



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:48 PM UTC

PDB ID : 8Q69 / pdb_00008q69
Title : Crystal structure of HsRNMT complexed with inhibitor DDD1060606
Authors : Petit, A.P.; Fyfe, P.K.
Deposited on : 2023-08-11
Resolution : 1.96 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

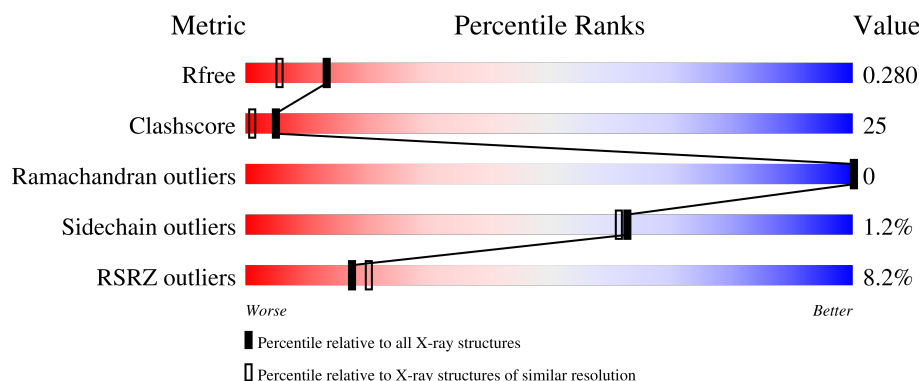
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	276	
1	B	276	

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
3	K7R	B	502	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4920 atoms, of which 1 is hydrogen 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.

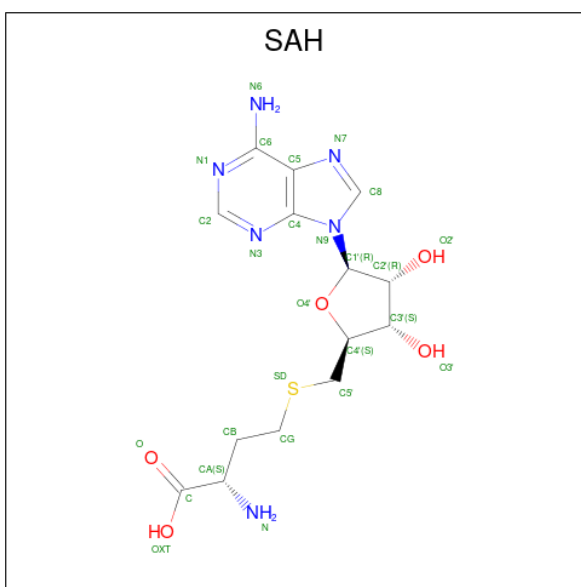
- Molecule 1 is a protein called mRNA cap guanine-N7 methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	1	0
			2239	1441	365	414	19			
1	B	264	Total	C	N	O	S	0	0	0
			2161	1392	353	397	19			

There are 8 discrepancies between the modelled and reference sequences:

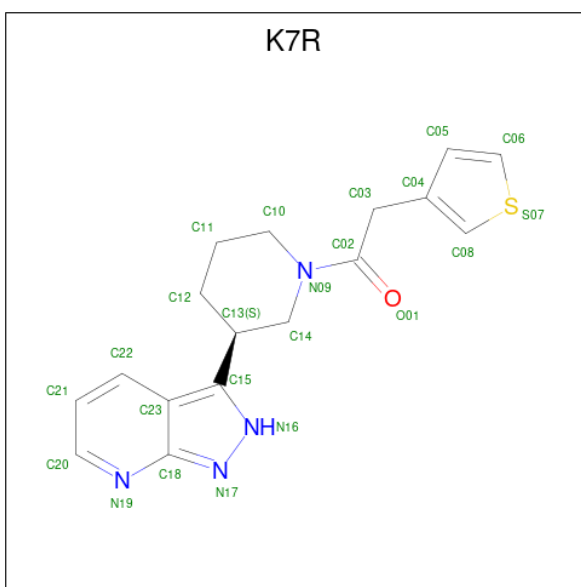
Chain	Residue	Modelled	Actual	Comment	Reference
A	416	GLY	-	linker	UNP O43148
A	417	LEU	-	linker	UNP O43148
A	418	GLY	-	linker	UNP O43148
A	419	CYS	-	linker	UNP O43148
B	416	GLY	-	linker	UNP O43148
B	417	LEU	-	linker	UNP O43148
B	418	GLY	-	linker	UNP O43148
B	419	CYS	-	linker	UNP O43148

- Molecule 2 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
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is 1-[(3 {S})-3-(2 {H})-pyrazolo[3,4-b]pyridin-3-yl)piperidin-1-yl]-2-thiophen-3-yl-ethanone (CCD ID: K7R) (formula: C₁₇H₁₈N₄OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			23	17	4	1	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			23	17	4	1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			7	3	1	3		

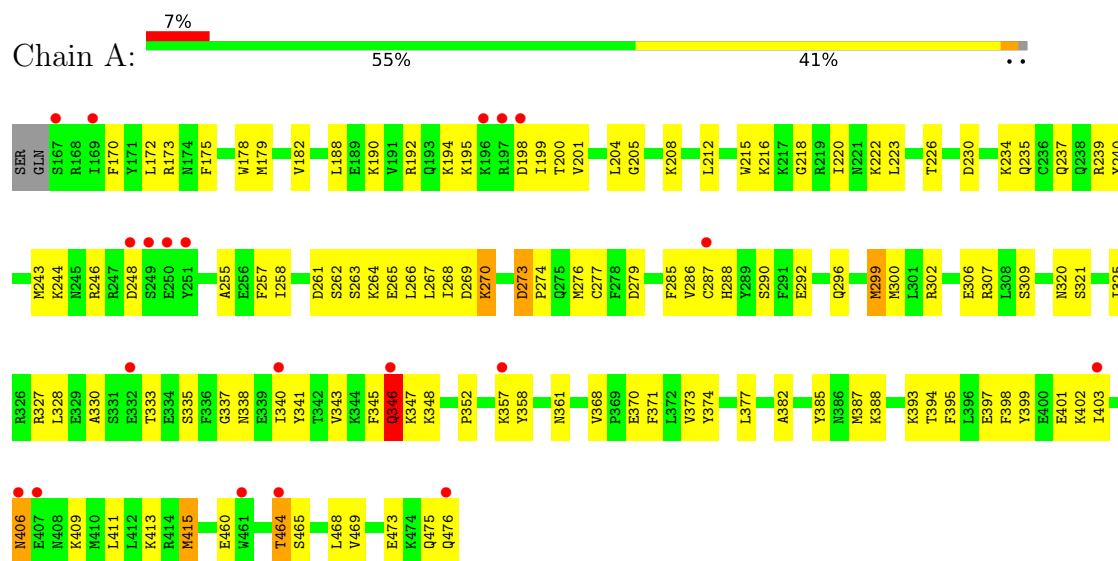
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	230	Total	O	0	0
			230	230		
6	B	175	Total	O	0	0
			175	175		

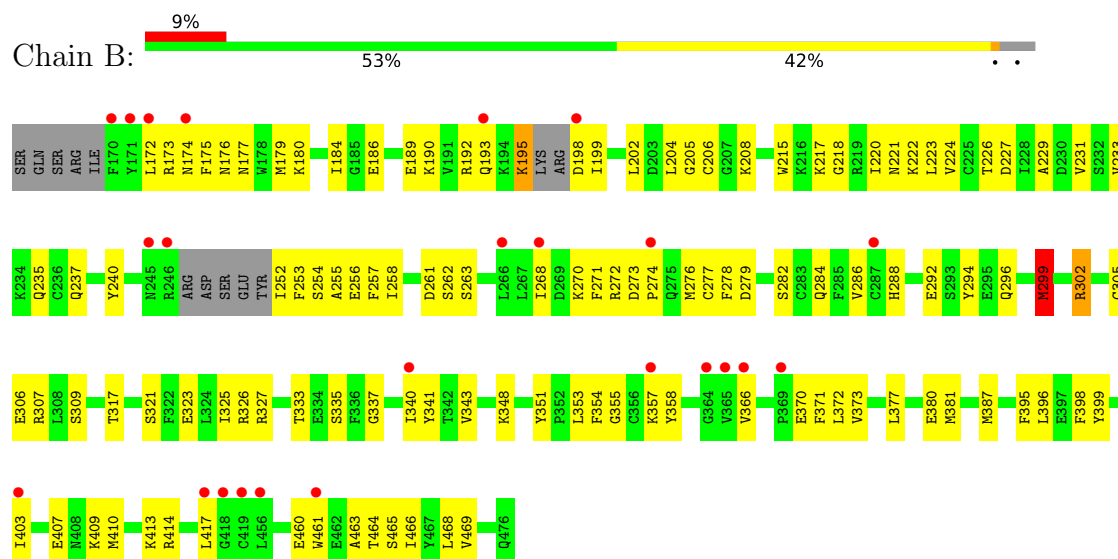
3 Residue-property plots

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: mRNA cap guanine-N7 methyltransferase



- Molecule 1: mRNA cap guanine-N7 methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.20Å 84.57Å 81.97Å 90.00° 99.03° 90.00°	Depositor
Resolution (Å)	40.47 – 1.96 40.47 – 1.96	Depositor EDS
% Data completeness (in resolution range)	96.6 (40.47-1.96) 97.2 (40.47-1.96)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.242 , 0.289 0.237 , 0.280	Depositor DCC
R_{free} test set	1731 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	26.5	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 23.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4920	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, SO4, K7R, 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	0.62	6/2288 (0.3%)	0.77	7/3068 (0.2%)
1	B	0.36	2/2204 (0.1%)	0.47	0/2952
All	All	0.51	8/4492 (0.2%)	0.64	7/6020 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	246	ARG	CA-C	-8.11	1.42	1.52
1	A	299	MET	C-O	-5.80	1.17	1.24
1	B	299	MET	C-O	-5.77	1.17	1.24
1	A	406[A]	ASN	CA-C	5.66	1.60	1.52
1	A	406[B]	ASN	CA-C	5.66	1.60	1.52
1	B	302	ARG	C-O	-5.41	1.17	1.24
1	A	346	GLN	C-O	-5.10	1.18	1.24
1	A	325	ILE	C-O	-5.06	1.18	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ASP	CA-C-N	11.71	134.48	119.84
1	A	273	ASP	C-N-CA	11.71	134.48	119.84
1	A	248	ASP	N-CA-C	-10.16	100.16	111.14
1	A	406[A]	ASN	CA-C-O	7.24	128.25	119.49
1	A	406[B]	ASN	CA-C-O	7.24	128.25	119.49
1	A	406[A]	ASN	N-CA-C	6.57	120.39	112.38
1	A	406[B]	ASN	N-CA-C	6.57	120.39	112.38

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	2239	0	2208	102	2
1	B	2161	0	2139	118	0
2	A	26	0	19	3	0
2	B	26	0	19	3	0
3	A	23	0	0	0	0
3	B	23	0	0	9	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
5	B	6	1	8	1	0
6	A	230	0	0	12	0
6	B	175	0	0	10	0
All	All	4919	1	4393	223	2

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 25.

All (223) 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:B:299:MET:HE1	1:B:302:ARG:HD3	1.59	0.84
1:A:346:GLN:H	1:A:346:GLN:HE21	1.24	0.83
1:A:338:ASN:HB2	6:A:613:HOH:O	1.78	0.83
1:B:395:PHE:HD2	1:B:464:THR:HG22	1.45	0.82
1:A:212:LEU:HD12	1:A:239:ARG:HG2	1.59	0.81
1:B:173:ARG:HD3	4:B:503:SO4:O2	1.80	0.81
1:B:174:ASN:HB3	1:B:417:LEU:HD21	1.60	0.81
1:B:205:GLY:HA3	1:B:286:VAL:HG21	1.65	0.78
1:B:366:VAL:HG21	3:B:502:K7R:C20	2.14	0.78
1:B:366:VAL:CG2	3:B:502:K7R:C20	2.62	0.78
1:B:176:ASN:ND2	3:B:502:K7R:O01	2.18	0.77
1:B:195:LYS:HD3	1:B:279:ASP:OD1	1.85	0.77
1:A:411:LEU:HG	1:A:415:MET:HE2	1.68	0.74
1:B:396:LEU:HB2	1:B:461:TRP:HZ2	1.52	0.74
1:B:261:ASP:OD2	6:B:601:HOH:O	2.06	0.73
1:A:190:LYS:O	1:A:194:LYS:HE3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:PHE:CD2	1:B:464:THR:HG21	2.26	0.71
1:B:273:ASP:HB3	1:B:276:MET:HB3	1.71	0.71
1:A:398:PHE:CD1	1:A:469:VAL:HG21	2.26	0.70
1:B:172:LEU:HD11	1:B:464:THR:OG1	1.92	0.70
1:B:299:MET:CE	1:B:302:ARG:HD3	2.21	0.69
1:B:398:PHE:CD1	1:B:469:VAL:HG21	2.28	0.68
1:A:395:PHE:HD2	1:A:464:THR:HG22	1.60	0.67
1:A:340:ILE:CD1	1:A:460:GLU:HG3	2.25	0.67
1:A:204:LEU:HD21	1:A:262:SER:OG	1.95	0.66
1:A:399:TYR:O	1:A:403:ILE:HG12	1.95	0.66
1:B:175:PHE:CE2	1:B:464:THR:HG21	2.31	0.66
1:B:333:THR:O	1:B:348:LYS:NZ	2.26	0.65
1:A:346:GLN:HE21	1:A:346:GLN:N	1.94	0.65
1:B:323:GLU:OE1	1:B:326:ARG:NH2	2.28	0.65
1:B:288:HIS:HA	1:B:373:VAL:CG2	2.28	0.64
1:A:340:ILE:HD13	1:A:460:GLU:HG3	1.79	0.64
1:A:172:LEU:HD21	1:A:464:THR:OG1	1.98	0.63
1:A:411:LEU:HG	1:A:415:MET:CE	2.28	0.62
1:B:192:ARG:NH2	1:B:218:GLY:O	2.32	0.62
1:A:195:LYS:HD3	1:A:279:ASP:OD1	2.00	0.62
1:B:299:MET:HE3	1:B:302:ARG:HB3	1.82	0.62
1:B:190:LYS:O	1:B:193:GLN:HB2	2.00	0.61
1:A:266:LEU:HD12	1:A:268:ILE:CG1	2.30	0.61
1:B:299:MET:HB2	6:B:650:HOH:O	2.01	0.60
1:B:325:ILE:HD11	1:B:372:LEU:HD21	1.82	0.60
1:B:172:LEU:HD21	1:B:463:ALA:HB3	1.83	0.60
1:B:202:LEU:HB2	1:B:278:PHE:CE1	2.37	0.59
1:B:366:VAL:HG23	3:B:502:K7R:C20	2.32	0.59
1:A:212:LEU:CD1	1:A:239:ARG:HG2	2.32	0.59
1:B:366:VAL:HB	3:B:502:K7R:C21	2.32	0.59
1:B:294:TYR:CE1	1:B:381:MET:HE3	2.36	0.59
1:B:173:ARG:HH11	1:B:177:ASN:ND2	2.01	0.59
1:A:290:SER:HB3	1:A:300:MET:SD	2.42	0.59
1:B:173:ARG:HH11	1:B:177:ASN:HD22	1.52	0.57
1:B:407:GLU:HA	1:B:410:MET:HE3	1.87	0.57
1:B:366:VAL:HG21	3:B:502:K7R:N19	2.20	0.57
1:B:335:SER:HA	1:B:343:VAL:O	2.05	0.57
1:B:222:LYS:HD2	1:B:254:SER:O	2.05	0.56
1:B:292:GLU:HB2	1:B:371:PHE:CE2	2.41	0.56
1:B:355:GLY:O	1:B:357:LYS:HG3	2.06	0.56
1:A:200:THR:HG23	1:A:222:LYS:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:TRP:HB2	1:A:415:MET:HE3	1.85	0.56
1:A:266:LEU:HD12	1:A:268:ILE:HG13	1.86	0.56
1:B:173:ARG:HD2	1:B:177:ASN:ND2	2.21	0.56
1:B:325:ILE:HD11	1:B:372:LEU:CD2	2.36	0.56
1:B:258:ILE:HG23	1:B:270:LYS:HD3	1.89	0.55
1:A:268:ILE:HD12	1:A:269:ASP:N	2.21	0.55
1:A:368:VAL:HB	6:A:607:HOH:O	2.06	0.55
1:A:287:CYS:HA	1:A:300:MET:SD	2.46	0.55
1:B:179:MET:HE2	1:B:395:PHE:CG	2.41	0.55
1:B:199:ILE:HA	1:B:279:ASP:OD2	2.07	0.55
1:B:327:ARG:NH2	1:B:465:SER:OG	2.40	0.55
1:B:268:ILE:HD11	1:B:274:PRO:O	2.07	0.54
1:A:266:LEU:HD22	1:A:299:MET:SD	2.47	0.54
1:A:302:ARG:HB2	1:A:385:TYR:CZ	2.42	0.54
1:B:461:TRP:HB3	6:B:611:HOH:O	2.06	0.54
1:A:476:GLN:H	1:A:476:GLN:CD	2.16	0.54
1:B:395:PHE:CD2	1:B:464:THR:HG22	2.33	0.54
1:A:223:LEU:O	1:A:255:ALA:HA	2.06	0.54
1:B:258:ILE:CG2	1:B:270:LYS:HD3	2.38	0.54
1:B:268:ILE:HD13	1:B:307:ARG:HG3	1.89	0.54
1:A:413:LYS:NZ	6:A:622:HOH:O	2.40	0.53
1:B:366:VAL:CG2	3:B:502:K7R:C21	2.85	0.53
1:A:337:GLY:HA2	1:A:341:TYR:CZ	2.43	0.53
1:B:396:LEU:HD13	1:B:461:TRP:CZ2	2.43	0.53
1:B:399:TYR:O	1:B:403:ILE:HG12	2.09	0.53
1:B:407:GLU:HA	1:B:410:MET:CE	2.40	0.52
1:A:192:ARG:HG3	1:A:199:ILE:HD11	1.91	0.52
1:A:302:ARG:HB2	1:A:385:TYR:OH	2.10	0.52
1:A:179:MET:HE2	1:A:395:PHE:CG	2.45	0.52
1:B:263:SER:HB2	1:B:296:GLN:HB3	1.92	0.52
1:B:237:GLN:HA	1:B:257:PHE:CE1	2.45	0.52
1:B:299:MET:HE3	1:B:299:MET:HA	1.91	0.51
1:B:299:MET:CE	1:B:302:ARG:HB3	2.40	0.51
1:A:237:GLN:HA	1:A:257:PHE:CE1	2.46	0.51
1:B:321:SER:O	1:B:325:ILE:HG12	2.10	0.51
1:B:252:ILE:N	6:B:621:HOH:O	2.43	0.51
1:B:217:LYS:NZ	6:B:615:HOH:O	2.39	0.51
1:B:337:GLY:HA2	1:B:341:TYR:CZ	2.45	0.51
1:B:357:LYS:HG2	1:B:371:PHE:CE1	2.46	0.50
1:B:272:ARG:NH1	6:B:624:HOH:O	2.45	0.50
2:B:501:SAH:SD	3:B:502:K7R:N16	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LYS:HD3	1:A:235:GLN:HE22	1.76	0.50
1:A:394:THR:OG1	1:A:397:GLU:HG3	2.11	0.50
1:A:302:ARG:NH2	6:A:606:HOH:O	2.44	0.50
1:A:346:GLN:HG2	1:A:347:LYS:N	2.26	0.50
1:A:205:GLY:HA3	1:A:286:VAL:HG21	1.94	0.50
1:B:175:PHE:HA	1:B:417:LEU:HD13	1.94	0.50
1:B:208:LYS:HD3	1:B:235:GLN:NE2	2.27	0.50
1:A:208:LYS:HD3	1:A:235:GLN:NE2	2.26	0.49
1:A:263:SER:HB2	1:A:296:GLN:HB3	1.95	0.49
1:A:188:LEU:HD13	1:A:218:GLY:HA3	1.95	0.49
1:B:268:ILE:HD13	1:B:307:ARG:CG	2.42	0.49
1:A:179:MET:HE2	1:A:395:PHE:CD2	2.47	0.49
1:A:306:GLU:HB2	6:A:606:HOH:O	2.12	0.49
1:A:204:LEU:HD22	1:A:226:THR:CG2	2.42	0.49
1:B:380:GLU:OE1	6:B:602:HOH:O	2.20	0.49
1:A:288:HIS:HA	1:A:373:VAL:CG2	2.43	0.49
1:A:170:PHE:CD1	1:A:173:ARG:HD3	2.48	0.49
1:B:341:TYR:CE1	1:B:466:ILE:HD11	2.48	0.48
1:B:208:LYS:HD3	1:B:235:GLN:HE22	1.77	0.48
1:B:220:ILE:O	1:B:253:PHE:HB3	2.14	0.48
1:A:395:PHE:CD2	1:A:464:THR:HG22	2.45	0.48
1:B:409:LYS:O	1:B:413:LYS:HG2	2.14	0.48
1:A:292:GLU:HB2	1:A:371:PHE:CE2	2.48	0.48
1:B:399:TYR:CE1	1:B:403:ILE:HG21	2.49	0.48
1:A:330:ALA:HA	6:A:755:HOH:O	2.12	0.48
1:A:182:VAL:HG11	1:A:402:LYS:HG3	1.96	0.47
1:A:266:LEU:CD2	1:A:299:MET:HE1	2.45	0.47
1:A:374:TYR:O	1:A:377:LEU:HB3	2.15	0.47
2:A:501:SAH:H2	6:A:630:HOH:O	2.15	0.47
1:A:216:LYS:HB2	1:A:243:MET:HE1	1.96	0.47
1:A:268:ILE:HG21	1:A:307:ARG:HD3	1.97	0.47
1:B:396:LEU:HB2	1:B:461:TRP:CZ2	2.42	0.47
1:B:354:PHE:CZ	1:B:377:LEU:HD21	2.50	0.47
1:B:414:ARG:NH1	6:B:615:HOH:O	2.39	0.47
1:B:206:CYS:SG	1:B:227:ASP:HB2	2.55	0.47
1:A:175:PHE:CE2	1:A:464:THR:HG21	2.50	0.46
1:A:393:LYS:HE2	1:A:401:GLU:OE1	2.14	0.46
1:B:184:ILE:HG23	1:B:215:TRP:CZ3	2.50	0.46
1:A:306:GLU:HG3	1:A:307:ARG:HD2	1.96	0.46
1:B:226:THR:HA	1:B:258:ILE:O	2.15	0.46
1:A:263:SER:O	1:A:296:GLN:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLN:HB3	6:A:766:HOH:O	2.16	0.45
1:B:396:LEU:CB	1:B:461:TRP:HZ2	2.27	0.45
1:A:258:ILE:HG23	1:A:270:LYS:HG2	1.98	0.45
1:B:186:GLU:O	1:B:190:LYS:HG3	2.16	0.45
1:B:288:HIS:HA	1:B:373:VAL:HG21	1.98	0.45
1:A:328:LEU:HD22	1:A:345:PHE:CG	2.51	0.45
1:B:192:ARG:HG2	1:B:199:ILE:HD11	1.98	0.45
1:B:198:ASP:HA	1:B:221:ASN:OD1	2.16	0.45
1:B:325:ILE:HD12	1:B:351:TYR:CE1	2.51	0.45
1:A:388:LYS:HE3	1:A:473:GLU:HB3	1.98	0.45
1:A:261:ASP:OD2	1:A:264:LYS:HG3	2.17	0.45
1:A:288:HIS:HA	1:A:373:VAL:HG21	1.98	0.45
1:B:358:TYR:CE2	1:B:370:GLU:HB2	2.51	0.45
1:A:268:ILE:HD12	1:A:269:ASP:OD1	2.17	0.45
1:A:409:LYS:HE2	1:A:409:LYS:HB2	1.68	0.44
1:B:189:GLU:HG3	6:B:742:HOH:O	2.16	0.44
1:B:302:ARG:O	1:B:306:GLU:HG2	2.18	0.44
1:B:284:GLN:O	1:B:286:VAL:HG23	2.17	0.44
1:B:357:LYS:HG2	1:B:371:PHE:HE1	1.82	0.43
1:A:172:LEU:HA	1:A:172:LEU:HD23	1.73	0.43
1:A:230:ASP:OD2	1:A:234:LYS:HE2	2.18	0.43
1:A:321:SER:HB3	1:A:373:VAL:O	2.18	0.43
1:A:358:TYR:CZ	1:A:370:GLU:HB2	2.53	0.43
1:B:396:LEU:HA	1:B:461:TRP:CH2	2.52	0.43
1:A:240:TYR:OH	1:A:244:LYS:HE2	2.17	0.43
1:B:468:LEU:HD12	1:B:468:LEU:C	2.43	0.43
1:A:194:LYS:HE2	6:A:654:HOH:O	2.19	0.43
1:A:406[A]:ASN:ND2	1:A:406[A]:ASN:H	2.17	0.43
1:A:341:TYR:HA	1:A:361:ASN:O	2.18	0.43
1:A:204:LEU:CD2	1:A:267:LEU:HD11	2.49	0.43
1:A:352:PRO:HA	6:B:713:HOH:O	2.18	0.43
1:A:182:VAL:HG11	1:A:402:LYS:CG	2.49	0.43
1:A:220:ILE:HD11	1:A:223:LEU:HB2	2.00	0.43
1:B:205:GLY:O	2:B:501:SAH:N	2.52	0.43
1:B:277:CYS:HB3	1:B:309:SER:OG	2.19	0.43
1:B:215:TRP:HZ2	1:B:282:SER:CB	2.32	0.42
1:B:276:MET:HE3	1:B:276:MET:HB2	1.92	0.42
1:A:388:LYS:NZ	6:A:641:HOH:O	2.52	0.42
1:A:286:VAL:HG22	2:A:501:SAH:O4'	2.19	0.42
1:A:327:ARG:NH2	1:A:465:SER:OG	2.50	0.42
1:A:415:MET:HE3	1:A:415:MET:HB2	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HD21	1:A:262:SER:CB	2.49	0.42
1:A:285:PHE:O	2:A:501:SAH:H5'2	2.19	0.42
1:B:204:LEU:HD21	1:B:262:SER:CB	2.49	0.42
1:A:382:ALA:HB1	1:A:387:MET:HB2	2.01	0.42
1:B:173:ARG:HD2	1:B:177:ASN:HD21	1.83	0.42
1:B:220:ILE:HD11	1:B:223:LEU:HB2	2.00	0.42
1:B:263:SER:O	1:B:296:GLN:HA	2.19	0.42
1:A:276:MET:HA	6:A:604:HOH:O	2.19	0.42
1:B:272:ARG:HE	1:B:272:ARG:HB3	1.55	0.42
1:A:192:ARG:CG	1:A:199:ILE:HD11	2.50	0.42
1:B:175:PHE:HD2	1:B:464:THR:HG21	1.79	0.42
1:B:317:THR:HG22	1:B:469:VAL:HG12	2.02	0.42
1:A:273:ASP:HA	1:A:274:PRO:HD2	1.41	0.42
1:B:229:ALA:O	1:B:233:VAL:HG23	2.20	0.42
1:A:277:CYS:HB3	1:A:309:SER:OG	2.20	0.41
1:A:468:LEU:C	1:A:468:LEU:HD12	2.44	0.41
1:B:172:LEU:HD12	1:B:172:LEU:HA	1.61	0.41
1:B:240:TYR:CE1	1:B:255:ALA:HB3	2.55	0.41
1:B:180:LYS:HD3	1:B:284:GLN:HB3	2.02	0.41
1:A:333:THR:O	1:A:348:LYS:NZ	2.35	0.41
1:B:353:LEU:HB3	1:B:377:LEU:HD22	2.03	0.41
1:B:396:LEU:HA	1:B:461:TRP:HH2	1.84	0.41
1:B:305:CYS:SG	1:B:387:MET:HG3	2.59	0.41
1:B:340:ILE:HD11	1:B:460:GLU:HG3	2.01	0.41
1:A:264:LYS:HE3	6:A:814:HOH:O	2.20	0.41
1:B:224:VAL:HG11	1:B:271:PHE:CE1	2.56	0.41
1:B:256:GLU:OE1	1:B:272:ARG:HG2	2.21	0.41
1:A:265:GLU:OE2	1:A:270:LYS:HE3	2.20	0.41
1:B:231:VAL:HG12	1:B:235:GLN:OE1	2.20	0.41
1:B:294:TYR:CD1	5:B:504:GOL:H2	2.56	0.41
1:A:201:VAL:HG11	1:A:215:TRP:CH2	2.55	0.41
1:A:320:ASN:HA	1:A:468:LEU:HD23	2.03	0.41
1:A:388:LYS:HG2	1:A:475:GLN:OE1	2.21	0.41
1:B:268:ILE:HD12	1:B:271:PHE:HD2	1.86	0.41
2:B:501:SAH:SD	3:B:502:K7R:C15	3.08	0.41
1:A:399:TYR:CE1	1:A:403:ILE:HG21	2.56	0.41
1:B:268:ILE:HD13	1:B:307:ARG:CD	2.51	0.41
1:A:399:TYR:CZ	1:A:403:ILE:HD13	2.56	0.40
1:A:204:LEU:HD22	1:A:226:THR:HG23	2.03	0.40
1:A:335:SER:HA	1:A:343:VAL:O	2.22	0.40
1:B:237:GLN:HA	1:B:257:PHE:CZ	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LYS:NZ	1:A:198:ASP:O	2.32	0.40
1:B:268:ILE:HD12	1:B:271:PHE:CD2	2.56	0.40

All (2) 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:357:LYS:NZ	1:A:476:GLN:NE2[1_655]	1.70	0.50
1:A:357:LYS:CE	1:A:476:GLN:NE2[1_655]	2.01	0.19

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	273/276 (99%)	260 (95%)	13 (5%)	0	100	100
1	B	258/276 (94%)	248 (96%)	10 (4%)	0	100	100
All	All	531/552 (96%)	508 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	245/252 (97%)	241 (98%)	4 (2%)	55	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	237/252 (94%)	235 (99%)	2 (1%)	73	74
All	All	482/504 (96%)	476 (99%)	6 (1%)	63	61

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	270	LYS
1	A	346	GLN
1	A	415	MET
1	A	464	THR
1	B	195	LYS
1	B	299	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	GLN
1	B	379	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 ligands are modelled in this entry.

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	504	-	5,5,5	0.92	0	5,5,5	1.10	0
4	SO4	A	503	-	4,4,4	0.24	0	6,6,6	0.07	0
2	SAH	A	501	-	27,28,28	2.04	10 (37%)	36,40,40	2.21	12 (33%)
2	SAH	B	501	-	27,28,28	1.08	4 (14%)	36,40,40	2.08	10 (27%)
3	K7R	B	502	-	23,26,26	2.31	5 (21%)	27,36,36	4.33	11 (40%)
4	SO4	B	503	-	4,4,4	0.23	0	6,6,6	0.09	0
3	K7R	A	502	-	23,26,26	2.09	8 (34%)	27,36,36	3.69	11 (40%)

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	504	-	-	1/4/4/4	-
2	SAH	A	501	-	-	0/15/31/31	0/3/3/3
2	SAH	B	501	-	-	1/15/31/31	0/3/3/3
3	K7R	B	502	-	-	1/12/22/22	0/4/4/4
3	K7R	A	502	-	-	3/12/22/22	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	K7R	C02-N09	6.86	1.48	1.35
3	B	502	K7R	C03-C04	5.18	1.55	1.50
3	A	502	K7R	C02-N09	4.60	1.44	1.35
2	A	501	SAH	C5-N7	-4.50	1.30	1.39
2	A	501	SAH	C8-N9	-4.43	1.30	1.37
3	A	502	K7R	C03-C04	4.31	1.54	1.50
3	B	502	K7R	C14-N09	4.02	1.51	1.46
2	A	501	SAH	C4-N9	-3.79	1.29	1.37
2	A	501	SAH	O4'-C4'	-3.66	1.36	1.45
3	A	502	K7R	O01-C02	-3.19	1.16	1.23
3	A	502	K7R	C20-N19	-3.03	1.28	1.34
3	A	502	K7R	C12-C13	-2.90	1.45	1.53
3	A	502	K7R	C18-C23	-2.68	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	K7R	C15-N16	-2.63	1.31	1.34
2	B	501	SAH	C2-N1	2.53	1.38	1.33
2	B	501	SAH	C2-N3	2.45	1.38	1.33
3	B	502	K7R	C10-N09	2.44	1.51	1.47
2	A	501	SAH	C2-N1	-2.44	1.29	1.33
2	A	501	SAH	OXT-C	-2.42	1.22	1.30
2	A	501	SAH	O2'-C2'	-2.29	1.37	1.43
2	A	501	SAH	C5'-SD	-2.27	1.72	1.81
3	B	502	K7R	C13-C15	2.25	1.56	1.49
2	B	501	SAH	OXT-C	-2.24	1.23	1.30
2	A	501	SAH	C5-C6	2.18	1.47	1.41
2	B	501	SAH	C8-N7	2.17	1.35	1.31
2	A	501	SAH	O4'-C1'	-2.14	1.37	1.42
3	A	502	K7R	C11-C12	-2.13	1.47	1.53

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	K7R	C12-C13-C15	-17.51	83.70	113.45
3	A	502	K7R	C12-C13-C15	-11.83	93.35	113.45
3	B	502	K7R	C14-C13-C15	10.20	129.65	110.17
3	A	502	K7R	C12-C11-C10	8.28	121.63	110.75
3	A	502	K7R	C14-C13-C15	6.36	122.31	110.17
3	A	502	K7R	C21-C22-C23	-6.34	115.55	121.80
2	B	501	SAH	N3-C2-N1	-5.65	120.03	128.58
2	A	501	SAH	N3-C4-N9	5.57	136.65	127.17
2	A	501	SAH	C4-N9-C8	5.01	111.00	105.74
2	A	501	SAH	C5-C4-N3	-4.72	120.22	126.72
2	B	501	SAH	C5-C4-N3	-4.29	120.81	126.72
2	B	501	SAH	C5'-SD-CG	-4.19	89.81	102.26
2	B	501	SAH	N9-C8-N7	-4.11	108.11	113.94
3	B	502	K7R	C20-N19-C18	3.92	121.30	116.64
3	A	502	K7R	C04-C08-S07	-3.77	104.79	112.19
2	A	501	SAH	N3-C2-N1	-3.74	122.92	128.58
3	B	502	K7R	C21-C22-C23	-3.70	118.16	121.80
2	A	501	SAH	C2-N3-C4	3.68	120.82	111.83
2	B	501	SAH	C5-N7-C8	3.50	108.95	103.45
3	B	502	K7R	C04-C08-S07	-3.50	105.32	112.19
3	A	502	K7R	C10-N09-C14	-3.42	106.47	113.07
2	B	501	SAH	C2-N3-C4	3.41	120.17	111.83
3	A	502	K7R	C03-C04-C05	-3.39	120.58	124.68
3	B	502	K7R	C18-N17-N16	3.35	109.31	103.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	SAH	C5-C6-N6	-3.27	115.19	123.29
3	B	502	K7R	C05-C04-C08	3.14	116.89	111.06
2	A	501	SAH	N6-C6-N1	3.12	125.34	118.38
3	A	502	K7R	C18-N17-N16	3.11	108.86	103.03
2	A	501	SAH	N9-C8-N7	-2.90	109.82	113.94
3	A	502	K7R	C05-C04-C08	2.72	116.10	111.06
2	B	501	SAH	N3-C4-N9	2.69	131.75	127.17
2	B	501	SAH	OXT-C-O	-2.64	118.08	124.08
2	A	501	SAH	C5-C4-N9	-2.62	102.96	105.81
3	B	502	K7R	C03-C04-C05	-2.60	121.53	124.68
3	B	502	K7R	C23-C18-N19	-2.59	121.66	125.91
2	B	501	SAH	C4-C5-N7	-2.54	107.68	110.58
2	A	501	SAH	C5-N7-C8	2.52	107.41	103.45
2	A	501	SAH	C4-N9-C1'	-2.26	121.36	126.63
3	A	502	K7R	C23-C18-N19	-2.17	122.35	125.91
2	B	501	SAH	O4'-C1'-N9	2.13	112.18	108.09
3	B	502	K7R	C21-C20-N19	-2.10	120.10	123.42
3	A	502	K7R	C10-N09-C02	2.06	129.61	122.83
3	B	502	K7R	C03-C04-C08	-2.04	121.58	124.12
2	A	501	SAH	C6-C5-N7	2.02	135.98	132.09

There are no chirality outliers.

All (6) torsion outliers are listed below:

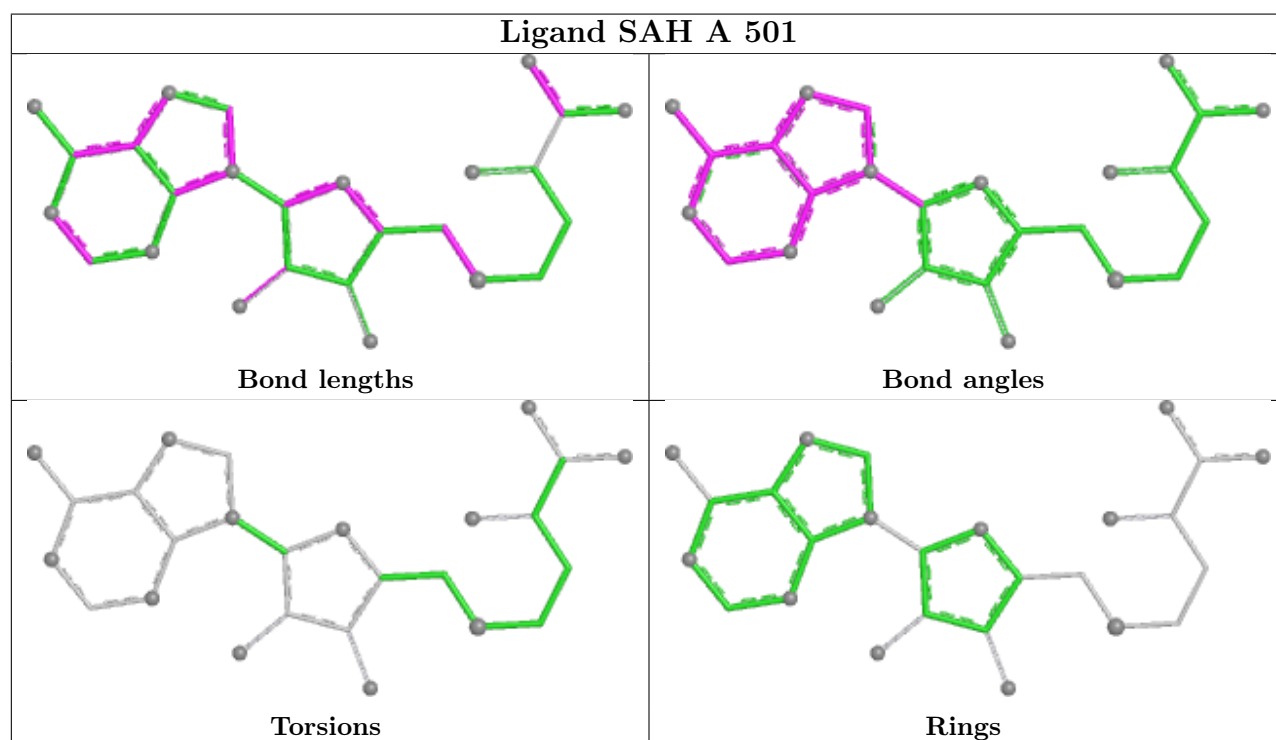
Mol	Chain	Res	Type	Atoms
3	A	502	K7R	C02-C03-C04-C05
3	A	502	K7R	C02-C03-C04-C08
5	B	504	GOL	O1-C1-C2-O2
2	B	501	SAH	CB-CG-SD-C5'
3	A	502	K7R	O01-C02-C03-C04
3	B	502	K7R	O01-C02-C03-C04

There are no ring outliers.

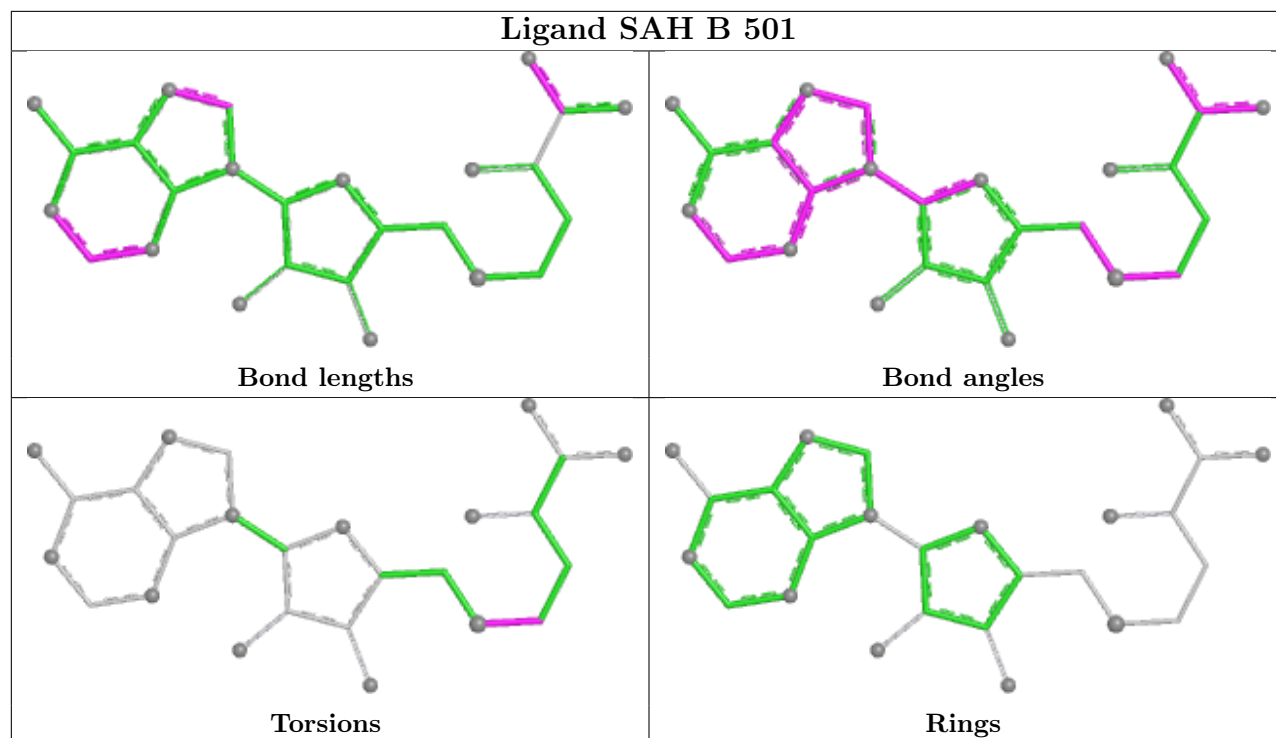
5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504	GOL	1	0
2	A	501	SAH	3	0
2	B	501	SAH	3	0
3	B	502	K7R	9	0
4	B	503	SO4	1	0

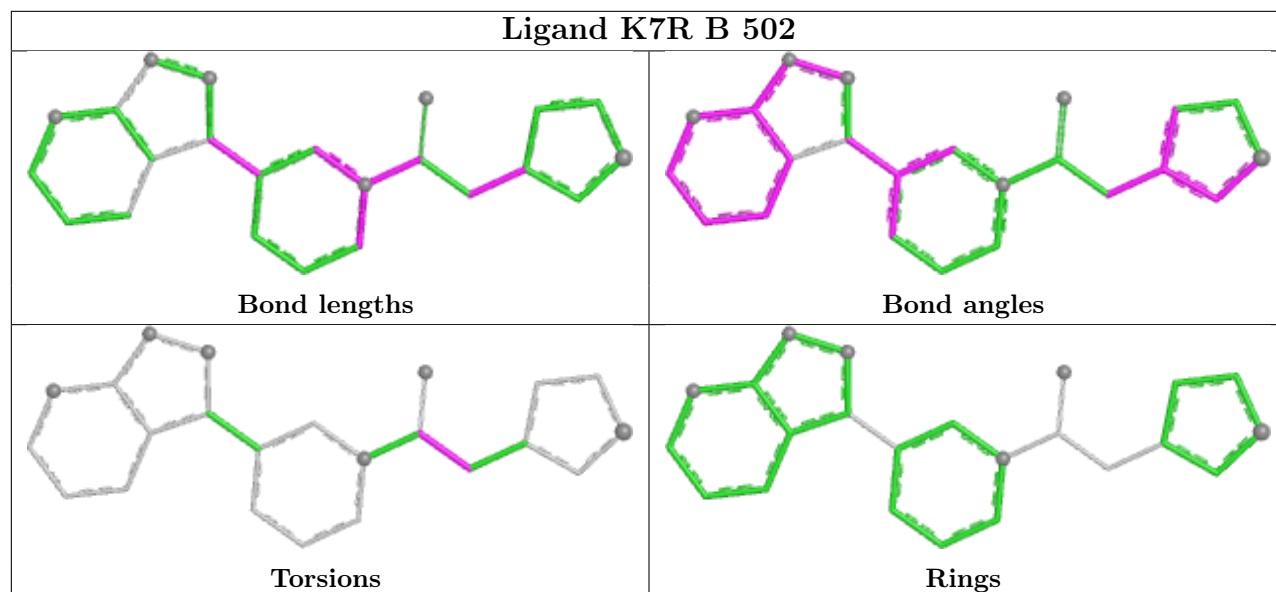
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

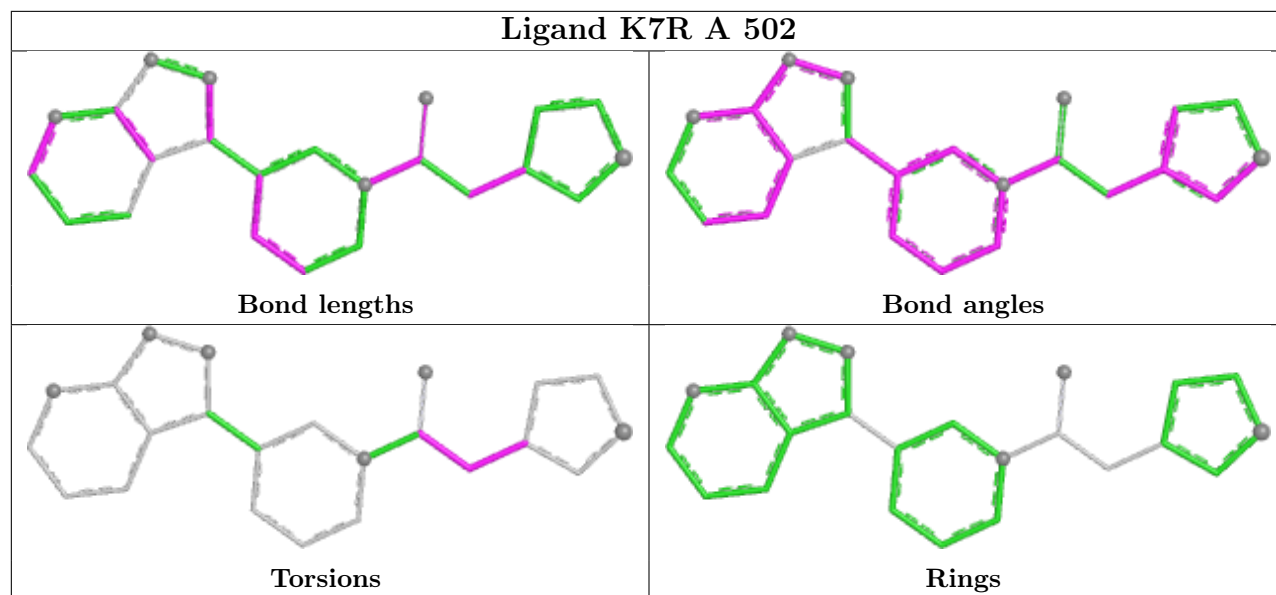


Ligand SAH B 501



Ligand K7R B 502





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	274/276 (99%)	0.73	20 (7%) 21 24	21, 27, 38, 51	1 (0%)
1	B	264/276 (95%)	0.93	24 (9%) 15 17	23, 32, 43, 54	0
All	All	538/552 (97%)	0.83	44 (8%) 17 20	21, 30, 42, 54	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	ARG	5.3
1	B	461	TRP	5.0
1	B	198	ASP	4.7
1	B	170	PHE	4.4
1	B	456	LEU	4.2
1	B	419	CYS	4.0
1	A	248	ASP	4.0
1	A	251	TYR	3.7
1	B	171	TYR	3.4
1	B	172	LEU	3.3
1	A	287	CYS	3.2
1	B	287	CYS	3.2
1	B	274	PRO	3.0
1	A	198	ASP	3.0
1	A	169	ILE	2.8
1	A	340	ILE	2.8
1	A	476	GLN	2.8
1	B	193	GLN	2.8
1	B	417	LEU	2.8
1	A	461	TRP	2.8
1	B	174	ASN	2.7
1	B	245	ASN	2.7
1	A	167	SER	2.7
1	A	403	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	249	SER	2.6
1	A	406[A]	ASN	2.5
1	B	246	ARG	2.5
1	A	332	GLU	2.5
1	B	266	LEU	2.4
1	B	365	VAL	2.4
1	A	346	GLN	2.4
1	B	364	GLY	2.4
1	B	357	LYS	2.3
1	A	196	LYS	2.3
1	A	250	GLU	2.2
1	B	366	VAL	2.2
1	A	407	GLU	2.1
1	A	357	LYS	2.1
1	B	268	ILE	2.1
1	B	340	ILE	2.1
1	B	403	ILE	2.0
1	B	418	GLY	2.0
1	A	464	THR	2.0
1	B	369	PRO	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	K7R	B	502	23/23	0.50	0.21	33,35,39,48	0
5	GOL	B	504	6/6	0.76	0.11	31,32,35,39	0
3	K7R	A	502	23/23	0.79	0.13	28,29,33,42	0

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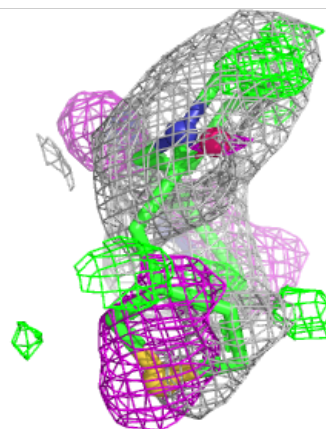
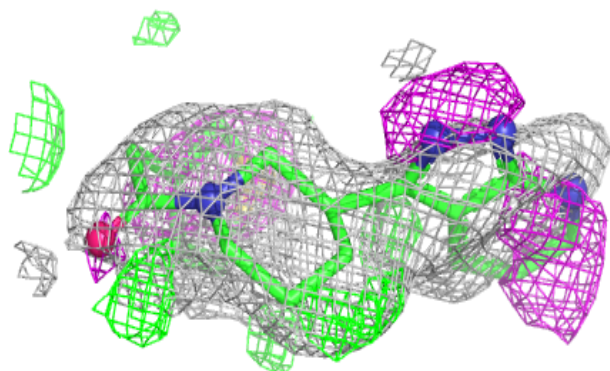
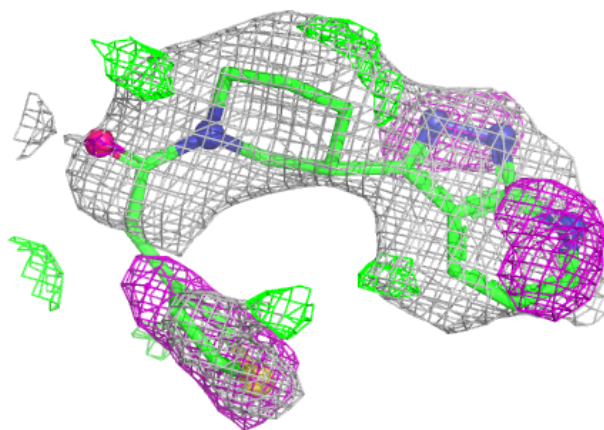
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	503	5/5	0.84	0.24	33,34,37,37	0
4	SO4	B	503	5/5	0.87	0.13	40,41,44,46	0
2	SAH	B	501	26/26	0.93	0.08	27,28,30,30	0
2	SAH	A	501	26/26	0.93	0.07	20,20,20,20	0

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.

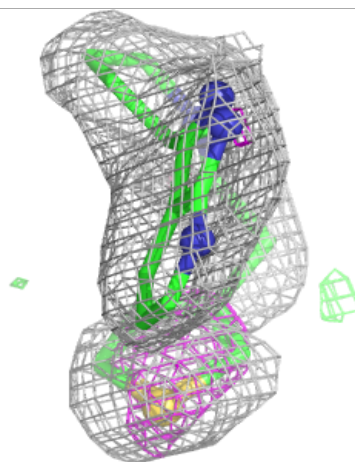
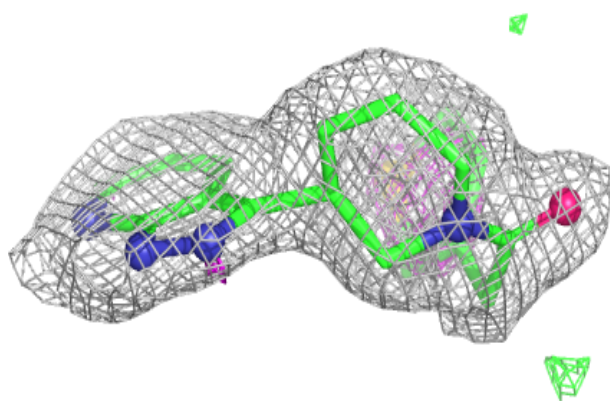
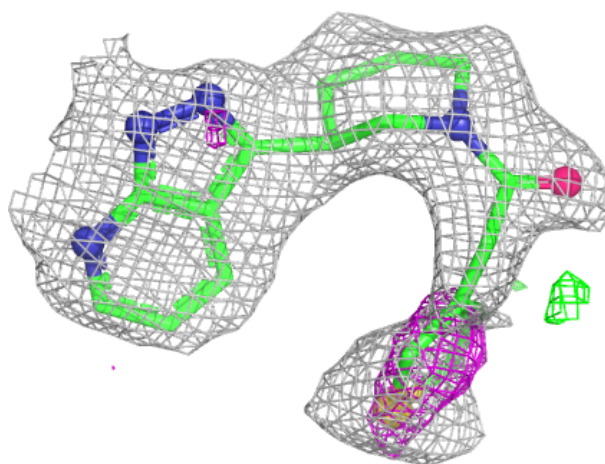
Electron density around K7R B 502:

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



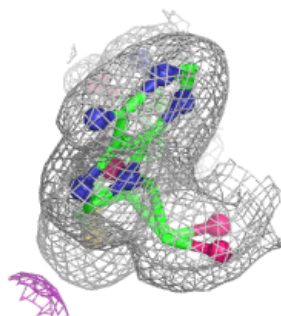
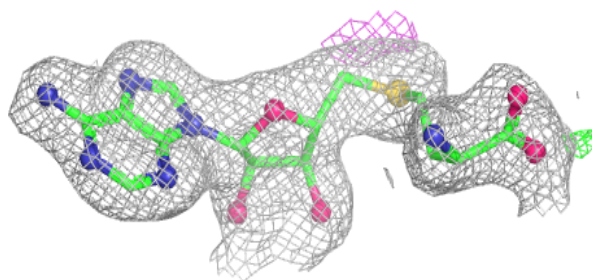
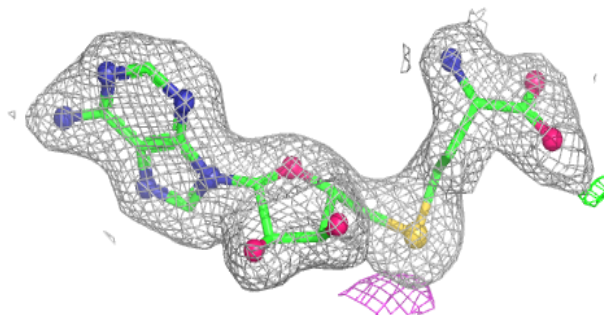
Electron density around K7R A 502:

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

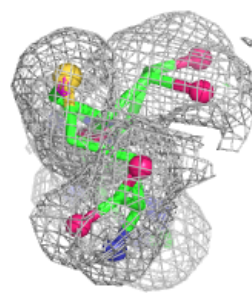
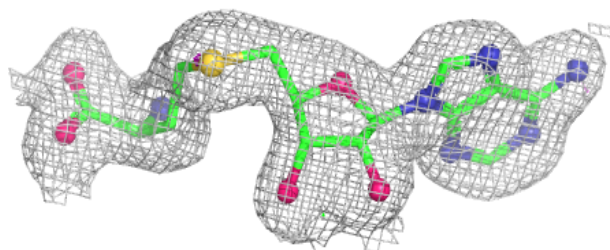
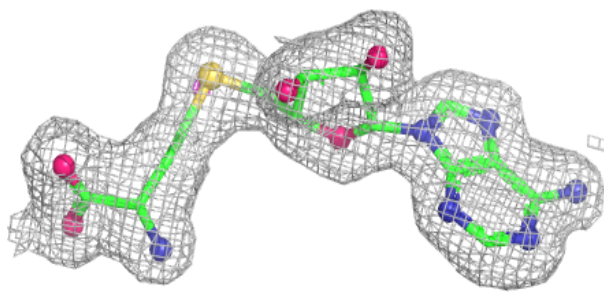


Electron density around SAH B 501:

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

**Electron density around SAH A 501:**

$2mF_o-DF_c$ (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.