	D	700	T13	OAN-CAV-CAP	2.78	118.19	116.26
7	D	600	GDP	C6-N1-C2	2.74	120.29	115.93
7	B	600	GDP	C6-N1-C2	2.72	120.25	115.93
7	D	600	GDP	PA-O3A-PB	-2.66	123.69	132.83
4	C	600	GTP	C5-C6-N1	-2.65	119.81	123.43
7	B	600	GDP	PA-O3A-PB	-2.65	123.74	132.83
7	D	600	GDP	C3'-C2'-C1'	2.62	104.92	100.98
4	A	600	GTP	O3'-C3'-C4'	-2.61	103.50	111.05
4	C	600	GTP	C1'-N9-C4	-2.51	122.22	126.64
4	C	600	GTP	C6-N1-C2	2.50	119.89	115.93
6	B	1241	T13	CAK-CAJ-CAO	-2.47	117.44	120.30
6	B	700	T13	CAL-CAP-CAV	-2.47	119.18	122.81
4	A	600	GTP	PA-O3A-PB	-2.46	124.37	132.83
4	A	600	GTP	C5-C6-N1	-2.46	120.07	123.43
4	A	600	GTP	N2-C2-N1	2.45	121.06	117.25
6	D	1241	T13	CAK-CAJ-CAO	-2.42	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1241	T13	FAG-CAS-CAQ	2.40	123.38	118.61
4	A	600	GTP	O3G-PG-O3B	2.39	112.64	104.64
7	D	600	GDP	O2B-PB-O3A	2.38	112.63	104.64
4	C	600	GTP	C4-C5-N7	-2.37	106.92	109.40
6	D	1241	T13	CAO-CAL-CAP	2.35	120.68	118.76
6	B	1241	T13	CAO-CAL-CAP	2.34	120.67	118.76
6	D	700	T13	FAD-CAP-CAL	2.33	123.25	118.61
6	B	700	T13	CAO-CAL-CAP	2.26	120.60	118.76
6	B	700	T13	CAK-CAJ-CAO	-2.25	117.69	120.30
7	B	600	GDP	O3B-PB-O3A	2.25	112.18	104.64
6	B	1241	T13	FAD-CAP-CAL	2.24	123.07	118.61
6	D	1241	T13	FAD-CAP-CAL	2.24	123.06	118.61
6	D	700	T13	CAO-NAM-SAX	2.22	130.16	123.24
7	B	600	GDP	C2'-C3'-C4'	2.21	106.93	102.64
7	B	600	GDP	O3'-C3'-C2'	-2.16	104.85	111.82
6	D	700	T13	OAN-CAV-CAK	-2.14	120.69	124.37
4	C	600	GTP	O3G-PG-O3B	2.14	111.82	104.64
6	D	700	T13	CAR-CAT-CAW	-2.13	119.03	121.74
6	D	700	T13	CAL-CAP-CAV	-2.10	119.73	122.81
6	B	700	T13	FAD-CAP-CAL	2.05	122.69	118.61
6	D	1241	T13	FAG-CAS-CAQ	2.04	122.68	118.61

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	1241	T13	CAP-CAV-OAN-CAA
6	D	700	T13	CAP-CAV-OAN-CAA
6	D	700	T13	CAU-CAW-SAX-OAB
6	B	700	T13	CAP-CAV-OAN-CAA
6	B	700	T13	CAO-NAM-SAX-CAW
4	A	600	GTP	C5'-O5'-PA-O1A
4	C	600	GTP	C5'-O5'-PA-O1A
6	D	1241	T13	CAP-CAV-OAN-CAA
6	D	700	T13	CAO-NAM-SAX-OAC
6	B	700	T13	CAO-NAM-SAX-OAB
6	B	1241	T13	CAO-NAM-SAX-CAW
6	D	700	T13	CAO-NAM-SAX-CAW
6	D	1241	T13	CAO-NAM-SAX-CAW
6	B	700	T13	CAO-NAM-SAX-OAC
7	B	600	GDP	C3'-C4'-C5'-O5'
6	B	1241	T13	CAK-CAV-OAN-CAA

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Mol	Chain	Res	Type	Atoms
6	D	1241	T13	CAK-CAV-OAN-CAA
6	B	700	T13	CAK-CAV-OAN-CAA
7	B	600	GDP	O4'-C4'-C5'-O5'
6	D	700	T13	CAO-NAM-SAX-OAB
7	D	600	GDP	C3'-C4'-C5'-O5'
4	C	600	GTP	PB-O3B-PG-O1G
6	D	700	T13	CAK-CAV-OAN-CAA
7	D	600	GDP	O4'-C4'-C5'-O5'
6	B	1241	T13	CAO-NAM-SAX-OAC
7	B	600	GDP	PA-O3A-PB-O3B
4	C	600	GTP	PB-O3B-PG-O3G
7	B	600	GDP	C5'-O5'-PA-O3A
7	D	600	GDP	C5'-O5'-PA-O3A
4	A	600	GTP	C5'-O5'-PA-O3A
4	C	600	GTP	C5'-O5'-PA-O3A
4	A	600	GTP	C5'-O5'-PA-O2A
4	C	600	GTP	C5'-O5'-PA-O2A
6	D	700	T13	CAT-CAW-SAX-OAB
4	A	600	GTP	PB-O3B-PG-O1G
4	A	600	GTP	PB-O3A-PA-O2A
4	C	600	GTP	PB-O3A-PA-O2A
7	B	600	GDP	PA-O3A-PB-O2B
7	D	600	GDP	PA-O3A-PB-O3B
7	B	600	GDP	C5'-O5'-PA-O1A
7	D	600	GDP	C5'-O5'-PA-O1A

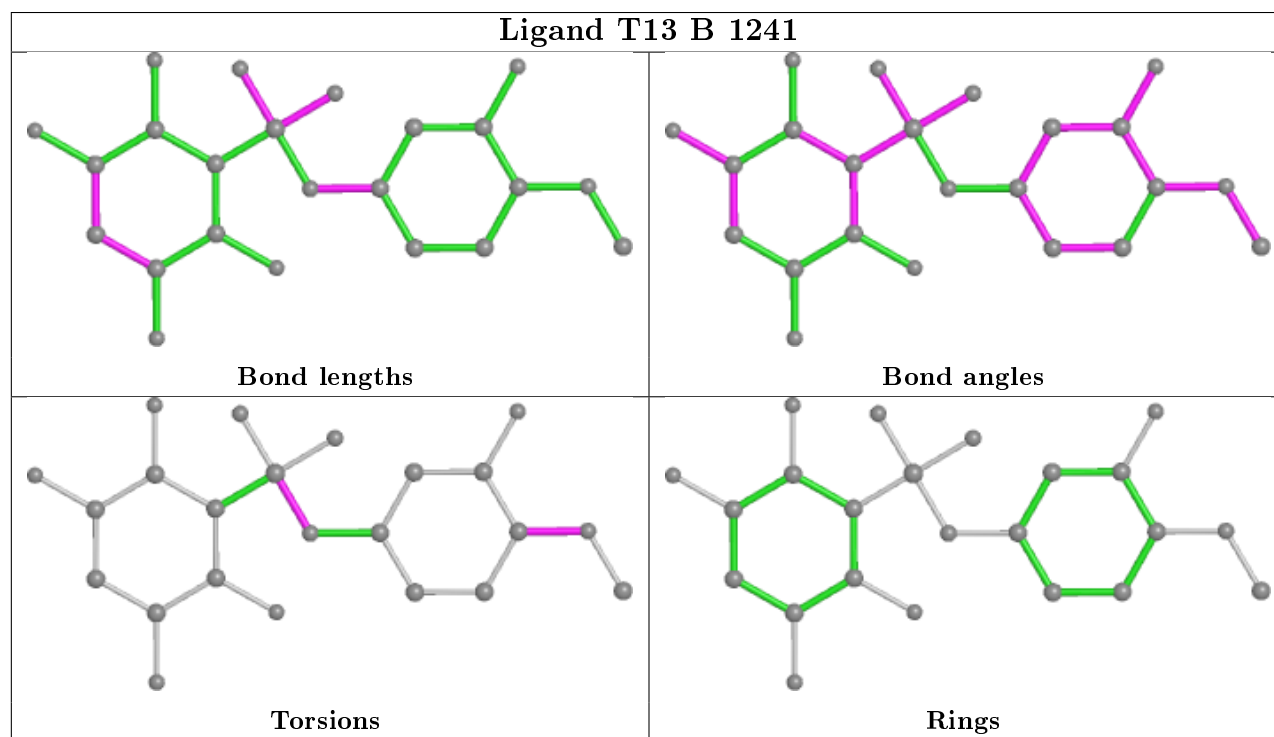
There are no ring outliers.

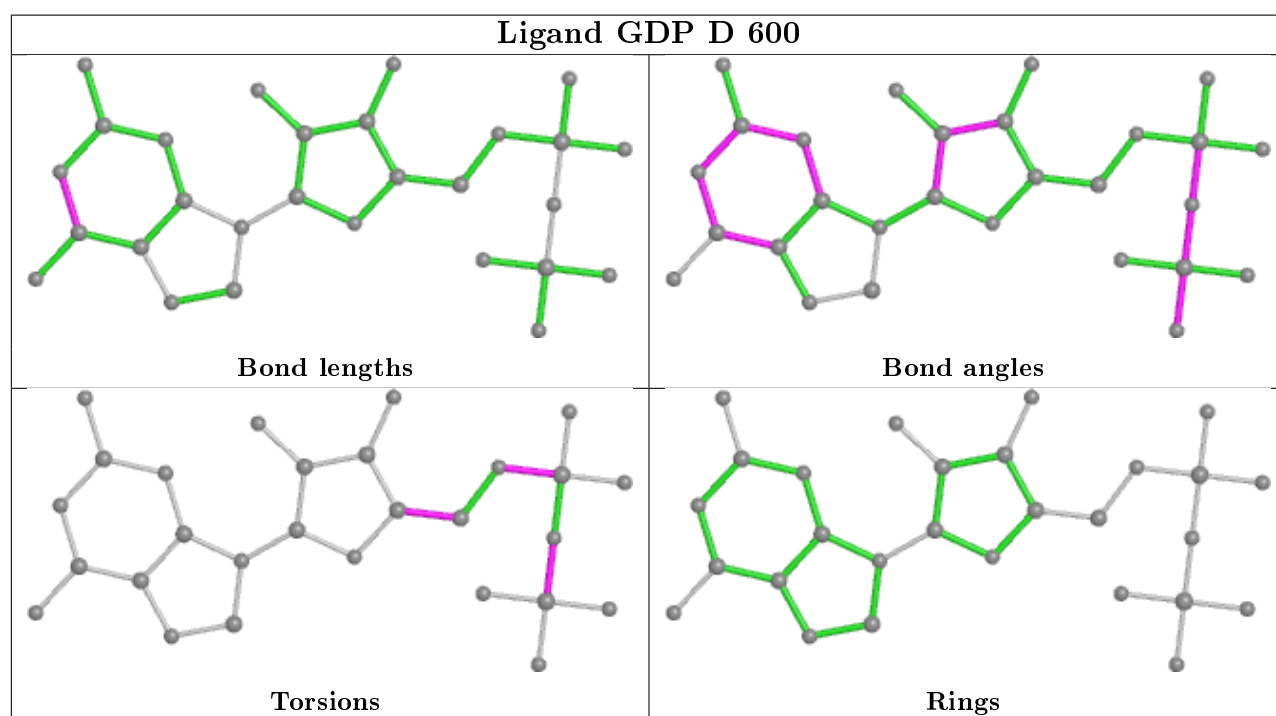
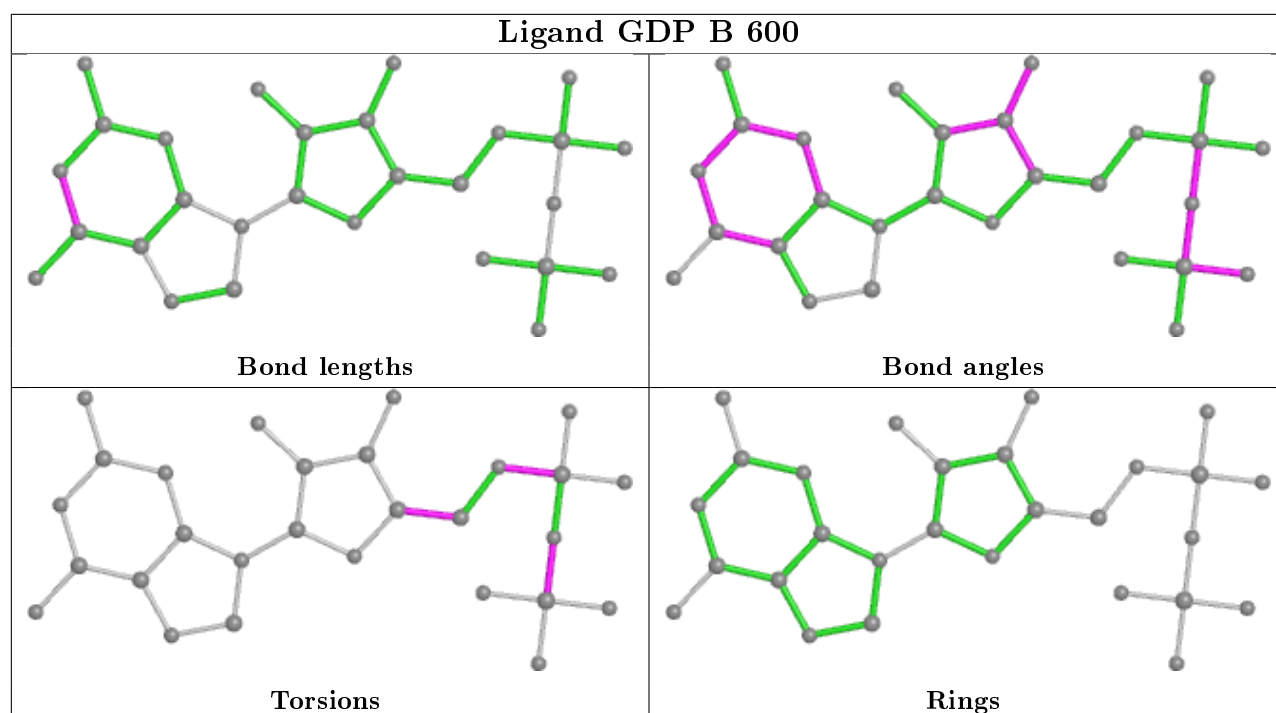
8 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1241	T13	4	0
7	B	600	GDP	5	0
7	D	600	GDP	4	0
6	D	700	T13	1	0
6	B	700	T13	2	0
4	A	600	GTP	4	0
4	C	600	GTP	4	0
6	D	1241	T13	5	0

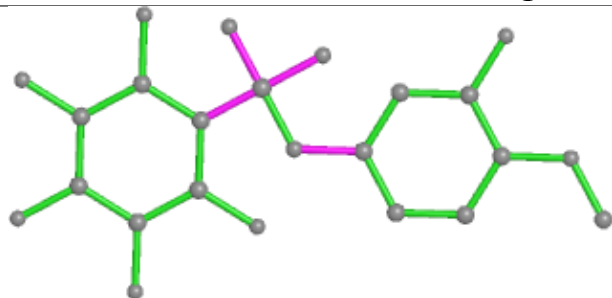
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

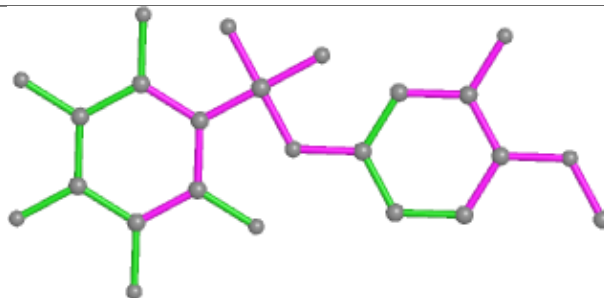




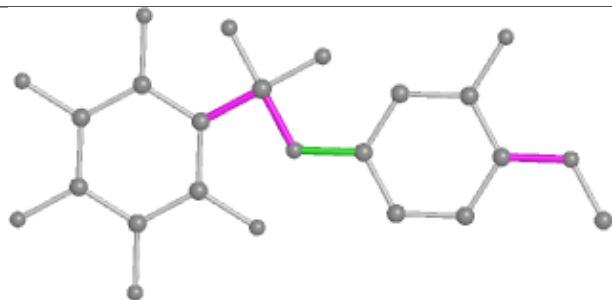
Ligand T13 D 700



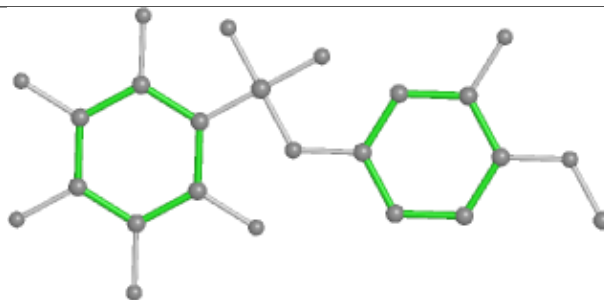
Bond lengths



Bond angles

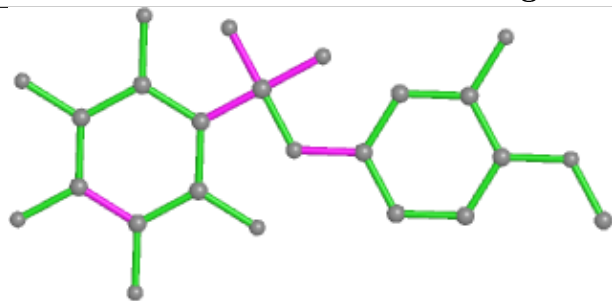


Torsions

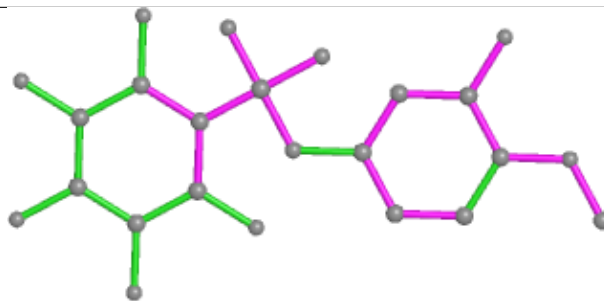


Rings

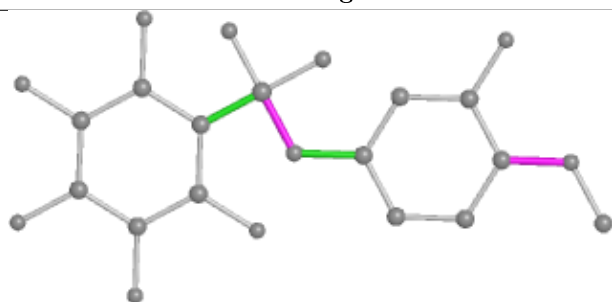
Ligand T13 B 700



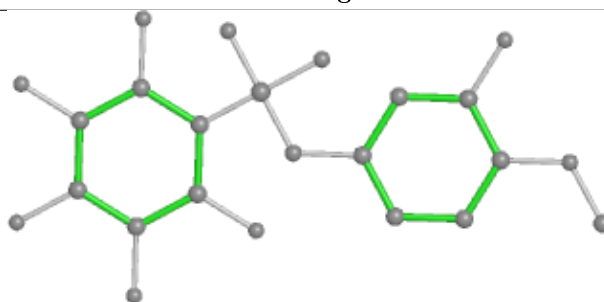
Bond lengths



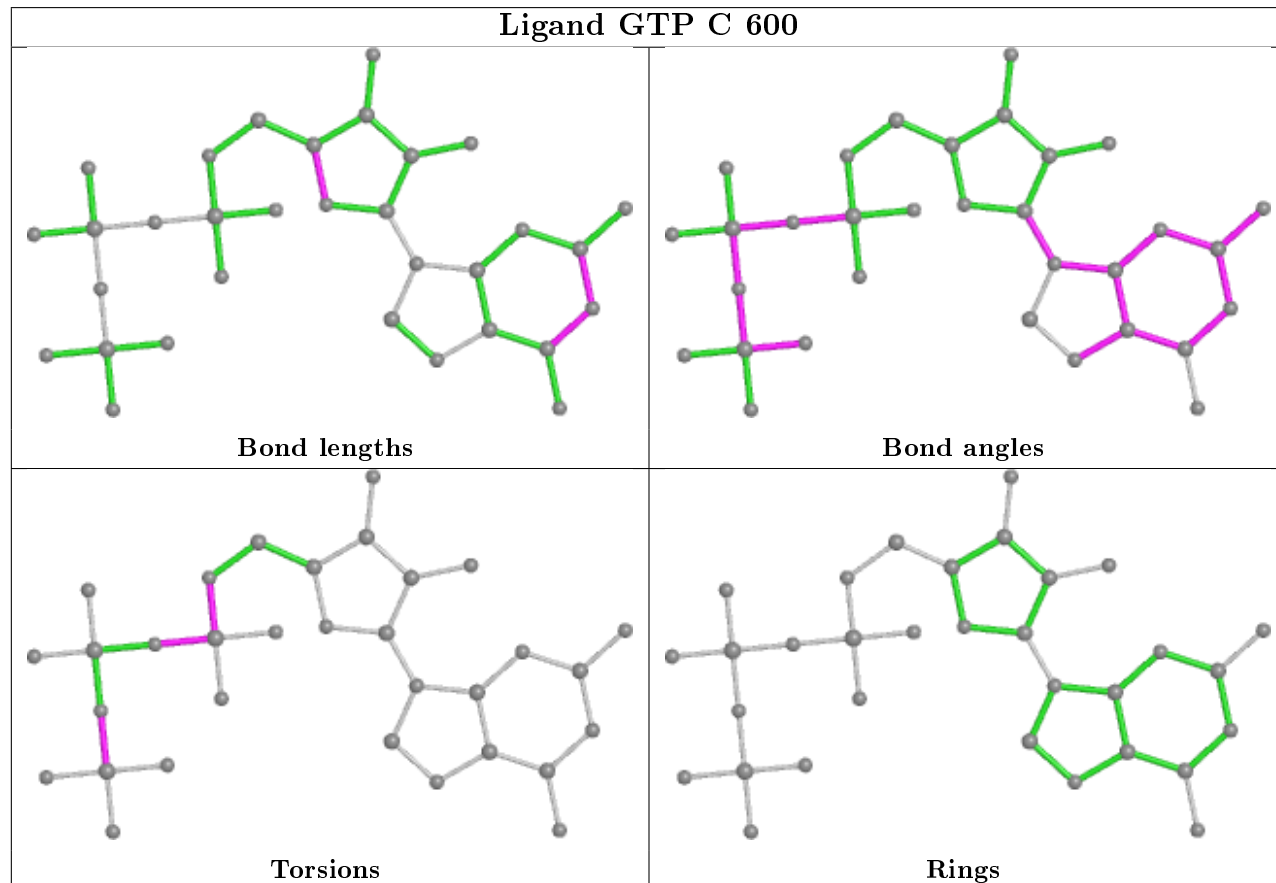
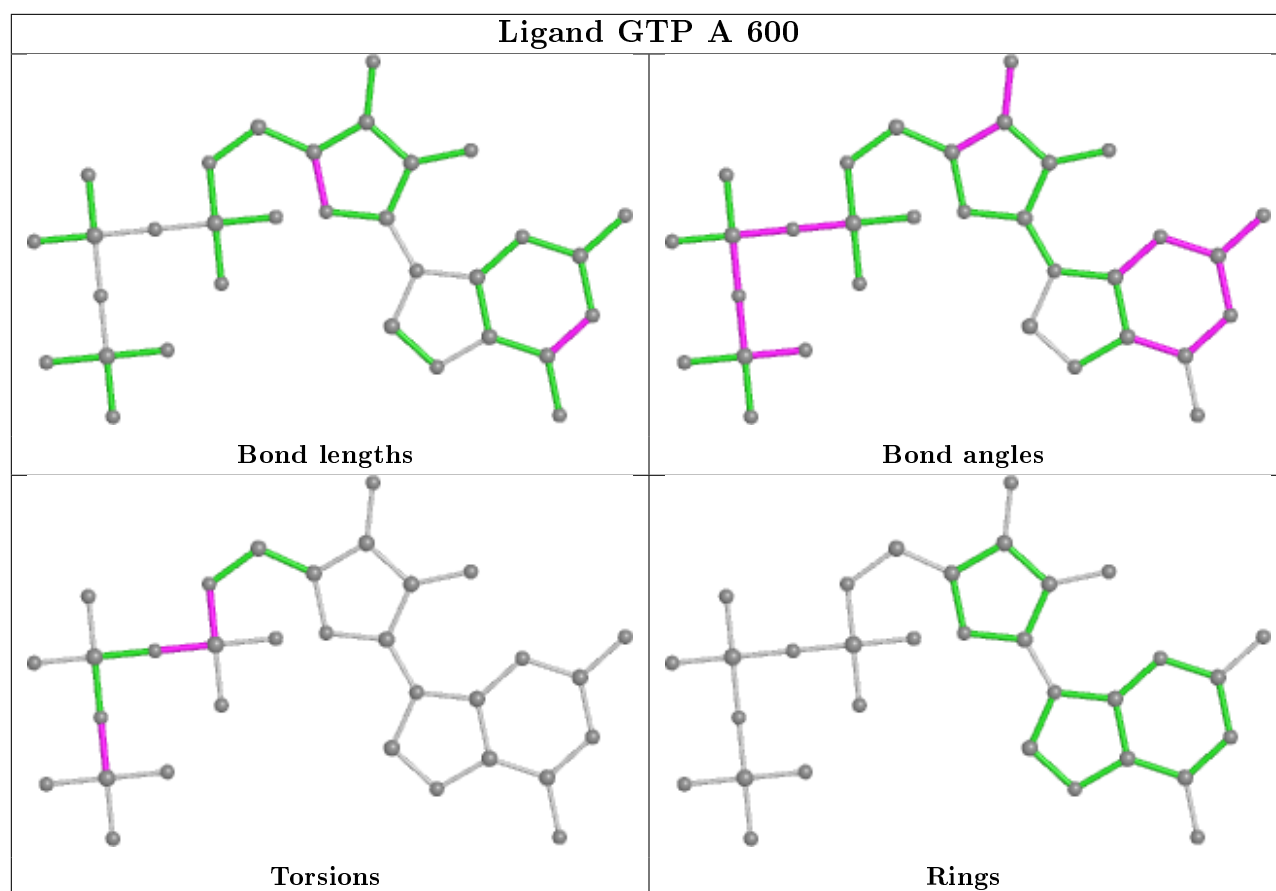
Bond angles

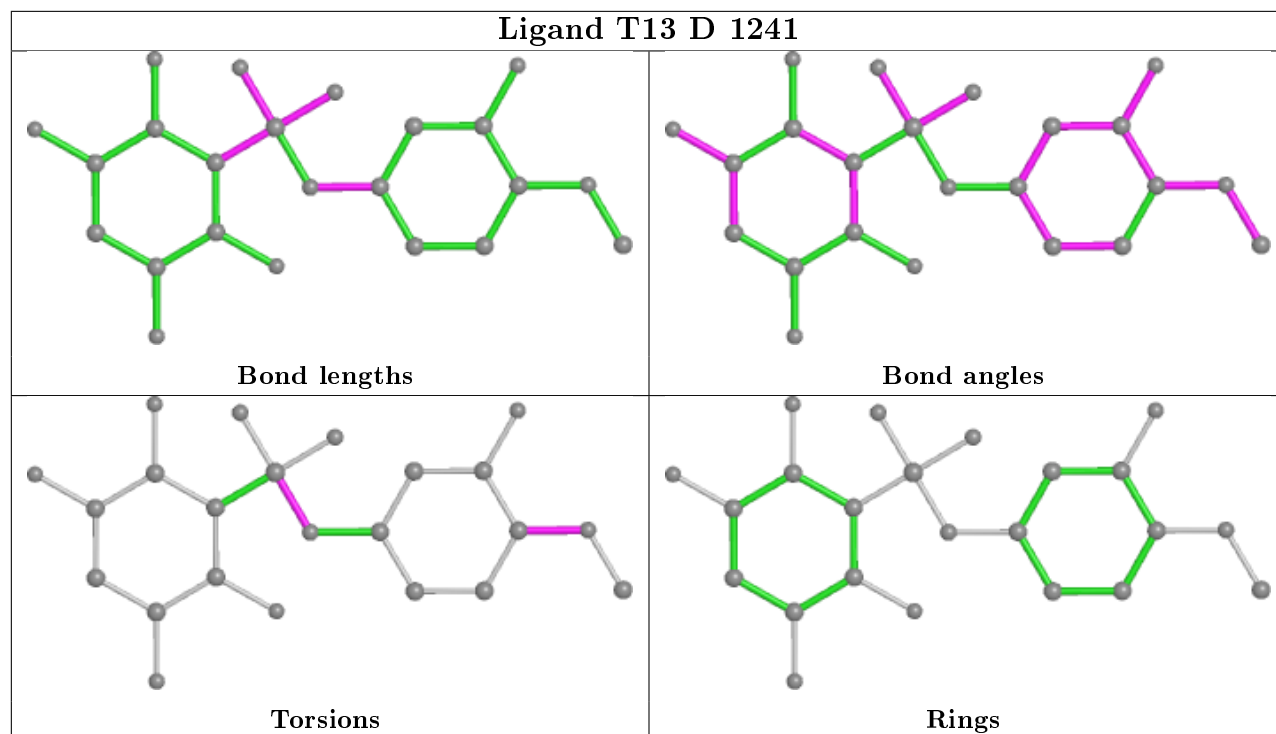


Torsions



Rings





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.34	2 (0%) 91 83	63, 66, 67, 73	0
1	C	428/451 (94%)	-0.13	7 (1%) 72 57	60, 66, 67, 77	0
2	B	420/445 (94%)	-0.18	4 (0%) 82 70	64, 66, 67, 72	0
2	D	427/445 (95%)	-0.26	4 (0%) 84 73	64, 66, 67, 73	0
3	E	124/142 (87%)	-0.47	1 (0%) 86 75	59, 66, 71, 74	0
All	All	1826/1934 (94%)	-0.24	18 (0%) 82 70	59, 66, 68, 77	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	279	GLY	3.9
1	C	30	ILE	3.0
1	C	370	LYS	2.6
2	B	57	THR	2.6
1	A	351	PHE	2.6
1	C	302	MET	2.5
2	B	276	THR	2.4
1	C	247	ALA	2.4
3	E	4	ALA	2.3
1	C	276	ILE	2.2
2	B	35	SER	2.2
1	C	245	ASP	2.2
2	B	56	ALA	2.2
1	A	178	SER	2.1
2	D	312	TYR	2.1
1	C	37	PRO	2.0
2	D	399	PHE	2.0
2	D	280	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

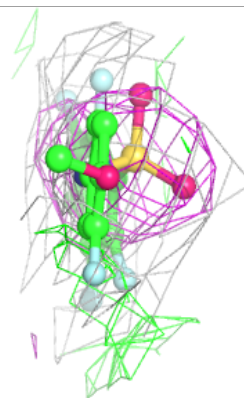
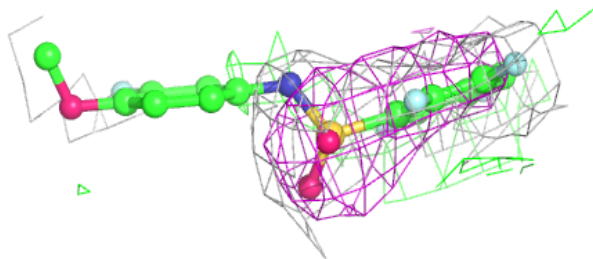
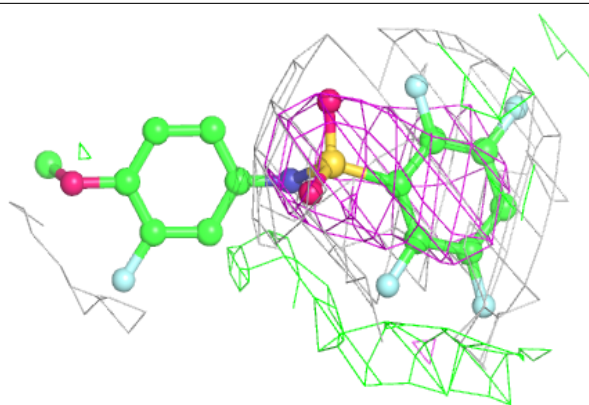
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	T13	B	1241	23/24	0.84	0.28	68,69,100,100	23
6	T13	B	700	24/24	0.89	0.24	62,71,76,77	24
6	T13	D	700	24/24	0.90	0.23	61,65,67,69	24
6	T13	D	1241	23/24	0.93	0.15	64,66,100,100	23
4	GTP	C	600	32/32	0.94	0.15	63,65,66,66	0
7	GDP	B	600	28/28	0.94	0.12	64,65,67,67	0
7	GDP	D	600	28/28	0.96	0.13	64,65,67,67	0
5	MG	B	601	1/1	0.97	1.03	53,53,53,53	0
4	GTP	A	600	32/32	0.97	0.13	63,65,66,66	0
5	MG	C	601	1/1	0.98	0.19	30,30,30,30	0
5	MG	A	601	1/1	0.99	0.11	30,30,30,30	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.

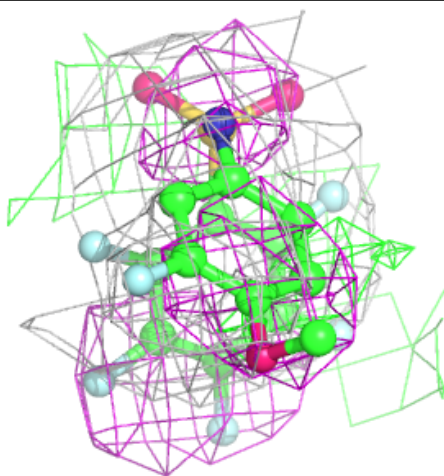
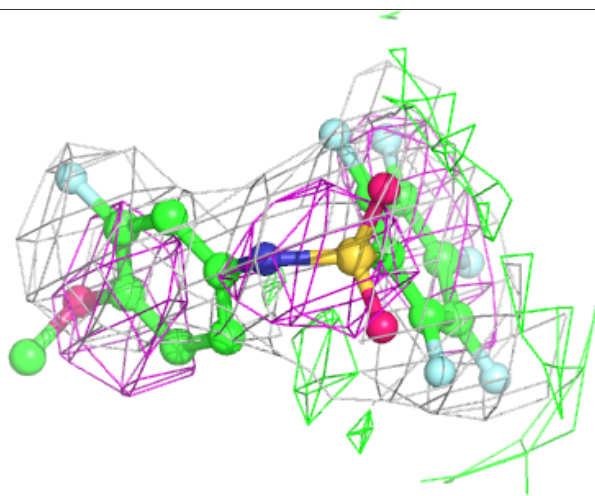
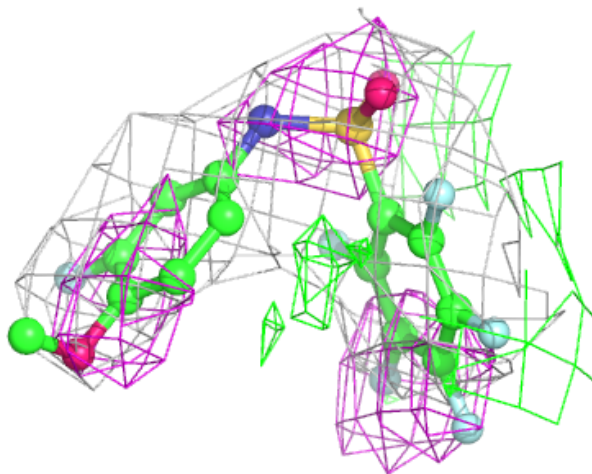
Electron density around T13 B 1241:

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



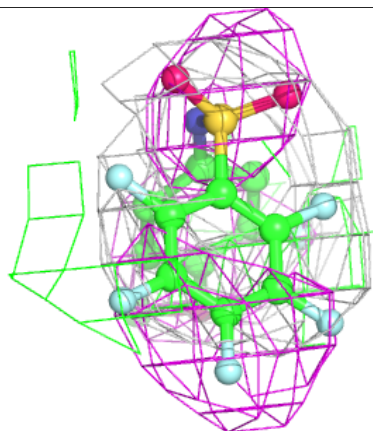
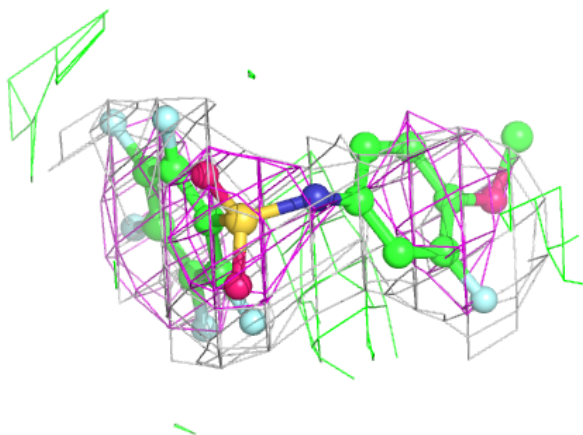
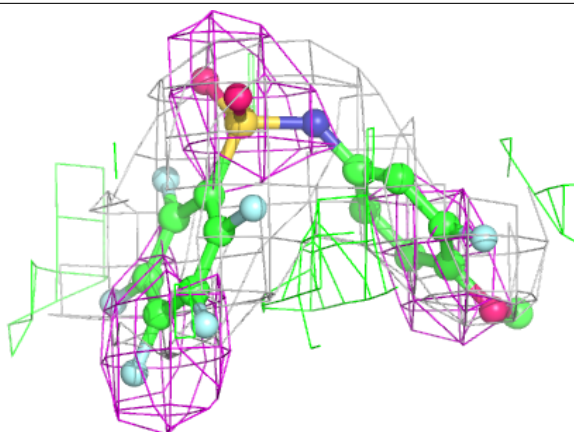
Electron density around T13 B 700:

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

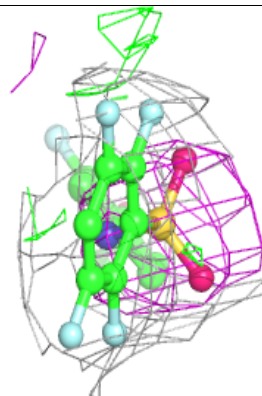
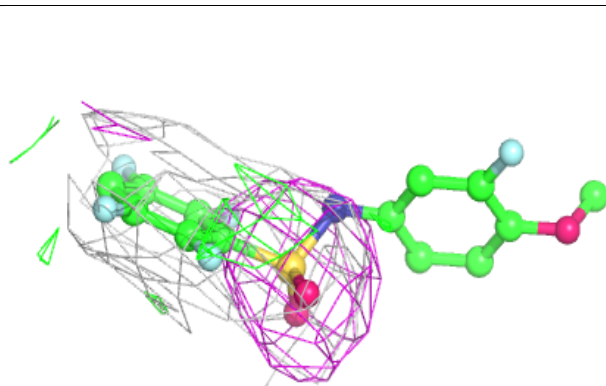
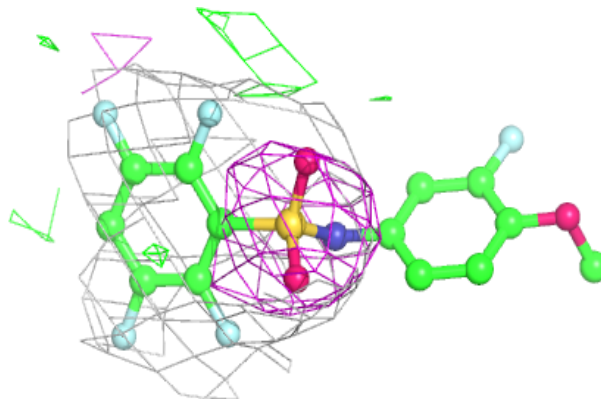


Electron density around T13 D 700:

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

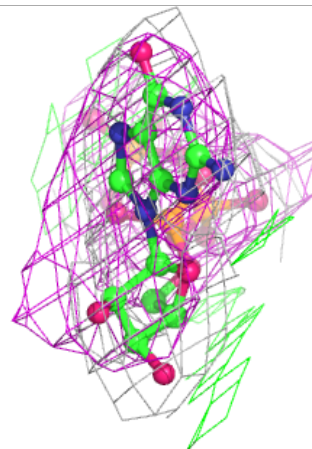
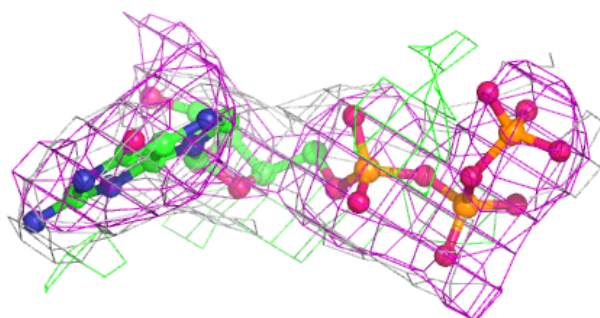
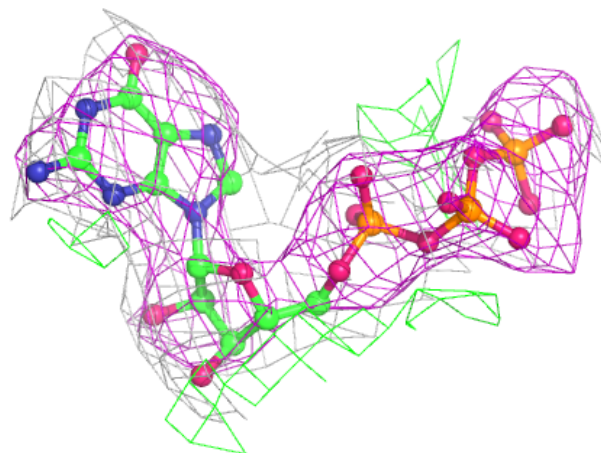
**Electron density around T13 D 1241:**

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



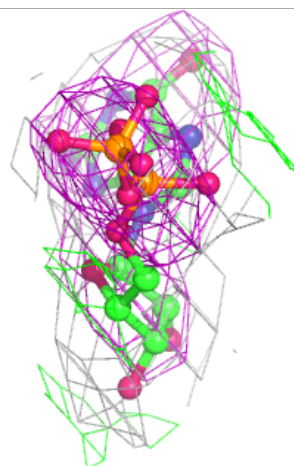
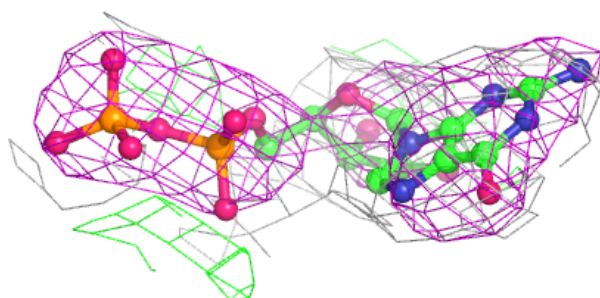
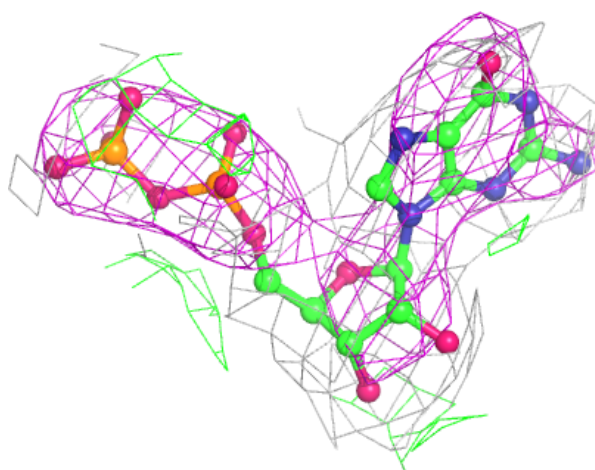
Electron density around GTP C 600:

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



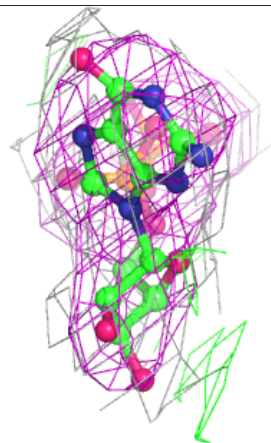
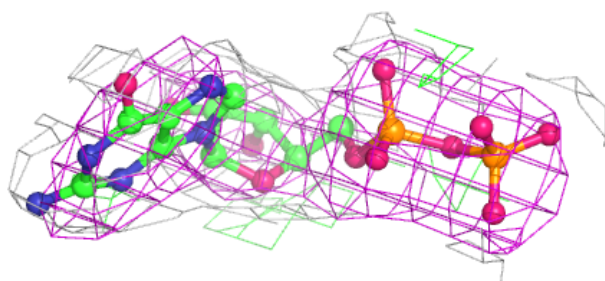
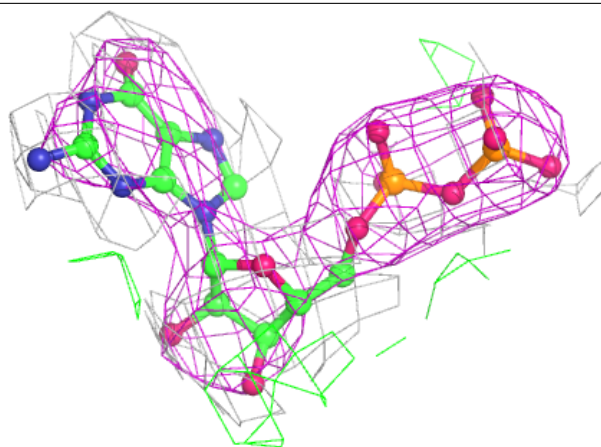
Electron density around GDP B 600:

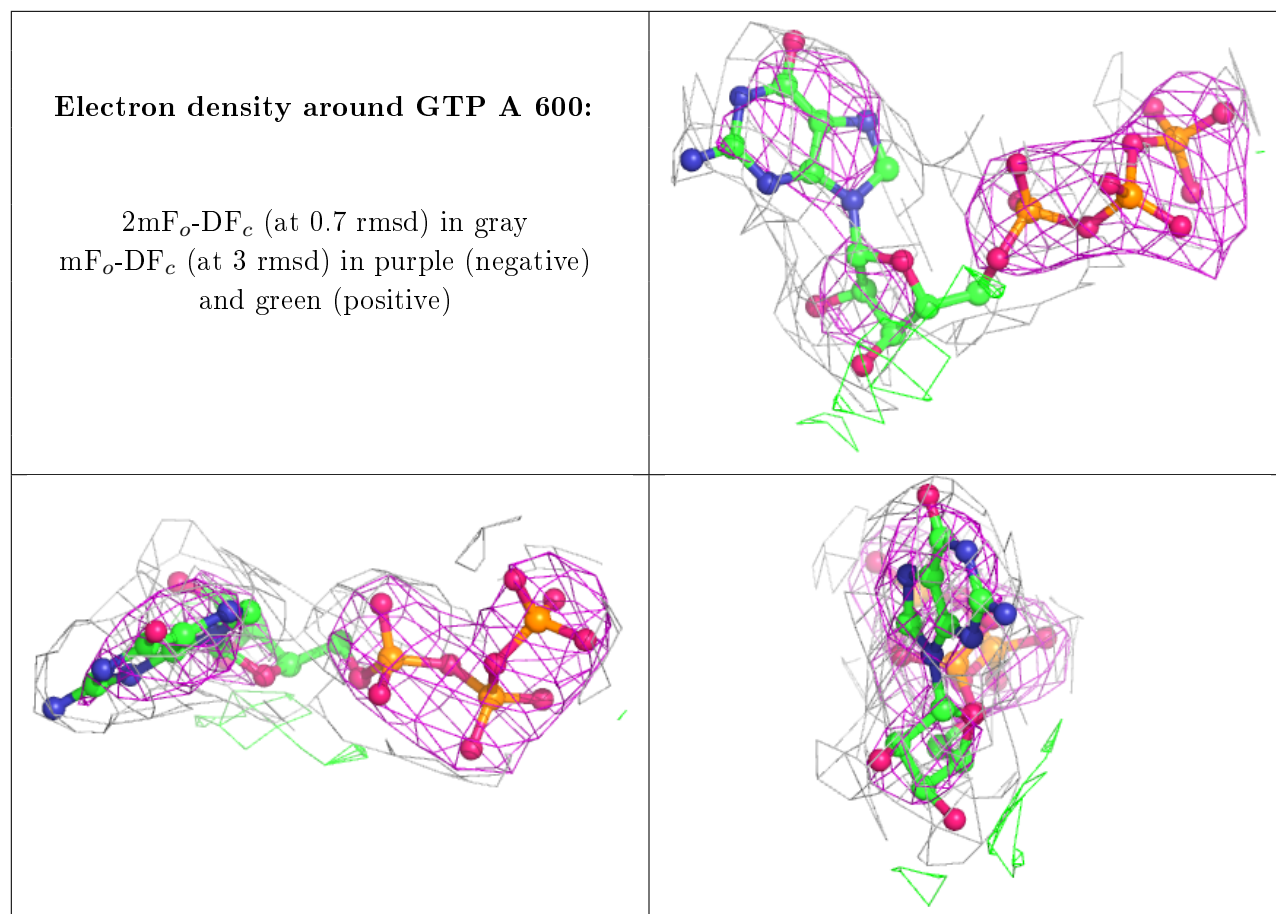
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.