



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:17 AM UTC

PDB ID : 6KR3 / pdb_00006kr3
Title : Crystal structure of Dengue virus nonstructural protein NS5 (form 2)
Authors : Wu, J.; Lu, G.; Ye, H.Q.; Gong, P.
Deposited on : 2019-08-20
Resolution : 2.93 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

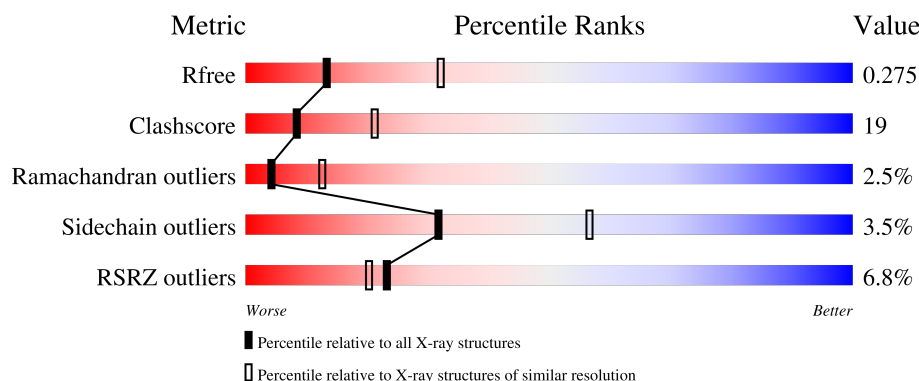
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	1159 (2.96-2.92)
Clashscore	190562	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)
RSRZ outliers	180081	1159 (2.96-2.92)

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	911	5% 60% 30% • 8%
1	B	911	8% 58% 32% • 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	GOL	B	1009	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12957 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 Genome polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	842	Total	C	N	O	S	0	0	0
			6452	4064	1149	1197	42			
1	B	836	Total	C	N	O	S	0	0	0
			6305	3968	1123	1170	44			

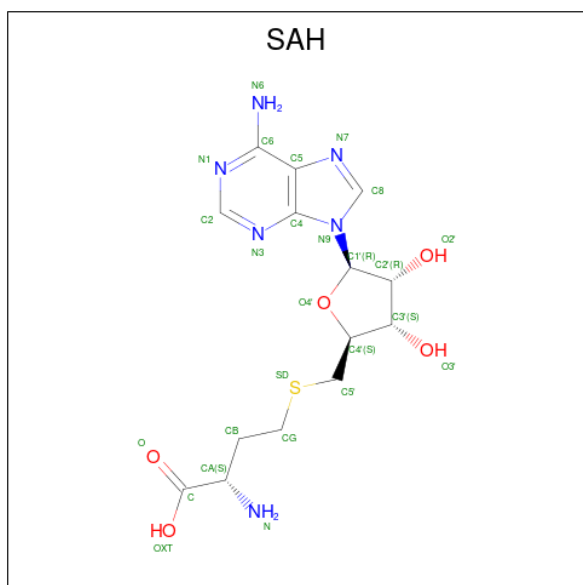
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q91H74
A	901	GLY	-	expression tag	UNP Q91H74
A	902	SER	-	expression tag	UNP Q91H74
A	903	SER	-	expression tag	UNP Q91H74
A	904	SER	-	expression tag	UNP Q91H74
A	905	HIS	-	expression tag	UNP Q91H74
A	906	HIS	-	expression tag	UNP Q91H74
A	907	HIS	-	expression tag	UNP Q91H74
A	908	HIS	-	expression tag	UNP Q91H74
A	909	HIS	-	expression tag	UNP Q91H74
A	910	HIS	-	expression tag	UNP Q91H74
B	0	MET	-	initiating methionine	UNP Q91H74
B	901	GLY	-	expression tag	UNP Q91H74
B	902	SER	-	expression tag	UNP Q91H74
B	903	SER	-	expression tag	UNP Q91H74
B	904	SER	-	expression tag	UNP Q91H74
B	905	HIS	-	expression tag	UNP Q91H74
B	906	HIS	-	expression tag	UNP Q91H74
B	907	HIS	-	expression tag	UNP Q91H74
B	908	HIS	-	expression tag	UNP Q91H74
B	909	HIS	-	expression tag	UNP Q91H74
B	910	HIS	-	expression tag	UNP Q91H74

- Molecule 2 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total I 12 12	0	0
2	B	3	Total I 3 3	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).

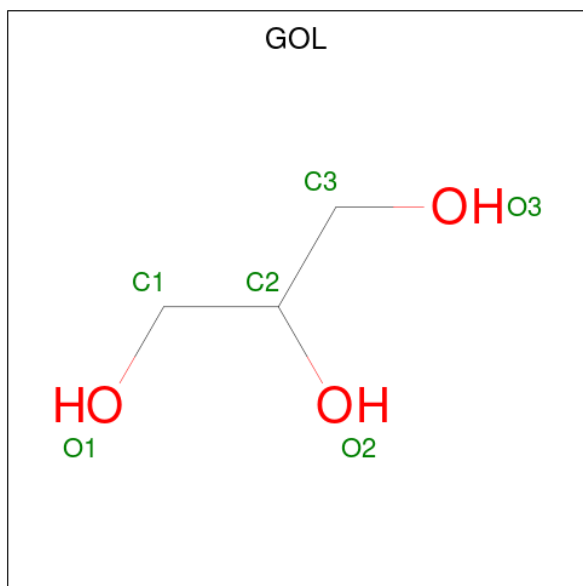


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 26 14 6 5 1	0	0
3	A	1	Total C N O S 26 14 6 5 1	0	0
3	B	1	Total C N O S 26 14 6 5 1	0	0
3	B	1	Total C N O S 26 14 6 5 1	0	0

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Zn 2 2	0	0
4	B	2	Total Zn 2 2	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0

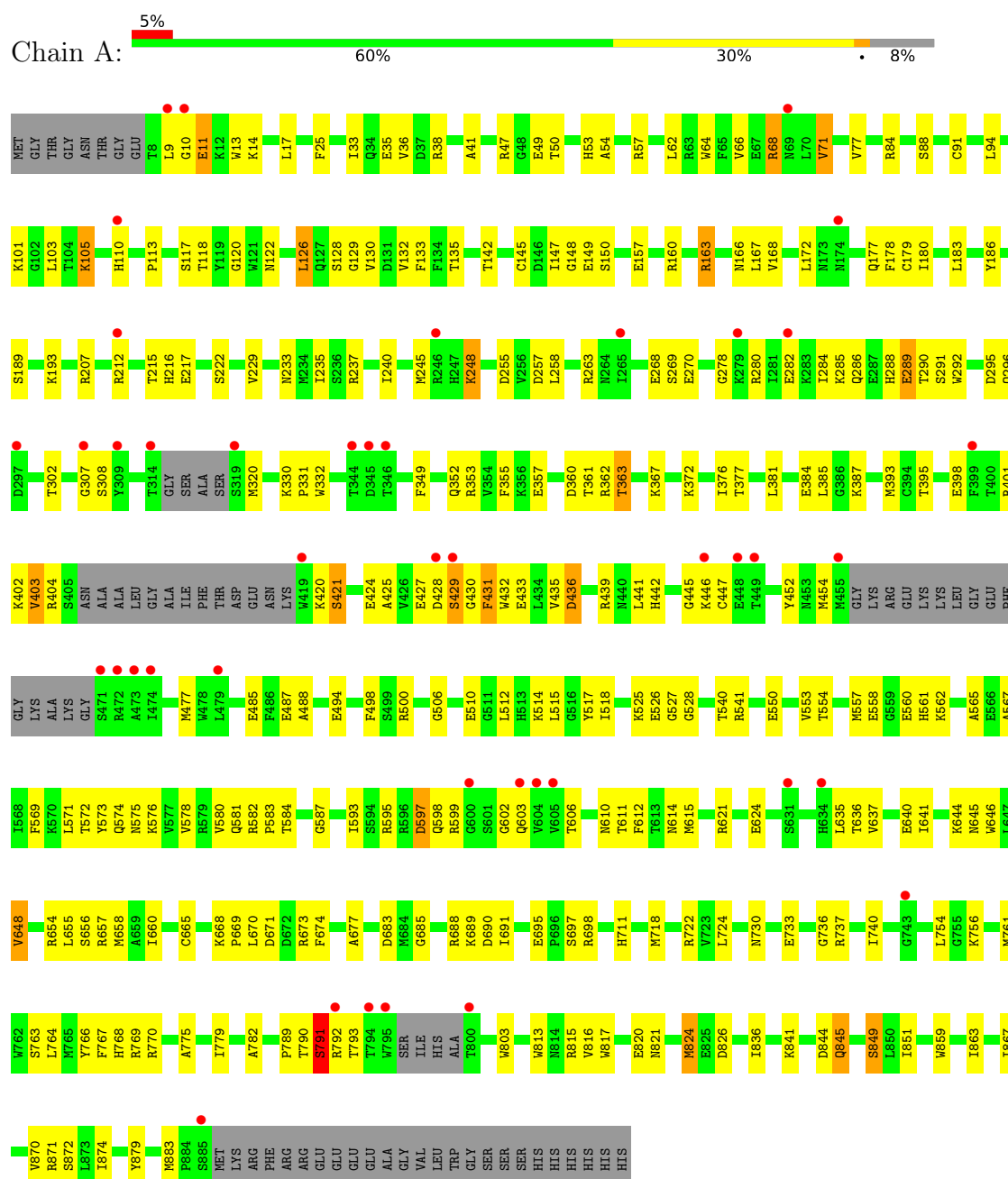
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	31	Total O 31 31	0	0
6	B	16	Total O 16 16	0	0

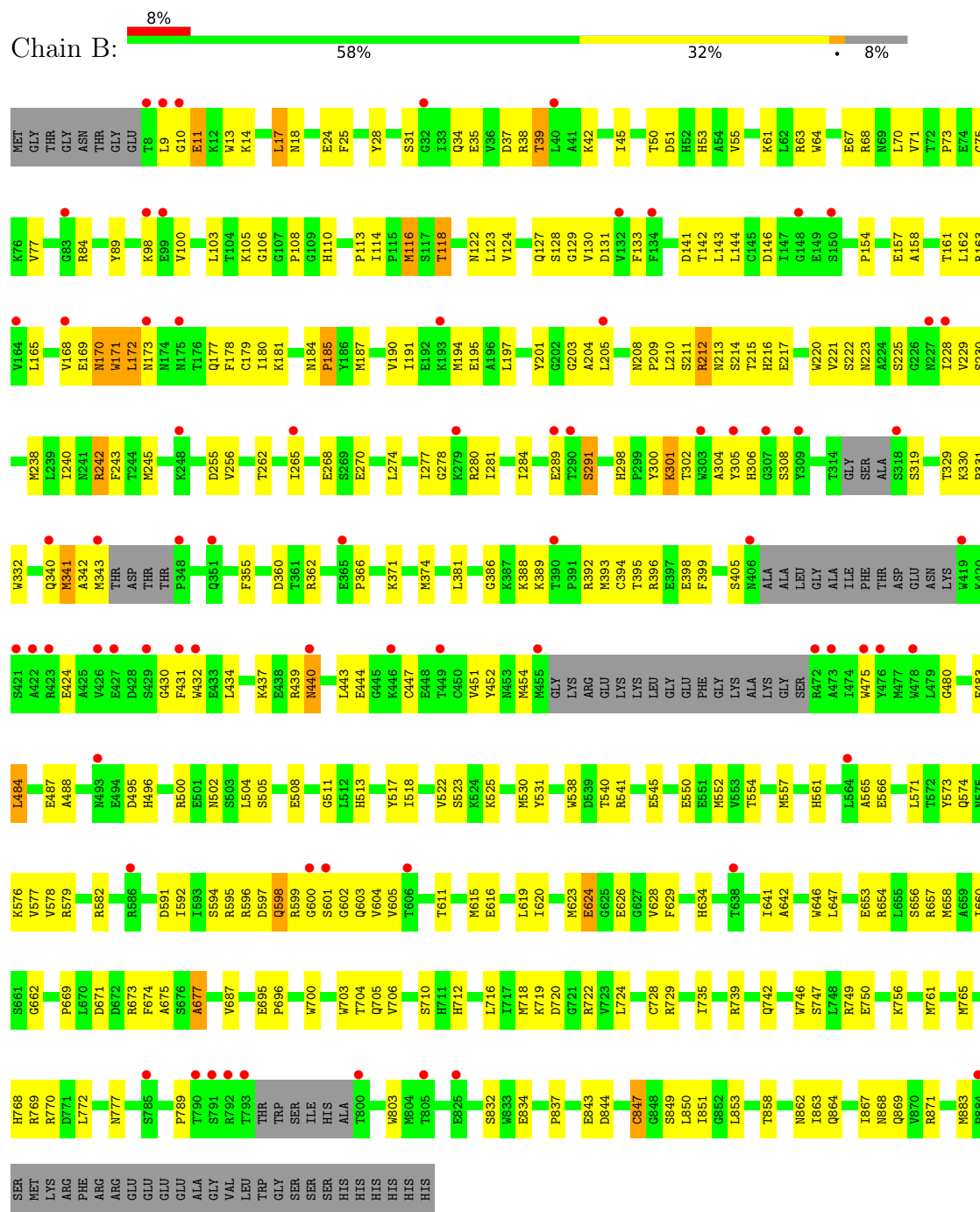
3 Residue-property plots

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



• Molecule 1: Genome polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	178.84Å 209.97Å 157.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 2.93 49.81 – 2.93	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.81-2.93) 99.8 (49.81-2.93)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.233 , 0.268 0.242 , 0.275	Depositor DCC
R_{free} test set	3164 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	64.3	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12957	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: IOD, SAH, ZN, GOL

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	0.58	8/6601 (0.1%)	0.74	0/8968
1	B	0.59	7/6453 (0.1%)	0.72	3/8787 (0.0%)
All	All	0.58	15/13054 (0.1%)	0.73	3/17755 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	ARG	NE-CZ	-12.83	1.19	1.33
1	A	698	ARG	NE-CZ	-11.52	1.20	1.33
1	B	212	ARG	CZ-NH2	-11.41	1.18	1.33
1	B	242	ARG	NE-CZ	-8.96	1.23	1.33
1	A	68	ARG	NE-CZ	-8.84	1.23	1.33
1	B	212	ARG	CD-NE	-8.84	1.33	1.46
1	B	847	CYS	CA-C	8.52	1.64	1.52
1	A	68	ARG	CZ-NH1	-8.29	1.21	1.32
1	A	698	ARG	CZ-NH1	-8.18	1.21	1.32
1	B	212	ARG	CZ-NH1	-7.87	1.21	1.32
1	B	242	ARG	CZ-NH2	-7.68	1.23	1.33
1	A	698	ARG	CD-NE	-7.66	1.35	1.46
1	A	698	ARG	CZ-NH2	-7.58	1.23	1.33
1	A	68	ARG	CD-NE	-6.09	1.37	1.46
1	A	68	ARG	CZ-NH2	-5.77	1.25	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	600	GLY	N-CA-C	-5.95	99.08	113.18
1	B	265	ILE	CA-C-N	5.85	127.45	120.14
1	B	265	ILE	C-N-CA	5.85	127.45	120.14

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	6452	0	5986	233	1
1	B	6305	0	5713	239	0
2	A	12	0	0	2	0
2	B	3	0	0	0	0
3	A	52	0	38	1	0
3	B	52	0	38	5	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	12	0	16	3	0
5	B	18	0	24	4	0
6	A	31	0	0	2	0
6	B	16	0	0	1	0
All	All	12957	0	11815	471	1

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 19.

All (471) 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:A:57:ARG:NH1	1:A:212:ARG:NH1	1.93	1.16
1:A:57:ARG:HH11	1:A:212:ARG:NH1	1.41	1.16
1:B:165:LEU:HD21	1:B:197:LEU:HD12	1.26	1.14
1:B:238:MET:HE3	1:B:242:ARG:NH1	1.66	1.09
1:B:165:LEU:HD21	1:B:197:LEU:CD1	1.93	0.99
1:B:238:MET:CE	1:B:242:ARG:NH1	2.28	0.96
1:A:525:LYS:NZ	1:A:656:SER:OG	2.00	0.94
1:A:57:ARG:NH1	1:A:212:ARG:CZ	2.31	0.92
1:B:165:LEU:CD2	1:B:197:LEU:HD12	1.99	0.91
1:A:35:GLU:OE2	1:A:212:ARG:NH1	2.04	0.90
1:B:392:ARG:NH2	1:B:495:ASP:OD1	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:VAL:HG13	1:B:221:VAL:HG23	1.57	0.84
1:A:817:TRP:O	1:A:821:ASN:ND2	2.12	0.82
1:B:624:GLU:HB3	1:B:677:ALA:HB1	1.61	0.82
1:A:764:LEU:HD11	1:A:816:VAL:HG21	1.61	0.81
1:B:756:LYS:HG2	1:B:789:PRO:HG3	1.65	0.79
1:A:35:GLU:CD	1:A:212:ARG:HH11	1.91	0.79
1:B:579:ARG:HB3	1:B:592:ILE:HG22	1.66	0.78
1:A:574:GLN:C	1:A:575:ASN:HD22	1.92	0.77
1:A:101:LYS:HD3	1:A:103:LEU:HD21	1.67	0.77
1:B:864:GLN:O	1:B:868:ASN:ND2	2.18	0.76
1:B:133:PHE:CE1	1:B:163:ARG:HG2	2.21	0.75
1:B:440:ASN:HA	1:B:443:LEU:HD23	1.69	0.74
1:A:212:ARG:HH21	1:A:212:ARG:HG3	1.52	0.74
1:B:394:CYS:HB2	1:B:487:GLU:HA	1.70	0.73
1:B:769:ARG:NH2	1:B:844:ASP:OD1	2.22	0.73
1:A:756:LYS:HD3	1:A:789:PRO:HG3	1.70	0.73
1:A:57:ARG:HH12	1:A:212:ARG:CZ	2.01	0.73
1:A:611:THR:HG23	1:A:660:ILE:HG22	1.71	0.73
1:A:35:GLU:OE2	1:A:57:ARG:NH1	2.23	0.72
1:A:595:ARG:HE	1:A:597:ASP:HB2	1.55	0.71
1:B:695:GLU:OE1	1:B:696:PRO:HD2	1.91	0.71
1:B:238:MET:HE3	1:B:242:ARG:CZ	2.20	0.71
1:A:428:ASP:O	1:A:430:GLY:N	2.23	0.71
1:B:165:LEU:CD2	1:B:197:LEU:CD1	2.64	0.71
1:B:439:ARG:HH22	1:B:487:GLU:CD	2.00	0.70
1:B:452:TYR:HB2	1:B:578:VAL:HG22	1.74	0.69
1:B:278:GLY:HA2	1:B:281:ILE:HD12	1.74	0.69
1:A:38:ARG:NH1	1:A:54:ALA:O	2.19	0.69
1:B:177:GLN:OE1	1:B:223:ASN:ND2	2.25	0.69
1:B:9:LEU:H	1:B:11:GLU:HG3	1.57	0.69
1:B:70:LEU:HB3	1:B:221:VAL:HG21	1.75	0.69
1:A:526:GLU:O	1:A:657:ARG:NH2	2.25	0.69
1:A:541:ARG:HD3	1:A:685:GLY:O	1.93	0.68
1:A:145:CYS:SG	1:A:147:ILE:HD12	2.32	0.68
1:A:421:SER:O	1:A:424:GLU:N	2.27	0.68
1:A:432:TRP:HA	1:A:435:VAL:HG12	1.75	0.68
1:A:207:ARG:NH1	1:A:215:THR:O	2.27	0.68
1:A:599:ARG:NH1	1:A:610:ASN:OD1	2.22	0.67
1:B:157:GLU:O	1:B:161:THR:HG22	1.94	0.67
1:A:872:SER:HB3	1:B:746:TRP:O	1.95	0.67
1:B:340:GLN:O	1:B:342:ALA:N	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:LEU:HD22	1:B:853:LEU:HD12	1.76	0.67
1:A:599:ARG:HD3	1:A:606:THR:HB	1.77	0.67
1:A:737:ARG:HD2	2:A:1012:IOD:I	2.64	0.67
1:A:149:GLU:HB3	1:A:160:ARG:NH2	2.09	0.67
1:A:50:THR:O	1:A:117:SER:N	2.23	0.66
1:A:282:GLU:O	1:A:286:GLN:HG3	1.95	0.66
1:B:304:ALA:HB3	1:B:594:SER:HB2	1.76	0.66
1:B:14:LYS:O	1:B:18:ASN:ND2	2.29	0.66
1:A:229:VAL:O	1:A:233:ASN:ND2	2.29	0.66
1:A:189:SER:OG	2:A:1011:IOD:I	2.84	0.66
1:A:245:MET:O	1:A:248:LYS:HE3	1.97	0.65
1:A:718:MET:HE2	1:A:724:LEU:HD21	1.77	0.65
1:A:576:LYS:NZ	1:A:597:ASP:O	2.29	0.65
1:B:194:MET:HE2	1:B:205:LEU:HD21	1.79	0.65
1:B:302:THR:OG1	1:B:595:ARG:NH1	2.29	0.65
1:A:722:ARG:HD2	1:A:824:MET:SD	2.37	0.64
1:B:169:GLU:OE1	1:B:197:LEU:HD21	1.96	0.64
1:B:451:VAL:HG12	1:B:577:VAL:HG13	1.78	0.64
1:B:63:ARG:CZ	1:B:256:VAL:HG22	2.28	0.64
1:A:730:ASN:HB3	1:A:733:GLU:HG3	1.80	0.63
1:B:277:ILE:HD12	1:B:281:ILE:HD11	1.79	0.63
1:B:530:MET:HE2	1:B:706:VAL:HG11	1.80	0.63
1:B:355:PHE:CD2	1:B:454:MET:HE1	2.34	0.63
1:A:295:ASP:OD1	1:A:296:GLN:N	2.31	0.63
1:A:851:ILE:HD12	1:A:851:ILE:H	1.63	0.63
1:A:101:LYS:NZ	6:A:1101:HOH:O	2.26	0.63
1:A:550:GLU:CD	1:A:599:ARG:HH22	2.05	0.63
1:B:146:ASP:HB3	3:B:1005:SAH:HN1	1.64	0.63
1:A:432:TRP:O	1:A:436:ASP:HB2	1.99	0.62
1:A:349:PHE:O	1:A:353:ARG:HG3	1.98	0.62
1:A:770:ARG:HD2	1:A:844:ASP:OD2	2.00	0.62
1:B:671:ASP:OD2	1:B:673:ARG:NE	2.29	0.62
1:B:573:TYR:O	1:B:576:LYS:NZ	2.32	0.62
1:A:393:MET:HE1	1:A:560:GLU:HG2	1.81	0.61
1:B:170:ASN:O	1:B:172:LEU:N	2.32	0.61
1:B:280:ARG:HE	1:B:447:CYS:HB2	1.64	0.61
1:A:867:ILE:HG22	1:A:871:ARG:HD2	1.82	0.61
1:A:381:LEU:HD23	1:A:612:PHE:CE1	2.36	0.61
1:B:735:ILE:O	1:B:739:ARG:HG2	2.00	0.61
1:A:77:VAL:HG22	1:A:142:THR:CG2	2.31	0.61
1:B:110:HIS:HB3	3:B:1005:SAH:O2'	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:TYR:O	1:B:306:HIS:ND1	2.33	0.61
1:A:215:THR:OG1	1:A:217:GLU:HG3	2.00	0.61
1:B:500:ARG:NH2	1:B:658:MET:O	2.34	0.60
1:A:569:PHE:O	1:A:574:GLN:HG3	2.02	0.60
1:A:567:ALA:O	1:A:571:LEU:HB2	2.02	0.60
1:B:430:GLY:O	1:B:434:LEU:HD12	2.02	0.60
1:A:355:PHE:HD2	1:A:454:MET:HE1	1.66	0.60
1:A:128:SER:OG	1:A:129:GLY:N	2.33	0.60
1:B:61:LYS:HA	1:B:208:ASN:HD21	1.66	0.60
1:B:154:PRO:O	1:B:187:MET:HE1	2.01	0.60
1:B:268:GLU:O	1:B:362:ARG:NH2	2.35	0.60
1:B:242:ARG:HG3	1:B:245:MET:HE2	1.83	0.60
1:B:611:THR:CG2	1:B:662:GLY:H	2.15	0.60
1:B:284:ILE:HD11	1:B:592:ILE:HG12	1.85	0.59
1:B:484:LEU:HD12	1:B:484:LEU:H	1.67	0.59
1:B:611:THR:HG23	1:B:662:GLY:H	1.67	0.59
1:B:371:LYS:HD3	1:B:545:GLU:HG3	1.84	0.59
1:B:274:LEU:HD23	1:B:274:LEU:H	1.67	0.59
1:B:626:GLU:CD	1:B:654:ARG:HH21	2.11	0.59
1:A:290:THR:OG1	1:A:291:SER:N	2.35	0.59
1:A:280:ARG:HH21	1:A:447:CYS:HB2	1.67	0.59
1:A:439:ARG:NH1	1:A:487:GLU:OE1	2.35	0.59
1:B:602:GLY:O	1:B:604:VAL:N	2.36	0.59
1:B:280:ARG:NH1	1:B:571:LEU:O	2.36	0.58
1:A:574:GLN:O	1:A:575:ASN:ND2	2.32	0.58
1:B:122:ASN:HD22	1:B:262:THR:HB	1.68	0.58
1:A:770:ARG:HB2	1:A:851:ILE:HD11	1.86	0.58
1:A:527:GLY:HA2	1:A:670:LEU:O	2.03	0.58
1:B:343:MET:HE3	5:B:1009:GOL:O1	2.04	0.58
1:A:567:ALA:HA	1:A:571:LEU:HD23	1.84	0.58
1:B:165:LEU:CG	1:B:197:LEU:HD12	2.34	0.58
1:A:177:GLN:OE1	1:A:222:SER:OG	2.21	0.58
1:A:688:ARG:NH1	1:A:697:SER:OG	2.37	0.58
1:A:761:MET:HE3	1:A:766:TYR:HE2	1.68	0.58
1:A:57:ARG:NH1	1:A:212:ARG:HH11	1.98	0.57
1:B:184:ASN:OD1	1:B:187:MET:HE2	2.04	0.57
1:A:240:ILE:HD13	5:A:1017:GOL:H2	1.87	0.57
1:A:167:LEU:HD11	6:A:1108:HOH:O	2.05	0.57
1:B:280:ARG:HE	1:B:447:CYS:CB	2.18	0.57
1:A:133:PHE:CD1	1:A:167:LEU:HD22	2.39	0.57
1:B:716:LEU:HD11	1:B:837:PRO:HG2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:GLU:HB3	1:A:183:LEU:CD1	2.35	0.56
1:A:331:PRO:HG2	1:A:332:TRP:CE3	2.40	0.56
1:A:33:ILE:HD13	1:A:212:ARG:HD3	1.86	0.56
1:A:35:GLU:HG3	1:A:36:VAL:H	1.70	0.56
1:A:157:GLU:HB3	1:A:183:LEU:HD12	1.87	0.56
1:B:554:THR:HA	1:B:557:MET:SD	2.46	0.56
1:B:31:SER:HB3	1:B:245:MET:HE3	1.87	0.56
1:B:84:ARG:HB3	1:B:114:ILE:HG13	1.86	0.56
1:B:396:ARG:HG2	1:B:483:PHE:CZ	2.41	0.56
1:B:770:ARG:HD2	1:B:851:ILE:HD13	1.87	0.56
1:A:355:PHE:CD2	1:A:454:MET:HE1	2.40	0.55
1:B:89:TYR:HB3	1:B:118:THR:HG21	1.86	0.55
1:B:366:PRO:O	1:B:371:LYS:NZ	2.31	0.55
1:B:381:LEU:HD21	1:B:615:MET:HE2	1.87	0.55
1:B:582:ARG:HH11	1:B:591:ASP:CG	2.13	0.55
1:B:270:GLU:HG2	1:B:362:ARG:HH12	1.70	0.55
1:B:623:MET:HE2	1:B:647:LEU:HD21	1.88	0.55
1:B:51:ASP:O	1:B:53:HIS:N	2.37	0.55
1:A:817:TRP:C	1:A:821:ASN:ND2	2.63	0.55
1:B:37:ASP:OD2	1:B:39:THR:OG1	2.06	0.55
1:B:500:ARG:HH11	1:B:518:ILE:HG23	1.72	0.55
1:B:641:ILE:HD12	1:B:642:ALA:N	2.21	0.55
1:A:212:ARG:HH21	1:A:212:ARG:CG	2.19	0.55
1:B:389:LYS:HE3	1:B:502:ASN:HD22	1.71	0.55
1:A:330:LYS:HB3	5:B:1009:GOL:H32	1.89	0.55
1:A:602:GLY:O	1:A:606:THR:HG23	2.06	0.55
1:A:775:ALA:O	1:A:779:ILE:HG13	2.07	0.55
1:A:782:ALA:HB2	1:A:867:ILE:HG23	1.88	0.55
1:A:871:ARG:HG2	1:A:879:TYR:CE2	2.42	0.55
1:B:355:PHE:CE2	1:B:454:MET:HE1	2.42	0.55
1:A:64:TRP:CD1	1:A:68:ARG:HH12	2.24	0.54
1:A:288:HIS:C	1:A:290:THR:H	2.15	0.54
1:A:384:GLU:HA	1:A:387:LYS:HD2	1.88	0.54
1:B:143:LEU:HD13	1:B:171:TRP:HB3	1.89	0.54
1:A:292:TRP:CD1	1:A:292:TRP:C	2.85	0.54
1:A:512:LEU:HD23	1:A:515:LEU:HD12	1.90	0.54
1:B:343:MET:CE	5:B:1009:GOL:O1	2.55	0.54
1:B:703:TRP:C	1:B:705:GLN:H	2.15	0.54
1:A:550:GLU:OE1	1:A:599:ARG:NH2	2.41	0.54
1:B:128:SER:O	1:B:130:VAL:HG23	2.07	0.54
1:B:146:ASP:HA	1:B:181:LYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:ARG:HA	1:A:113:PRO:HA	1.89	0.54
1:B:331:PRO:HG2	1:B:332:TRP:CZ3	2.43	0.54
1:B:194:MET:CE	1:B:205:LEU:HD21	2.37	0.54
1:B:710:SER:HB3	1:B:729:ARG:HH21	1.73	0.54
1:B:158:ALA:HB2	1:B:187:MET:HE3	1.90	0.54
1:B:17:LEU:HD11	1:B:25:PHE:HE1	1.72	0.53
1:B:747:SER:OG	1:B:750:GLU:HG3	2.08	0.53
1:B:832:SER:OG	1:B:834:GLU:HG3	2.08	0.53
1:A:133:PHE:HD1	1:A:167:LEU:HD22	1.74	0.53
1:B:172:LEU:HD13	1:B:201:TYR:CD1	2.43	0.53
1:B:191:ILE:O	1:B:195:GLU:HG3	2.07	0.53
1:A:41:ALA:HA	1:A:53:HIS:ND1	2.24	0.53
1:A:402:LYS:C	1:A:404:ARG:H	2.15	0.53
1:B:574:GLN:O	1:B:596:ARG:HB3	2.09	0.53
1:A:282:GLU:OE1	1:A:286:GLN:NE2	2.39	0.53
1:B:179:CYS:HA	1:B:220:TRP:O	2.09	0.53
1:A:103:LEU:HB3	1:A:130:VAL:HG11	1.91	0.53
1:A:126:LEU:HB2	5:A:1018:GOL:H31	1.91	0.53
1:A:292:TRP:CH2	1:A:307:GLY:HA3	2.44	0.53
1:B:747:SER:O	1:B:749:ARG:N	2.38	0.53
1:B:215:THR:OG1	1:B:217:GLU:HG3	2.09	0.52
1:B:513:HIS:ND1	1:B:765:MET:HE1	2.25	0.52
1:B:716:LEU:HD11	1:B:837:PRO:CG	2.39	0.52
1:A:94:LEU:O	1:A:263:ARG:NH2	2.42	0.52
1:B:843:GLU:OE1	1:B:843:GLU:N	2.35	0.52
1:A:36:VAL:HG21	1:A:255:ASP:HA	1.91	0.52
1:A:454:MET:HG3	1:A:578:VAL:CG1	2.40	0.52
1:B:240:ILE:HA	1:B:243:PHE:CD2	2.45	0.52
1:A:331:PRO:HG2	1:A:332:TRP:CZ3	2.45	0.52
1:A:718:MET:HG2	1:A:724:LEU:HD11	1.92	0.52
1:A:257:ASP:HB3	1:A:357:GLU:HB3	1.92	0.52
1:A:452:TYR:CD2	1:A:477:MET:HE3	2.45	0.52
1:B:270:GLU:OE1	1:B:596:ARG:HG3	2.09	0.52
1:B:500:ARG:NH1	1:B:518:ILE:HG23	2.25	0.51
1:A:133:PHE:CE1	1:A:163:ARG:HD2	2.45	0.51
1:B:213:ASN:O	1:B:215:THR:N	2.41	0.51
1:B:184:ASN:O	1:B:190:VAL:HG21	2.11	0.51
1:A:500:ARG:NH2	1:A:658:MET:O	2.44	0.51
1:A:761:MET:SD	1:A:793:THR:HG21	2.51	0.51
1:B:488:ALA:O	1:B:561:HIS:HE1	1.93	0.51
1:A:863:ILE:HG21	1:A:883:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:868:ASN:HA	1:B:871:ARG:HB2	1.93	0.51
1:A:863:ILE:O	1:A:867:ILE:HG13	2.11	0.51
1:B:185:PRO:HA	1:B:190:VAL:HG11	1.91	0.51
1:A:14:LYS:HD2	1:A:186:TYR:OH	2.11	0.51
1:B:143:LEU:O	1:B:178:PHE:HA	2.10	0.51
1:A:688:ARG:NH2	1:A:695:GLU:O	2.38	0.51
1:B:289:GLU:C	1:B:291:SER:H	2.18	0.51
1:A:36:VAL:CG2	1:A:255:ASP:HA	2.40	0.51
1:A:671:ASP:CG	1:A:673:ARG:HE	2.18	0.51
1:B:10:GLY:O	1:B:13:TRP:HB3	2.11	0.51
1:B:538:TRP:CD1	1:B:538:TRP:C	2.89	0.51
1:A:105:LYS:HD3	1:A:110:HIS:CE1	2.47	0.50
1:A:557:MET:HE3	1:A:561:HIS:CD2	2.47	0.50
1:A:813:TRP:CZ2	1:A:836:ILE:HG12	2.47	0.50
1:B:51:ASP:C	1:B:53:HIS:H	2.20	0.50
1:B:475:TRP:HZ3	1:B:576:LYS:HD2	1.75	0.50
1:B:255:ASP:OD2	1:B:256:VAL:N	2.37	0.50
1:A:381:LEU:HD21	1:A:615:MET:HE2	1.94	0.50
1:A:870:VAL:O	1:A:874:ILE:HG13	2.11	0.50
1:B:863:ILE:O	1:B:867:ILE:HG13	2.11	0.50
1:A:736:GLY:O	1:A:740:ILE:HD13	2.12	0.50
1:B:61:LYS:NZ	6:B:1104:HOH:O	2.44	0.50
1:B:213:ASN:C	1:B:215:THR:H	2.20	0.50
1:B:496:HIS:ND1	1:B:508:GLU:OE1	2.44	0.50
1:A:167:LEU:HD12	1:A:167:LEU:C	2.37	0.49
1:B:63:ARG:NH1	1:B:256:VAL:HG22	2.27	0.49
1:B:505:SER:HB2	1:B:615:MET:SD	2.52	0.49
1:A:280:ARG:O	1:A:284:ILE:HD12	2.13	0.49
1:A:557:MET:HE1	1:A:565:ALA:HB3	1.94	0.49
1:B:238:MET:CE	1:B:242:ARG:HH11	2.18	0.49
1:B:300:TYR:OH	1:B:591:ASP:OD1	2.27	0.49
1:A:168:VAL:HG11	1:A:180:ILE:HG12	1.94	0.49
1:A:35:GLU:HG3	1:A:36:VAL:N	2.27	0.49
1:A:302:THR:OG1	1:A:360:ASP:OD1	2.27	0.49
1:A:512:LEU:HD11	1:A:711:HIS:CE1	2.48	0.49
1:A:270:GLU:OE1	1:A:362:ARG:NH2	2.46	0.49
1:A:441:LEU:O	1:A:445:GLY:N	2.41	0.49
1:B:557:MET:HE3	1:B:561:HIS:CD2	2.48	0.49
1:B:624:GLU:HG3	1:B:629:PHE:CZ	2.48	0.49
1:B:654:ARG:HA	1:B:657:ARG:HG3	1.95	0.49
1:B:858:THR:O	1:B:862:ASN:ND2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLY:O	1:A:13:TRP:HB3	2.13	0.49
1:A:237:ARG:NH2	5:A:1017:GOL:O3	2.45	0.49
1:A:510:GLU:OE1	1:A:514:LYS:HD3	2.13	0.49
1:B:616:GLU:O	1:B:620:ILE:HG13	2.13	0.49
1:B:849:SER:OG	1:B:850:LEU:N	2.46	0.49
1:B:25:PHE:O	1:B:28:TYR:N	2.46	0.48
1:A:573:TYR:O	1:A:576:LYS:HD2	2.14	0.48
1:B:522:VAL:O	1:B:525:LYS:HB2	2.13	0.48
1:A:166:ASN:HD22	1:A:193:LYS:HZ3	1.62	0.48
1:B:646:TRP:CH2	1:B:654:ARG:HG3	2.48	0.48
1:A:557:MET:O	1:A:558:GLU:HB3	2.11	0.48
1:A:167:LEU:HD12	1:A:167:LEU:O	2.14	0.48
1:A:614:ASN:HD21	1:A:665:CYS:HB3	1.79	0.48
1:A:320:MET:HE2	1:B:869:GLN:HB2	1.95	0.48
1:B:331:PRO:HG2	1:B:332:TRP:CE3	2.49	0.48
1:B:626:GLU:OE1	1:B:654:ARG:NH2	2.44	0.48
1:A:71:VAL:HG21	1:A:179:CYS:HB2	1.95	0.47
1:A:285:LYS:O	1:A:289:GLU:N	2.47	0.47
1:B:280:ARG:NH2	1:B:577:VAL:HG12	2.29	0.47
1:A:454:MET:HG3	1:A:578:VAL:HG11	1.95	0.47
1:A:690:ASP:O	1:A:691:ILE:HG23	2.15	0.47
1:B:540:THR:HA	1:B:598:GLN:HG3	1.95	0.47
1:B:557:MET:HE3	1:B:561:HIS:CG	2.49	0.47
1:A:47:ARG:NH1	1:A:49:GLU:OE2	2.47	0.47
1:A:168:VAL:O	1:A:172:LEU:HG	2.15	0.47
1:A:292:TRP:CZ2	1:A:307:GLY:HA3	2.48	0.47
1:B:240:ILE:HA	1:B:243:PHE:HD2	1.78	0.47
1:B:451:VAL:HG12	1:B:577:VAL:CG1	2.42	0.47
1:A:582:ARG:HG2	1:A:583:PRO:HD2	1.97	0.47
1:B:64:TRP:CE2	1:B:209:PRO:HD2	2.49	0.47
1:A:38:ARG:HD2	1:A:57:ARG:HG2	1.96	0.47
1:A:558:GLU:HA	1:A:562:LYS:HB2	1.96	0.47
1:A:645:ASN:O	1:A:648:VAL:N	2.48	0.47
1:B:161:THR:HG23	1:B:162:LEU:N	2.30	0.47
1:B:735:ILE:HG22	1:B:739:ARG:HD3	1.96	0.47
1:A:57:ARG:HH11	1:A:212:ARG:HH12	1.50	0.47
1:A:207:ARG:HD2	1:A:235:ILE:HD12	1.97	0.47
1:B:37:ASP:O	1:B:38:ARG:HB2	2.14	0.47
1:B:557:MET:HE1	1:B:565:ALA:HB2	1.96	0.47
1:B:144:LEU:HD22	1:B:179:CYS:HB3	1.96	0.47
1:A:498:PHE:O	1:A:506:GLY:HA3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LEU:HD11	1:B:25:PHE:CE1	2.49	0.46
1:A:859:TRP:HB2	5:B:1009:GOL:H31	1.96	0.46
1:B:50:THR:HA	1:B:116:MET:CE	2.45	0.46
1:B:212:ARG:H	1:B:212:ARG:HG2	1.52	0.46
1:B:742:GLN:O	1:B:746:TRP:NE1	2.31	0.46
1:B:777:ASN:HB3	1:B:883:MET:SD	2.55	0.46
1:A:361:THR:O	1:A:595:ARG:NH1	2.44	0.46
1:A:763:SER:O	1:A:767:PHE:HB3	2.14	0.46
1:B:280:ARG:NE	1:B:447:CYS:HB2	2.29	0.46
1:B:669:PRO:HG3	1:B:674:PHE:CB	2.44	0.46
1:A:500:ARG:NH1	1:A:518:ILE:HG23	2.29	0.46
1:B:100:VAL:HG13	1:B:124:VAL:HA	1.96	0.46
1:A:554:THR:HA	1:A:557:MET:SD	2.56	0.46
1:B:541:ARG:HH21	1:B:687:VAL:HG11	1.81	0.46
1:B:619:LEU:HD23	1:B:619:LEU:HA	1.71	0.46
1:B:277:ILE:HD13	1:B:594:SER:OG	2.15	0.46
1:B:576:LYS:HG3	1:B:595:ARG:O	2.16	0.46
1:A:268:GLU:HA	1:A:362:ARG:HD2	1.98	0.46
1:A:849:SER:HB3	1:A:851:ILE:HD12	1.98	0.46
1:B:362:ARG:HA	1:B:595:ARG:HH22	1.81	0.46
1:A:57:ARG:HH11	1:A:212:ARG:CZ	2.04	0.45
1:A:132:VAL:HG22	3:A:1013:SAH:N1	2.31	0.45
1:A:442:HIS:CD2	1:A:447:CYS:SG	3.07	0.45
1:B:42:LYS:HA	1:B:45:ILE:HG22	1.99	0.45
1:A:485:GLU:OE2	1:A:573:TYR:OH	2.27	0.45
1:B:73:PRO:HA	1:B:142:THR:HG21	1.99	0.45
1:B:768:HIS:CD2	1:B:768:HIS:H	2.33	0.45
1:A:120:GLY:HA2	1:A:263:ARG:HG3	1.98	0.45
1:A:401:ARG:C	1:A:403:VAL:H	2.24	0.45
1:A:431:PHE:C	1:A:431:PHE:CD2	2.93	0.45
1:A:595:ARG:CZ	1:A:598:GLN:HE21	2.29	0.45
1:B:68:ARG:HD3	3:B:1004:SAH:HG1	1.98	0.45
1:B:394:CYS:O	1:B:487:GLU:HG3	2.15	0.45
1:A:655:LEU:HA	1:A:658:MET:HE2	1.98	0.45
1:A:815:ARG:O	1:A:820:GLU:HB2	2.16	0.45
1:B:146:ASP:HB3	3:B:1005:SAH:HB2	1.97	0.45
1:B:170:ASN:C	1:B:172:LEU:H	2.25	0.45
1:A:352:GLN:NE2	1:A:582:ARG:HG3	2.32	0.45
1:A:553:VAL:O	1:A:557:MET:HG3	2.17	0.45
1:A:57:ARG:HH12	1:A:212:ARG:NE	2.13	0.45
1:A:402:LYS:HE3	1:A:494:GLU:OE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:ASP:C	1:A:849:SER:HB2	2.42	0.45
1:B:14:LYS:HA	1:B:17:LEU:HB3	1.99	0.45
1:B:615:MET:HG3	1:B:660:ILE:HD12	1.98	0.45
1:B:768:HIS:ND1	1:B:769:ARG:HD3	2.31	0.45
1:A:425:ALA:C	1:A:427:GLU:H	2.25	0.45
1:A:768:HIS:CD2	1:A:768:HIS:H	2.34	0.45
1:B:208:ASN:OD1	1:B:210:LEU:HB2	2.17	0.45
1:B:768:HIS:CE1	1:B:769:ARG:HD3	2.51	0.45
1:B:205:LEU:HD22	1:B:220:TRP:HA	1.99	0.45
1:B:284:ILE:CD1	1:B:592:ILE:HG21	2.45	0.45
1:B:238:MET:HE3	1:B:242:ARG:HH12	1.72	0.45
1:A:280:ARG:NH1	1:A:571:LEU:O	2.45	0.44
1:A:584:THR:OG1	1:A:587:GLY:O	2.34	0.44
1:A:646:TRP:CZ2	1:A:654:ARG:HG3	2.52	0.44
1:B:197:LEU:HD23	1:B:197:LEU:HA	1.78	0.44
1:A:367:LYS:HG2	1:A:683:ASP:OD2	2.18	0.44
1:B:330:LYS:N	1:B:331:PRO:HD2	2.32	0.44
1:B:550:GLU:OE1	1:B:599:ARG:NH2	2.48	0.44
1:A:288:HIS:O	1:A:290:THR:HG23	2.17	0.44
1:A:372:LYS:HE3	1:A:640:GLU:OE1	2.17	0.44
1:A:761:MET:HE3	1:A:766:TYR:CE2	2.51	0.44
1:B:55:VAL:CG1	1:B:84:ARG:HB2	2.47	0.44
1:B:389:LYS:HG3	1:B:502:ASN:ND2	2.32	0.44
1:B:602:GLY:O	1:B:605:VAL:N	2.51	0.44
1:A:178:PHE:HB2	1:A:180:ILE:CD1	2.46	0.44
1:A:330:LYS:N	1:A:331:PRO:HD2	2.33	0.44
1:B:77:VAL:HB	1:B:100:VAL:HG23	1.98	0.44
1:B:844:ASP:OD1	1:B:849:SER:HB2	2.18	0.44
3:B:1005:SAH:H4'	3:B:1005:SAH:HG1	1.76	0.44
1:A:278:GLY:C	1:A:280:ARG:N	2.75	0.44
1:A:441:LEU:HD22	1:A:446:LYS:CB	2.47	0.44
1:B:68:ARG:HB2	1:B:70:LEU:HG	1.98	0.44
1:B:511:GLY:HA3	1:B:513:HIS:CE1	2.53	0.44
1:A:557:MET:HE3	1:A:561:HIS:NE2	2.33	0.44
1:B:13:TRP:CZ2	1:B:17:LEU:HD22	2.52	0.44
1:B:340:GLN:C	1:B:342:ALA:H	2.26	0.44
1:B:392:ARG:HD2	1:B:393:MET:O	2.18	0.44
1:A:816:VAL:HG23	1:A:817:TRP:N	2.33	0.44
1:B:168:VAL:HG21	1:B:180:ILE:HG12	1.99	0.44
1:B:386:GLY:HA2	1:B:389:LYS:HB2	1.99	0.44
1:B:105:LYS:O	1:B:129:GLY:HA2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:THR:HG23	1:B:162:LEU:H	1.83	0.44
1:B:374:MET:HB3	1:B:616:GLU:OE2	2.17	0.44
1:B:480:GLY:O	1:B:484:LEU:HD12	2.17	0.44
1:A:454:MET:HE3	1:A:454:MET:HB3	1.75	0.43
1:B:653:GLU:O	1:B:656:SER:OG	2.28	0.43
1:A:133:PHE:CD1	1:A:167:LEU:CD2	3.02	0.43
1:A:689:LYS:O	1:A:690:ASP:HB2	2.17	0.43
1:A:764:LEU:HD11	1:A:816:VAL:CG2	2.42	0.43
1:B:178:PHE:HB2	1:B:180:ILE:HD11	2.01	0.43
1:B:178:PHE:HB2	1:B:180:ILE:CD1	2.48	0.43
1:B:439:ARG:NH2	1:B:487:GLU:OE2	2.51	0.43
1:A:363:THR:HG23	1:A:541:ARG:CZ	2.47	0.43
1:A:817:TRP:O	1:A:824:MET:HE3	2.19	0.43
1:B:720:ASP:OD1	1:B:722:ARG:HG3	2.19	0.43
1:A:381:LEU:HD23	1:A:612:PHE:CD1	2.52	0.43
1:A:572:THR:O	1:A:576:LYS:HG3	2.18	0.43
1:A:599:ARG:HD2	1:A:610:ASN:OD1	2.19	0.43
1:B:431:PHE:O	1:B:434:LEU:N	2.51	0.43
1:B:863:ILE:HG21	1:B:883:MET:HE2	2.00	0.43
1:B:84:ARG:HA	1:B:113:PRO:HA	2.01	0.43
1:B:483:PHE:O	1:B:487:GLU:N	2.49	0.43
1:A:376:ILE:HG13	1:A:377:THR:N	2.33	0.43
1:A:11:GLU:H	1:A:11:GLU:HG3	1.60	0.43
1:B:712:HIS:CD2	1:B:728:CYS:HB3	2.54	0.43
1:A:624:GLU:HB3	1:A:677:ALA:HB1	2.01	0.42
1:B:395:THR:OG1	1:B:398:GLU:HG3	2.19	0.42
1:B:703:TRP:C	1:B:705:GLN:N	2.77	0.42
1:A:637:VAL:O	1:A:641:ILE:HG13	2.19	0.42
1:A:640:GLU:O	1:A:644:LYS:HG3	2.19	0.42
1:B:165:LEU:CD2	1:B:197:LEU:HD11	2.48	0.42
1:A:288:HIS:O	1:A:290:THR:N	2.49	0.42
1:A:761:MET:HB2	1:A:803:TRP:CD1	2.53	0.42
1:A:841:LYS:O	1:A:845:GLN:HG2	2.19	0.42
1:B:240:ILE:O	1:B:243:PHE:HB2	2.19	0.42
1:A:621:ARG:HG2	1:A:674:PHE:CE2	2.54	0.42
1:B:341:MET:HB2	1:B:341:MET:HE3	1.70	0.42
1:A:54:ALA:HA	1:A:258:LEU:HD12	2.01	0.42
1:B:517:TYR:OH	1:B:724:LEU:HA	2.20	0.42
1:A:395:THR:O	1:A:398:GLU:HB3	2.19	0.42
1:B:541:ARG:HH21	1:B:687:VAL:CG1	2.32	0.42
1:B:761:MET:HB2	1:B:803:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:ARG:HD2	1:A:518:ILE:HD13	2.01	0.42
1:B:531:TYR:CE2	1:B:675:ALA:HB2	2.55	0.42
1:B:623:MET:HB3	1:B:628:VAL:HG22	2.00	0.42
1:B:203:GLY:O	1:B:225:SER:HA	2.19	0.42
1:B:399:PHE:HD2	1:B:432:TRP:HH2	1.68	0.42
1:A:77:VAL:HG13	1:A:142:THR:HG23	2.02	0.42
1:B:28:TYR:O	1:B:213:ASN:ND2	2.40	0.42
1:A:17:LEU:HD11	1:A:25:PHE:CE1	2.54	0.42
1:A:540:THR:HA	1:A:598:GLN:HG2	2.02	0.42
1:A:754:LEU:HD13	1:A:791:SER:CB	2.50	0.41
1:A:122:ASN:OD1	1:A:122:ASN:N	2.53	0.41
1:A:430:GLY:O	1:A:431:PHE:C	2.62	0.41
1:A:557:MET:HE1	1:A:565:ALA:CB	2.49	0.41
1:A:57:ARG:HE	1:A:57:ARG:HB3	1.38	0.41
1:A:488:ALA:HB1	1:A:565:ALA:HB2	2.01	0.41
1:B:13:TRP:CE3	1:B:216:HIS:HD2	2.37	0.41
1:B:35:GLU:CD	1:B:212:ARG:NH2	2.78	0.41
1:A:33:ILE:CD1	1:A:212:ARG:HD3	2.49	0.41
1:A:372:LYS:O	1:A:376:ILE:HG23	2.21	0.41
1:A:427:GLU:C	1:A:429:SER:H	2.29	0.41
1:A:669:PRO:HG3	1:A:674:PHE:CG	2.56	0.41
1:A:718:MET:HG3	1:A:722:ARG:O	2.20	0.41
1:B:98:LYS:O	1:B:123:LEU:HD13	2.21	0.41
1:B:393:MET:HE3	1:B:393:MET:HB3	1.72	0.41
1:B:772:LEU:HD23	1:B:772:LEU:HA	1.87	0.41
1:B:554:THR:HG21	1:B:566:GLU:HG2	2.02	0.41
1:A:528:GLY:O	1:A:668:LYS:HE2	2.21	0.41
1:A:580:VAL:HG22	1:A:581:GLN:O	2.20	0.41
1:B:55:VAL:HG11	1:B:84:ARG:HB2	2.01	0.41
1:B:170:ASN:C	1:B:172:LEU:N	2.79	0.41
1:B:298:HIS:CD2	1:B:305:TYR:CD2	3.09	0.41
1:B:440:ASN:CA	1:B:443:LEU:HD23	2.45	0.41
1:B:700:TRP:CB	1:B:706:VAL:HG12	2.51	0.41
1:A:216:HIS:O	1:A:217:GLU:C	2.63	0.41
1:A:430:GLY:O	1:A:433:GLU:N	2.53	0.41
1:A:782:ALA:HA	1:A:871:ARG:HG3	2.03	0.41
1:B:75:GLY:HA3	1:B:141:ASP:OD1	2.21	0.41
1:B:103:LEU:HD22	1:B:127:GLN:NE2	2.35	0.41
1:B:388:LYS:O	1:B:389:LYS:HG2	2.21	0.41
1:A:770:ARG:HD2	1:A:770:ARG:HH11	1.69	0.40
1:A:824:MET:HE2	1:A:824:MET:HB2	1.95	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:CYS:HA	1:A:94:LEU:HD12	2.03	0.40
1:B:242:ARG:HD2	1:B:245:MET:HE1	2.03	0.40
1:B:301:LYS:HG3	1:B:360:ASP:OD1	2.21	0.40
1:A:62:LEU:O	1:A:66:VAL:HG23	2.22	0.40
1:A:517:TYR:OH	1:A:724:LEU:HA	2.22	0.40
1:B:749:ARG:HH11	1:B:749:ARG:HD2	1.74	0.40
1:B:178:PHE:CZ	1:B:222:SER:HA	2.57	0.40
1:A:286:GLN:C	1:A:288:HIS:N	2.79	0.40
1:A:688:ARG:NH1	1:A:691:ILE:HD11	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:NH1	1:A:826:ASP:OD2[6_445]	2.11	0.09

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	832/911 (91%)	738 (89%)	81 (10%)	13 (2%)	7	21
1	B	824/911 (90%)	703 (85%)	92 (11%)	29 (4%)	3	7
All	All	1656/1822 (91%)	1441 (87%)	173 (10%)	42 (2%)	4	12

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	597	ASP
1	A	791	SER
1	A	792	ARG
1	B	171	TRP

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Mol	Chain	Res	Type
1	B	214	SER
1	B	341	MET
1	B	405	SER
1	B	603	GLN
1	A	9	LEU
1	A	403	VAL
1	A	421	SER
1	B	24	GLU
1	B	131	ASP
1	B	173	ASN
1	B	229	VAL
1	B	424	GLU
1	B	597	ASP
1	B	847	CYS
1	A	429	SER
1	A	431	PHE
1	A	603	GLN
1	B	170	ASN
1	B	172	LEU
1	B	204	ALA
1	B	228	ILE
1	B	437	LYS
1	B	440	ASN
1	B	601	SER
1	A	420	LYS
1	B	39	THR
1	B	291	SER
1	B	552	MET
1	A	269	SER
1	A	289	GLU
1	B	17	LEU
1	B	106	GLY
1	B	185	PRO
1	B	504	LEU
1	B	677	ALA
1	B	704	THR
1	A	148	GLY
1	B	108	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	638/790 (81%)	614 (96%)	24 (4%)	29	54
1	B	605/790 (77%)	586 (97%)	19 (3%)	35	60
All	All	1243/1580 (79%)	1200 (96%)	43 (4%)	32	56

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	71	VAL
1	A	88	SER
1	A	105	LYS
1	A	118	THR
1	A	126	LEU
1	A	135	THR
1	A	150	SER
1	A	163	ARG
1	A	248	LYS
1	A	308	SER
1	A	363	THR
1	A	385	LEU
1	A	436	ASP
1	A	593	ILE
1	A	635	LEU
1	A	636	THR
1	A	648	VAL
1	A	769	ARG
1	A	790	THR
1	A	791	SER
1	A	824	MET
1	A	845	GLN
1	A	849	SER
1	B	11	GLU
1	B	34	GLN
1	B	67	GLU

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Mol	Chain	Res	Type
1	B	116	MET
1	B	118	THR
1	B	211	SER
1	B	230	SER
1	B	301	LYS
1	B	308	SER
1	B	319	SER
1	B	329	THR
1	B	444	GLU
1	B	484	LEU
1	B	523	SER
1	B	598	GLN
1	B	624	GLU
1	B	634	HIS
1	B	718	MET
1	B	719	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	110	HIS
1	A	166	ASN
1	A	306	HIS
1	A	575	ASN
1	A	614	ASN
1	A	618	GLN
1	A	622	GLN
1	A	701	ASN
1	A	868	ASN
1	B	18	ASN
1	B	110	HIS
1	B	127	GLN
1	B	153	ASN
1	B	502	ASN
1	B	561	HIS
1	B	581	GLN
1	B	622	GLN
1	B	711	HIS
1	B	731	GLN
1	B	869	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 28 ligands modelled in this entry, 19 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
5	GOL	B	1008	-	5,5,5	0.57	0	5,5,5	0.91	0
5	GOL	A	1017	-	5,5,5	0.51	0	5,5,5	0.93	0
5	GOL	A	1018	-	5,5,5	0.46	0	5,5,5	0.48	0
3	SAH	A	1014	-	27,28,28	1.13	3 (11%)	36,40,40	2.59	16 (44%)
3	SAH	A	1013	-	27,28,28	1.06	2 (7%)	36,40,40	2.27	12 (33%)
3	SAH	B	1005	-	27,28,28	1.17	3 (11%)	36,40,40	2.33	11 (30%)
5	GOL	B	1010	-	5,5,5	0.58	0	5,5,5	0.45	0
5	GOL	B	1009	-	5,5,5	0.53	0	5,5,5	0.92	0
3	SAH	B	1004	-	27,28,28	1.37	3 (11%)	36,40,40	2.38	14 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	1008	-	-	4/4/4/4	-
5	GOL	A	1017	-	-	4/4/4/4	-
5	GOL	A	1018	-	-	2/4/4/4	-
3	SAH	A	1014	-	-	1/15/31/31	0/3/3/3
3	SAH	A	1013	-	-	6/15/31/31	0/3/3/3
3	SAH	B	1005	-	-	7/15/31/31	0/3/3/3
5	GOL	B	1010	-	-	3/4/4/4	-
5	GOL	B	1009	-	-	2/4/4/4	-
3	SAH	B	1004	-	-	8/15/31/31	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1004	SAH	C2-N3	3.70	1.40	1.33
3	B	1005	SAH	C2-N1	3.24	1.39	1.33
3	B	1004	SAH	C2-N1	3.23	1.39	1.33
3	B	1004	SAH	C8-N7	3.06	1.37	1.31
3	A	1014	SAH	C2-N3	2.53	1.38	1.33
3	A	1014	SAH	C5-N7	-2.38	1.34	1.39
3	B	1005	SAH	C8-N7	2.32	1.36	1.31
3	A	1014	SAH	C8-N7	2.28	1.36	1.31
3	B	1005	SAH	C2-N3	2.28	1.38	1.33
3	A	1013	SAH	OXT-C	-2.04	1.24	1.30
3	A	1013	SAH	O4'-C4'	-2.01	1.40	1.45

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1014	SAH	N3-C2-N1	-6.36	118.96	128.58
3	B	1004	SAH	C5-C4-N3	-6.08	118.34	126.72
3	A	1013	SAH	C5'-SD-CG	-5.65	85.50	102.26
3	A	1013	SAH	N3-C2-N1	-5.42	120.38	128.58
3	B	1005	SAH	N3-C2-N1	-5.41	120.40	128.58
3	B	1004	SAH	N3-C2-N1	-4.83	121.27	128.58
3	B	1004	SAH	C5'-SD-CG	-4.76	88.14	102.26
3	A	1014	SAH	C5-C4-N3	-4.74	120.19	126.72
3	A	1013	SAH	C5-C4-N3	-4.70	120.25	126.72
3	A	1013	SAH	O4'-C1'-N9	4.68	117.08	108.09
3	A	1014	SAH	N9-C8-N7	-4.68	107.30	113.94
3	B	1005	SAH	C5'-SD-CG	-4.46	89.01	102.26
3	A	1014	SAH	N3-C4-N9	4.40	134.66	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1005	SAH	N3-C4-N9	4.31	134.50	127.17
3	B	1004	SAH	N3-C4-N9	4.26	134.41	127.17
3	B	1005	SAH	N9-C8-N7	-4.15	108.04	113.94
3	B	1005	SAH	C5-C4-N3	-4.00	121.21	126.72
3	B	1005	SAH	C4-N9-C8	3.96	109.90	105.74
3	B	1005	SAH	N6-C6-N1	3.93	127.13	118.38
3	B	1004	SAH	C2-N3-C4	3.82	121.17	111.83
3	A	1014	SAH	C2-N3-C4	3.74	120.97	111.83
3	A	1014	SAH	C4-N9-C8	3.69	109.61	105.74
3	A	1014	SAH	OXT-C-O	-3.67	115.75	124.08
3	A	1014	SAH	C4'-C5'-SD	-3.56	101.07	113.78
3	A	1013	SAH	C2-N3-C4	3.51	120.40	111.83
3	B	1005	SAH	C5-C6-N6	-3.39	114.90	123.29
3	A	1013	SAH	N9-C8-N7	-3.38	109.15	113.94
3	A	1013	SAH	C5-N7-C8	3.36	108.73	103.45
3	A	1014	SAH	C5-C6-N6	-3.22	115.31	123.29
3	B	1004	SAH	C5-N7-C8	3.15	108.40	103.45
3	A	1014	SAH	CB-CA-C	3.13	118.73	110.45
3	B	1004	SAH	N9-C8-N7	-3.08	109.57	113.94
3	B	1004	SAH	O4'-C1'-N9	3.00	113.86	108.09
3	B	1005	SAH	C2-N3-C4	3.00	119.15	111.83
3	A	1014	SAH	O3'-C3'-C2'	-2.95	102.36	111.82
3	A	1014	SAH	C5-N7-C8	2.71	107.71	103.45
3	A	1013	SAH	N3-C4-N9	2.66	131.69	127.17
3	B	1005	SAH	C5-N7-C8	2.57	107.48	103.45
3	A	1013	SAH	C4-C5-N7	-2.54	107.68	110.58
3	A	1014	SAH	C2'-C1'-N9	-2.42	107.30	113.30
3	B	1005	SAH	C6-C5-C4	2.40	120.45	117.18
3	B	1004	SAH	C4-C5-N7	-2.37	107.87	110.58
3	B	1004	SAH	C6-C5-C4	2.35	120.38	117.18
3	A	1014	SAH	N6-C6-N1	2.30	123.50	118.38
3	A	1014	SAH	CB-CG-SD	-2.27	108.39	113.45
3	A	1013	SAH	OXT-C-O	-2.23	119.02	124.08
3	A	1013	SAH	C2'-C3'-C4'	2.22	106.89	102.61
3	B	1004	SAH	OXT-C-O	-2.20	119.09	124.08
3	B	1004	SAH	O4'-C1'-C2'	-2.11	102.11	106.62
3	B	1004	SAH	C4'-C5'-SD	-2.07	106.40	113.78
3	A	1013	SAH	C5-C4-N9	2.07	108.06	105.81
3	B	1004	SAH	C4'-O4'-C1'	-2.03	104.98	109.47
3	A	1014	SAH	C5'-SD-CG	-2.01	96.31	102.26

There are no chirality outliers.

All (37) torsion outliers are listed below:

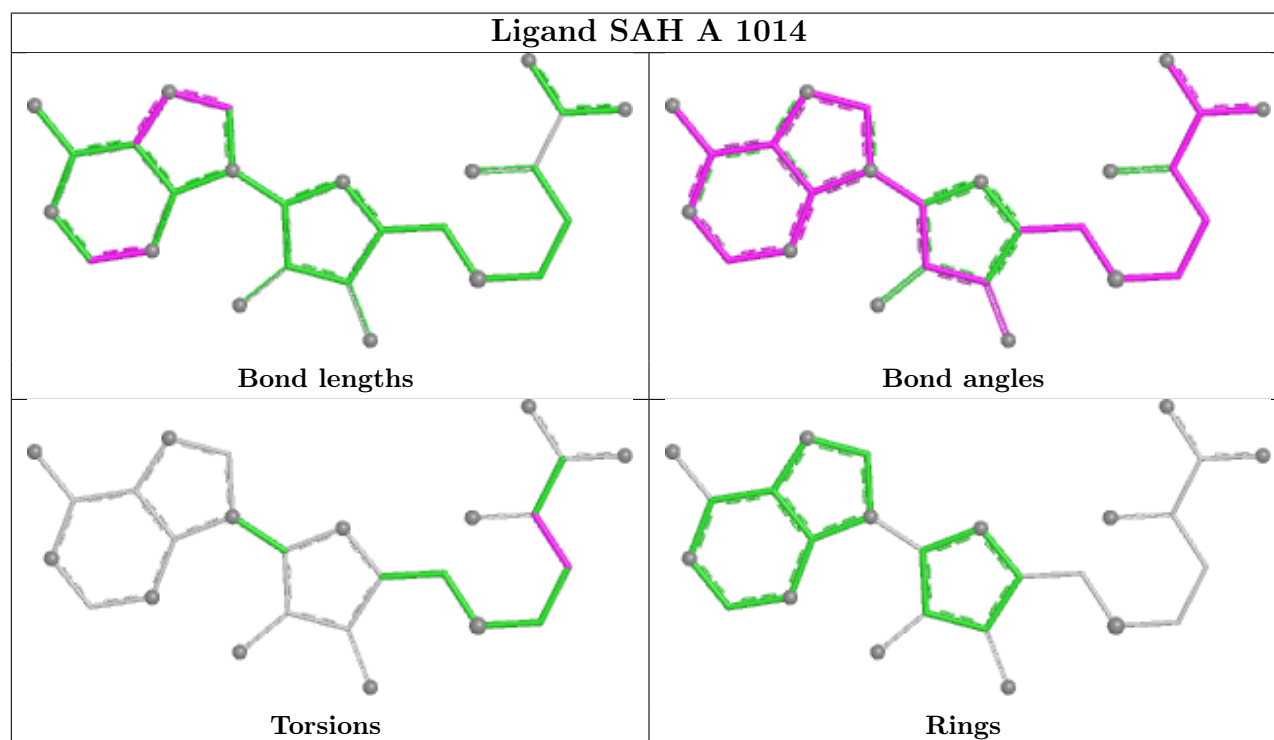
Mol	Chain	Res	Type	Atoms
3	B	1004	SAH	O4'-C4'-C5'-SD
3	B	1004	SAH	C3'-C4'-C5'-SD
5	A	1017	GOL	O1-C1-C2-C3
5	A	1018	GOL	O1-C1-C2-C3
5	B	1008	GOL	O1-C1-C2-C3
5	B	1009	GOL	C1-C2-C3-O3
5	B	1010	GOL	O1-C1-C2-C3
3	B	1004	SAH	CA-CB-CG-SD
5	A	1017	GOL	C1-C2-C3-O3
5	B	1008	GOL	C1-C2-C3-O3
5	B	1010	GOL	O1-C1-C2-O2
3	B	1005	SAH	C-CA-CB-CG
5	A	1018	GOL	O1-C1-C2-O2
5	B	1008	GOL	O1-C1-C2-O2
5	B	1009	GOL	O2-C2-C3-O3
5	A	1017	GOL	O1-C1-C2-O2
5	B	1010	GOL	O2-C2-C3-O3
3	B	1004	SAH	O4'-C1'-N9-C4
3	A	1013	SAH	C2'-C1'-N9-C8
3	B	1005	SAH	C2'-C1'-N9-C8
3	B	1005	SAH	N-CA-CB-CG
3	B	1004	SAH	O4'-C1'-N9-C8
5	A	1017	GOL	O2-C2-C3-O3
3	B	1004	SAH	O-C-CA-CB
3	B	1004	SAH	OXT-C-CA-CB
3	A	1013	SAH	C-CA-CB-CG
3	A	1014	SAH	C-CA-CB-CG
3	A	1013	SAH	CA-CB-CG-SD
5	B	1008	GOL	O2-C2-C3-O3
3	B	1004	SAH	CB-CG-SD-C5'
3	A	1013	SAH	O4'-C1'-N9-C8
3	B	1005	SAH	O4'-C1'-N9-C8
3	B	1005	SAH	OXT-C-CA-N
3	B	1005	SAH	CB-CG-SD-C5'
3	A	1013	SAH	OXT-C-CA-CB
3	B	1005	SAH	C2'-C1'-N9-C4
3	A	1013	SAH	O-C-CA-CB

There are no ring outliers.

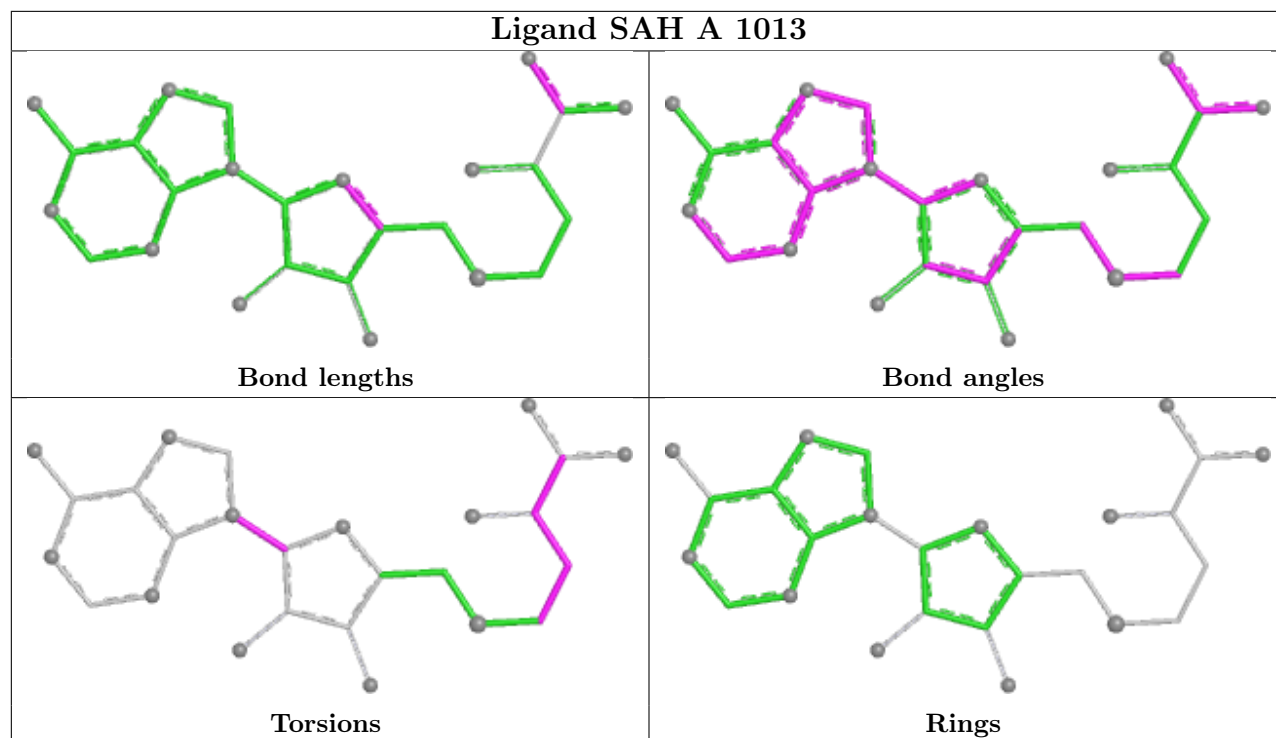
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1017	GOL	2	0
5	A	1018	GOL	1	0
3	A	1013	SAH	1	0
3	B	1005	SAH	4	0
5	B	1009	GOL	4	0
3	B	1004	SAH	1	0

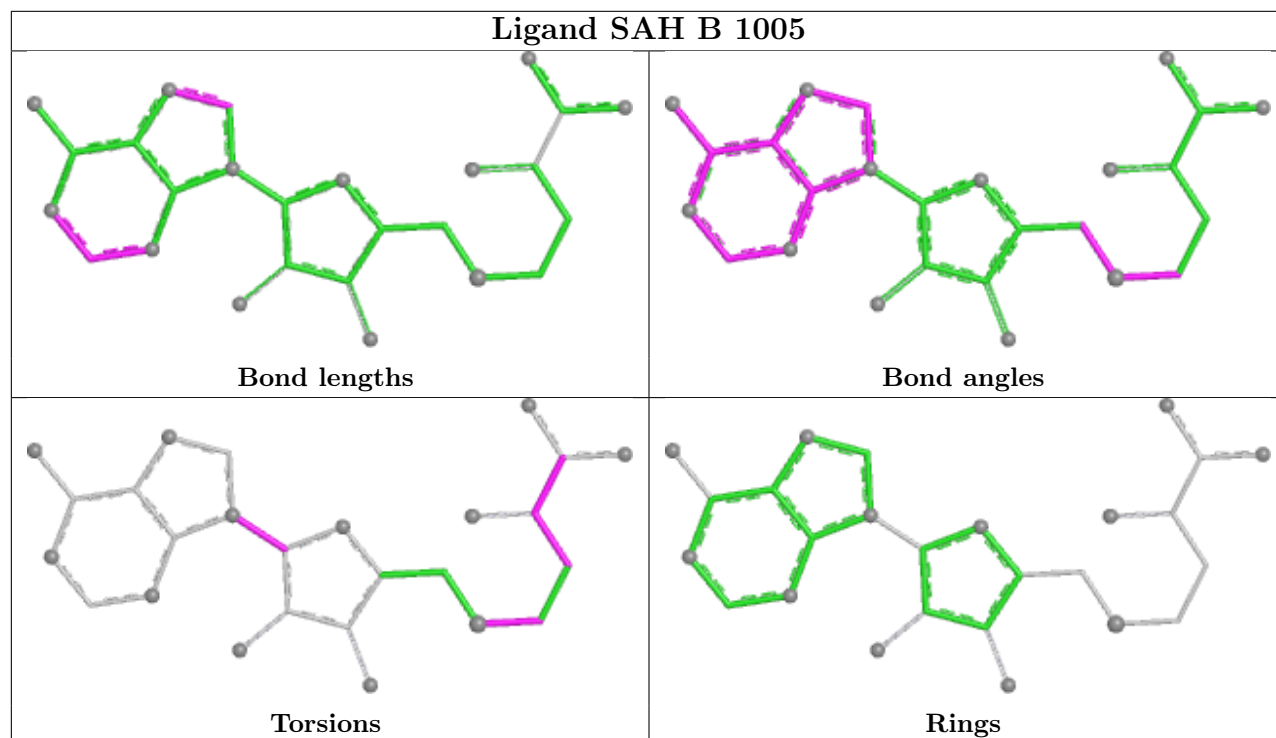
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

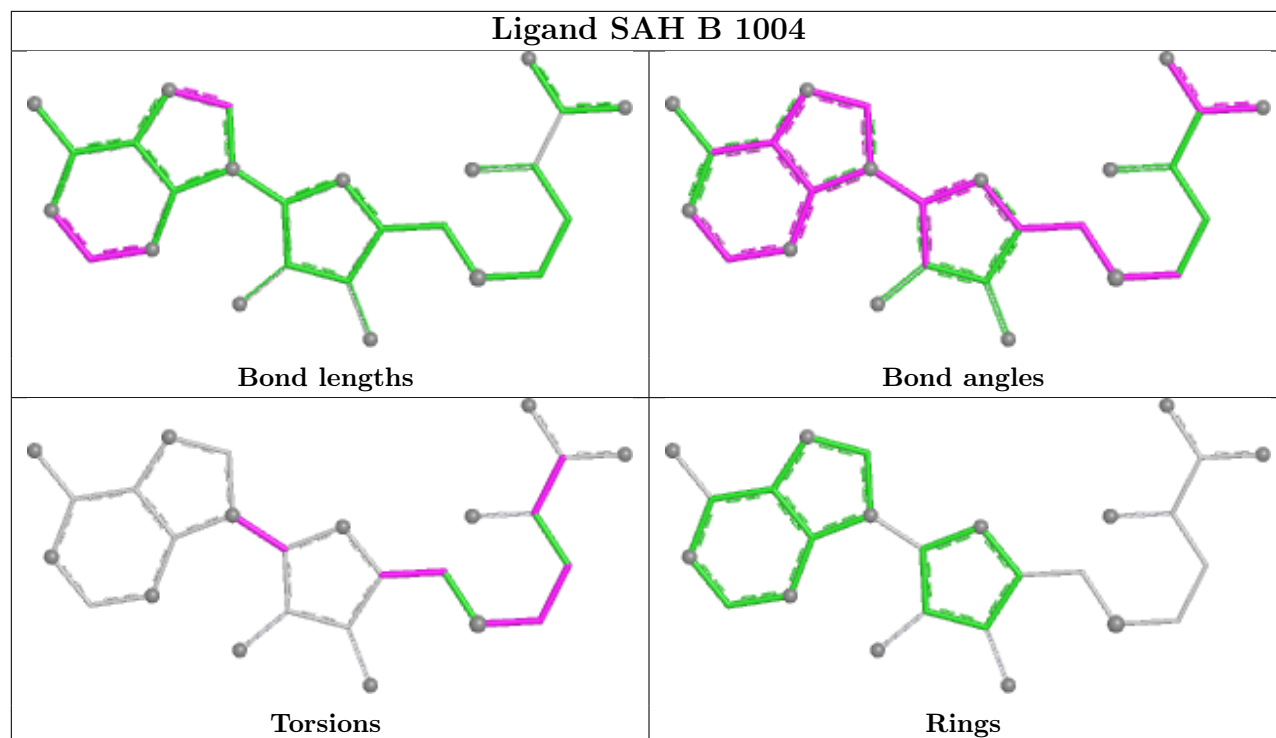


Ligand SAH A 1013



Ligand SAH B 1005





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	842/911 (92%)	0.31	43 (5%)	33 27	33, 51, 78, 97	0
1	B	836/911 (91%)	0.79	71 (8%)	16 15	37, 69, 88, 104	0
All	All	1678/1822 (92%)	0.55	114 (6%)	23 20	33, 59, 85, 104	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	792	ARG	6.6
1	A	795	TRP	5.8
1	A	419	TRP	5.3
1	B	348	PRO	4.9
1	B	419	TRP	4.8
1	B	473	ALA	4.4
1	B	475	TRP	4.2
1	B	601	SER	4.1
1	B	790	THR	4.0
1	B	800	THR	4.0
1	A	246	ARG	3.9
1	B	884	PRO	3.9
1	B	455	MET	3.8
1	B	307	GLY	3.8
1	B	318	SER	3.7
1	A	794	THR	3.7
1	A	473	ALA	3.5
1	A	455	MET	3.4
1	B	164	VAL	3.4
1	B	791	SER	3.4
1	A	471	SER	3.4
1	A	600	GLY	3.3
1	B	805	THR	3.2
1	A	345	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	227	ASN	3.2
1	A	449	THR	3.2
1	A	319	SER	3.2
1	A	314	THR	3.2
1	B	785	SER	3.1
1	B	343	MET	3.1
1	A	792	ARG	3.1
1	B	426	VAL	3.0
1	B	478	TRP	3.0
1	A	9	LEU	3.0
1	A	297	ASP	2.9
1	B	9	LEU	2.9
1	B	148	GLY	2.8
1	B	421	SER	2.8
1	A	605	VAL	2.8
1	B	423	ARG	2.8
1	B	600	GLY	2.8
1	A	265	ILE	2.8
1	B	32	GLY	2.8
1	B	446	LYS	2.7
1	A	474	ILE	2.7
1	B	8	THR	2.6
1	B	10	GLY	2.6
1	B	476	TYR	2.6
1	B	132	VAL	2.5
1	B	606	THR	2.5
1	A	174	ASN	2.5
1	B	586	ARG	2.5
1	A	279	LYS	2.5
1	A	631	SER	2.5
1	B	638	THR	2.5
1	B	793	THR	2.5
1	B	173	ASN	2.5
1	A	448	GLU	2.5
1	B	493	ASN	2.4
1	B	265	ILE	2.4
1	A	307	GLY	2.4
1	B	303	TRP	2.4
1	B	825	GLU	2.4
1	B	279	LYS	2.4
1	B	431	PHE	2.4
1	A	603	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	40	LEU	2.4
1	B	406	ASN	2.4
1	B	168	VAL	2.4
1	A	472	ARG	2.3
1	B	427	GLU	2.3
1	A	346	THR	2.3
1	B	98	LYS	2.3
1	A	479	LEU	2.3
1	A	800	THR	2.3
1	B	309	TYR	2.3
1	B	472	ARG	2.3
1	A	885	SER	2.3
1	B	99	GLU	2.3
1	B	289	GLU	2.3
1	B	422	ALA	2.3
1	B	248	LYS	2.3
1	B	390	THR	2.3
1	B	205	LEU	2.2
1	B	429	SER	2.2
1	B	134	PHE	2.2
1	A	69	ASN	2.2
1	B	351	GLN	2.2
1	A	344	THR	2.2
1	B	290	THR	2.2
1	A	446	LYS	2.2
1	A	309	TYR	2.1
1	A	429	SER	2.1
1	B	305	TYR	2.1
1	B	340	GLN	2.1
1	A	743	GLY	2.1
1	A	399	PHE	2.1
1	B	365	GLU	2.1
1	A	110	HIS	2.1
1	B	440	ASN	2.1
1	A	10	GLY	2.1
1	A	212	ARG	2.1
1	B	228	ILE	2.1
1	A	282	GLU	2.1
1	B	150	SER	2.0
1	B	83	GLY	2.0
1	B	449	THR	2.0
1	A	428	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	432	TRP	2.0
1	B	193	LYS	2.0
1	A	634	HIS	2.0
1	B	564	LEU	2.0
1	B	175	ASN	2.0
1	A	604	VAL	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.

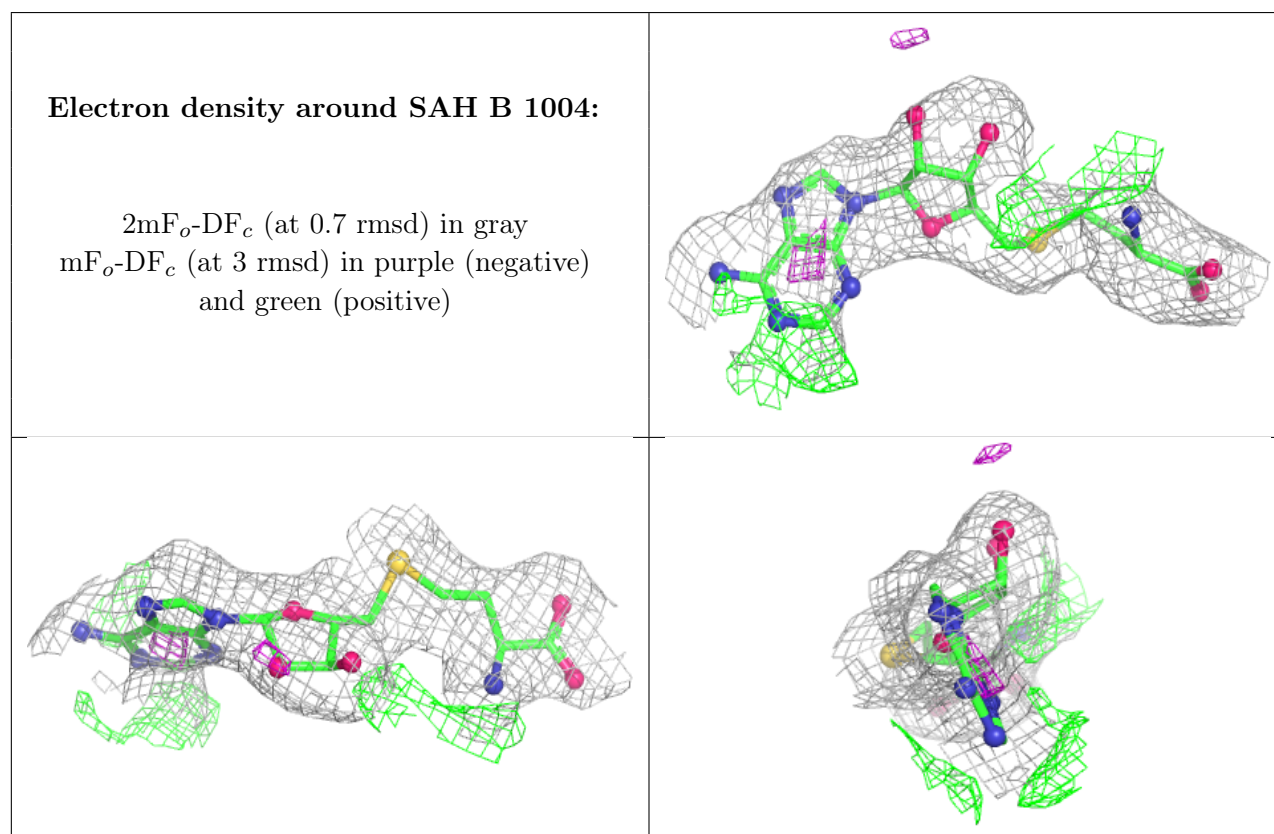
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SAH	B	1004	26/26	0.71	0.16	52,64,74,79	0
3	SAH	B	1005	26/26	0.74	0.17	72,78,84,90	26
3	SAH	A	1014	26/26	0.75	0.16	44,62,73,76	0
5	GOL	A	1017	6/6	0.85	0.15	43,46,48,51	0
5	GOL	B	1008	6/6	0.90	0.14	46,48,50,53	0
5	GOL	B	1010	6/6	0.92	0.13	44,46,48,53	6
5	GOL	B	1009	6/6	0.93	0.11	39,42,43,58	0
5	GOL	A	1018	6/6	0.93	0.13	42,46,48,51	6
3	SAH	A	1013	26/26	0.94	0.10	41,44,54,64	0
2	IOD	A	1011	1/1	0.94	0.08	91,91,91,91	1
2	IOD	B	1002	1/1	0.94	0.09	108,108,108,108	1
2	IOD	A	1007	1/1	0.96	0.07	109,109,109,109	1
2	IOD	A	1012	1/1	0.96	0.10	91,91,91,91	1
2	IOD	A	1008	1/1	0.96	0.13	101,101,101,101	1
4	ZN	B	1006	1/1	0.97	0.07	121,121,121,121	0
2	IOD	B	1003	1/1	0.97	0.12	113,113,113,113	1
2	IOD	A	1003	1/1	0.97	0.06	76,76,76,76	0

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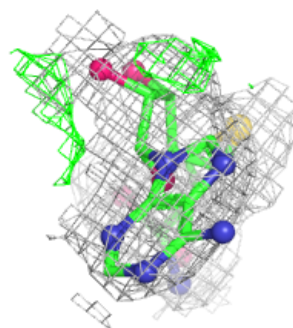
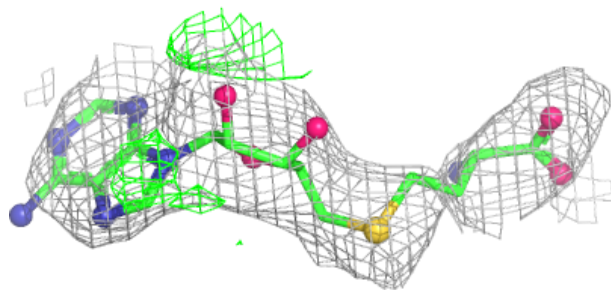
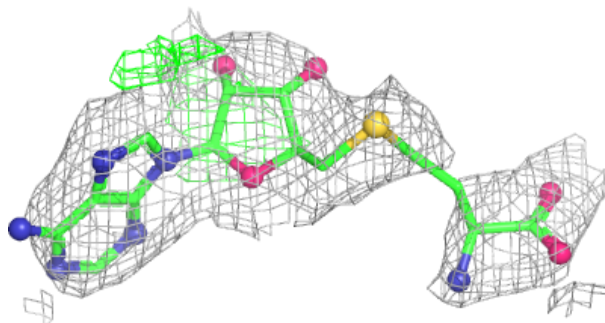
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	IOD	A	1006	1/1	0.97	0.06	94,94,94,94	1
2	IOD	B	1001	1/1	0.97	0.07	117,117,117,117	1
2	IOD	A	1010	1/1	0.97	0.07	91,91,91,91	1
2	IOD	A	1002	1/1	0.98	0.06	76,76,76,76	0
2	IOD	A	1009	1/1	0.98	0.11	103,103,103,103	1
2	IOD	A	1005	1/1	0.98	0.05	76,76,76,76	0
4	ZN	A	1016	1/1	0.99	0.04	55,55,55,55	1
2	IOD	A	1004	1/1	0.99	0.12	76,76,76,76	0
4	ZN	B	1007	1/1	0.99	0.04	62,62,62,62	1
4	ZN	A	1015	1/1	0.99	0.04	127,127,127,127	0
2	IOD	A	1001	1/1	1.00	0.03	76,76,76,76	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.

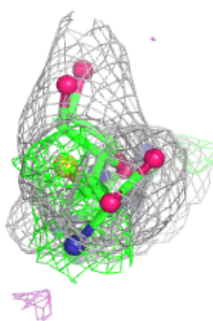
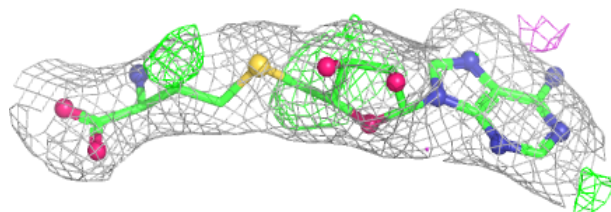
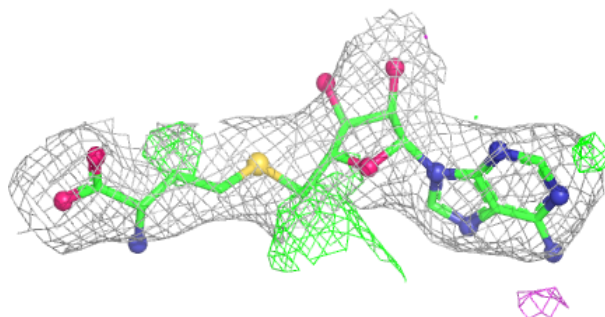


Electron density around SAH B 1005:

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

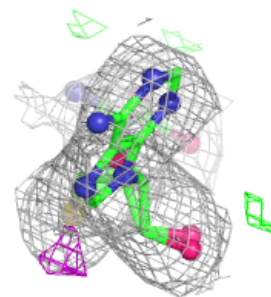
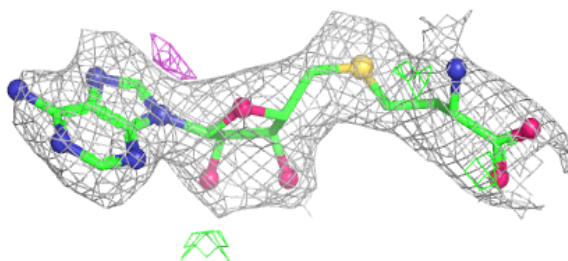
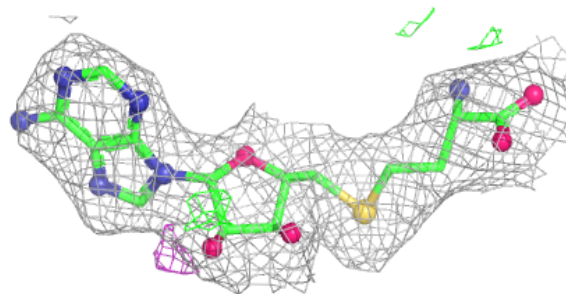
**Electron density around SAH A 1014:**

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



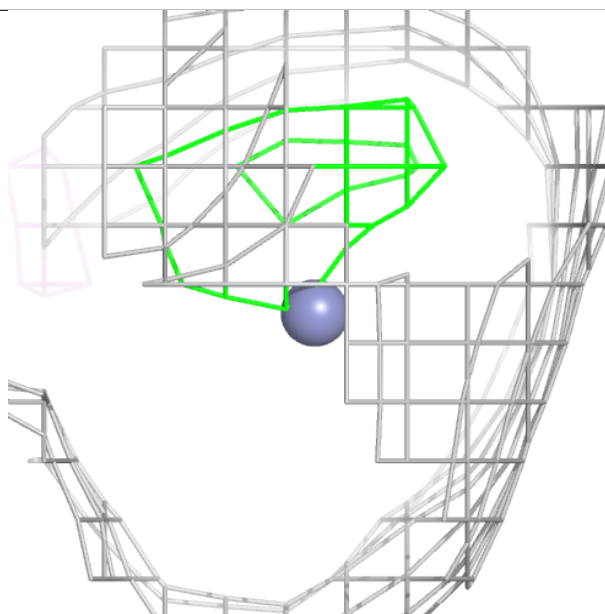
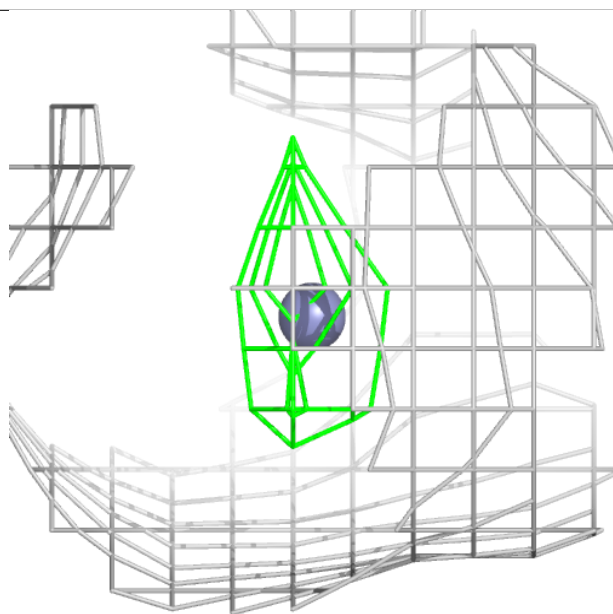
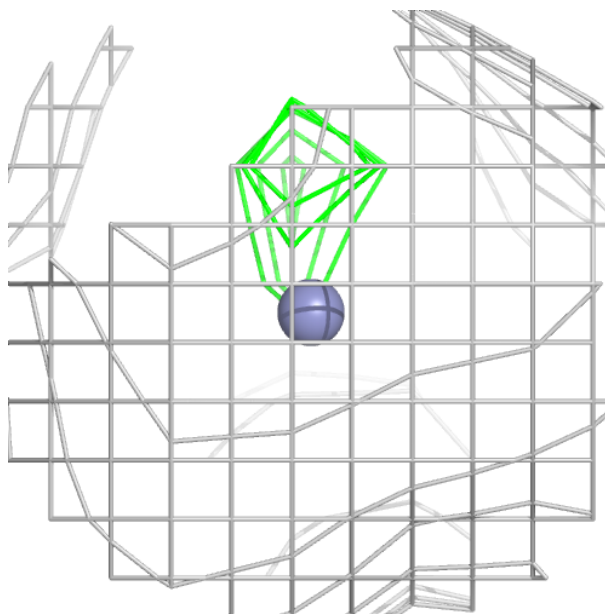
Electron density around SAH A 1013:

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



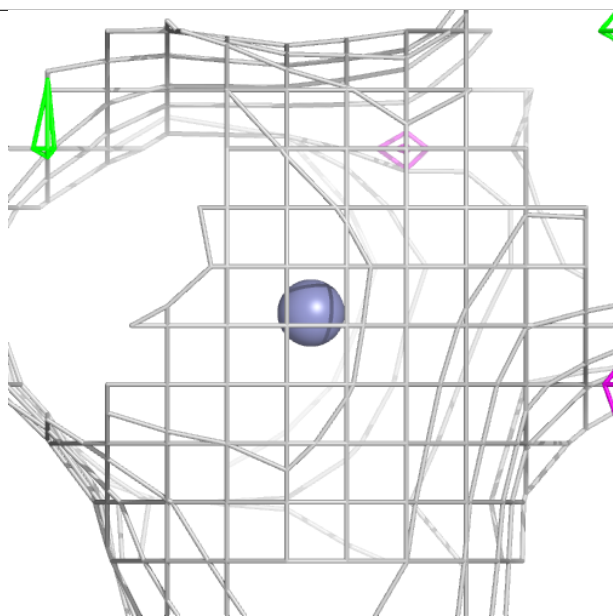
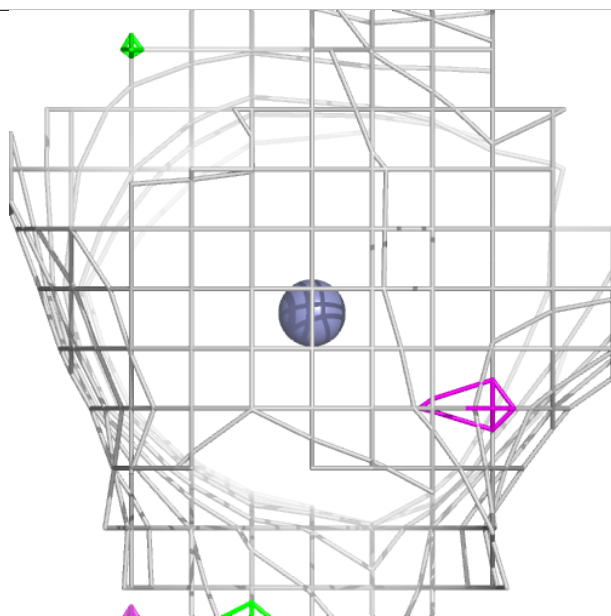
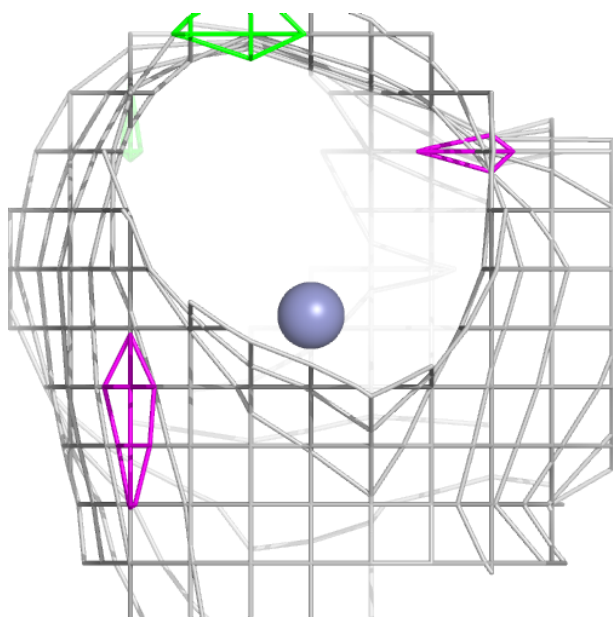
Electron density around ZN B 1006:

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



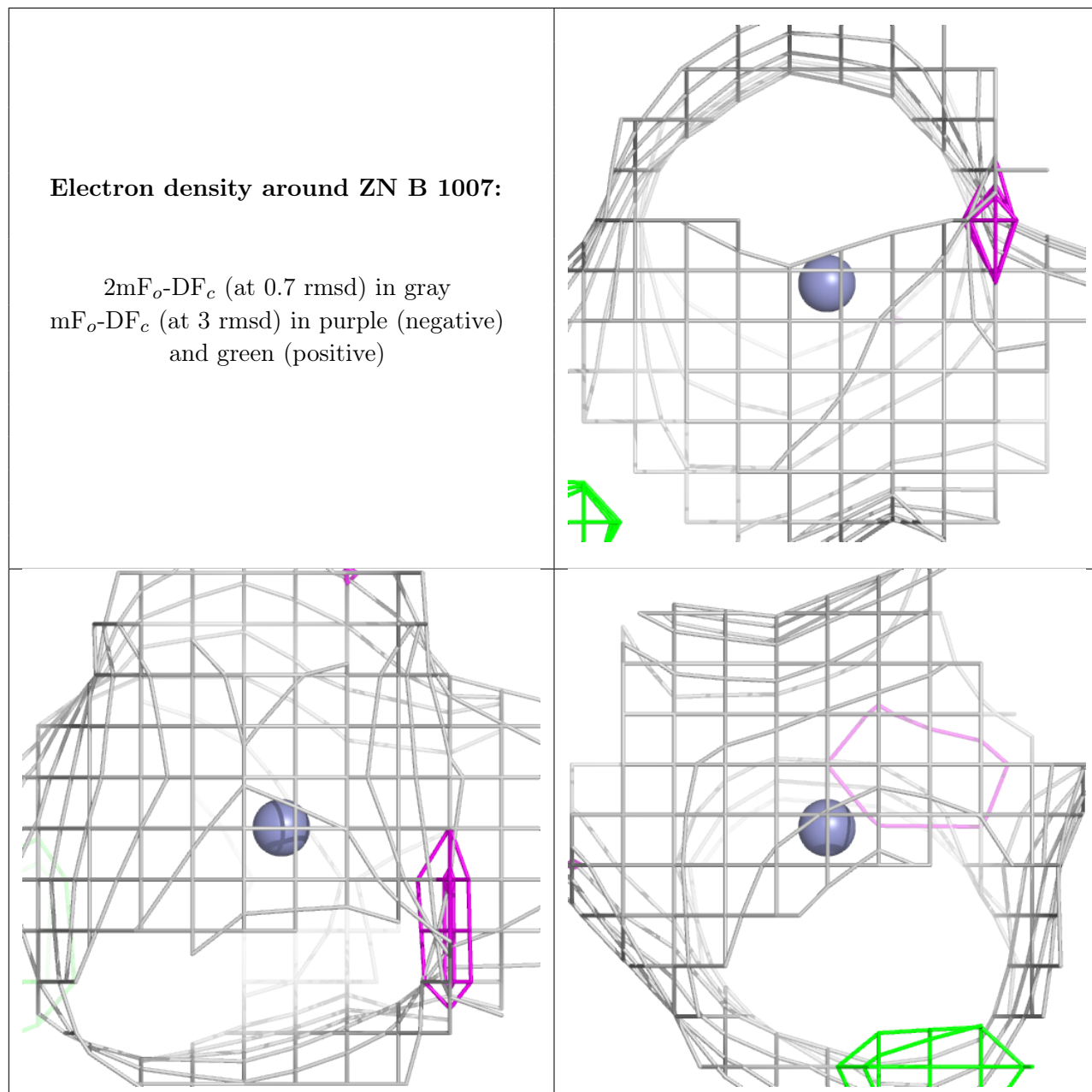
Electron density around ZN A 1016:

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



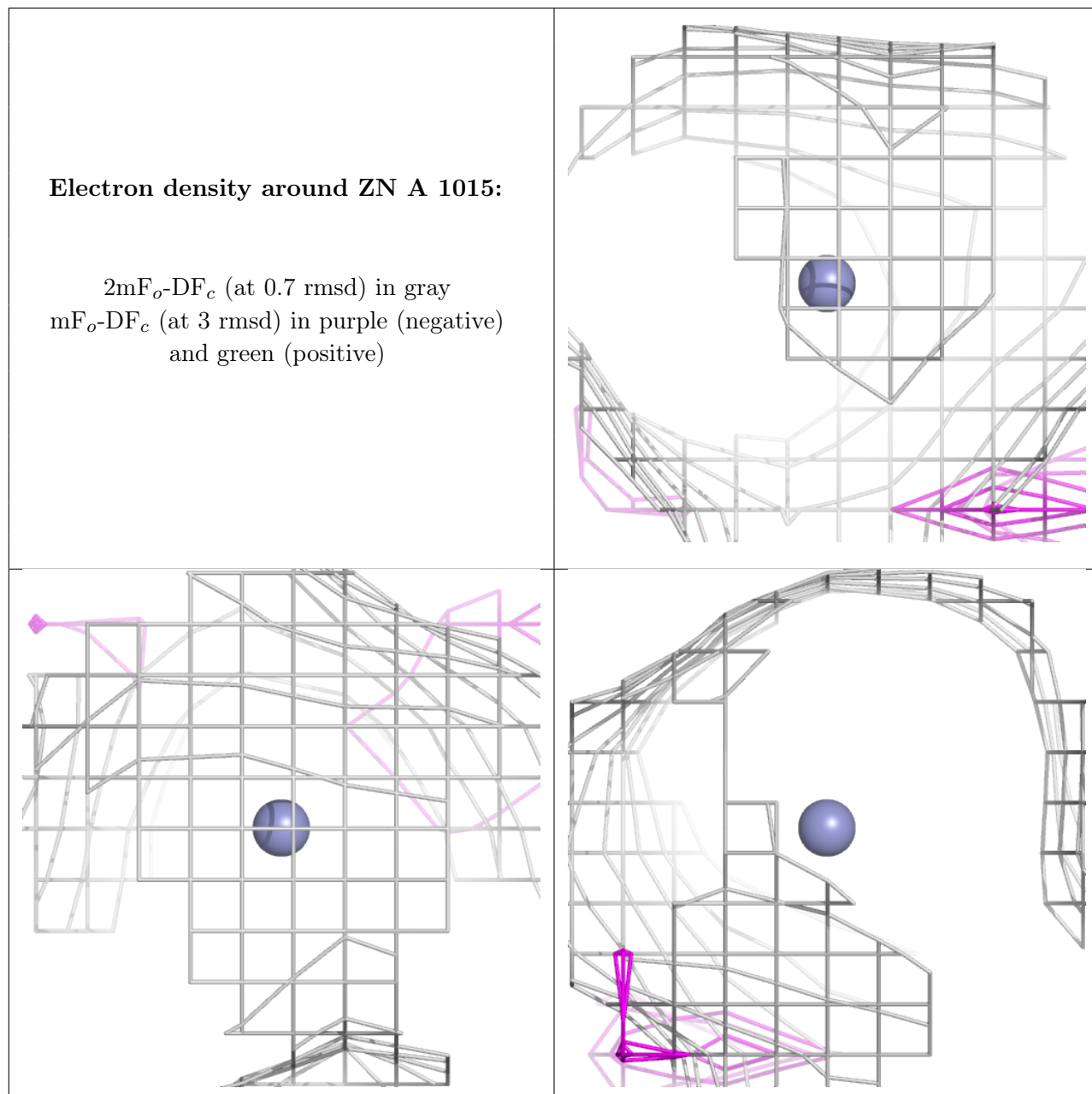
Electron density around ZN B 1007:

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



Electron density around ZN A 1015:

$2mF_o-DF_c$ (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.