Full wwPDB X-ray Structure Validation Report (i)

Mar 6, 2025 – 03:47 pm GMT

PDB ID	:	8Q69
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 (i) 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 (i)) were used in the production of this report:

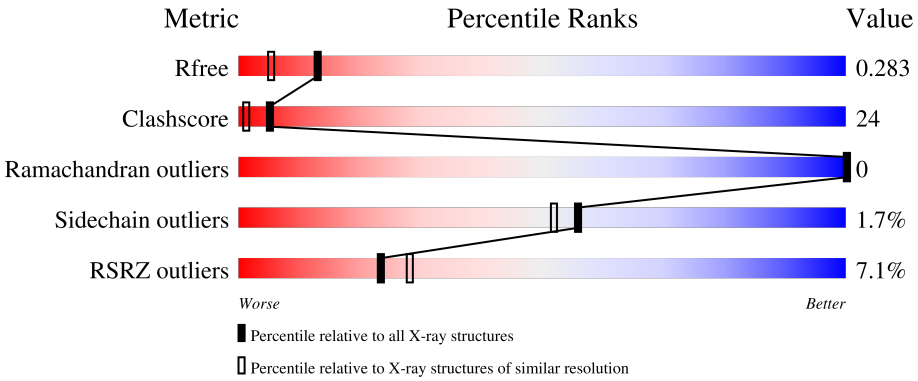
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

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}	164625	3187 (1.96-1.96)
Clashscore	180529	3412 (1.96-1.96)
Ramachandran outliers	177936	3390 (1.96-1.96)
Sidechain outliers	177891	3390 (1.96-1.96)
RSRZ outliers	164620	3186 (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 <=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	7% 57% 40%
1	B	276	7% 54% 40%

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 (i)

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.

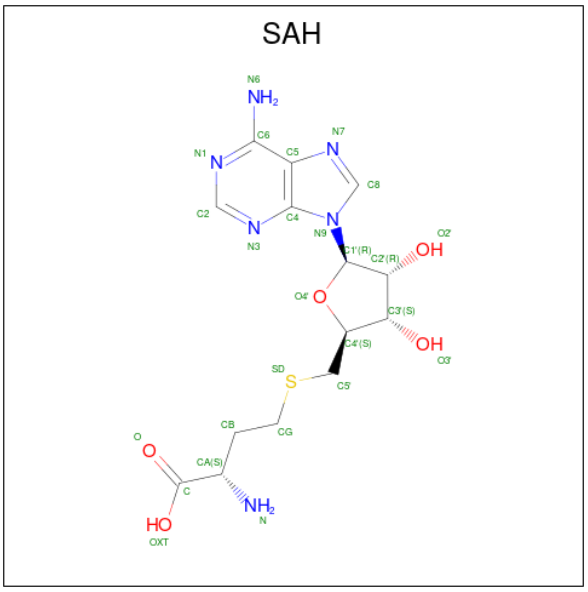
- Molecule 1 is a protein called mRNA cap guanine-N7 methyltransferase.

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:

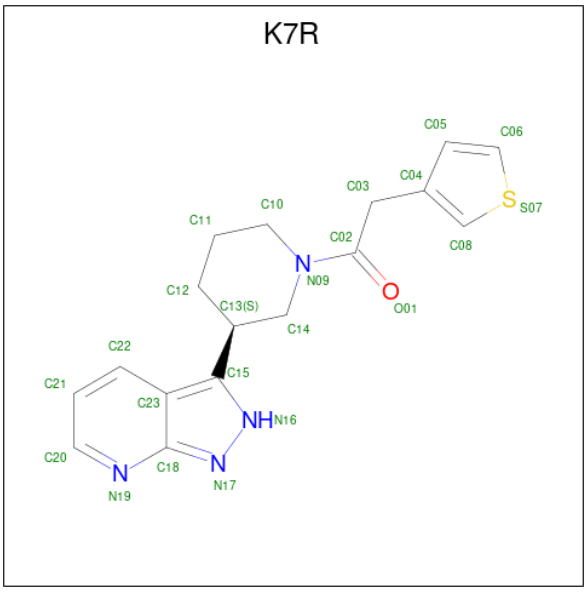
Chain	Residue	Modelled	Actual	Comment	Reference
A	416	GLY	-	linker	UNP O43148
A	417	LEU	-	linker	UNP O43148
A	418	GLY	-	linker	UNP O43148
A	419	CYS	-	linker	UNP O43148
B	416	GLY	-	linker	UNP O43148
B	417	LEU	-	linker	UNP O43148
B	418	GLY	-	linker	UNP O43148
B	419	CYS	-	linker	UNP O43148

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: 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 (three-letter code: K7R) (formula: $C_{17}H_{18}N_4OS$) (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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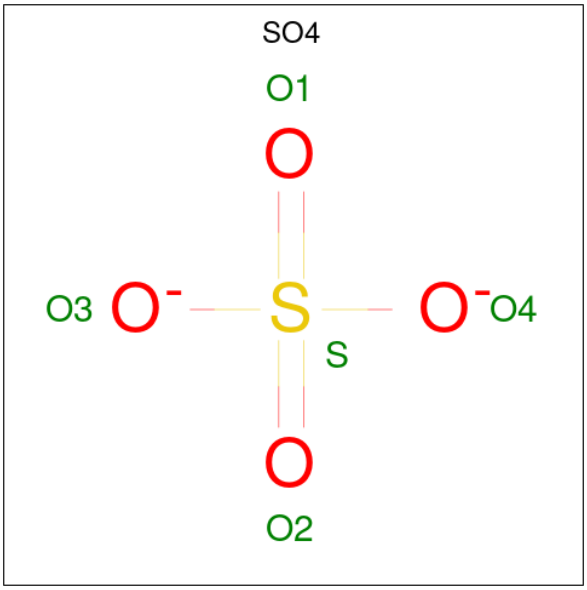
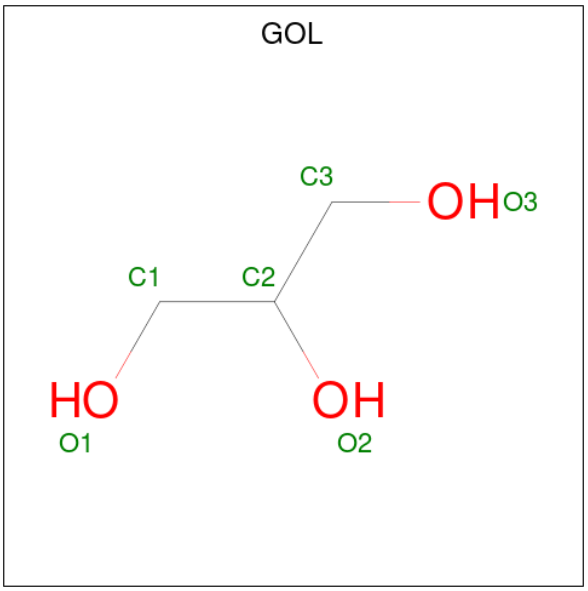
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			23	17	4	1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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 (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

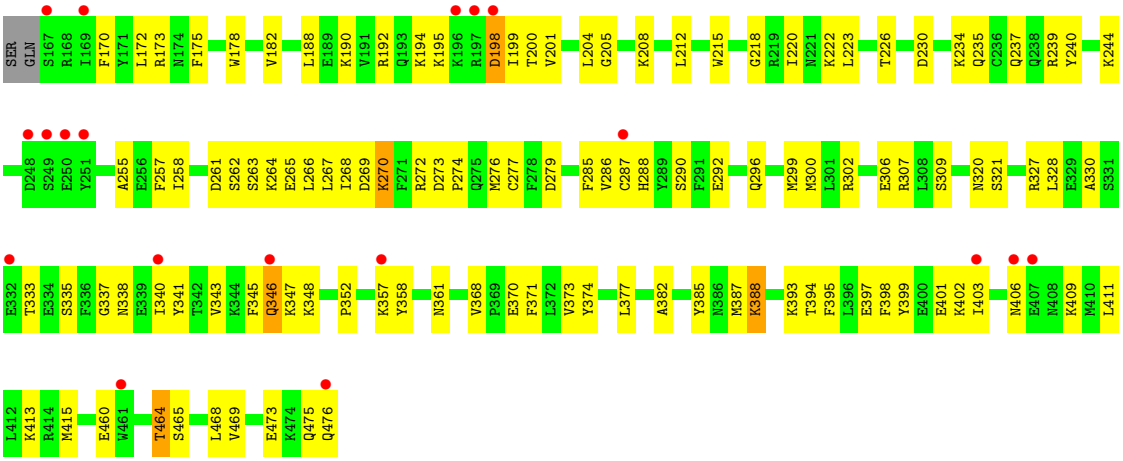
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	230	Total O 230 230	0	0
6	B	175	Total O 175 175	0	0

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.

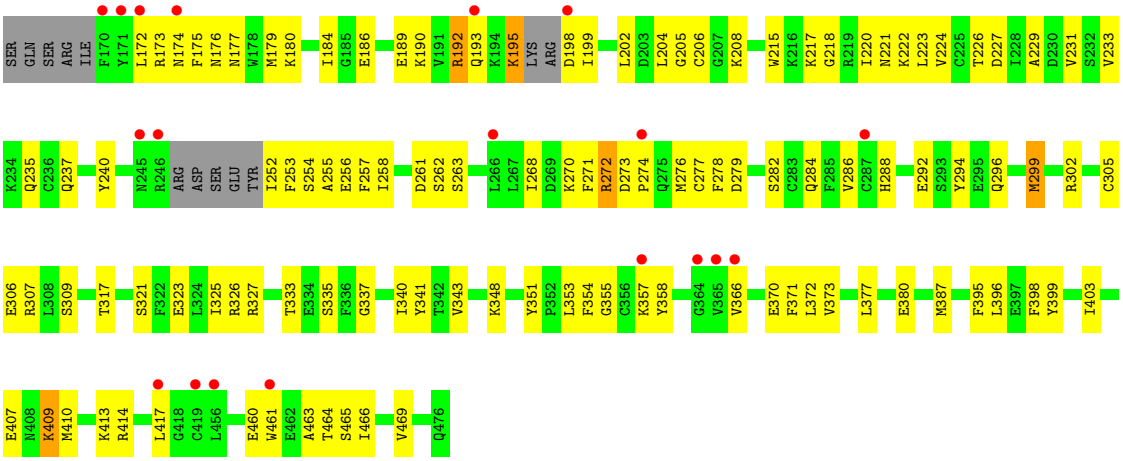
• Molecule 1: mRNA cap guanine-N7 methyltransferase

Chain A:



• Molecule 1: mRNA cap guanine-N7 methyltransferase

Chain B:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.12 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.242 , 0.289 0.239 , 0.283	Depositor DCC
R_{free} test set	1787 reflections (4.69%)	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]	$< \|L\| > = 0.53$, $< L^2 > = 0.36$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, K7R, SAH, 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	0.48	0/2288	0.59	1/3068 (0.0%)
1	B	0.34	0/2204	0.50	2/2952 (0.1%)
All	All	0.42	0/4492	0.55	3/6020 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	299	MET	CG-SD-CE	6.33	110.33	100.20
1	A	272	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	B	192	ARG	NE-CZ-NH2	-5.33	117.63	120.30

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	97	2
1	B	2161	0	2139	115	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	215	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 24.

All (215) 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: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: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
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:178:TRP:HB2	1:A:415:MET:HE3	1.77	0.66
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:299:MET:HE1	1:B:302:ARG:HD3	1.78	0.65
1:A:346:GLN:HE21	1:A:346:GLN:N	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:411:LEU:HG	1:A:415:MET:HE2	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: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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:299:MET:HE3	1:B:302:ARG:HD3	1.89	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:B:333:THR:O	1:B:348:LYS:NZ	2.26	0.52
1:A:302:ARG:HB2	1:A:385:TYR:OH	2.10	0.52
1:B:299:MET:HE3	1:B:302:ARG:HB3	1.92	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: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: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
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:476:GLN:H	1:A:476:GLN:CD	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:268:ILE:HG21	1:A:307:ARG:HD3	1.97	0.47
1:B:179:MET:HE3	1:B:398:PHE:CD2	2.50	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
1:B:407:GLU:HA	1:B:410:MET:HE2	1.96	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:411:LEU:HG	1:A:415:MET:HE1	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:217:LYS:NZ	6:B:615:HOH:O	2.39	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
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%)	240 (98%)	5 (2%)	50	44
1	B	237/252 (94%)	234 (99%)	3 (1%)	65	62
All	All	482/504 (96%)	474 (98%)	8 (2%)	56	52

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	ASP
1	A	270	LYS
1	A	346	GLN
1	A	388	LYS
1	A	464	THR
1	B	195	LYS
1	B	272	ARG
1	B	409	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	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

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	$\#\|Z\| > 2$
4	SO4	A	503	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SAH	B	501	-	24,28,28	1.19	3 (12%)	25,40,40	1.73	4 (16%)
2	SAH	A	501	-	24,28,28	1.76	8 (33%)	25,40,40	1.61	6 (24%)
5	GOL	B	504	-	5,5,5	0.89	0	5,5,5	1.02	0
4	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.07	0
3	K7R	A	502	-	24,26,26	2.16	10 (41%)	19,36,36	4.69	8 (42%)
3	K7R	B	502	-	24,26,26	2.31	8 (33%)	19,36,36	5.27	5 (26%)

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
2	SAH	B	501	-	-	1/11/31/31	0/3/3/3
2	SAH	A	501	-	-	0/11/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	504	-	-	1/4/4/4	-
3	K7R	A	502	-	-	0/8/22/22	0/4/4/4
3	K7R	B	502	-	-	0/8/22/22	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	K7R	C02-N09	6.48	1.48	1.35
3	A	502	K7R	C08-C04	5.18	1.40	1.37
3	A	502	K7R	C02-N09	4.34	1.44	1.35
3	B	502	K7R	C08-C04	4.22	1.39	1.37
3	B	502	K7R	C14-N09	3.90	1.51	1.46
2	B	501	SAH	C2-N3	3.84	1.38	1.32
2	A	501	SAH	C8-N7	-3.74	1.28	1.34
2	A	501	SAH	O4'-C4'	-3.64	1.36	1.45
3	B	502	K7R	C15-C13	3.41	1.56	1.51
3	A	502	K7R	O01-C02	-3.12	1.16	1.23
2	A	501	SAH	O4'-C1'	-2.89	1.37	1.41
3	A	502	K7R	C12-C13	-2.74	1.45	1.53
3	A	502	K7R	C23-C18	-2.68	1.35	1.43
3	B	502	K7R	C03-C02	2.57	1.55	1.52
3	B	502	K7R	C10-N09	2.47	1.51	1.47
2	A	501	SAH	C5-N7	-2.44	1.30	1.39
3	A	502	K7R	C18-N19	-2.43	1.33	1.37
2	B	501	SAH	C2-N1	2.43	1.38	1.33
2	A	501	SAH	O2'-C2'	-2.42	1.37	1.43
2	A	501	SAH	OXT-C	-2.33	1.22	1.30
2	A	501	SAH	C2-N1	-2.31	1.29	1.33
3	A	502	K7R	C15-N16	-2.20	1.31	1.34
2	A	501	SAH	C5'-SD	-2.16	1.72	1.80
3	B	502	K7R	C03-C04	2.16	1.55	1.51
2	B	501	SAH	OXT-C	-2.15	1.23	1.30
3	A	502	K7R	C20-N19	-2.15	1.28	1.32
3	B	502	K7R	C08-S07	2.05	1.73	1.70
3	A	502	K7R	C14-C13	-2.04	1.51	1.53
3	A	502	K7R	C11-C12	-2.03	1.47	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	K7R	C12-C13-C15	-19.30	83.70	111.44
3	A	502	K7R	C12-C13-C15	-12.59	93.35	111.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	K7R	C04-C08-S07	-11.64	104.79	112.29
3	B	502	K7R	C04-C08-S07	-10.81	105.32	112.29
3	A	502	K7R	C12-C11-C10	7.69	121.63	110.85
2	B	501	SAH	N3-C2-N1	-5.53	120.03	128.68
2	B	501	SAH	C5'-SD-CG	-4.15	89.81	102.27
3	A	502	K7R	C21-C22-C23	-3.85	115.55	120.89
3	B	502	K7R	C20-N19-C18	3.81	121.30	116.60
2	A	501	SAH	N3-C2-N1	-3.68	122.92	128.68
3	A	502	K7R	C04-C03-C02	-3.58	106.29	112.61
2	A	501	SAH	C5-C6-N6	-3.39	115.19	120.35
3	A	502	K7R	C10-N09-C14	-3.29	106.47	113.06
2	A	501	SAH	N6-C6-N1	3.26	125.34	118.57
2	A	501	SAH	C1'-N9-C4	-3.01	121.36	126.64
3	A	502	K7R	C06-S07-C08	2.86	98.21	92.37
2	B	501	SAH	OXT-C-O	-2.64	118.08	124.09
3	B	502	K7R	C21-C20-N19	-2.51	120.10	123.94
2	A	501	SAH	O-C-CA	-2.29	114.06	122.14
2	B	501	SAH	OXT-C-CA	2.25	121.04	113.38
3	B	502	K7R	C06-S07-C08	2.20	96.86	92.37
2	A	501	SAH	OXT-C-CA	2.19	120.84	113.38
3	A	502	K7R	C10-N09-C02	2.08	129.61	122.81

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	504	GOL	O1-C1-C2-O2
2	B	501	SAH	CB-CG-SD-C5'

There are no ring outliers.

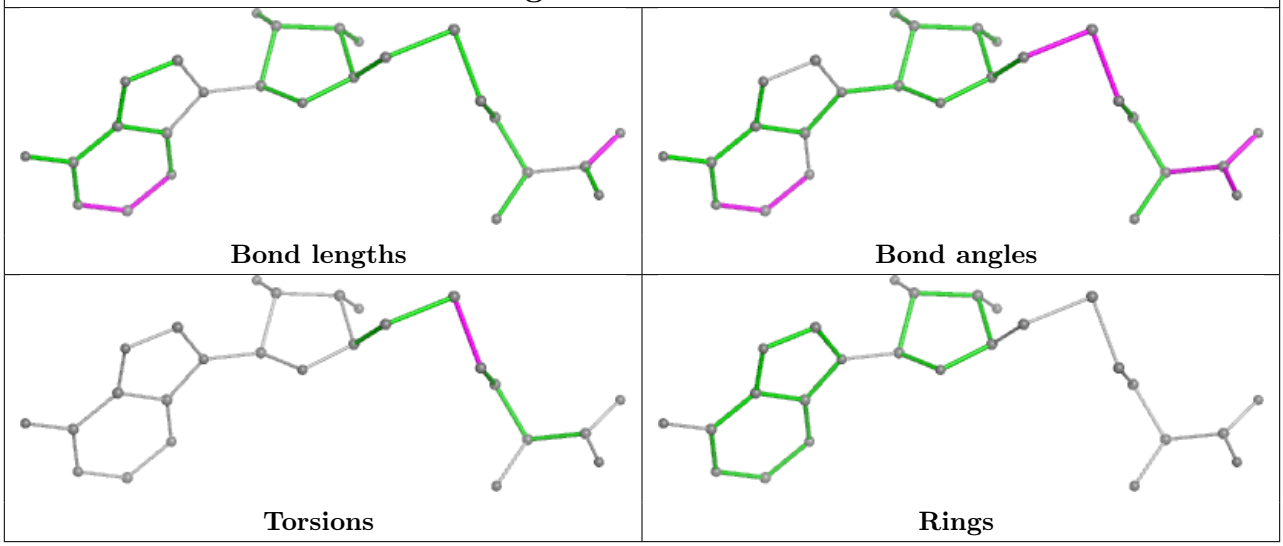
5 monomers are involved in 15 short contacts:

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

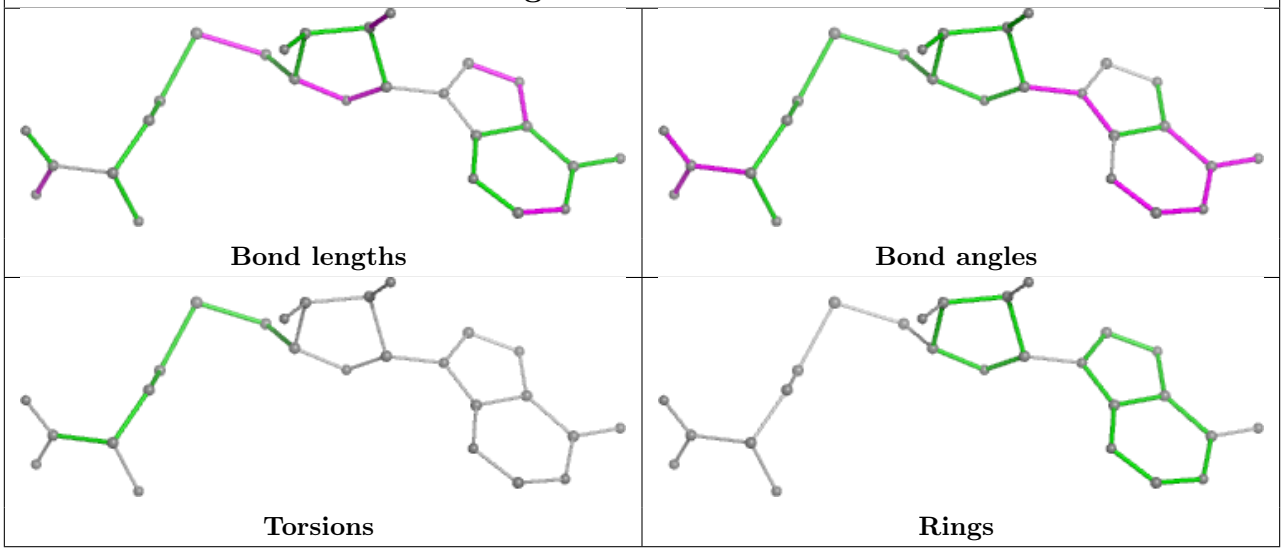
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

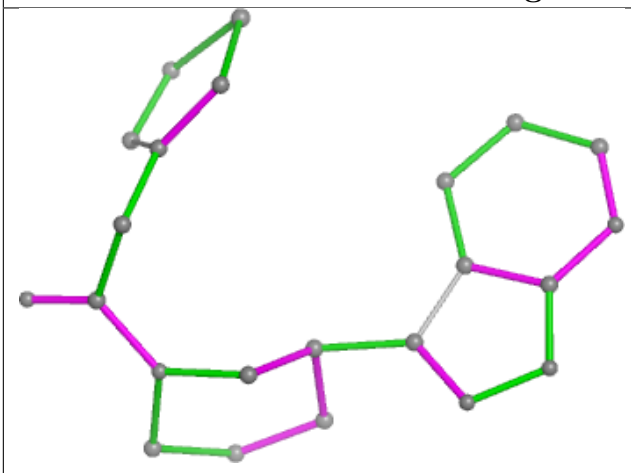
Ligand SAH B 501



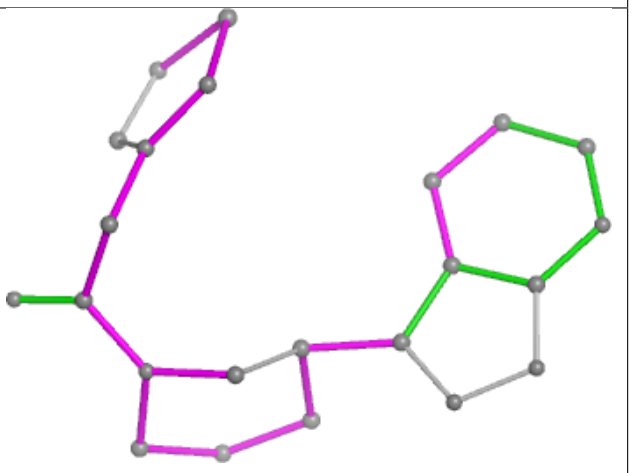
Ligand SAH A 501



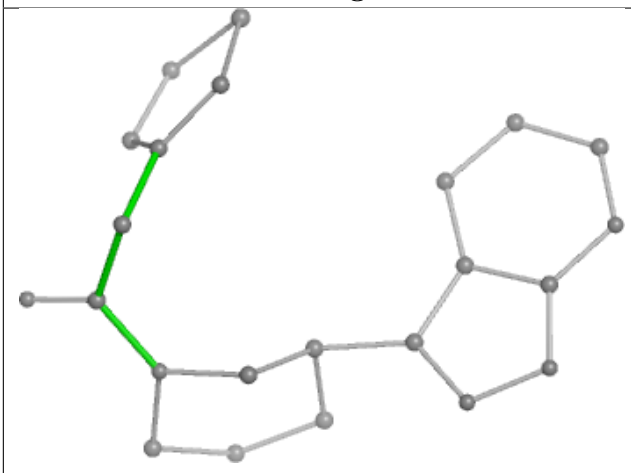
Ligand K7R A 502



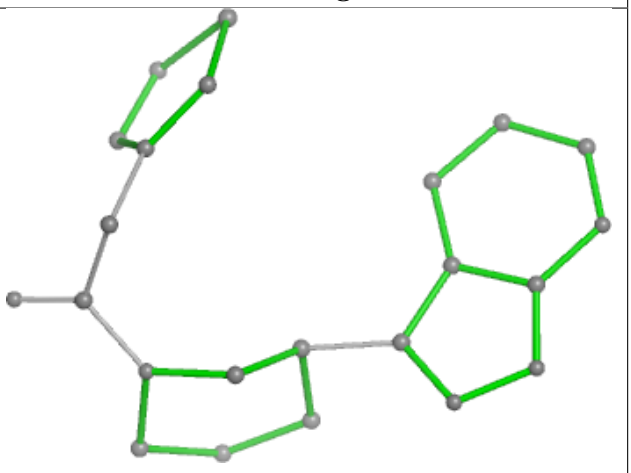
Bond lengths



Bond angles

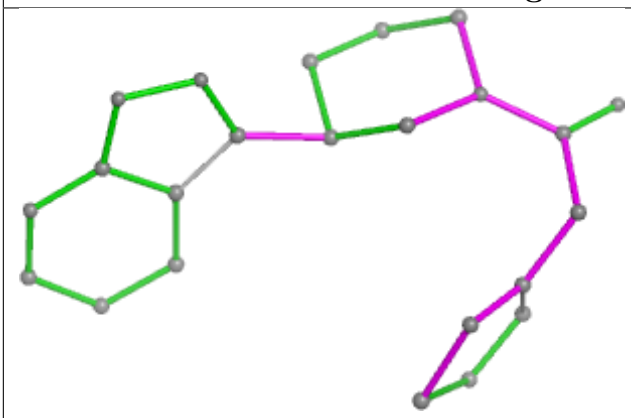


Torsions

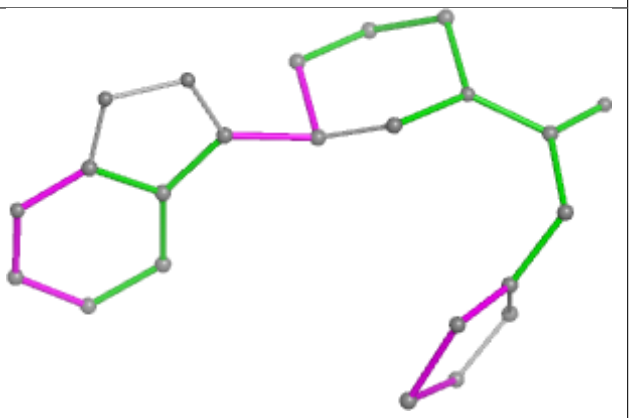


Rings

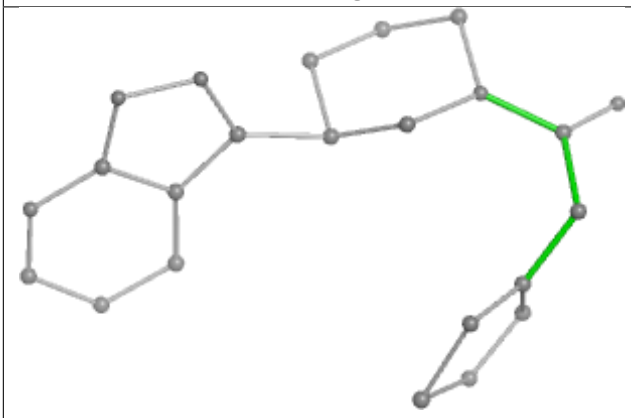
Ligand K7R B 502



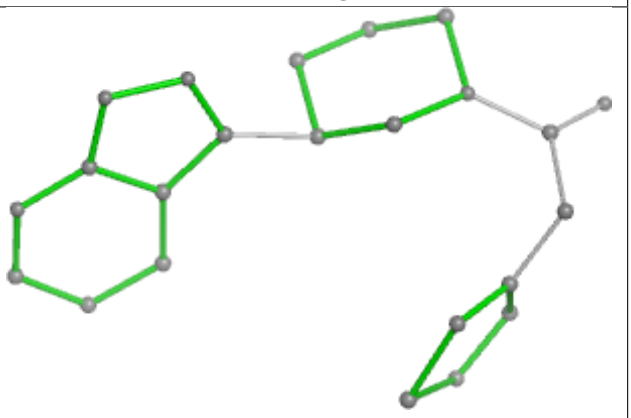
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.62	19 (6%)	24	29	21, 27, 38, 51	1 (0%)
1	B	264/276 (95%)	0.82	19 (7%)	23	27	23, 32, 43, 54	0
All	All	538/552 (97%)	0.72	38 (7%)	23	28	21, 30, 42, 54	1 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	ARG	5.2
1	B	461	TRP	4.7
1	B	198	ASP	4.6
1	B	170	PHE	4.2
1	B	456	LEU	4.0
1	A	248	ASP	3.9
1	B	419	CYS	3.9
1	A	251	TYR	3.6
1	B	171	TYR	3.2
1	B	172	LEU	3.1
1	A	287	CYS	3.0
1	B	287	CYS	3.0
1	A	198	ASP	2.8
1	B	274	PRO	2.8
1	A	169	ILE	2.7
1	A	476	GLN	2.7
1	B	193	GLN	2.7
1	A	340	ILE	2.6
1	B	174	ASN	2.6
1	B	417	LEU	2.6
1	B	245	ASN	2.6
1	A	461	TRP	2.5
1	A	167	SER	2.5
1	A	403	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	249	SER	2.4
1	A	332	GLU	2.4
1	B	246	ARG	2.4
1	A	406[A]	ASN	2.4
1	A	346	GLN	2.3
1	B	266	LEU	2.3
1	B	365	VAL	2.2
1	B	357	LYS	2.2
1	A	196	LYS	2.2
1	B	364	GLY	2.2
1	A	250	GLU	2.2
1	B	366	VAL	2.1
1	A	407	GLU	2.1
1	A	357	LYS	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 monosaccharides 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, 95^{th} 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.

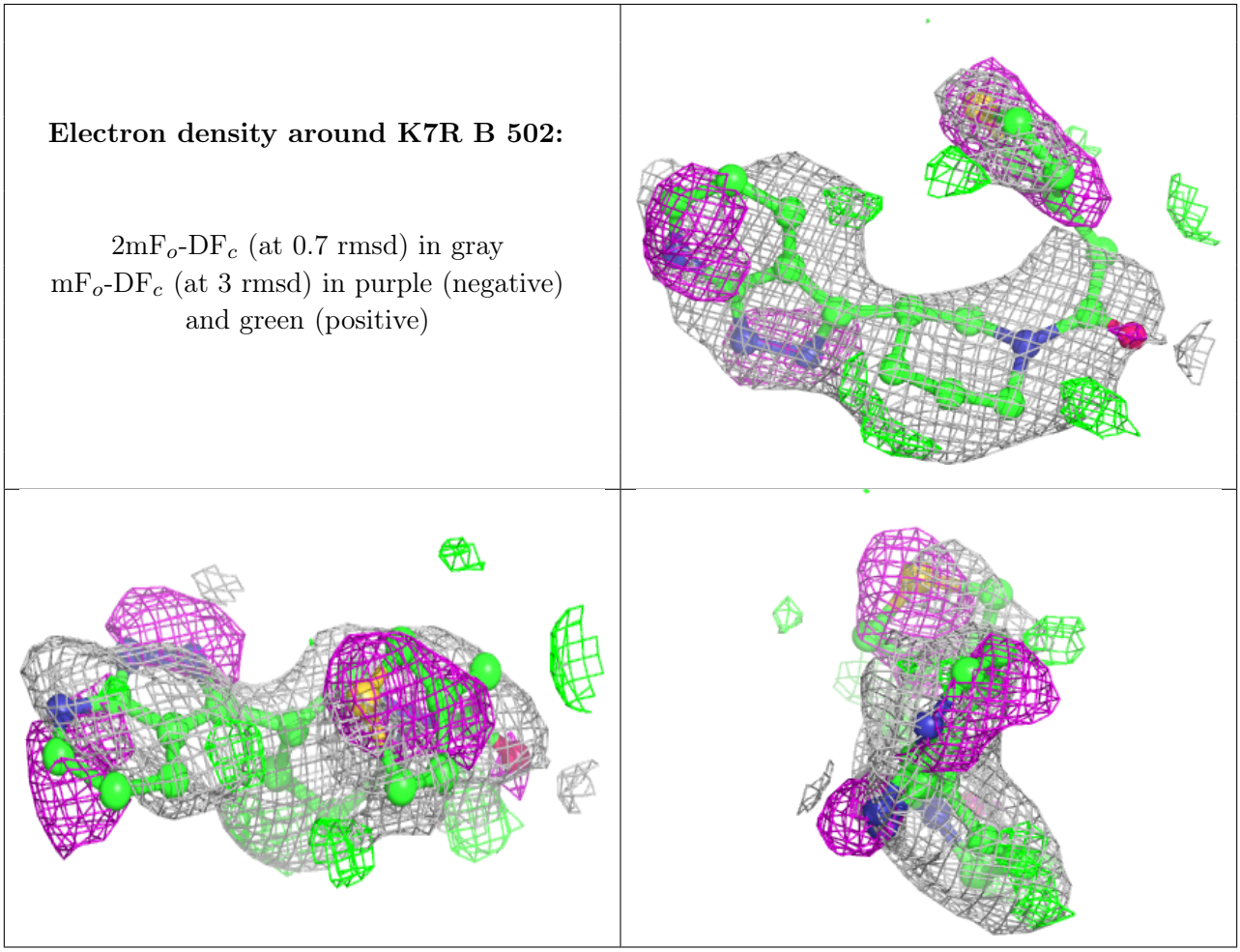
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	K7R	B	502	23/23	0.50	0.21	33,35,39,48	0
5	GOL	B	504	6/6	0.76	0.11	31,32,35,39	0
3	K7R	A	502	23/23	0.79	0.13	28,29,33,42	0
4	SO4	A	503	5/5	0.84	0.24	33,34,37,37	0
4	SO4	B	503	5/5	0.87	0.13	40,41,44,46	0
2	SAH	B	501	26/26	0.93	0.08	27,28,30,30	0
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.

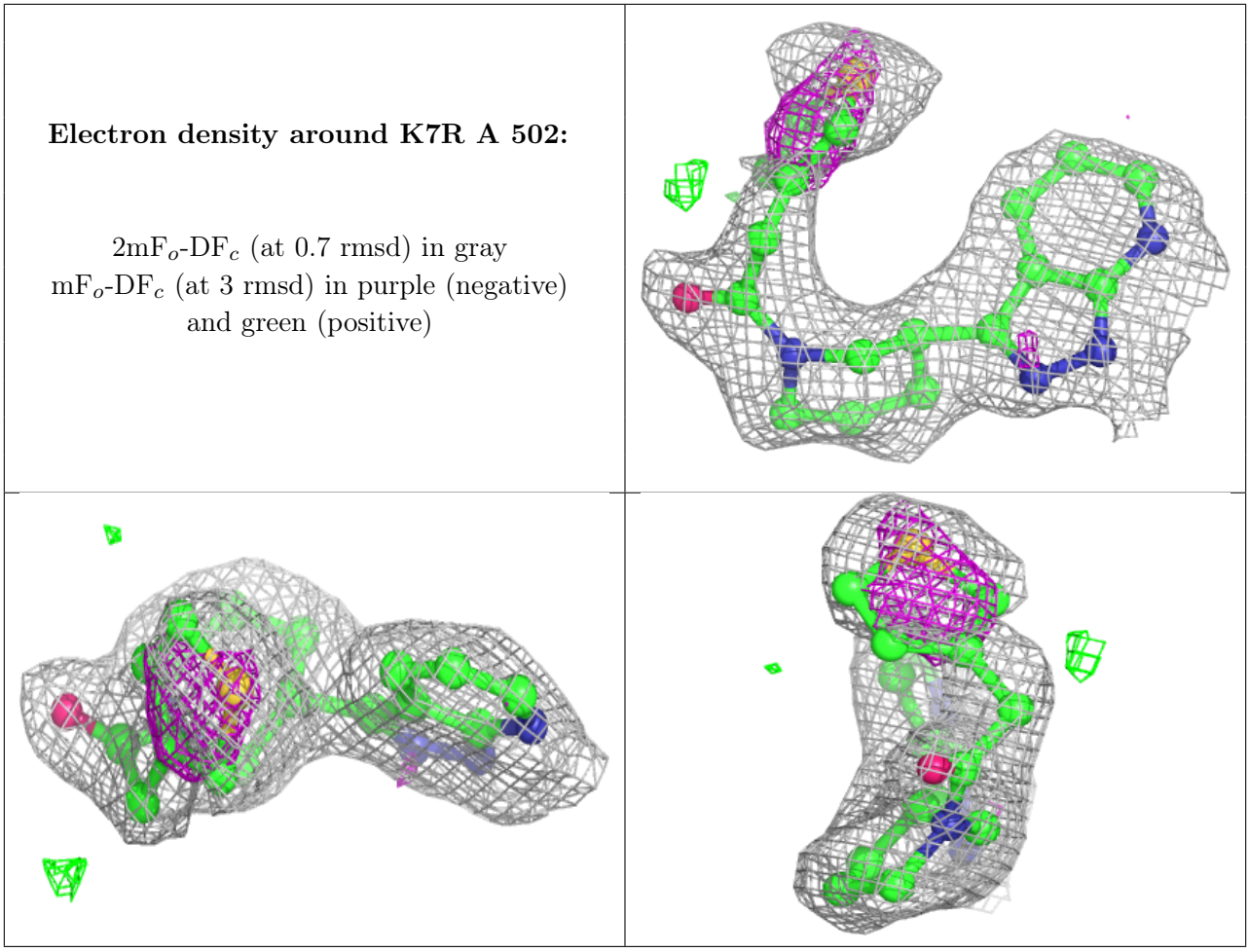
Electron density around K7R B 502:

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



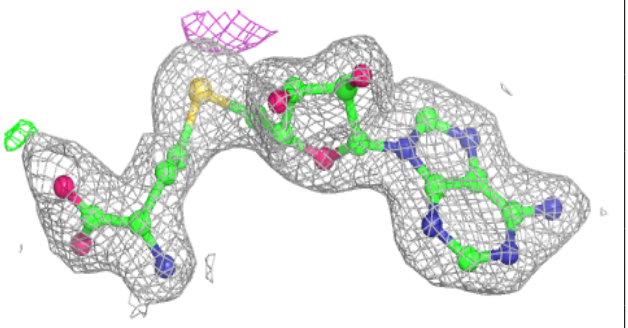
Electron density around K7R A 502:

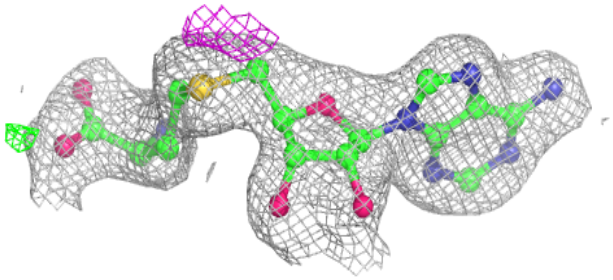
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

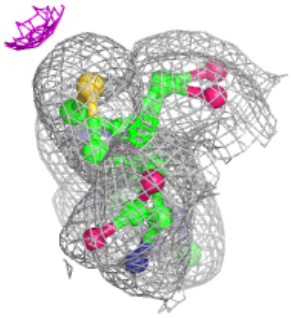


Electron density around SAH B 501:

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

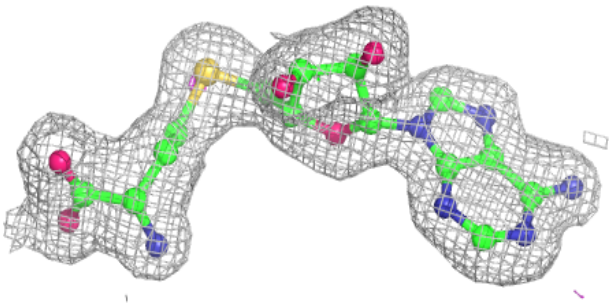


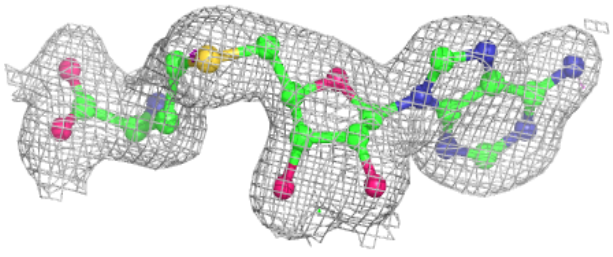


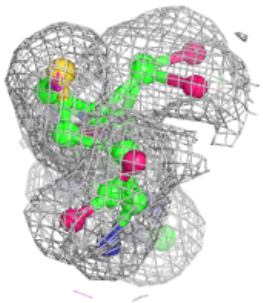


Electron density around SAH A 501:

$2mF_o$-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.