



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:19 PM UTC

PDB ID : 4G3M / pdb_00004g3m
Title : Complex Structure of Bacillus subtilis RibG: The Deamination Process in Riboflavin Biosynthesis
Authors : Chen, S.C.; Shen, C.Y.; Yen, T.M.; Yu, H.C.; Chang, T.H.; Lai, W.L.; Liaw, S.H.
Deposited on : 2012-07-15
Resolution : 2.56 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

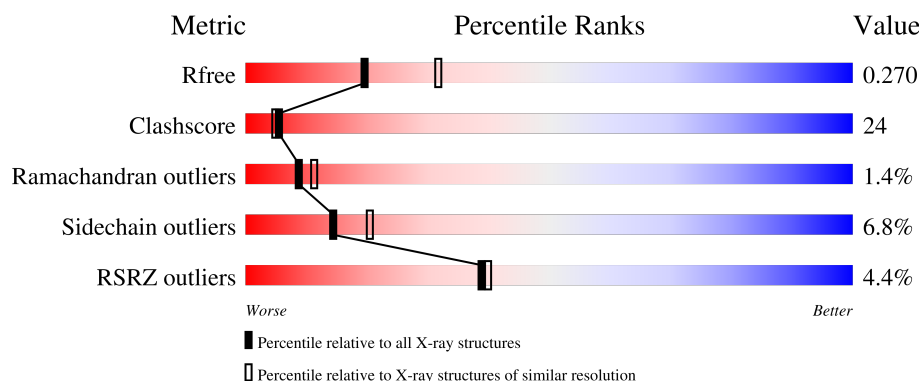
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	373	0% 68% 26% • •
1	B	373	2% 57% 35% 5% • • •
1	C	373	5% 57% 33% 6% •
1	D	373	9% 53% 37% 6% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11519 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 Riboflavin biosynthesis protein RibD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2756	1749	472	520	15			
1	B	361	Total	C	N	O	S	0	0	0
			2751	1745	471	520	15			
1	C	361	Total	C	N	O	S	0	0	0
			2751	1745	471	520	15			
1	D	361	Total	C	N	O	S	0	0	0
			2751	1745	471	520	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P17618
A	-10	ARG	-	expression tag	UNP P17618
A	-9	GLY	-	expression tag	UNP P17618
A	-8	SER	-	expression tag	UNP P17618
A	-7	HIS	-	expression tag	UNP P17618
A	-6	HIS	-	expression tag	UNP P17618
A	-5	HIS	-	expression tag	UNP P17618
A	-4	HIS	-	expression tag	UNP P17618
A	-3	HIS	-	expression tag	UNP P17618
A	-2	HIS	-	expression tag	UNP P17618
A	-1	GLY	-	expression tag	UNP P17618
A	0	SER	-	expression tag	UNP P17618
B	-11	MET	-	expression tag	UNP P17618
B	-10	ARG	-	expression tag	UNP P17618
B	-9	GLY	-	expression tag	UNP P17618
B	-8	SER	-	expression tag	UNP P17618
B	-7	HIS	-	expression tag	UNP P17618
B	-6	HIS	-	expression tag	UNP P17618
B	-5	HIS	-	expression tag	UNP P17618
B	-4	HIS	-	expression tag	UNP P17618
B	-3	HIS	-	expression tag	UNP P17618

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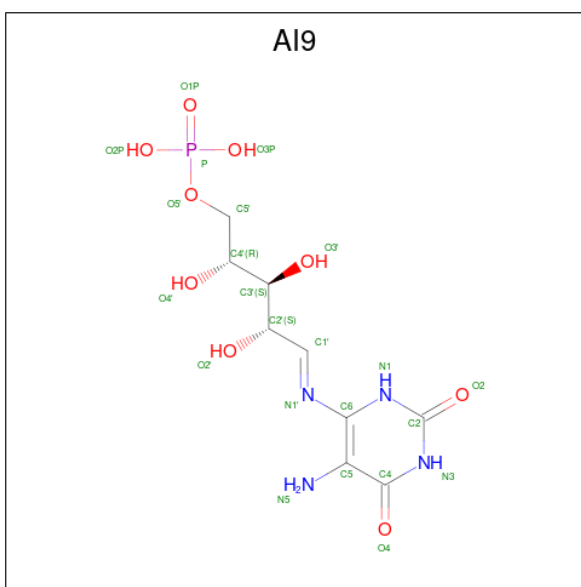
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP P17618
B	-1	GLY	-	expression tag	UNP P17618
B	0	SER	-	expression tag	UNP P17618
C	-11	MET	-	expression tag	UNP P17618
C	-10	ARG	-	expression tag	UNP P17618
C	-9	GLY	-	expression tag	UNP P17618
C	-8	SER	-	expression tag	UNP P17618
C	-7	HIS	-	expression tag	UNP P17618
C	-6	HIS	-	expression tag	UNP P17618
C	-5	HIS	-	expression tag	UNP P17618
C	-4	HIS	-	expression tag	UNP P17618
C	-3	HIS	-	expression tag	UNP P17618
C	-2	HIS	-	expression tag	UNP P17618
C	-1	GLY	-	expression tag	UNP P17618
C	0	SER	-	expression tag	UNP P17618
D	-11	MET	-	expression tag	UNP P17618
D	-10	ARG	-	expression tag	UNP P17618
D	-9	GLY	-	expression tag	UNP P17618
D	-8	SER	-	expression tag	UNP P17618
D	-7	HIS	-	expression tag	UNP P17618
D	-6	HIS	-	expression tag	UNP P17618
D	-5	HIS	-	expression tag	UNP P17618
D	-4	HIS	-	expression tag	UNP P17618
D	-3	HIS	-	expression tag	UNP P17618
D	-2	HIS	-	expression tag	UNP P17618
D	-1	GLY	-	expression tag	UNP P17618
D	0	SER	-	expression tag	UNP P17618

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

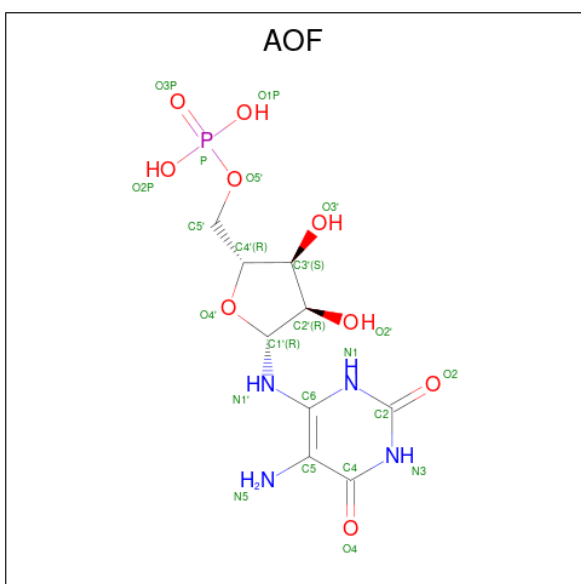
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is [(2R,3S,4S,5E)-5-[[5-azanyl-2,4-bis(oxidanylidene)-1H-pyrimidin-6-yl]imino]-2,3,4-tris(oxidanyl)pentyl] dihydrogen phosphate (CCD ID: AI9) (formula: C₉H₁₅N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			23	9	4	9	1		

- Molecule 4 is N-(5-amino-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl)-5-O-phosphono-beta-D-ribofuranosylamine (CCD ID: AOF) (formula: $C_9H_{15}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
4	C	1	Total	C	N	O	P	0	0
			23	9	4	9	1		
4	D	1	Total	C	N	O	P	0	0
			23	9	4	9	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	115	Total	O	0	0
			115	115		
5	B	70	Total	O	0	0
			70	70		
5	C	86	Total	O	0	0
			86	86		
5	D	74	Total	O	0	0
			74	74		

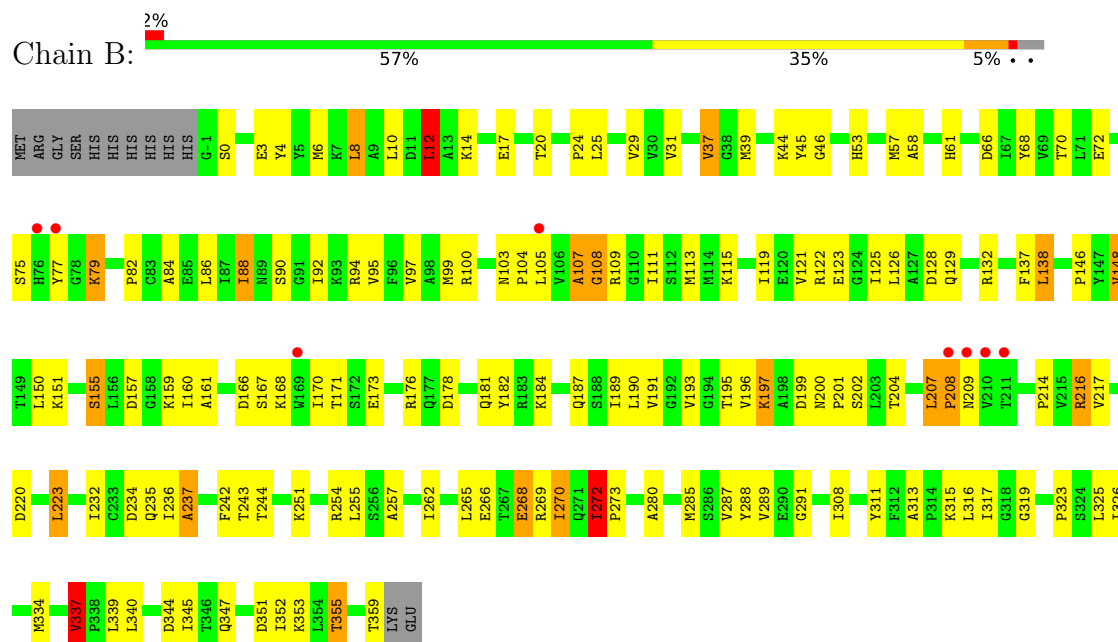
3 Residue-property plots [i](#)

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

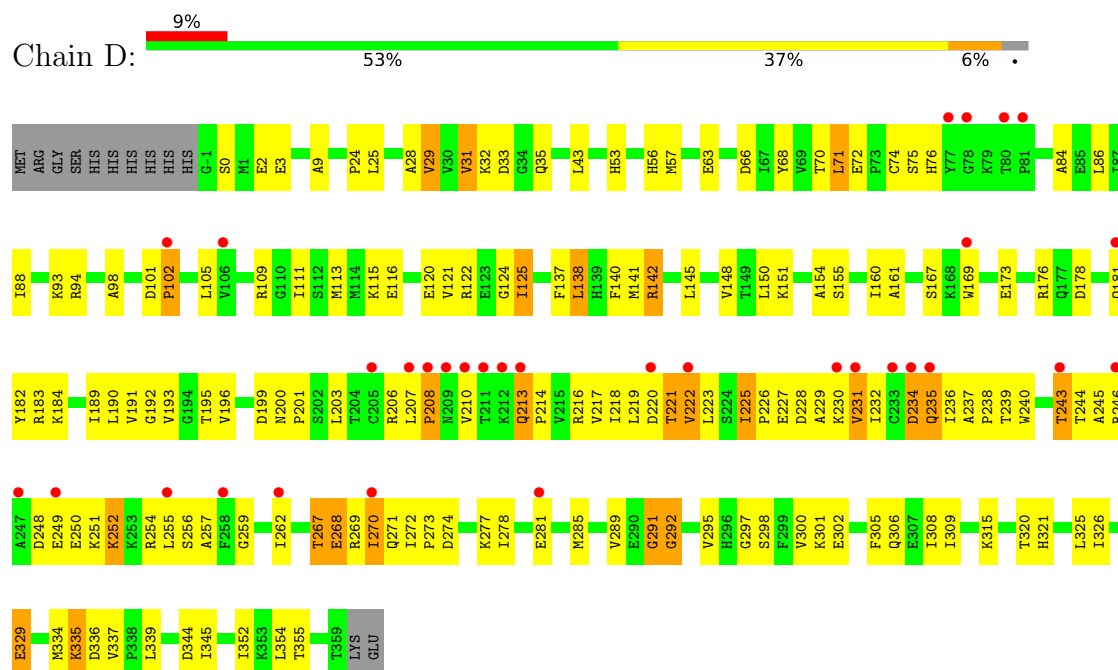
• Molecule 1: Riboflavin biosynthesis protein RibD



• Molecule 1: Riboflavin biosynthesis protein RibD



• Molecule 1: Riboflavin biosynthesis protein RibD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.01Å 109.19Å 189.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.72 – 2.56 29.72 – 2.56	Depositor EDS
% Data completeness (in resolution range)	94.7 (29.72-2.56) 95.0 (29.72-2.56)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.222 , 0.270 0.222 , 0.270	Depositor DCC
R_{free} test set	5958 reflections (10.16%)	wwPDB-VP
Wilson B-factor (Å ²)	56.2	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11519	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: AOF, ZN, AI9

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	0.50	0/2807	1.00	12/3797 (0.3%)
1	B	0.46	1/2802 (0.0%)	0.94	12/3791 (0.3%)
1	C	0.45	1/2802 (0.0%)	0.94	9/3791 (0.2%)
1	D	0.47	0/2802	0.94	9/3791 (0.2%)
All	All	0.47	2/11213 (0.0%)	0.96	42/15170 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	272	ILE	CA-CB	6.60	1.57	1.54
1	C	272	ILE	CA-CB	5.05	1.56	1.54

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	ILE	N-CA-C	-12.27	101.26	111.81
1	A	320	THR	N-CA-C	-7.02	103.67	111.82
1	D	268	GLU	N-CA-C	-6.79	105.03	113.38
1	A	325	LEU	N-CA-C	6.68	118.22	111.07
1	B	148	VAL	N-CA-C	6.31	117.01	108.17
1	C	211	THR	CB-CA-C	-6.27	109.36	116.63
1	A	148	VAL	N-CA-C	6.20	116.78	108.11
1	A	21	GLU	CB-CA-C	-5.98	109.10	117.23
1	D	145	LEU	CA-C-N	5.97	125.98	119.89
1	D	145	LEU	C-N-CA	5.97	125.98	119.89
1	A	190	LEU	N-CA-C	5.94	119.23	109.72
1	C	121	VAL	N-CA-C	5.81	115.10	106.85
1	D	291	GLY	N-CA-C	5.81	118.16	111.36
1	D	256	SER	N-CA-C	-5.67	106.20	113.01
1	A	172	SER	N-CA-C	5.64	117.97	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	ILE	N-CA-C	5.62	116.22	107.28
1	D	229	ALA	N-CA-C	5.59	115.93	108.38
1	C	48	ALA	N-CA-C	5.51	118.02	110.24
1	B	291	GLY	N-CA-C	5.49	120.33	111.38
1	A	304	CYS	N-CA-C	5.42	118.69	112.57
1	D	142	ARG	N-CA-C	5.42	117.18	111.28
1	D	124	GLY	N-CA-C	5.41	121.52	115.08
1	B	325	LEU	N-CA-C	5.39	117.58	111.11
1	C	21	GLU	CB-CA-C	-5.39	110.38	116.63
1	B	237	ALA	N-CA-C	5.38	114.49	108.25
1	B	337	VAL	CA-C-N	5.33	125.27	119.78
1	B	337	VAL	C-N-CA	5.33	125.27	119.78
1	C	262	ILE	N-CA-C	5.31	115.61	108.17
1	A	65	ALA	N-CA-C	5.31	116.77	110.19
1	B	155	SER	N-CA-C	-5.28	103.56	110.53
1	B	20	THR	N-CA-C	5.21	119.27	113.02
1	B	207	LEU	CA-C-N	5.20	126.34	119.84
1	B	207	LEU	C-N-CA	5.20	126.34	119.84
1	C	178	ASP	N-CA-C	-5.17	105.82	111.82
1	B	12	LEU	N-CA-C	-5.17	105.82	111.82
1	A	124	GLY	N-CA-C	5.17	120.84	114.69
1	C	85	GLU	N-CA-C	-5.17	105.56	111.14
1	D	183	ARG	N-CA-C	-5.15	107.03	113.15
1	A	193	VAL	CB-CA-C	-5.11	104.59	112.05
1	C	4	TYR	N-CA-C	-5.10	105.80	111.36
1	A	293	SER	N-CA-C	-5.07	105.75	111.28
1	C	148	VAL	N-CA-C	5.02	116.19	108.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2756	0	2800	96	0
1	B	2751	0	2790	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2751	0	2790	140	0
1	D	2751	0	2790	193	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	23	0	15	1	0
3	B	23	0	15	2	0
3	C	23	0	15	0	0
3	D	23	0	15	0	0
4	B	23	0	15	0	0
4	C	23	0	15	1	0
4	D	23	0	15	0	0
5	A	115	0	0	5	0
5	B	70	0	0	4	0
5	C	86	0	0	4	0
5	D	74	0	0	6	0
All	All	11519	0	11275	534	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 24.

All (534) 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)
1:D:213:GLN:CG	1:D:237:ALA:HB2	1.52	1.39
1:C:230:LYS:O	1:C:234:ASP:HB2	1.29	1.27
1:D:213:GLN:HB3	1:D:237:ALA:CB	1.76	1.15
1:D:213:GLN:CB	1:D:237:ALA:HB2	1.76	1.15
1:D:213:GLN:HB3	1:D:237:ALA:HB1	1.31	1.12
1:C:20:THR:HG21	1:C:25:LEU:HD12	1.14	1.10
1:D:213:GLN:HG2	1:D:237:ALA:HB2	1.17	1.10
1:D:230:LYS:HG2	1:D:231:VAL:H	1.15	1.09
1:D:221:THR:O	1:D:222:VAL:HG22	1.51	1.08
1:D:270:ILE:HD13	1:D:270:ILE:H	1.14	1.06
1:D:125:ILE:HD12	1:D:125:ILE:H	1.21	1.05
1:C:20:THR:CG2	1:C:25:LEU:HD12	1.88	1.04
1:D:213:GLN:CB	1:D:237:ALA:CB	2.36	1.00
1:D:213:GLN:CG	1:D:237:ALA:CB	2.41	0.99
1:A:360:LYS:HE3	1:A:360:LYS:HA	1.44	0.99
1:C:125:ILE:HD12	1:C:125:ILE:H	1.27	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:THR:O	1:D:222:VAL:HG13	1.62	0.98
1:A:290:GLU:HG3	1:A:291:GLY:H	1.30	0.94
1:D:148:VAL:H	1:D:306:GLN:NE2	1.68	0.91
1:D:221:THR:O	1:D:222:VAL:CG2	2.22	0.88
1:D:250:GLU:O	1:D:254:ARG:HB2	1.73	0.88
1:D:270:ILE:H	1:D:270:ILE:CD1	1.87	0.86
1:A:243:THR:HG21	1:A:247:ALA:HB2	1.59	0.85
1:C:243:THR:HG22	1:C:244:THR:H	1.39	0.84
1:D:201:PRO:HG2	1:D:203:LEU:HD21	1.59	0.84
1:D:270:ILE:HD13	1:D:270:ILE:N	1.92	0.83
1:C:66:ASP:OD1	1:C:94:ARG:HB2	1.77	0.83
1:D:230:LYS:HG2	1:D:231:VAL:N	1.95	0.82
1:D:140:PHE:HD2	1:D:141:MET:HE2	1.45	0.82
1:D:160:ILE:HD11	1:D:325:LEU:HD23	1.60	0.81
1:B:37:VAL:HG22	1:B:58:ALA:HA	1.63	0.81
1:C:178:ASP:O	1:C:181:GLN:HG2	1.81	0.81
1:B:220:ASP:O	1:B:243:THR:HG22	1.80	0.80
1:D:221:THR:O	1:D:222:VAL:CG1	2.29	0.80
1:D:190:LEU:HD11	1:D:219:LEU:HG	1.64	0.80
1:B:6:MET:HE1	1:B:70:THR:HG22	1.64	0.79
1:B:111:ILE:HG23	1:B:121:VAL:HG11	1.63	0.79
1:C:193:VAL:HG11	1:C:220:ASP:CG	2.08	0.79
1:B:193:VAL:HG11	1:B:220:ASP:CG	2.07	0.79
1:D:0:SER:HB3	1:D:3:GLU:HG3	1.64	0.78
1:C:205:CYS:HB3	1:C:213:GLN:HE22	1.49	0.77
1:B:187:GLN:HE22	1:B:285:MET:HG3	1.50	0.76
1:D:230:LYS:HE3	1:D:231:VAL:HG22	1.67	0.76
1:C:20:THR:HB	1:C:23:ASN:O	1.84	0.76
1:D:150:LEU:HB2	1:D:308:ILE:HD13	1.69	0.75
1:B:193:VAL:HG11	1:B:220:ASP:OD2	1.87	0.74
1:B:197:LYS:HD3	5:B:511:HOH:O	1.87	0.74
1:B:37:VAL:HG21	1:B:61:HIS:HB2	1.68	0.74
1:C:7:LYS:HA	1:C:10:LEU:HD12	1.69	0.74
1:B:122:ARG:HB3	1:B:122:ARG:NH1	2.03	0.74
1:B:8:LEU:HD22	1:B:12:LEU:HD22	1.70	0.73
1:D:344:ASP:HB3	1:D:355:THR:CG2	2.18	0.73
1:C:102:PRO:HG2	1:C:138:LEU:HD12	1.70	0.73
1:D:231:VAL:HG21	1:D:239:THR:HG21	1.69	0.73
1:D:201:PRO:O	1:D:230:LYS:HG3	1.88	0.72
1:D:213:GLN:HG2	1:D:237:ALA:CB	2.09	0.72
1:C:134:ASN:O	1:C:138:LEU:HD22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:VAL:HG12	1:C:71:LEU:H	1.54	0.72
1:C:347:GLN:HG3	1:C:352:ILE:HD13	1.71	0.71
1:D:221:THR:C	1:D:222:VAL:HG13	2.15	0.71
1:D:334:MET:O	1:D:337:VAL:HG12	1.90	0.71
1:D:150:LEU:HD12	1:D:308:ILE:HD11	1.73	0.71
1:D:190:LEU:HD13	1:D:217:VAL:HG12	1.73	0.70
1:A:342:PHE:CE2	1:C:352:ILE:HG12	2.26	0.70
1:A:308:ILE:HD11	1:A:310:PHE:CZ	2.26	0.70
1:A:328:GLY:O	1:C:320:THR:HG22	1.92	0.70
1:D:111:ILE:HG23	1:D:121:VAL:HG11	1.73	0.70
1:D:148:VAL:HB	1:D:305:PHE:HA	1.74	0.70
1:C:205:CYS:HB3	1:C:213:GLN:NE2	2.07	0.70
1:A:106:VAL:HG22	1:A:109:ARG:NH2	2.07	0.69
1:C:220:ASP:O	1:C:243:THR:HG23	1.92	0.69
1:D:262:ILE:HD12	1:D:262:ILE:O	1.92	0.68
1:B:100:ARG:NH1	1:B:108:GLY:HA2	2.08	0.68
1:D:193:VAL:HG11	1:D:220:ASP:OD2	1.94	0.68
1:A:223:LEU:HB2	1:A:243:THR:HG21	1.75	0.68
1:A:290:GLU:HG3	1:A:291:GLY:N	2.07	0.68
1:B:105:LEU:HD23	1:B:105:LEU:H	1.58	0.68
1:C:343:THR:HB	1:C:355:THR:HG23	1.75	0.68
1:A:220:ASP:O	1:A:243:THR:HG23	1.93	0.68
1:D:140:PHE:CD2	1:D:141:MET:HE2	2.28	0.67
1:B:168:LYS:HE2	1:D:334:MET:HB3	1.75	0.67
1:C:7:LYS:HE3	5:C:534:HOH:O	1.95	0.67
1:D:125:ILE:H	1:D:125:ILE:CD1	1.96	0.67
1:A:122:ARG:HH11	1:A:122:ARG:HG2	1.58	0.67
1:B:84:ALA:O	1:B:88:ILE:HG12	1.94	0.67
1:B:334:MET:HE2	1:D:169:TRP:O	1.95	0.66
1:C:167:SER:O	1:C:169:TRP:N	2.28	0.66
1:C:125:ILE:HG22	1:C:126:LEU:HD13	1.77	0.66
1:D:178:ASP:O	1:D:181:GLN:HG2	1.95	0.66
1:D:231:VAL:HG23	1:D:232:ILE:N	2.10	0.66
1:A:360:LYS:HA	1:A:360:LYS:CE	2.24	0.66
1:A:317:ILE:HG12	1:C:337:VAL:HG21	1.77	0.66
1:B:216:ARG:HD2	1:B:237:ALA:HB3	1.79	0.65
1:A:96:PHE:CE1	1:A:122:ARG:HD2	2.32	0.65
1:C:191:VAL:HA	1:C:291:GLY:HA2	1.78	0.64
1:C:230:LYS:O	1:C:234:ASP:CB	2.25	0.64
1:A:75:SER:OG	1:A:109:ARG:HD2	1.97	0.64
1:C:102:PRO:CG	1:C:138:LEU:HD12	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LYS:HD2	1:B:207:LEU:HD12	1.80	0.64
1:D:267:THR:HG22	1:D:268:GLU:H	1.61	0.64
1:C:24:PRO:HG3	4:C:402:AOF:H9	1.78	0.64
1:D:221:THR:O	1:D:222:VAL:CB	2.44	0.64
1:C:71:LEU:HD23	1:C:72:GLU:H	1.63	0.64
1:D:193:VAL:HG11	1:D:220:ASP:CG	2.23	0.64
1:B:334:MET:O	1:B:337:VAL:HG13	1.98	0.64
1:D:196:VAL:HG13	1:D:230:LYS:HD3	1.80	0.64
1:D:191:VAL:CG1	1:D:195:THR:HB	2.28	0.63
1:D:218:ILE:HG12	1:D:230:LYS:HZ1	1.62	0.63
1:C:176:ARG:HG2	1:C:176:ARG:HH11	1.62	0.63
1:D:125:ILE:HD12	1:D:125:ILE:N	2.06	0.63
1:D:221:THR:C	1:D:222:VAL:HG22	2.22	0.63
1:D:218:ILE:HG12	1:D:230:LYS:NZ	2.15	0.62
1:D:272:ILE:HB	1:D:273:PRO:HD3	1.81	0.62
1:C:125:ILE:H	1:C:125:ILE:CD1	2.03	0.62
1:B:88:ILE:HG22	1:B:119:ILE:HD13	1.80	0.62
1:C:232:ILE:HD12	1:C:255:LEU:HD22	1.82	0.62
1:C:20:THR:OG1	1:C:25:LEU:HD11	1.99	0.62
1:C:184:LYS:NZ	1:C:184:LYS:HB2	2.14	0.61
1:D:63:GLU:HB3	5:D:532:HOH:O	2.00	0.61
1:B:46:GLY:HA2	1:B:79:LYS:HE2	1.81	0.61
1:B:148:VAL:HG22	1:B:287:VAL:CG1	2.30	0.61
1:B:334:MET:HA	1:B:337:VAL:CG1	2.31	0.61
1:D:217:VAL:C	1:D:218:ILE:HD12	2.26	0.61
1:D:274:ASP:O	1:D:278:ILE:HG12	2.00	0.60
1:D:138:LEU:O	1:D:142:ARG:HG3	2.00	0.60
1:B:232:ILE:HD13	1:B:255:LEU:HD22	1.84	0.60
1:D:231:VAL:HB	1:D:239:THR:OG1	2.01	0.60
1:A:152:ALA:HB3	1:A:310:PHE:CE1	2.36	0.60
1:C:347:GLN:O	1:C:348:ILE:HD13	2.01	0.60
1:A:243:THR:CG2	1:A:247:ALA:HB2	2.30	0.60
1:A:159:LYS:HE2	5:C:508:HOH:O	2.01	0.59
1:B:187:GLN:HE22	1:B:285:MET:CG	2.14	0.59
1:A:184:LYS:HE3	1:A:207:LEU:HD12	1.83	0.59
1:C:274:ASP:O	1:C:278:ILE:HG12	2.03	0.59
1:D:268:GLU:HG3	1:D:269:ARG:HG2	1.85	0.59
1:C:102:PRO:O	1:C:104:PRO:HD3	2.03	0.58
1:D:111:ILE:HG22	1:D:115:LYS:HE2	1.85	0.58
1:B:190:LEU:HD13	1:B:191:VAL:N	2.16	0.58
1:C:93:LYS:HD2	1:C:94:ARG:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ASP:OD1	1:C:168:LYS:HG3	2.02	0.58
1:B:344:ASP:HB3	1:B:355:THR:HG23	1.84	0.58
1:B:269:ARG:HD3	5:B:546:HOH:O	2.03	0.58
1:C:84:ALA:O	1:C:88:ILE:HG13	2.03	0.58
1:D:32:LYS:HE2	1:D:33:ASP:OD2	2.04	0.58
1:D:76:HIS:HB3	1:D:109:ARG:HH12	1.68	0.58
1:B:122:ARG:HB3	1:B:122:ARG:CZ	2.33	0.58
1:B:168:LYS:CE	1:D:334:MET:HB3	2.32	0.58
1:C:32:LYS:HE3	1:C:33:ASP:OD2	2.04	0.58
1:D:250:GLU:CB	1:D:254:ARG:HH21	2.17	0.58
1:A:8:LEU:HD11	1:A:39:MET:HE3	1.85	0.57
1:C:199:ASP:HB3	1:C:201:PRO:HD3	1.86	0.57
1:D:151:LYS:C	1:D:151:LYS:HD3	2.29	0.57
1:A:193:VAL:HG22	1:A:219:LEU:O	2.05	0.57
1:D:210:VAL:HG23	1:D:210:VAL:O	2.04	0.57
1:A:246:ARG:HH11	1:A:246:ARG:HB3	1.69	0.57
1:D:216:ARG:CZ	1:D:231:VAL:HG12	2.34	0.57
1:A:355:THR:HG23	5:A:559:HOH:O	2.04	0.57
1:C:3:GLU:HB2	1:C:126:LEU:HD11	1.87	0.57
1:B:184:LYS:CD	1:B:207:LEU:HD12	2.35	0.57
1:D:232:ILE:HD12	1:D:255:LEU:HD22	1.85	0.57
1:B:12:LEU:HD21	1:B:39:MET:HB3	1.86	0.57
1:B:75:SER:HB2	1:B:113:MET:CE	2.35	0.56
1:B:146:PRO:HD3	1:B:280:ALA:HB2	1.87	0.56
1:D:154:ALA:HB2	1:D:160:ILE:HD13	1.87	0.56
1:C:20:THR:CG2	1:C:25:LEU:CD1	2.75	0.56
1:C:93:LYS:HD2	1:C:94:ARG:N	2.20	0.56
1:C:193:VAL:HG11	1:C:220:ASP:OD2	2.06	0.56
1:B:24:PRO:HD3	1:B:137:PHE:CE2	2.41	0.56
1:B:97:VAL:O	1:B:123:GLU:HA	2.06	0.56
1:C:44:LYS:HE2	5:C:546:HOH:O	2.06	0.56
1:C:308:ILE:HD11	1:C:310:PHE:CZ	2.41	0.56
1:A:246:ARG:HB3	1:A:246:ARG:NH1	2.19	0.56
1:B:207:LEU:HB3	1:B:208:PRO:CD	2.35	0.56
1:B:344:ASP:HB3	1:B:355:THR:CG2	2.35	0.56
1:B:223:LEU:HD23	1:B:243:THR:CG2	2.36	0.56
1:B:345:ILE:O	1:B:345:ILE:HG13	2.05	0.56
1:D:148:VAL:H	1:D:306:GLN:HE21	1.51	0.56
1:D:191:VAL:HA	1:D:291:GLY:HA3	1.88	0.56
1:D:234:ASP:OD1	1:D:236:ILE:HD13	2.06	0.56
1:D:148:VAL:H	1:D:306:GLN:HE22	1.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:ASP:HB3	1:D:355:THR:HG21	1.87	0.56
1:A:122:ARG:HG2	1:A:122:ARG:NH1	2.20	0.56
1:C:125:ILE:HD12	1:C:125:ILE:N	2.09	0.56
1:D:230:LYS:HE3	1:D:231:VAL:CG2	2.36	0.56
1:A:51:GLU:H	1:A:51:GLU:CD	2.14	0.55
1:B:265:LEU:HD23	5:B:537:HOH:O	2.06	0.55
1:D:102:PRO:HG3	1:D:138:LEU:HD12	1.89	0.55
1:A:272:ILE:HB	1:A:273:PRO:HD3	1.88	0.55
1:C:234:ASP:O	1:C:235:GLN:HB3	2.07	0.55
1:C:20:THR:OG1	1:C:25:LEU:CD1	2.54	0.55
1:C:347:GLN:HG3	1:C:352:ILE:CD1	2.36	0.55
1:B:196:VAL:HA	1:B:201:PRO:HD2	1.88	0.55
1:B:315:LYS:HE2	1:D:339:LEU:HD13	1.89	0.55
1:C:6:MET:HB3	1:C:126:LEU:HD22	1.89	0.55
1:C:83:CYS:O	1:C:87:ILE:HG12	2.07	0.55
1:C:65:ALA:O	1:C:92:ILE:HG23	2.06	0.55
1:D:150:LEU:HD23	1:D:289:VAL:HB	1.89	0.55
1:D:320:THR:O	1:D:321:HIS:HB2	2.05	0.54
1:B:150:LEU:HD23	1:B:289:VAL:HB	1.89	0.54
1:D:298:SER:O	1:D:302:GLU:HG2	2.08	0.54
1:A:106:VAL:HG22	1:A:109:ARG:HH21	1.72	0.54
1:A:222:VAL:HG12	1:A:222:VAL:O	2.06	0.54
1:C:234:ASP:HB3	1:C:236:ILE:HG12	1.88	0.54
1:D:190:LEU:HD13	1:D:217:VAL:CG1	2.37	0.54
1:B:242:PHE:HD2	1:B:265:LEU:HD11	1.72	0.54
1:D:291:GLY:O	1:D:292:GLY:O	2.24	0.54
1:B:167:SER:HA	1:D:334:MET:HE3	1.90	0.54
1:A:2:GLU:HB3	1:A:125:ILE:HD13	1.90	0.54
1:A:345:ILE:HG23	1:A:354:LEU:CD2	2.38	0.54
1:B:159:LYS:HE2	5:D:533:HOH:O	2.07	0.54
1:C:344:ASP:H	1:C:355:THR:HG22	1.73	0.54
1:D:102:PRO:CG	1:D:138:LEU:HD12	2.38	0.54
1:A:326:ILE:HG22	5:A:572:HOH:O	2.08	0.54
1:D:71:LEU:HD23	1:D:72:GLU:H	1.72	0.53
1:A:35:GLN:OE1	1:B:44:LYS:NZ	2.40	0.53
1:A:278:ILE:O	1:A:282:GLU:HG2	2.08	0.53
1:B:0:SER:HB3	1:B:3:GLU:HB3	1.89	0.53
1:C:347:GLN:C	1:C:348:ILE:HD13	2.33	0.53
1:D:231:VAL:CG2	1:D:232:ILE:N	2.71	0.53
1:D:235:GLN:H	1:D:235:GLN:CD	2.16	0.53
1:A:310:PHE:CD2	1:C:156:LEU:HG	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:VAL:O	1:C:211:THR:OG1	2.20	0.53
1:C:232:ILE:HG22	1:C:233:CYS:SG	2.48	0.53
1:D:71:LEU:HD23	1:D:72:GLU:N	2.24	0.53
1:B:311:TYR:CE1	1:B:353:LYS:HD2	2.44	0.53
1:A:243:THR:HG22	1:A:244:THR:H	1.74	0.53
1:D:227:GLU:CD	1:D:251:LYS:HE3	2.34	0.53
1:D:189:ILE:HG13	1:D:214:PRO:HB2	1.90	0.53
1:A:169:TRP:N	1:A:169:TRP:CE3	2.77	0.53
1:A:201:PRO:HB3	3:A:402:AI9:H8	1.91	0.53
1:C:169:TRP:HA	1:C:169:TRP:HE3	1.73	0.52
1:D:203:LEU:HD22	1:D:203:LEU:N	2.24	0.52
1:D:335:LYS:HG3	1:D:336:ASP:OD1	2.09	0.52
1:A:272:ILE:O	1:A:275:VAL:HG22	2.10	0.52
1:C:148:VAL:HG22	1:C:287:VAL:CG1	2.39	0.52
1:A:310:PHE:HD2	1:C:156:LEU:HG	1.75	0.52
1:C:41:ALA:O	1:C:43:LEU:HD22	2.09	0.52
1:D:230:LYS:HE3	1:D:231:VAL:HG13	1.91	0.52
1:C:169:TRP:HA	1:C:169:TRP:CE3	2.45	0.52
1:D:72:GLU:OE1	1:D:111:ILE:HG12	2.10	0.52
1:C:202:SER:HB2	1:C:204:THR:HG23	1.92	0.52
1:C:222:VAL:HG12	1:C:222:VAL:O	2.09	0.52
1:C:181:GLN:HG3	1:C:182:TYR:N	2.24	0.52
1:C:243:THR:HG22	1:C:244:THR:N	2.17	0.52
1:C:55:ILE:HD11	1:C:67:ILE:HD12	1.92	0.52
1:D:221:THR:OG1	1:D:270:ILE:HD12	2.10	0.52
1:B:347:GLN:HG3	1:B:351:ASP:O	2.09	0.52
1:D:235:GLN:O	1:D:235:GLN:HG2	2.10	0.52
1:A:331:PHE:HB2	1:A:337:VAL:HG12	1.92	0.51
1:B:187:GLN:NE2	1:B:285:MET:HB2	2.24	0.51
1:B:129:GLN:HG2	1:B:132:ARG:HH21	1.75	0.51
1:D:102:PRO:HG2	1:D:137:PHE:HE1	1.75	0.51
1:D:277:LYS:O	1:D:281:GLU:HG3	2.11	0.51
1:A:51:GLU:OE1	1:A:51:GLU:N	2.35	0.51
1:C:159:LYS:HD2	1:C:322:ALA:HB3	1.92	0.51
1:D:235:GLN:OE1	1:D:235:GLN:N	2.42	0.51
1:A:12:LEU:HD11	1:A:39:MET:HE2	1.92	0.51
1:A:57:MET:HG3	1:B:53:HIS:CD2	2.45	0.51
1:D:84:ALA:O	1:D:88:ILE:HG13	2.10	0.51
1:D:267:THR:HG22	1:D:268:GLU:N	2.26	0.51
1:A:57:MET:HE2	1:B:53:HIS:HB3	1.93	0.51
1:B:199:ASP:O	1:B:200:ASN:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ILE:HD12	1:B:262:ILE:N	2.26	0.51
1:D:230:LYS:HG2	1:D:231:VAL:HG13	1.92	0.51
1:D:320:THR:O	1:D:321:HIS:CB	2.58	0.51
1:C:187:GLN:HE22	1:C:285:MET:HG3	1.75	0.51
1:C:152:ALA:HB3	1:C:310:PHE:CD1	2.46	0.51
1:C:202:SER:CB	1:C:204:THR:HG23	2.41	0.51
1:B:4:TYR:CD1	1:B:4:TYR:C	2.89	0.51
1:B:31:VAL:CG2	1:B:66:ASP:HB2	2.41	0.51
1:D:246:ARG:HD2	1:D:246:ARG:O	2.11	0.51
1:B:182:TYR:C	1:B:184:LYS:H	2.19	0.51
1:B:223:LEU:HD23	1:B:243:THR:HG21	1.91	0.51
1:B:254:ARG:O	1:B:257:ALA:HB3	2.11	0.51
1:D:193:VAL:HG13	1:D:219:LEU:O	2.11	0.51
1:D:74:CYS:HB2	1:D:76:HIS:CE1	2.46	0.50
1:B:150:LEU:CD2	1:B:289:VAL:HB	2.41	0.50
1:B:168:LYS:NZ	1:D:335:LYS:HB3	2.26	0.50
1:D:243:THR:HG22	1:D:244:THR:H	1.76	0.50
1:B:189:ILE:HD11	1:B:214:PRO:HG3	1.92	0.50
1:A:152:ALA:HB3	1:A:310:PHE:CD1	2.47	0.50
1:A:353:LYS:HG2	5:A:559:HOH:O	2.11	0.50
1:C:234:ASP:OD1	1:C:236:ILE:CG1	2.60	0.50
1:D:271:GLN:HB2	1:D:274:ASP:OD2	2.12	0.50
1:B:207:LEU:HB3	1:B:208:PRO:HD2	1.94	0.50
1:C:176:ARG:HG2	1:C:176:ARG:NH1	2.27	0.50
1:D:155:SER:HB2	1:D:315:LYS:O	2.12	0.50
1:D:111:ILE:HD12	1:D:121:VAL:HG11	1.95	0.49
1:A:193:VAL:HG22	1:A:220:ASP:HA	1.95	0.49
1:B:88:ILE:HG22	1:B:119:ILE:CD1	2.42	0.49
1:B:190:LEU:HD12	1:B:289:VAL:HG13	1.94	0.49
1:C:10:LEU:CD1	1:C:126:LEU:HD23	2.43	0.49
1:C:71:LEU:HD23	1:C:72:GLU:N	2.26	0.49
1:C:344:ASP:HB3	1:C:355:THR:CG2	2.43	0.49
1:D:252:LYS:NZ	1:D:252:LYS:HB2	2.26	0.49
1:D:230:LYS:O	1:D:231:VAL:C	2.56	0.49
1:C:151:LYS:HD3	1:C:151:LYS:C	2.38	0.49
1:A:271:GLN:HG3	5:A:575:HOH:O	2.11	0.49
1:B:178:ASP:O	1:B:181:GLN:HG2	2.13	0.49
1:B:202:SER:O	1:B:204:THR:HG23	2.12	0.49
1:D:150:LEU:HD12	1:D:308:ILE:CD1	2.41	0.49
1:A:82:PRO:HG2	1:A:85:GLU:HB2	1.95	0.49
1:D:291:GLY:O	1:D:295:VAL:HB	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:GLU:CD	1:B:268:GLU:H	2.20	0.49
1:C:151:LYS:HA	1:C:309:ILE:O	2.13	0.49
1:D:201:PRO:CG	1:D:203:LEU:HD21	2.35	0.49
1:D:227:GLU:HA	1:D:232:ILE:HG13	1.95	0.49
1:A:169:TRP:HE3	1:A:169:TRP:HA	1.78	0.48
1:B:173:GLU:OE2	1:B:176:ARG:HD2	2.13	0.48
1:C:102:PRO:HB2	1:C:141:MET:CB	2.42	0.48
1:C:290:GLU:O	1:C:291:GLY:O	2.30	0.48
1:D:140:PHE:CD1	1:D:285:MET:HA	2.48	0.48
1:D:223:LEU:O	1:D:251:LYS:NZ	2.46	0.48
1:B:103:ASN:OD1	1:B:104:PRO:HD2	2.13	0.48
1:D:102:PRO:HG2	1:D:137:PHE:CE1	2.48	0.48
1:A:169:TRP:CE3	1:A:169:TRP:CA	2.96	0.48
1:A:345:ILE:HG12	1:A:354:LEU:HD22	1.96	0.48
1:D:231:VAL:CG2	1:D:239:THR:HG21	2.39	0.48
1:A:9:ALA:O	1:A:27:GLY:HA3	2.13	0.48
1:A:67:ILE:HB	1:A:92:ILE:HD13	1.95	0.48
1:B:223:LEU:HB2	1:B:243:THR:HG21	1.94	0.48
1:C:103:ASN:O	1:C:107:ALA:N	2.45	0.48
1:D:161:ALA:HB2	1:D:167:SER:HB3	1.96	0.48
1:B:90:SER:OG	1:B:92:ILE:HG12	2.14	0.48
1:C:131:GLU:OE1	1:C:142:ARG:NH1	2.44	0.48
1:A:169:TRP:CE3	1:A:169:TRP:HA	2.49	0.48
1:A:337:VAL:HG23	1:A:337:VAL:O	2.13	0.48
1:D:244:THR:O	1:D:245:ALA:C	2.57	0.48
1:B:266:GLU:CD	1:B:266:GLU:H	2.21	0.48
1:D:182:TYR:C	1:D:184:LYS:H	2.22	0.48
1:B:193:VAL:HG11	1:B:220:ASP:CB	2.44	0.48
1:C:184:LYS:NZ	1:C:205:CYS:SG	2.86	0.48
1:D:66:ASP:OD1	1:D:94:ARG:HB3	2.13	0.48
1:C:333:SER:HB2	1:C:336:ASP:OD2	2.13	0.47
1:D:70:THR:O	1:D:98:ALA:HB3	2.13	0.47
1:D:207:LEU:HD23	1:D:208:PRO:HD2	1.94	0.47
1:A:223:LEU:HD13	1:A:251:LYS:HD3	1.96	0.47
1:B:75:SER:HB2	1:B:113:MET:HE1	1.95	0.47
1:C:92:ILE:O	1:C:119:ILE:HD12	2.14	0.47
1:A:308:ILE:HG22	1:A:356:ALA:O	2.13	0.47
1:C:8:LEU:HG	1:C:12:LEU:CD2	2.43	0.47
1:D:160:ILE:O	1:D:160:ILE:HG22	2.15	0.47
1:B:6:MET:HB3	1:B:126:LEU:HD12	1.97	0.47
1:D:267:THR:HG22	1:D:269:ARG:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:ILE:HG22	1:B:115:LYS:HE3	1.97	0.47
1:D:31:VAL:HA	1:D:35:GLN:O	2.15	0.47
1:A:69:VAL:HG12	1:A:71:LEU:H	1.79	0.47
1:A:221:THR:O	1:A:243:THR:HG22	2.14	0.47
1:B:107:ALA:C	1:B:109:ARG:H	2.22	0.47
1:B:160:ILE:O	1:B:161:ALA:HB2	2.15	0.47
1:B:223:LEU:CD1	1:B:251:LYS:HE2	2.45	0.47
1:B:223:LEU:HD11	1:B:255:LEU:CD1	2.44	0.47
1:D:230:LYS:O	1:D:232:ILE:N	2.48	0.47
1:C:164:THR:HG22	1:C:164:THR:O	2.13	0.47
1:D:75:SER:OG	1:D:109:ARG:HD2	2.15	0.47
1:D:120:GLU:HG3	5:D:569:HOH:O	2.14	0.47
1:B:66:ASP:OD1	1:B:94:ARG:HG3	2.15	0.47
1:C:268:GLU:CD	1:C:268:GLU:H	2.23	0.46
1:C:187:GLN:NE2	1:C:285:MET:HB2	2.30	0.46
1:D:191:VAL:HG12	1:D:192:GLY:N	2.30	0.46
1:C:227:GLU:HB2	5:C:575:HOH:O	2.15	0.46
1:B:190:LEU:HD13	1:B:190:LEU:C	2.40	0.46
1:C:53:HIS:HB3	1:D:57:MET:HE2	1.96	0.46
1:D:337:VAL:HG13	1:D:337:VAL:O	2.16	0.46
1:C:243:THR:HG21	1:C:247:ALA:HB2	1.97	0.46
1:D:216:ARG:NE	1:D:231:VAL:HG12	2.29	0.46
1:D:308:ILE:O	1:D:355:THR:HA	2.15	0.46
1:A:43:LEU:HD21	1:B:39:MET:HE2	1.97	0.46
1:B:339:LEU:O	1:B:359:THR:HG22	2.16	0.46
1:C:182:TYR:C	1:C:184:LYS:H	2.23	0.46
1:D:225:ILE:HD13	1:D:226:PRO:N	2.31	0.46
1:D:222:VAL:H	1:D:243:THR:HG22	1.80	0.46
1:C:220:ASP:CG	1:C:223:LEU:HA	2.41	0.45
1:C:344:ASP:HB3	1:C:355:THR:HG21	1.97	0.45
1:D:196:VAL:HA	1:D:201:PRO:HD2	1.98	0.45
1:A:76:HIS:O	1:A:82:PRO:HB3	2.16	0.45
1:B:6:MET:HE3	1:B:6:MET:O	2.15	0.45
1:A:167:SER:O	1:A:169:TRP:N	2.48	0.45
1:A:47:GLU:OE2	1:B:61:HIS:HE1	1.99	0.45
1:B:10:LEU:HD23	1:B:70:THR:CG2	2.46	0.45
1:C:56:HIS:NE2	1:D:56:HIS:CE1	2.84	0.45
1:C:191:VAL:HA	1:C:291:GLY:CA	2.45	0.45
1:D:101:ASP:OD1	1:D:102:PRO:HD2	2.16	0.45
1:C:258:PHE:N	1:C:258:PHE:CD1	2.84	0.45
1:B:223:LEU:HD11	1:B:255:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:LYS:HB2	1:C:184:LYS:HZ2	1.81	0.45
1:C:230:LYS:HB3	1:C:234:ASP:OD2	2.17	0.45
1:D:24:PRO:HD3	1:D:137:PHE:CE2	2.52	0.45
1:D:138:LEU:HB3	1:D:142:ARG:NH1	2.32	0.45
1:C:19:GLN:HB2	1:C:43:LEU:O	2.17	0.45
1:C:209:ASN:O	1:C:211:THR:HG23	2.16	0.45
1:A:53:HIS:HB3	1:B:57:MET:HE2	1.99	0.45
1:B:160:ILE:HG12	1:B:323:PRO:O	2.17	0.45
1:D:226:PRO:C	1:D:228:ASP:N	2.74	0.45
1:D:248:ASP:OD1	1:D:249:GLU:N	2.50	0.45
1:D:102:PRO:HB3	1:D:141:MET:HB2	1.99	0.44
1:D:250:GLU:HB3	1:D:254:ARG:HH21	1.82	0.44
1:B:100:ARG:HH11	1:B:108:GLY:HA2	1.78	0.44
1:C:17:GLU:HA	1:C:25:LEU:HD21	1.99	0.44
1:D:0:SER:OG	1:D:2:GLU:HG2	2.17	0.44
1:D:225:ILE:HG23	1:D:225:ILE:O	2.17	0.44
1:D:300:VAL:HG21	1:D:326:ILE:HD13	1.98	0.44
1:C:101:ASP:HA	1:C:102:PRO:HD3	1.81	0.44
1:C:234:ASP:OD1	1:C:236:ILE:HD11	2.17	0.44
1:C:272:ILE:HB	1:C:273:PRO:HD3	1.99	0.44
1:A:28:ALA:HA	1:A:68:TYR:O	2.17	0.44
1:B:268:GLU:CD	1:B:269:ARG:H	2.25	0.44
1:D:297:GLY:HA2	1:D:326:ILE:HG23	1.98	0.44
1:A:7:LYS:NZ	1:A:129:GLN:NE2	2.66	0.44
1:B:14:LYS:HG3	5:B:514:HOH:O	2.17	0.44
1:B:166:ASP:OD1	1:D:334:MET:HB2	2.17	0.44
1:B:170:ILE:HB	3:B:403:AI9:O4	2.18	0.44
1:B:190:LEU:CD2	1:B:217:VAL:HB	2.47	0.44
1:B:345:ILE:HG21	1:D:352:ILE:HD12	2.00	0.44
1:C:125:ILE:CG2	1:C:126:LEU:HD13	2.45	0.44
1:D:250:GLU:HB2	1:D:254:ARG:HH21	1.82	0.44
1:A:32:LYS:HG3	1:A:61:HIS:O	2.18	0.44
1:D:190:LEU:HD12	1:D:191:VAL:N	2.32	0.44
1:D:239:THR:C	1:D:240:TRP:HD1	2.26	0.44
1:B:191:VAL:HG21	1:B:195:THR:HG21	2.00	0.44
1:C:344:ASP:H	1:C:355:THR:CG2	2.30	0.44
1:B:269:ARG:O	1:B:270:ILE:C	2.61	0.43
1:D:182:TYR:CZ	1:D:309:ILE:HD13	2.53	0.43
1:C:51:GLU:O	1:C:55:ILE:HD13	2.18	0.43
1:C:258:PHE:N	1:C:258:PHE:HD1	2.16	0.43
1:D:150:LEU:HB2	1:D:308:ILE:CD1	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:ARG:NH2	5:D:531:HOH:O	2.51	0.43
1:A:96:PHE:HE1	1:A:122:ARG:HD2	1.80	0.43
1:A:169:TRP:N	1:A:169:TRP:CD2	2.85	0.43
1:C:134:ASN:C	1:C:138:LEU:HD22	2.43	0.43
1:A:106:VAL:O	1:A:109:ARG:HB2	2.18	0.43
1:A:178:ASP:O	1:A:181:GLN:HB2	2.18	0.43
1:B:181:GLN:HG3	1:B:182:TYR:N	2.33	0.43
1:B:243:THR:HB	1:B:244:THR:H	1.60	0.43
1:B:339:LEU:C	1:B:340:LEU:HD12	2.44	0.43
1:A:190:LEU:HD23	1:A:190:LEU:C	2.43	0.43
1:B:17:GLU:HA	1:B:25:LEU:HD11	1.99	0.43
1:B:319:GLY:HA2	1:D:329:GLU:O	2.18	0.43
1:D:199:ASP:O	1:D:200:ASN:HB3	2.19	0.43
1:D:228:ASP:O	1:D:228:ASP:OD1	2.37	0.43
1:B:45:TYR:CZ	1:B:79:LYS:HE3	2.53	0.43
1:B:166:ASP:OD1	1:B:168:LYS:HG2	2.18	0.43
1:C:223:LEU:HB2	1:C:243:THR:HG21	2.01	0.43
1:A:193:VAL:CG2	1:A:220:ASP:HA	2.48	0.43
1:D:113:MET:O	1:D:116:GLU:HB3	2.19	0.43
1:A:180:GLN:OE1	1:A:205:CYS:HA	2.18	0.43
1:B:189:ILE:HD11	1:B:214:PRO:CG	2.49	0.43
1:B:316:LEU:O	1:D:337:VAL:HG23	2.19	0.43
1:B:352:ILE:HD13	1:D:345:ILE:HD12	2.01	0.43
1:A:340:LEU:N	1:A:340:LEU:HD12	2.34	0.42
1:D:28:ALA:HA	1:D:68:TYR:O	2.19	0.42
1:D:220:ASP:OD1	1:D:221:THR:N	2.52	0.42
1:A:12:LEU:HD11	1:A:39:MET:CE	2.49	0.42
1:A:275:VAL:HG23	1:A:276:LEU:N	2.34	0.42
1:B:99:MET:HE1	1:B:138:LEU:HD21	2.00	0.42
1:B:151:LYS:HD2	1:B:288:TYR:OH	2.19	0.42
1:D:105:LEU:HD13	1:D:105:LEU:C	2.43	0.42
1:D:236:ILE:HG12	5:D:515:HOH:O	2.20	0.42
1:C:57:MET:HG3	1:D:53:HIS:CD2	2.54	0.42
1:D:230:LYS:HE2	1:D:230:LYS:HB3	1.92	0.42
1:D:230:LYS:CE	1:D:231:VAL:HG22	2.43	0.42
1:D:71:LEU:HB2	5:D:554:HOH:O	2.19	0.42
1:A:53:HIS:CD2	1:B:57:MET:HG3	2.55	0.42
1:A:170:ILE:HA	1:C:334:MET:HE2	2.02	0.42
1:C:245:ALA:C	1:C:247:ALA:H	2.27	0.42
1:A:210:VAL:O	1:A:210:VAL:HG23	2.20	0.42
1:A:222:VAL:O	1:A:222:VAL:CG1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLY:HA2	1:A:326:ILE:CG2	2.49	0.42
1:C:200:ASN:HD21	1:C:230:LYS:HG3	1.84	0.42
1:D:137:PHE:HD2	1:D:285:MET:HE1	1.84	0.42
1:D:226:PRO:C	1:D:228:ASP:H	2.26	0.42
1:B:171:THR:HG22	1:B:313:ALA:HB2	2.01	0.42
1:B:173:GLU:OE2	1:B:176:ARG:NH1	2.53	0.42
1:B:201:PRO:HB3	3:B:403:AI9:H8	2.01	0.42
1:B:234:ASP:C	1:B:236:ILE:H	2.27	0.42
1:B:272:ILE:N	1:B:273:PRO:CD	2.83	0.42
1:D:345:ILE:HD12	1:D:354:LEU:HD22	2.02	0.42
1:C:173:GLU:HG2	1:C:176:ARG:HH21	1.84	0.42
1:D:201:PRO:HG2	1:D:203:LEU:CD2	2.40	0.42
1:C:21:GLU:OE2	1:C:212:LYS:NZ	2.53	0.42
1:D:237:ALA:HB1	1:D:238:PRO:CD	2.50	0.42
1:A:311:TYR:CE1	1:A:353:LYS:HD2	2.55	0.41
1:B:234:ASP:OD2	1:B:236:ILE:HB	2.21	0.41
1:D:254:ARG:O	1:D:257:ALA:HB3	2.19	0.41
1:B:79:LYS:NZ	1:B:79:LYS:CB	2.83	0.41
1:B:190:LEU:HD22	1:B:217:VAL:HB	2.01	0.41
1:C:296:HIS:HB3	1:C:326:ILE:HD12	2.02	0.41
1:A:132:ARG:NE	1:A:132:ARG:HA	2.35	0.41
1:A:177:GLN:O	1:A:180:GLN:HB3	2.21	0.41
1:A:302:GLU:OE1	1:A:302:GLU:HA	2.20	0.41
1:B:216:ARG:HD2	1:B:237:ALA:CB	2.49	0.41
1:C:199:ASP:O	1:C:200:ASN:C	2.63	0.41
1:C:248:ASP:OD2	1:C:250:GLU:HB2	2.20	0.41
1:C:97:VAL:O	1:C:123:GLU:HA	2.21	0.41
1:D:206:ARG:HG3	1:D:206:ARG:HH11	1.86	0.41
1:D:225:ILE:HA	1:D:226:PRO:HD3	1.91	0.41
1:A:7:LYS:NZ	1:A:129:GLN:HE22	2.19	0.41
1:C:200:ASN:CG	1:C:200:ASN:O	2.64	0.41
1:C:317:ILE:HG22	1:C:318:GLY:O	2.21	0.41
1:C:337:VAL:HA	1:C:338:PRO:HD3	1.90	0.41
1:B:6:MET:HE1	1:B:70:THR:CG2	2.41	0.41
1:B:66:ASP:OD1	1:B:94:ARG:CG	2.69	0.41
1:B:157:ASP:OD1	1:B:316:LEU:HA	2.20	0.41
1:A:161:ALA:HB2	1:A:167:SER:HB3	2.03	0.41
1:C:103:ASN:HB2	1:C:106:VAL:HB	2.03	0.41
1:C:212:LYS:NZ	1:C:212:LYS:HB2	2.35	0.41
1:A:84:ALA:HB3	1:A:113:MET:HE2	2.03	0.41
1:A:93:LYS:HD3	1:A:93:LYS:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:MET:HE2	1:D:43:LEU:HD21	2.02	0.41
1:D:191:VAL:HG11	1:D:195:THR:HB	2.00	0.41
1:A:329:GLU:N	5:A:585:HOH:O	2.54	0.41
1:A:345:ILE:CD1	1:C:352:ILE:HD12	2.51	0.41
1:B:77:TYR:CD1	1:B:82:PRO:HD3	2.56	0.41
1:B:148:VAL:HG22	1:B:287:VAL:HG13	1.99	0.41
1:D:191:VAL:CG1	1:D:192:GLY:N	2.83	0.41
1:D:206:ARG:HG3	1:D:206:ARG:NH1	2.36	0.41
1:A:170:ILE:HG12	1:C:334:MET:CE	2.50	0.40
1:B:68:TYR:CD1	1:B:68:TYR:N	2.89	0.40
1:B:79:LYS:HB3	1:B:79:LYS:HZ3	1.85	0.40
1:C:190:LEU:HD23	1:C:191:VAL:N	2.36	0.40
1:D:161:ALA:CB	1:D:167:SER:HB3	2.51	0.40
1:C:200:ASN:ND2	1:C:230:LYS:HG3	2.36	0.40
1:D:344:ASP:C	1:D:345:ILE:HD13	2.46	0.40
1:B:31:VAL:HG22	1:B:66:ASP:HB2	2.03	0.40
1:B:88:ILE:HG12	1:B:88:ILE:H	1.58	0.40
1:C:1:MET:HE2	1:C:1:MET:HA	2.02	0.40
1:D:227:GLU:HG2	1:D:255:LEU:HD21	2.02	0.40
1:B:103:ASN:OD1	1:B:105:LEU:HD23	2.22	0.40
1:B:155:SER:HB3	1:B:317:ILE:HG12	2.03	0.40
1:D:9:ALA:HB2	1:D:29:VAL:HG13	2.03	0.40
1:A:345:ILE:HD11	1:C:352:ILE:CD1	2.51	0.40
1:C:75:SER:HA	1:C:82:PRO:HB3	2.03	0.40
1:C:243:THR:CG2	1:C:244:THR:H	2.20	0.40
1:D:2:GLU:HG2	1:D:2:GLU:H	1.57	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	359/373 (96%)	341 (95%)	17 (5%)	1 (0%)	36	44
1	B	359/373 (96%)	320 (89%)	32 (9%)	7 (2%)	6	7
1	C	359/373 (96%)	330 (92%)	25 (7%)	4 (1%)	11	15
1	D	359/373 (96%)	322 (90%)	29 (8%)	8 (2%)	5	5
All	All	1436/1492 (96%)	1313 (91%)	103 (7%)	20 (1%)	9	11

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	168	LYS
1	C	291	GLY
1	D	222	VAL
1	D	231	VAL
1	D	267	THR
1	D	292	GLY
1	B	270	ILE
1	C	198	ALA
1	D	329	GLU
1	A	168	LYS
1	C	199	ASP
1	D	234	ASP
1	D	259	GLY
1	B	107	ALA
1	B	209	ASN
1	B	208	PRO
1	B	235	GLN
1	B	108	GLY
1	B	125	ILE
1	D	102	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/305 (97%)	279 (95%)	16 (5%)	20	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	294/305 (96%)	275 (94%)	19 (6%)	15	22
1	C	294/305 (96%)	269 (92%)	25 (8%)	10	14
1	D	294/305 (96%)	274 (93%)	20 (7%)	14	20
All	All	1177/1220 (96%)	1097 (93%)	80 (7%)	14	20

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	71	LEU
1	A	86	LEU
1	A	135	GLU
1	A	138	LEU
1	A	181	GLN
1	A	193	VAL
1	A	223	LEU
1	A	243	THR
1	A	246	ARG
1	A	261	ASN
1	A	301	LYS
1	A	343	THR
1	A	350	ARG
1	A	355	THR
1	A	360	LYS
1	B	8	LEU
1	B	12	LEU
1	B	29	VAL
1	B	37	VAL
1	B	72	GLU
1	B	79	LYS
1	B	86	LEU
1	B	88	ILE
1	B	95	VAL
1	B	128	ASP
1	B	138	LEU
1	B	197	LYS
1	B	216	ARG
1	B	223	LEU
1	B	268	GLU
1	B	272	ILE
1	B	308	ILE

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Mol	Chain	Res	Type
1	B	337	VAL
1	B	355	THR
1	C	12	LEU
1	C	14	LYS
1	C	20	THR
1	C	43	LEU
1	C	71	LEU
1	C	85	GLU
1	C	86	LEU
1	C	106	VAL
1	C	116	GLU
1	C	125	ILE
1	C	128	ASP
1	C	138	LEU
1	C	169	TRP
1	C	176	ARG
1	C	184	LYS
1	C	193	VAL
1	C	199	ASP
1	C	212	LYS
1	C	228	ASP
1	C	234	ASP
1	C	264	THR
1	C	268	GLU
1	C	275	VAL
1	C	320	THR
1	C	340	LEU
1	D	25	LEU
1	D	29	VAL
1	D	31	VAL
1	D	71	LEU
1	D	86	LEU
1	D	93	LYS
1	D	122	ARG
1	D	125	ILE
1	D	138	LEU
1	D	173	GLU
1	D	208	PRO
1	D	213	GLN
1	D	221	THR
1	D	225	ILE
1	D	235	GLN

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Mol	Chain	Res	Type
1	D	243	THR
1	D	252	LYS
1	D	270	ILE
1	D	301	LYS
1	D	335	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	53	HIS
1	A	129	GLN
1	A	139	HIS
1	A	181	GLN
1	A	187	GLN
1	A	296	HIS
1	B	23	ASN
1	B	53	HIS
1	B	61	HIS
1	B	129	GLN
1	B	180	GLN
1	B	187	GLN
1	B	235	GLN
1	B	271	GLN
1	B	341	GLN
1	C	23	ASN
1	C	187	GLN
1	C	332	GLN
1	C	341	GLN
1	D	53	HIS
1	D	89	ASN
1	D	129	GLN
1	D	180	GLN
1	D	186	HIS
1	D	213	GLN
1	D	261	ASN
1	D	306	GLN
1	D	332	GLN
1	D	347	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	AOF	D	402	2	22,24,24	1.62	5 (22%)	31,36,36	4.50	20 (64%)
3	AI9	B	403	-	20,23,23	2.41	6 (30%)	25,33,33	1.96	7 (28%)
3	AI9	A	402	-	20,23,23	2.27	6 (30%)	25,33,33	1.94	8 (32%)
4	AOF	C	402	2	22,24,24	1.79	5 (22%)	31,36,36	4.31	20 (64%)
4	AOF	B	402	2	22,24,24	1.72	4 (18%)	31,36,36	4.37	19 (61%)
3	AI9	C	403	-	20,23,23	2.34	6 (30%)	25,33,33	1.88	6 (24%)
3	AI9	D	403	-	20,23,23	2.45	6 (30%)	25,33,33	1.96	7 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	AOF	D	402	2	-	3/10/26/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AI9	B	403	-	-	4/15/19/19	0/1/1/1
3	AI9	A	402	-	-	4/15/19/19	0/1/1/1
4	AOF	C	402	2	-	2/10/26/26	0/2/2/2
4	AOF	B	402	2	-	3/10/26/26	0/2/2/2
3	AI9	C	403	-	-	0/15/19/19	0/1/1/1
3	AI9	D	403	-	-	3/15/19/19	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	AI9	O4-C4	5.50	1.34	1.23
3	B	403	AI9	O2-C2	5.44	1.34	1.23
3	A	402	AI9	O4-C4	5.05	1.33	1.23
3	D	403	AI9	O2-C2	4.98	1.33	1.23
3	B	403	AI9	O4-C4	4.97	1.33	1.23
3	C	403	AI9	O2-C2	4.75	1.33	1.23
3	A	402	AI9	O2-C2	4.69	1.33	1.23
3	B	403	AI9	P-O1P	4.65	1.64	1.50
3	C	403	AI9	O4-C4	4.56	1.32	1.23
3	D	403	AI9	P-O1P	4.51	1.64	1.50
4	C	402	AOF	C2-N3	4.51	1.44	1.37
3	C	403	AI9	C5'-C4'	4.47	1.57	1.51
3	A	402	AI9	P-O1P	4.31	1.63	1.50
4	C	402	AOF	C6-N1	4.19	1.43	1.37
3	C	403	AI9	P-O1P	4.19	1.63	1.50
4	D	402	AOF	C2-N3	4.18	1.44	1.37
4	B	402	AOF	C2-N3	4.10	1.44	1.37
4	B	402	AOF	C6-N1	4.01	1.43	1.37
4	B	402	AOF	C2-N1	3.99	1.44	1.37
3	D	403	AI9	C5'-C4'	3.72	1.56	1.51
4	C	402	AOF	C2-N1	3.71	1.43	1.37
3	A	402	AI9	C5'-C4'	3.65	1.56	1.51
4	D	402	AOF	C6-N1	3.61	1.42	1.37
3	B	403	AI9	C5'-C4'	3.51	1.56	1.51
3	C	403	AI9	P-O2P	3.40	1.67	1.54
3	D	403	AI9	P-O3P	3.33	1.67	1.54
3	D	403	AI9	P-O2P	3.33	1.67	1.54
3	B	403	AI9	P-O2P	3.27	1.67	1.54
3	B	403	AI9	P-O3P	3.20	1.66	1.54
4	D	402	AOF	C2-N1	3.08	1.42	1.37
3	A	402	AI9	P-O2P	3.05	1.66	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	AI9	P-O3P	2.99	1.65	1.54
3	C	403	AI9	P-O3P	2.93	1.65	1.54
4	C	402	AOF	C4-N3	2.70	1.43	1.38
4	D	402	AOF	C4-N3	2.60	1.43	1.38
4	B	402	AOF	C4-N3	2.45	1.43	1.38
4	D	402	AOF	P-O1P	2.15	1.62	1.54
4	C	402	AOF	P-O1P	2.13	1.62	1.54

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	AOF	O2-C2-N1	-15.93	93.56	121.86
4	C	402	AOF	O2-C2-N1	-15.45	94.40	121.86
4	B	402	AOF	O2-C2-N1	-15.44	94.42	121.86
4	B	402	AOF	O2-C2-N3	-9.02	105.83	121.86
4	D	402	AOF	O2-C2-N3	-8.85	106.13	121.86
4	C	402	AOF	O2-C2-N3	-8.60	106.58	121.86
4	D	402	AOF	O4'-C1'-N1'	-7.75	101.44	110.22
4	C	402	AOF	O4'-C1'-N1'	-6.85	102.46	110.22
4	B	402	AOF	O4'-C1'-N1'	-5.82	103.63	110.22
4	B	402	AOF	O3'-C3'-C4'	-5.79	94.44	111.08
4	D	402	AOF	O3'-C3'-C4'	-5.56	95.12	111.08
4	B	402	AOF	C5-C4-N3	5.35	121.32	111.10
4	B	402	AOF	C4-N3-C2	-5.32	119.04	126.37
4	C	402	AOF	C5-C4-N3	5.30	121.22	111.10
4	C	402	AOF	C4-N3-C2	-5.24	119.16	126.37
4	D	402	AOF	C5-C4-N3	5.16	120.96	111.10
4	D	402	AOF	C4-N3-C2	-5.00	119.48	126.37
4	C	402	AOF	O3'-C3'-C4'	-4.80	97.30	111.08
4	D	402	AOF	O4'-C4'-C5'	-4.31	95.51	109.33
3	C	403	AI9	C5-C4-N3	4.26	119.24	111.10
4	C	402	AOF	O1P-P-O5'	-4.20	95.72	106.67
3	B	403	AI9	C5-C4-N3	4.20	119.12	111.10
4	C	402	AOF	O4'-C4'-C5'	-4.17	95.99	109.33
4	B	402	AOF	O1P-P-O5'	-4.15	95.84	106.67
3	D	403	AI9	C5-C4-N3	4.11	118.96	111.10
4	D	402	AOF	O1P-P-O5'	-4.08	96.02	106.67
3	A	402	AI9	C5-C4-N3	4.08	118.90	111.10
4	B	402	AOF	O4'-C4'-C5'	-4.03	96.42	109.33
4	B	402	AOF	O4'-C1'-C2'	-3.75	102.39	106.29
4	D	402	AOF	C1'-N1'-C6	3.73	131.30	123.53
3	C	403	AI9	C4-N3-C2	-3.73	121.24	126.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	402	AOF	C1'-N1'-C6	3.69	131.22	123.53
4	D	402	AOF	O4'-C1'-C2'	-3.62	102.52	106.29
3	A	402	AI9	O5'-P-O1P	3.57	116.10	106.44
3	A	402	AI9	C4-N3-C2	-3.51	121.53	126.37
3	D	403	AI9	C1'-N1'-C6	3.51	126.43	120.60
3	D	403	AI9	C4-N3-C2	-3.42	121.66	126.37
3	B	403	AI9	C4-N3-C2	-3.37	121.73	126.37
4	D	402	AOF	N1-C2-N3	3.35	121.00	115.74
3	B	403	AI9	C1'-N1'-C6	3.34	126.16	120.60
4	B	402	AOF	N1-C2-N3	3.31	120.94	115.74
3	B	403	AI9	O5'-P-O1P	3.30	115.35	106.44
4	C	402	AOF	N1-C2-N3	3.22	120.80	115.74
3	A	402	AI9	C1'-N1'-C6	3.21	125.94	120.60
4	B	402	AOF	O2P-P-O5'	3.18	114.96	106.67
4	B	402	AOF	C3'-C2'-C1'	3.12	107.35	101.46
4	C	402	AOF	C3'-C2'-C1'	3.11	107.33	101.46
3	D	403	AI9	O5'-P-O1P	3.02	114.60	106.44
4	D	402	AOF	O2P-P-O5'	3.00	114.48	106.67
4	D	402	AOF	O3'-C3'-C2'	2.98	121.38	111.82
4	C	402	AOF	O2P-P-O5'	2.98	114.43	106.67
3	B	403	AI9	O4-C4-C5	-2.95	120.04	127.48
4	C	402	AOF	C1'-N1'-C6	2.93	129.64	123.53
4	D	402	AOF	C3'-C2'-C1'	2.93	106.99	101.46
3	D	403	AI9	N1-C2-N3	2.90	120.30	115.74
3	A	402	AI9	N1-C2-N3	2.89	120.28	115.74
3	C	403	AI9	N1-C2-N3	2.84	120.21	115.74
3	C	403	AI9	O4-C4-C5	-2.82	120.37	127.48
4	C	402	AOF	O3'-C3'-C2'	2.81	120.82	111.82
4	C	402	AOF	C4'-O4'-C1'	2.77	114.38	108.63
4	B	402	AOF	C5'-C4'-C3'	2.72	125.01	115.21
4	D	402	AOF	C4'-O4'-C1'	2.68	114.19	108.63
4	B	402	AOF	O3'-C3'-C2'	2.67	120.39	111.82
4	B	402	AOF	C4'-O4'-C1'	2.67	114.17	108.63
3	D	403	AI9	O4-C4-C5	-2.67	120.75	127.48
4	D	402	AOF	O2'-C2'-C1'	2.63	119.13	110.10
3	A	402	AI9	O4-C4-C5	-2.59	120.95	127.48
4	B	402	AOF	O2'-C2'-C1'	2.52	118.77	110.10
3	C	403	AI9	O5'-P-O1P	2.52	113.25	106.44
4	D	402	AOF	C5-C6-N1	2.52	123.93	118.51
4	D	402	AOF	C5'-C4'-C3'	2.48	124.12	115.21
3	B	403	AI9	N1-C2-N3	2.46	119.61	115.74
3	C	403	AI9	C1'-N1'-C6	2.41	124.60	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	402	AOF	C5'-C4'-C3'	2.38	123.78	115.21
3	A	402	AI9	O4'-C4'-C5'	-2.37	104.75	109.99
3	B	403	AI9	C5'-C4'-C3'	-2.36	107.77	112.22
4	C	402	AOF	C5-C6-N1	2.33	123.52	118.51
4	D	402	AOF	N1-C6-N1'	-2.32	115.28	118.66
3	A	402	AI9	O3'-C3'-C2'	-2.27	104.92	109.13
4	C	402	AOF	O2'-C2'-C1'	2.23	117.78	110.10
4	B	402	AOF	C5-C6-N1	2.17	123.19	118.51
4	C	402	AOF	O4-C4-C5	-2.15	122.06	127.48
4	D	402	AOF	O4-C4-C5	-2.13	122.10	127.48
4	C	402	AOF	O4'-C1'-C2'	-2.13	104.07	106.29
4	B	402	AOF	O4-C4-C5	-2.08	122.22	127.48
4	C	402	AOF	N1-C6-N1'	-2.01	115.74	118.66
3	D	403	AI9	O3'-C3'-C2'	-2.01	105.40	109.13

There are no chirality outliers.

All (19) torsion outliers are listed below:

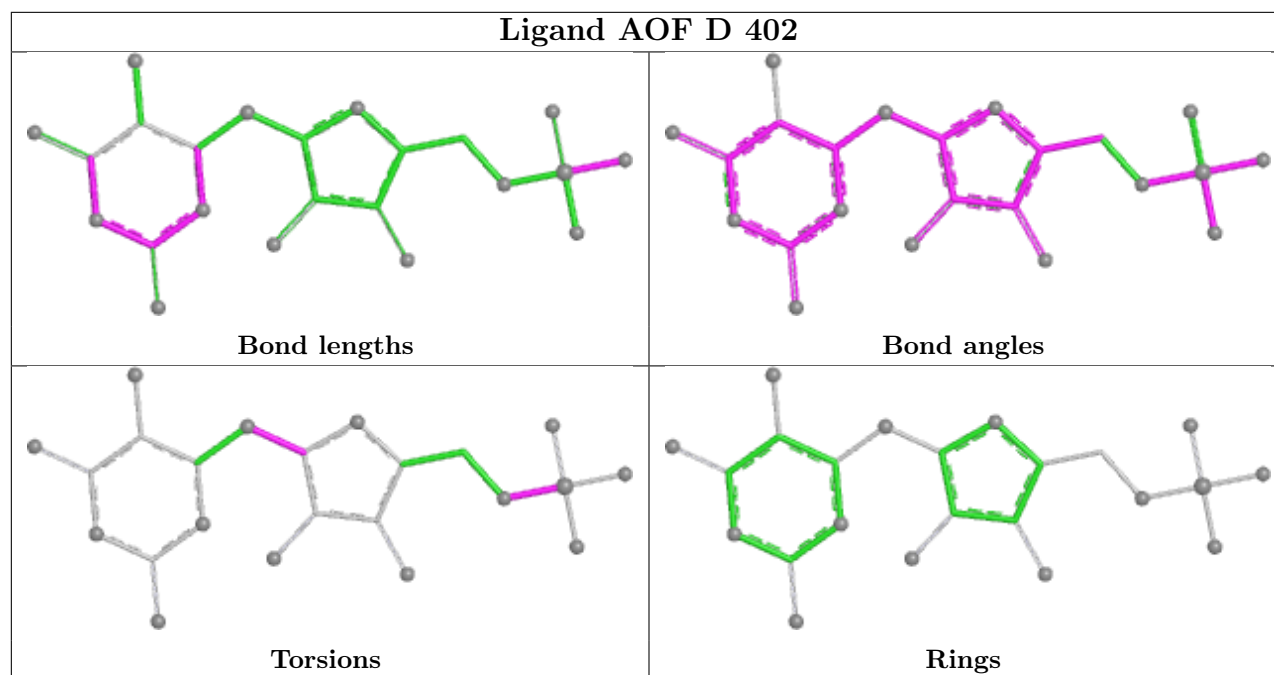
Mol	Chain	Res	Type	Atoms
3	A	402	AI9	C5'-O5'-P-O2P
3	A	402	AI9	C5'-O5'-P-O3P
3	A	402	AI9	C2'-C1'-N1'-C6
3	B	403	AI9	C5'-O5'-P-O1P
3	B	403	AI9	C5'-O5'-P-O2P
3	B	403	AI9	C5'-O5'-P-O3P
3	B	403	AI9	C2'-C1'-N1'-C6
3	D	403	AI9	C5'-O5'-P-O2P
3	D	403	AI9	C5'-O5'-P-O3P
4	B	402	AOF	C5'-O5'-P-O1P
4	B	402	AOF	C5'-O5'-P-O2P
4	D	402	AOF	C5'-O5'-P-O1P
4	D	402	AOF	O4'-C1'-N1'-C6
3	D	403	AI9	C5'-O5'-P-O1P
4	D	402	AOF	C5'-O5'-P-O2P
4	B	402	AOF	O4'-C1'-N1'-C6
4	C	402	AOF	O4'-C1'-N1'-C6
3	A	402	AI9	C5'-O5'-P-O1P
4	C	402	AOF	C5'-O5'-P-O2P

There are no ring outliers.

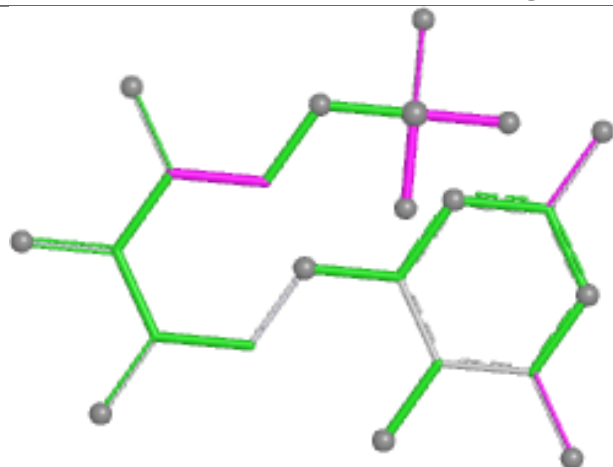
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	403	AI9	2	0
3	A	402	AI9	1	0
4	C	402	AOF	1	0

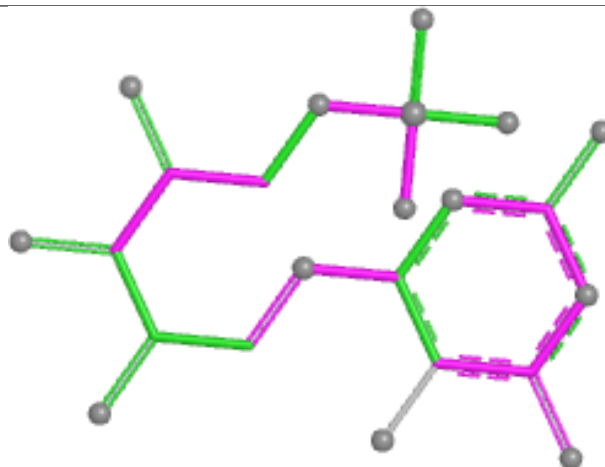
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



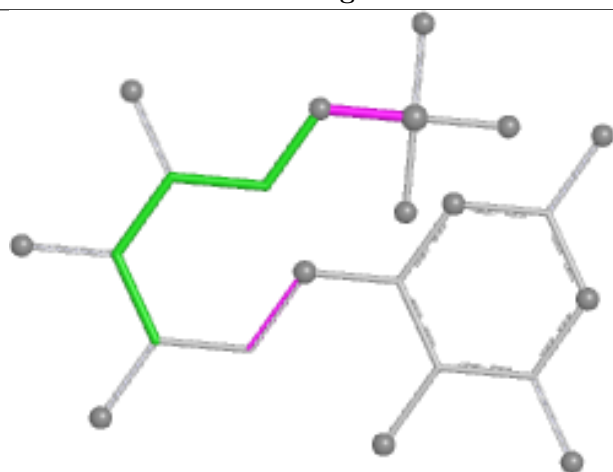
Ligand AI9 B 403



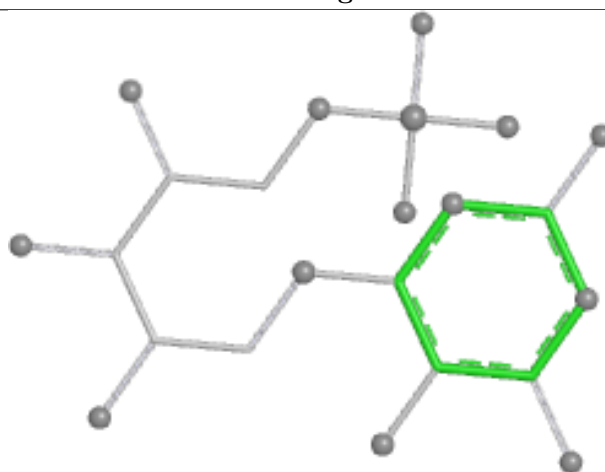
Bond lengths



Bond angles

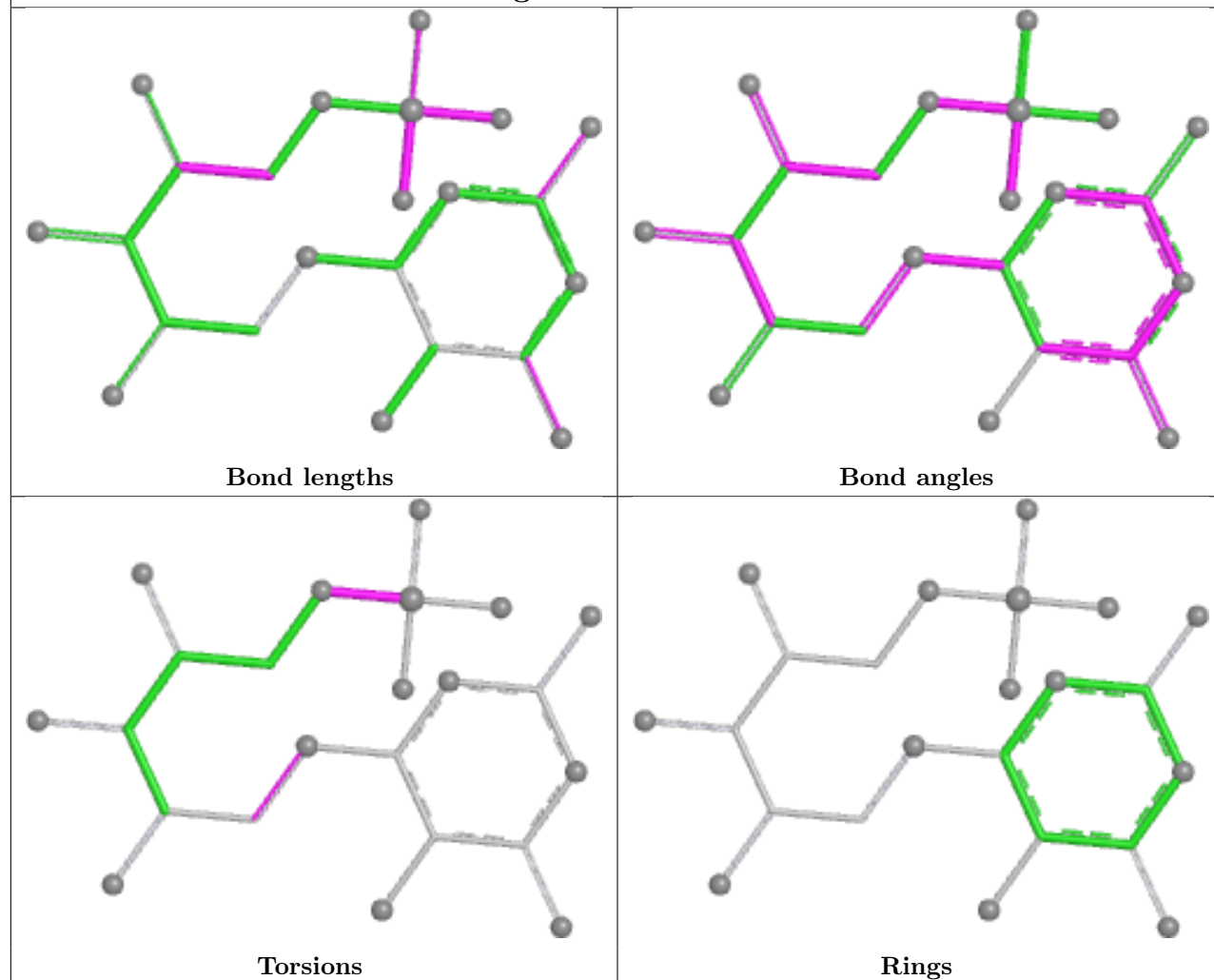


Torsions

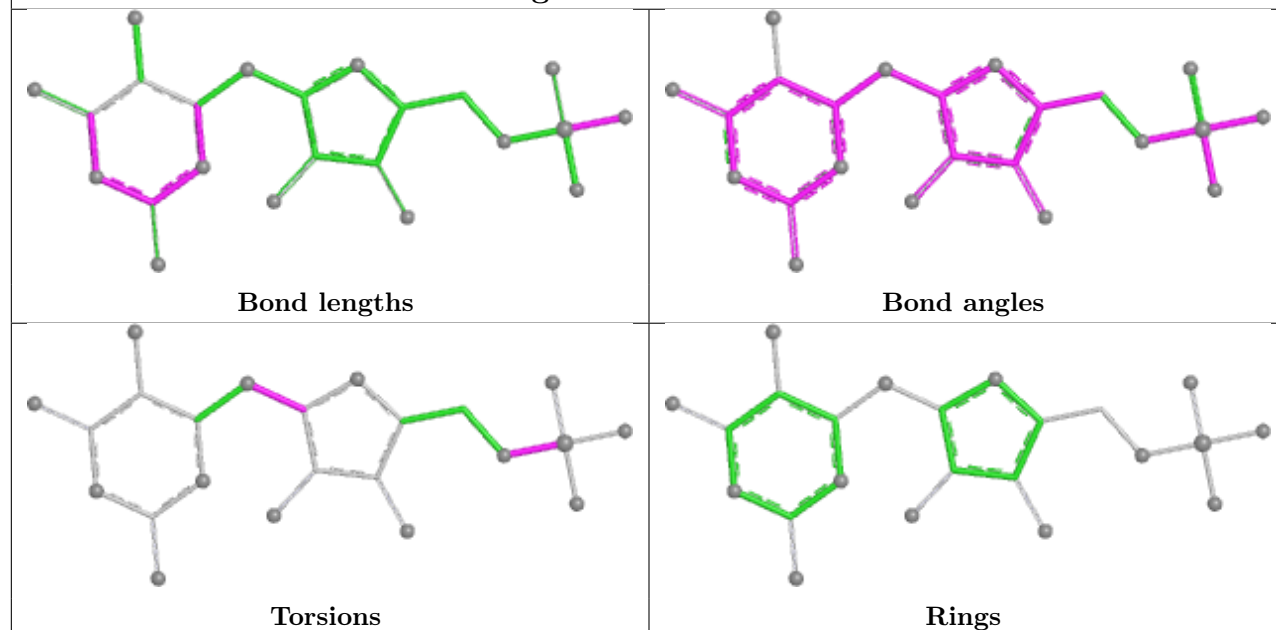


Rings

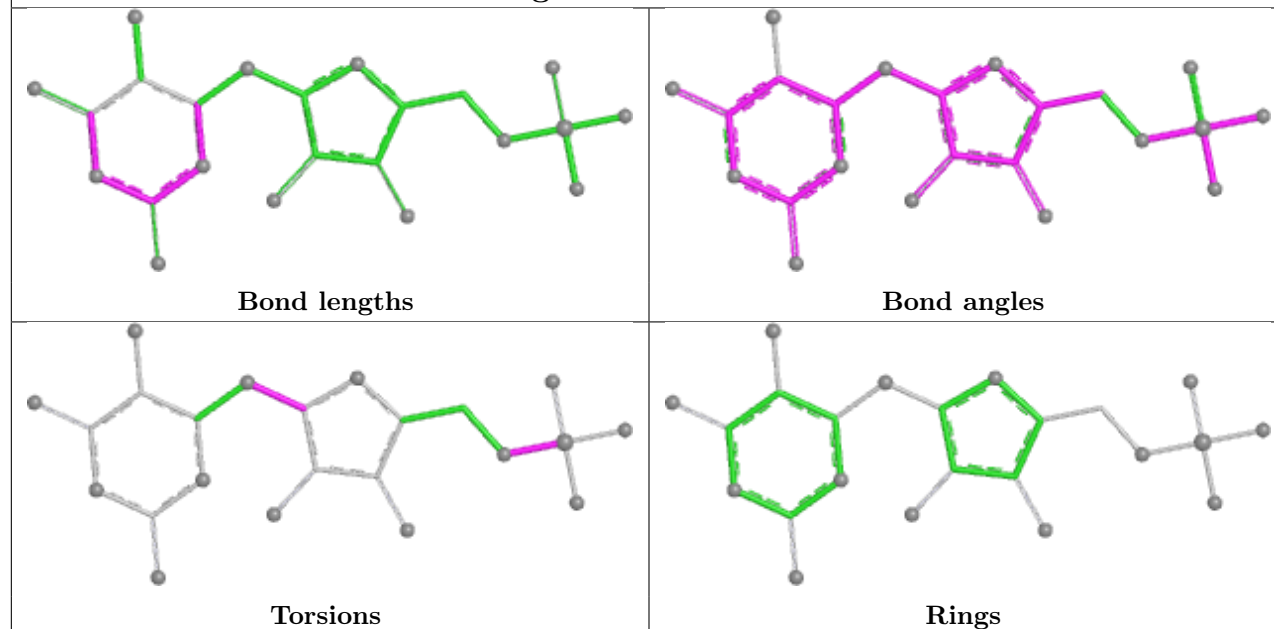
Ligand AI9 A 402



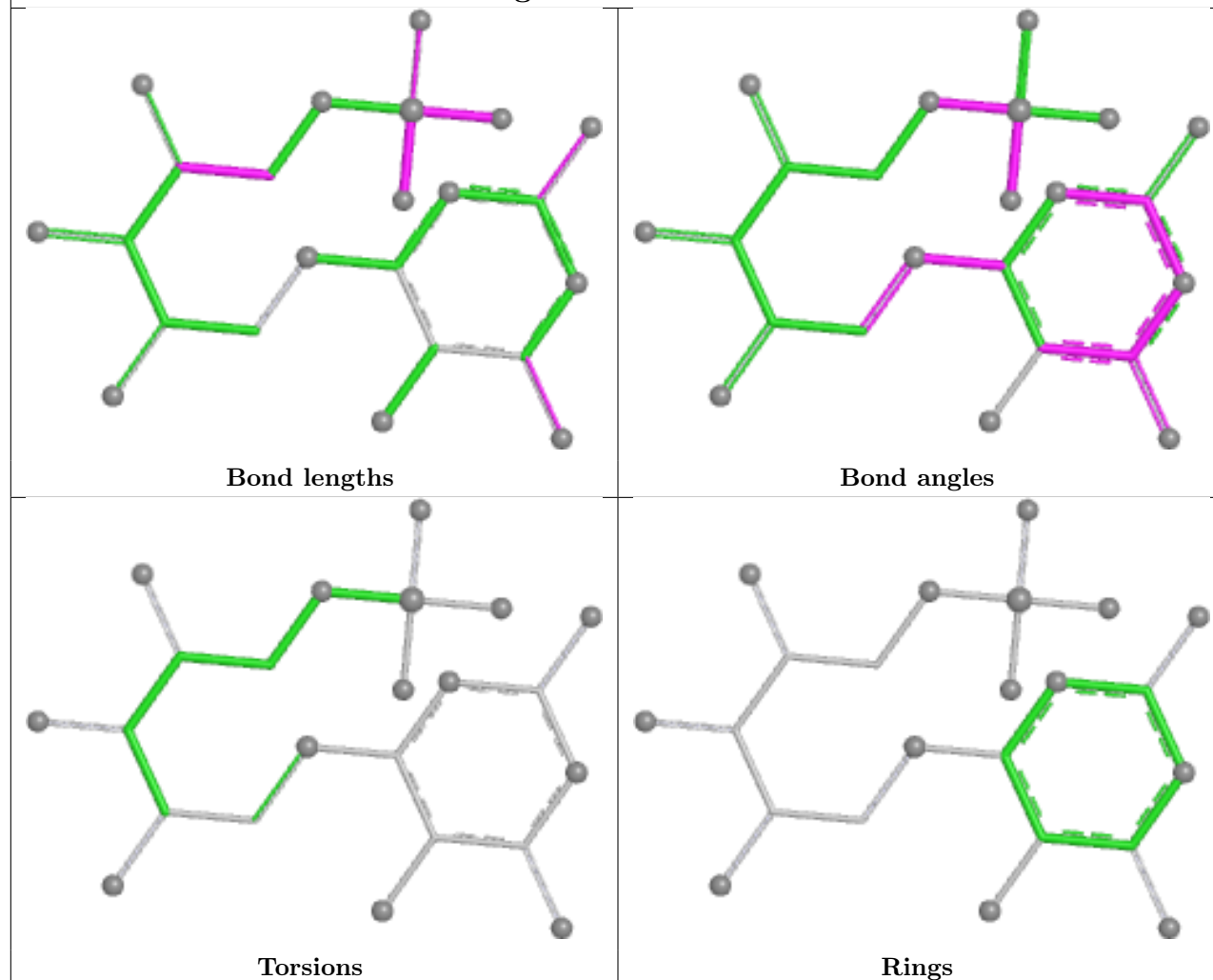
Ligand AOF C 402

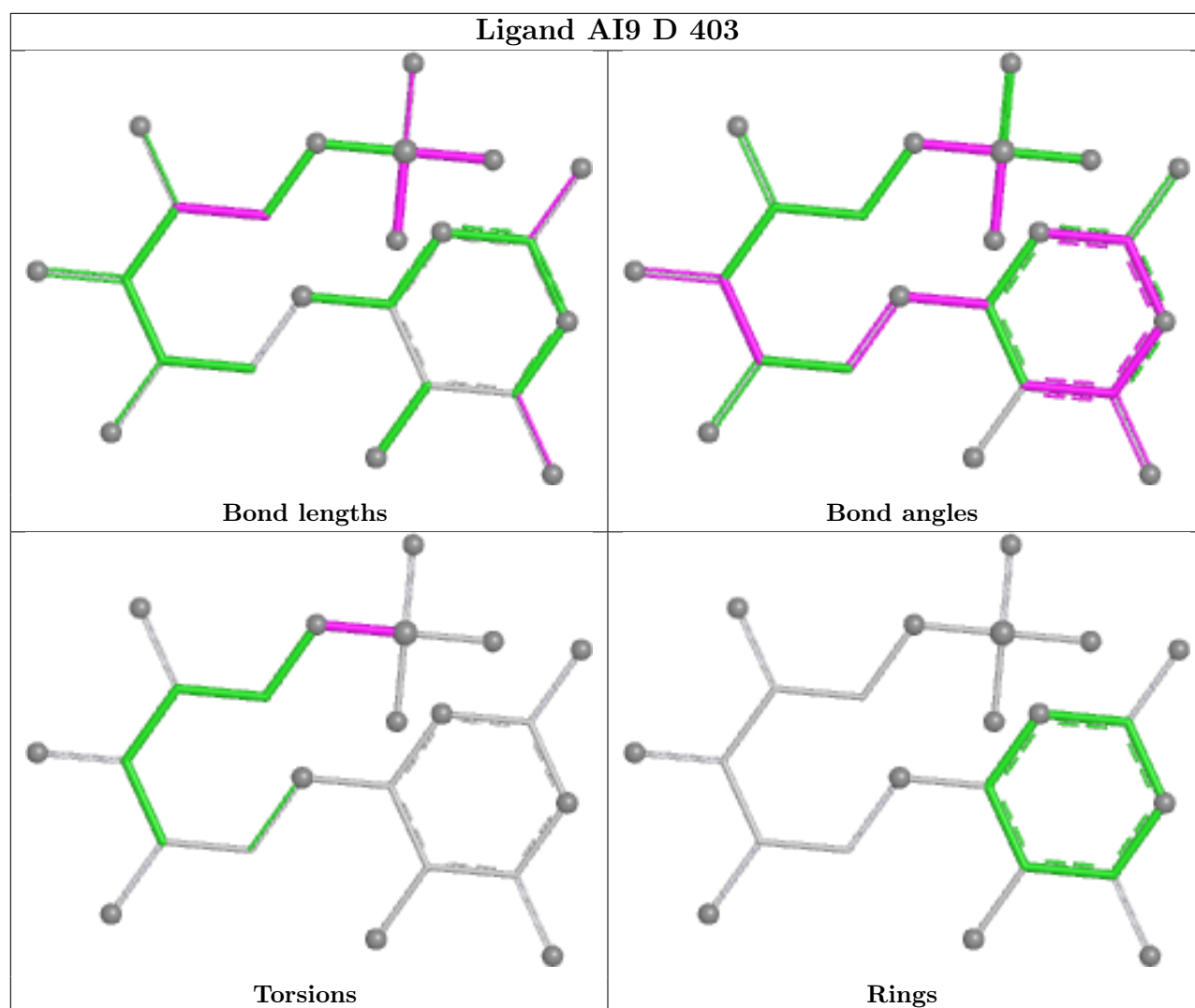


Ligand AOF B 402



Ligand AI9 C 403





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	361/373 (96%)	-0.10	5 (1%) 73 75	33, 49, 64, 78	0
1	B	361/373 (96%)	0.22	8 (2%) 62 63	40, 58, 73, 85	0
1	C	361/373 (96%)	0.33	18 (4%) 34 34	42, 60, 77, 84	0
1	D	361/373 (96%)	0.50	32 (8%) 15 15	37, 61, 82, 87	0
All	All	1444/1492 (96%)	0.24	63 (4%) 39 40	33, 56, 77, 87	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	106	VAL	5.4
1	D	80	THR	5.0
1	D	169	TRP	5.0
1	C	20	THR	4.8
1	D	247	ALA	4.4
1	D	230	LYS	4.3
1	C	210	VAL	4.3
1	B	169	TRP	4.3
1	D	208	PRO	4.1
1	A	235	GLN	4.0
1	D	78	GLY	3.9
1	D	211	THR	3.7
1	D	213	GLN	3.6
1	C	104	PRO	3.5
1	C	291	GLY	3.4
1	D	81	PRO	3.3
1	D	210	VAL	3.2
1	C	211	THR	3.1
1	D	249	GLU	3.1
1	C	105	LEU	3.1
1	D	77	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	207	LEU	3.0
1	D	106	VAL	2.7
1	B	77	TYR	2.7
1	C	21	GLU	2.7
1	A	317	ILE	2.6
1	D	102	PRO	2.6
1	D	258	PHE	2.6
1	B	210	VAL	2.6
1	B	209	ASN	2.6
1	D	209	ASN	2.6
1	D	235	GLN	2.6
1	D	205	CYS	2.5
1	C	82	PRO	2.5
1	C	77	TYR	2.5
1	B	211	THR	2.4
1	C	81	PRO	2.4
1	D	220	ASP	2.4
1	D	222	VAL	2.4
1	C	80	THR	2.4
1	C	102	PRO	2.3
1	A	291	GLY	2.3
1	D	233	CYS	2.3
1	C	234	ASP	2.3
1	D	281	GLU	2.3
1	D	243	THR	2.3
1	D	231	VAL	2.3
1	A	211	THR	2.3
1	D	181	GLN	2.2
1	B	105	LEU	2.2
1	C	103	ASN	2.2
1	B	76	HIS	2.2
1	D	212	LYS	2.2
1	B	208	PRO	2.2
1	C	235	GLN	2.1
1	A	132	ARG	2.1
1	C	209	ASN	2.1
1	D	255	LEU	2.1
1	D	246	ARG	2.1
1	D	234	ASP	2.1
1	C	208	PRO	2.1
1	D	270	ILE	2.1
1	D	262	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

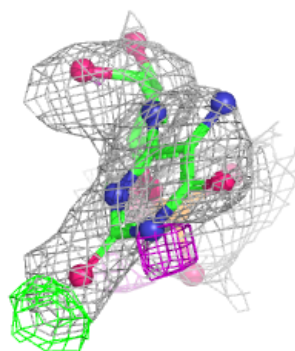
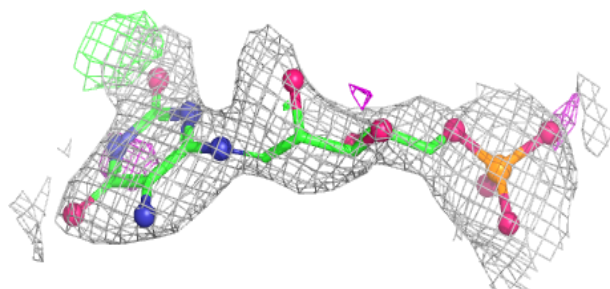
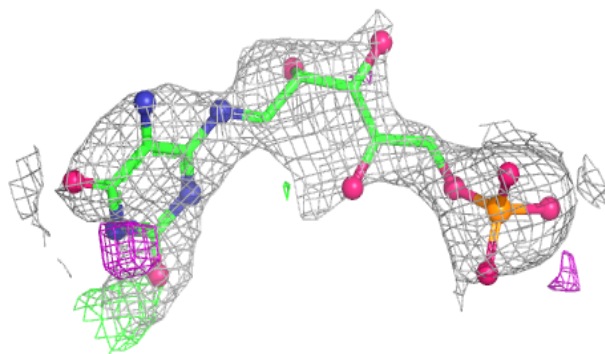
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AI9	B	403	23/23	0.74	0.14	70,78,81,83	0
3	AI9	D	403	23/23	0.83	0.12	75,77,81,81	0
4	AOF	D	402	23/23	0.84	0.12	71,73,76,77	0
4	AOF	C	402	23/23	0.87	0.11	67,72,74,74	0
3	AI9	C	403	23/23	0.87	0.13	62,73,80,81	0
4	AOF	B	402	23/23	0.92	0.10	63,66,69,72	0
3	AI9	A	402	23/23	0.93	0.08	52,60,62,63	0
2	ZN	B	401	1/1	0.98	0.03	63,63,63,63	0
2	ZN	C	401	1/1	0.99	0.03	69,69,69,69	0
2	ZN	A	401	1/1	0.99	0.04	39,39,39,39	0
2	ZN	D	401	1/1	1.00	0.05	53,53,53,53	0

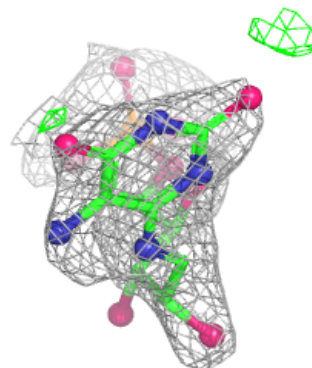
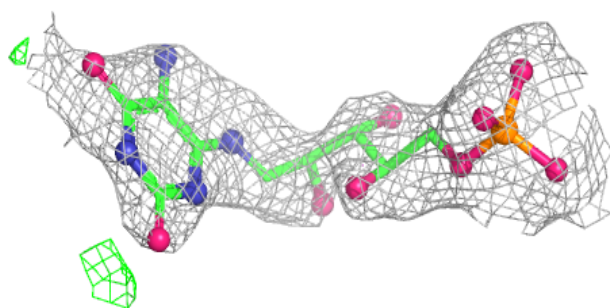
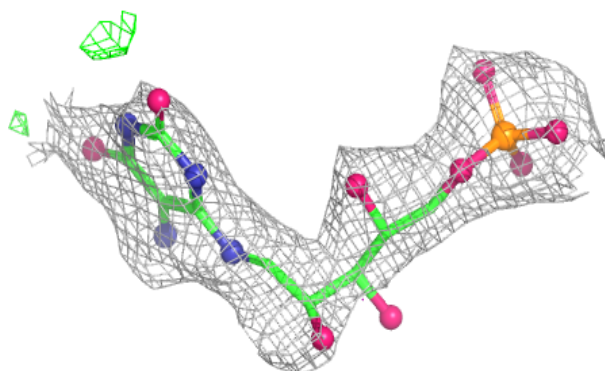
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AI9 B 403:

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

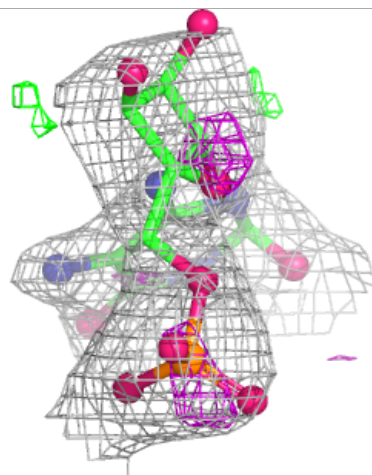
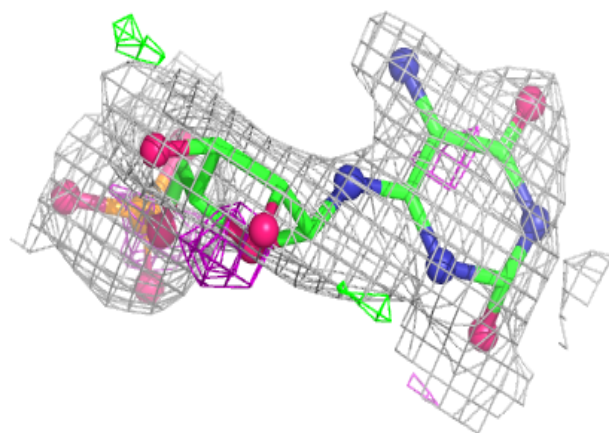
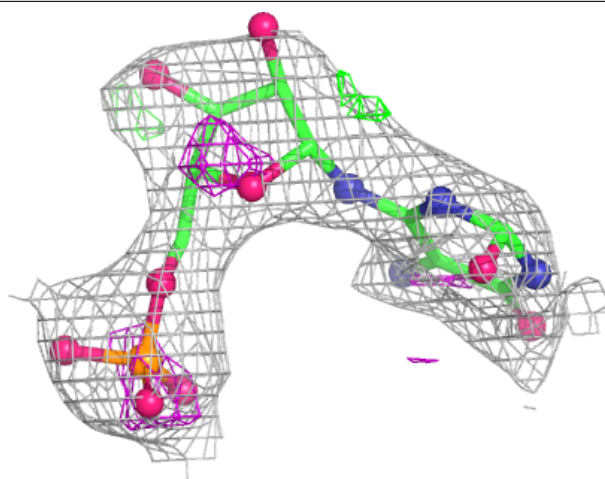
**Electron density around AI9 D 403:**

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



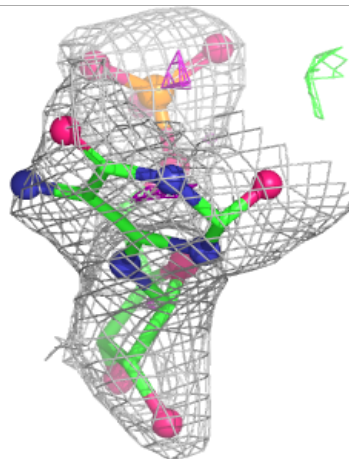
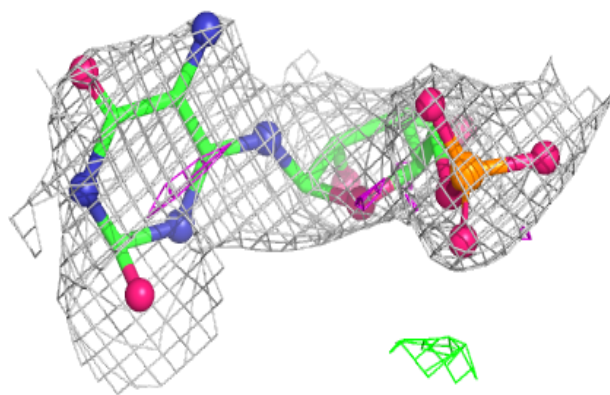
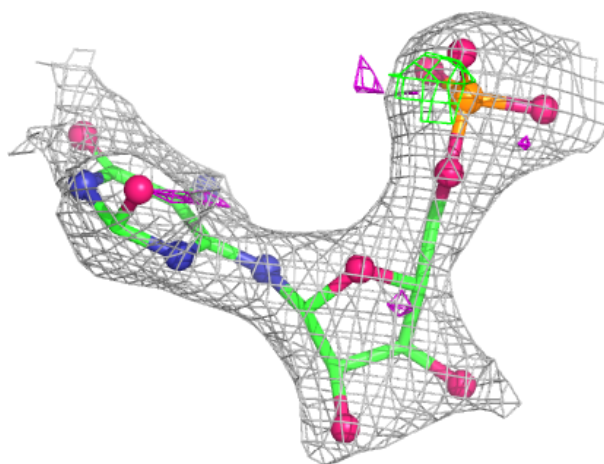
Electron density around AOF D 402:

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



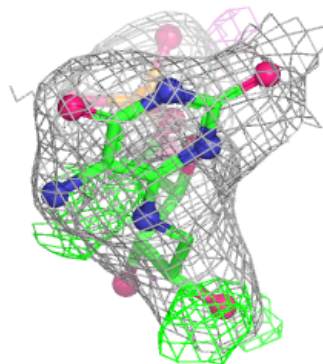
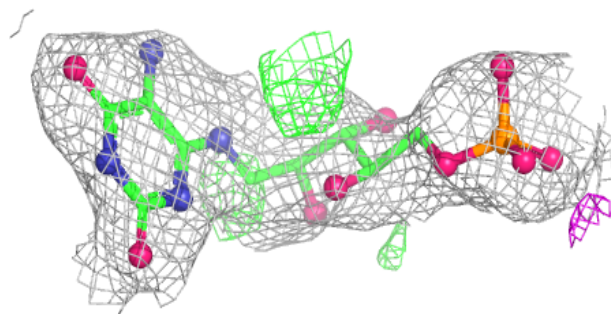
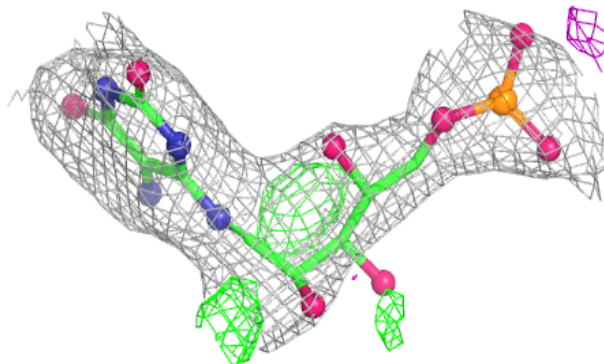
Electron density around AOF C 402:

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



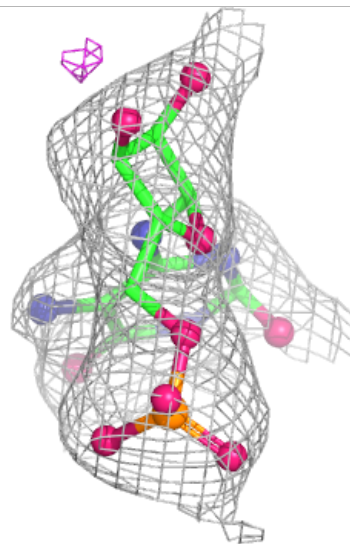
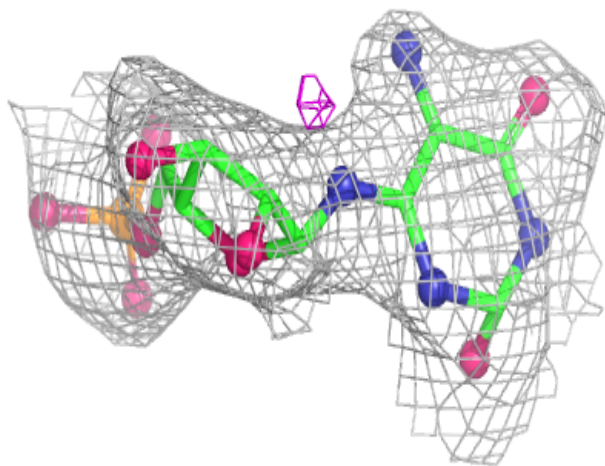
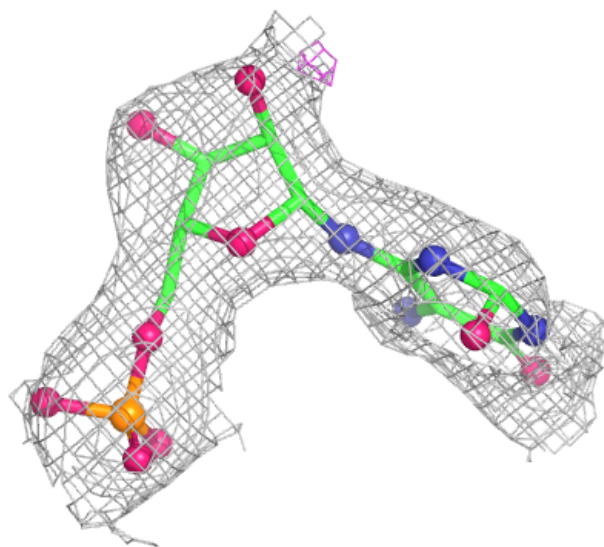
Electron density around AI9 C 403:

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



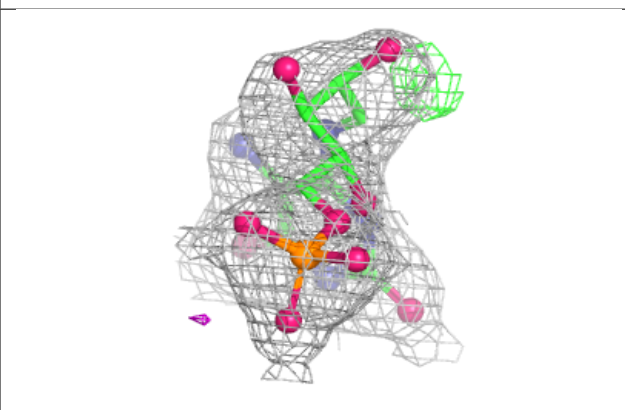
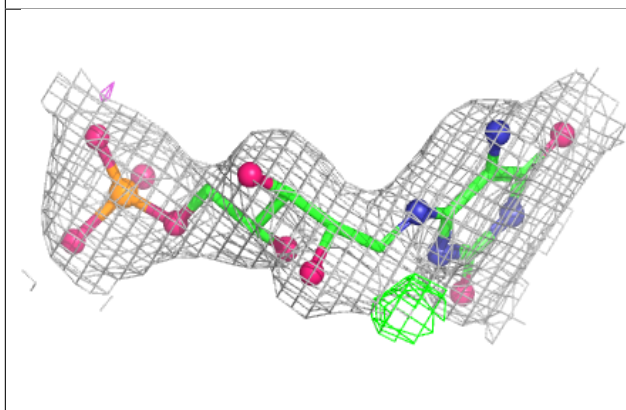
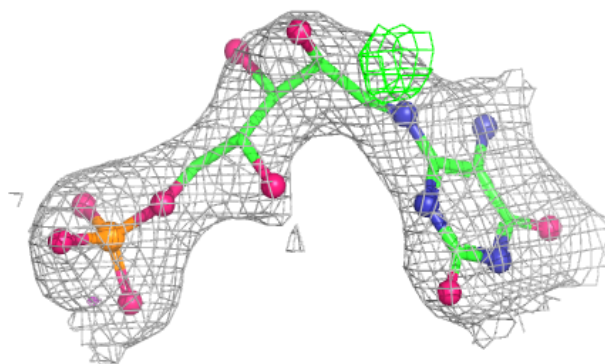
Electron density around AOF B 402:

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



Electron density around AI9 A 402:

$2mF_o-DF_c$ (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.