



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:21 PM UTC

PDB ID : 2PTR / pdb_00002ptr
Title : Crystal structure of Escherichia coli adenylosuccinate lyase mutant H171A with bound adenylosuccinate substrate
Authors : Tsai, M.; Howell, P.L.
Deposited on : 2007-05-08
Resolution : 1.85 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

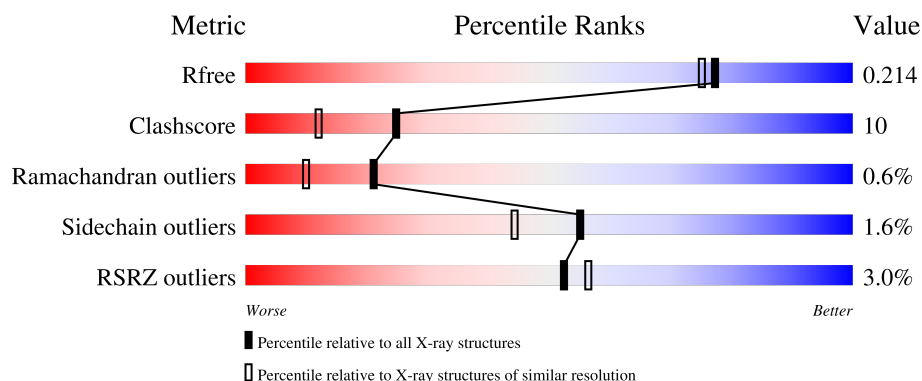
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	462	<div> <div>3%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	B	462	<div> <div>3%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7856 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.

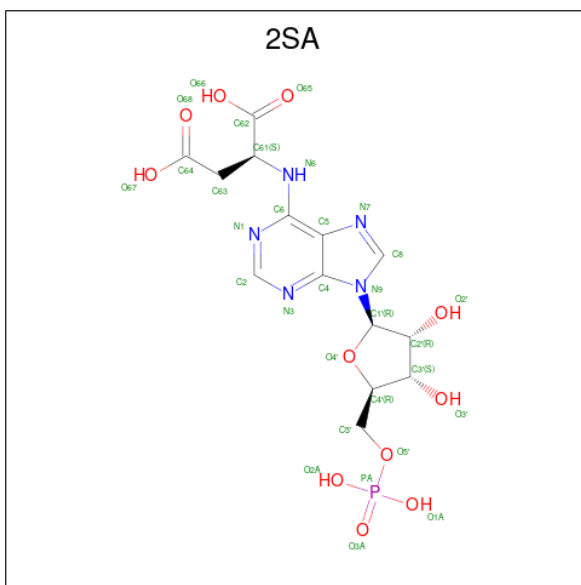
- Molecule 1 is a protein called Adenylosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	454	Total	C	N	O	S	0	0	0
			3559	2268	618	662	11			
1	B	456	Total	C	N	O	S	0	0	0
			3625	2311	629	674	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	LEU	ILE	conflict	UNP P0AB89
A	171	ALA	HIS	engineered mutation	UNP P0AB89
A	457	HIS	-	expression tag	UNP P0AB89
A	458	HIS	-	expression tag	UNP P0AB89
A	459	HIS	-	expression tag	UNP P0AB89
A	460	HIS	-	expression tag	UNP P0AB89
A	461	HIS	-	expression tag	UNP P0AB89
A	462	HIS	-	expression tag	UNP P0AB89
B	154	LEU	ILE	conflict	UNP P0AB89
B	171	ALA	HIS	engineered mutation	UNP P0AB89
B	457	HIS	-	expression tag	UNP P0AB89
B	458	HIS	-	expression tag	UNP P0AB89
B	459	HIS	-	expression tag	UNP P0AB89
B	460	HIS	-	expression tag	UNP P0AB89
B	461	HIS	-	expression tag	UNP P0AB89
B	462	HIS	-	expression tag	UNP P0AB89

- Molecule 2 is 2-[9-(3,4-DIHYDROXY-5-PHOSPHONOOXYMETHYL-TETRAHYDRO-FURAN-2-YL)-9H-PURIN-6-YLAMINO]-SUCCINIC ACID (CCD ID: 2SA) (formula: C₁₄H₁₈N₅O₁₁P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 31	C 14	N 5	O 11	P 1	0	0
2	B	1	Total 31	C 14	N 5	O 11	P 1	0	0

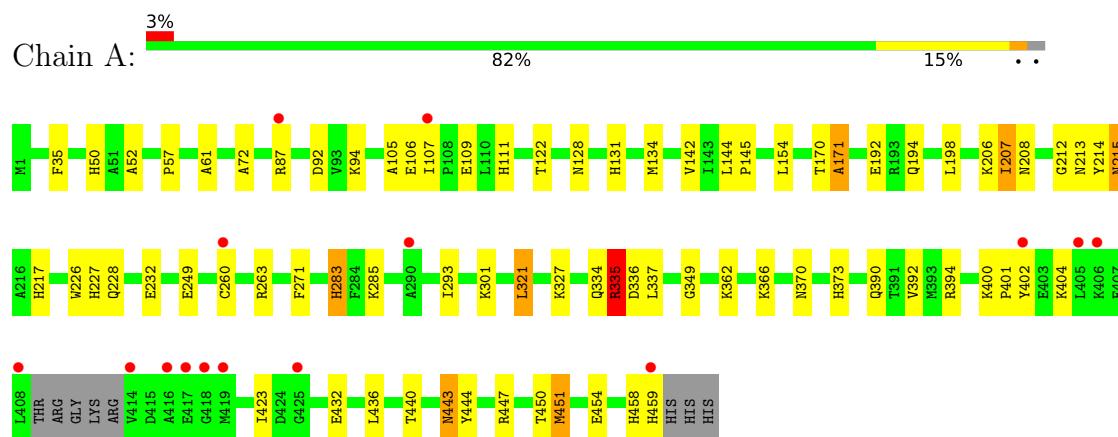
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	306	Total O 306 306	0	0
3	B	304	Total O 304 304	0	0

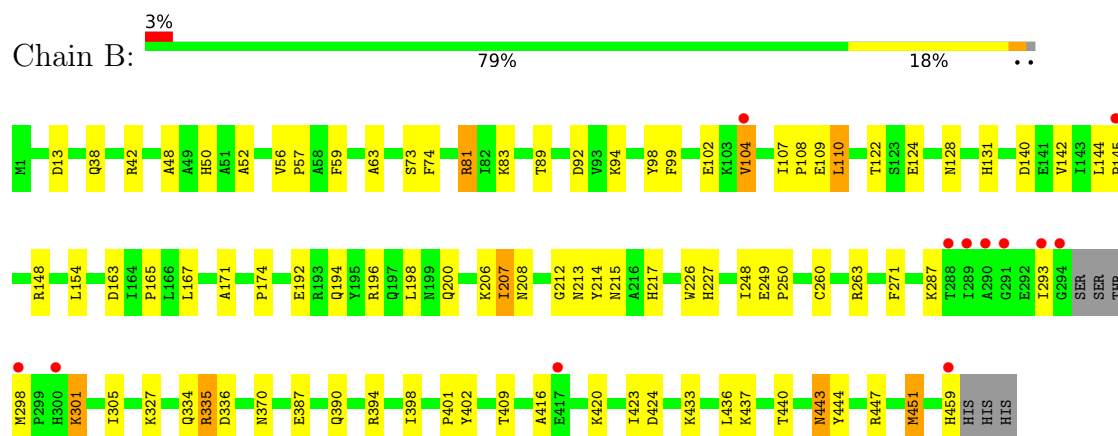
3 Residue-property plots

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: Adenylosuccinate lyase



• Molecule 1: Adenylosuccinate lyase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	98.40Å 143.19Å 69.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.00 – 1.85 44.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.00-1.85) 99.6 (44.00-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	6.80	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.04 (at 1.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.183 , 0.216 0.182 , 0.214	Depositor DCC
R_{free} test set	4220 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7856	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.17% 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: 2SA

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	0.41	0/3636	0.92	10/4940 (0.2%)
1	B	0.39	0/3703	0.94	12/5021 (0.2%)
All	All	0.40	0/7339	0.93	22/9961 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	GLU	N-CA-C	-12.40	94.03	109.65
1	A	249	GLU	N-CA-C	-12.00	94.53	109.65
1	B	301	LYS	N-CA-C	8.64	122.11	110.35
1	A	301	LYS	N-CA-C	7.69	121.67	110.28
1	B	298	MET	CA-C-N	7.33	127.04	119.56
1	B	298	MET	C-N-CA	7.33	127.04	119.56
1	A	171	ALA	N-CA-C	-6.75	104.62	112.86
1	B	122	THR	N-CA-C	-6.70	99.75	110.14
1	B	92	ASP	N-CA-C	6.43	118.29	111.28
1	B	409	THR	N-CA-C	6.38	121.72	113.88
1	A	122	THR	N-CA-C	-6.29	100.39	110.14
1	B	171	ALA	N-CA-C	-6.18	105.32	112.86
1	B	250	PRO	N-CA-C	5.81	121.40	113.84
1	B	89	THR	N-CA-C	5.80	118.54	111.82
1	A	336	ASP	N-CA-C	-5.67	100.89	109.85
1	A	61	ALA	N-CA-C	5.56	118.06	111.33
1	A	283	HIS	N-CA-C	-5.52	106.05	112.89
1	B	336	ASP	N-CA-C	-5.43	101.27	109.85
1	A	285	LYS	N-CA-C	-5.36	102.25	110.14
1	B	140	ASP	N-CA-C	5.26	117.92	111.82
1	A	92	ASP	N-CA-C	5.20	117.03	111.36
1	A	72	ALA	N-CA-C	5.00	116.73	111.28

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	3559	0	3492	69	0
1	B	3625	0	3597	77	0
2	B	62	0	26	0	0
3	A	306	0	0	4	0
3	B	304	0	0	7	0
All	All	7856	0	7115	141	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (141) 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:128:ASN:HD21	1:A:206:LYS:H	1.07	0.97
1:B:128:ASN:HD21	1:B:206:LYS:H	1.18	0.85
1:A:106:GLU:HG3	1:A:107:ILE:HD12	1.61	0.81
1:A:447:ARG:NH1	1:A:451:MET:HE3	1.95	0.80
1:A:194:GLN:HE22	1:A:263:ARG:HE	1.29	0.80
1:B:194:GLN:HE22	1:B:263:ARG:HE	1.32	0.78
1:B:447:ARG:NH1	1:B:451:MET:HE3	1.99	0.77
1:A:443:ASN:C	1:A:443:ASN:HD22	1.92	0.76
1:B:451:MET:HA	1:B:451:MET:CE	2.16	0.74
1:B:142:VAL:O	1:B:145:PRO:HG2	1.87	0.74
1:B:443:ASN:C	1:B:443:ASN:HD22	1.94	0.74
1:B:104:VAL:HG13	1:B:110:LEU:HB3	1.70	0.74
1:A:106:GLU:HG3	1:A:107:ILE:CD1	2.17	0.73
1:A:451:MET:CE	1:A:451:MET:HA	2.22	0.70
1:A:215:ASN:H	1:A:215:ASN:HD22	1.39	0.70
1:B:451:MET:HA	1:B:451:MET:HE2	1.73	0.69
1:A:283:HIS:HD2	1:A:373:HIS:HD2	1.40	0.69
1:A:451:MET:HA	1:A:451:MET:HE2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASN:HD21	1:A:206:LYS:N	1.89	0.67
1:A:213:ASN:HB2	1:A:215:ASN:HD21	1.58	0.67
1:A:128:ASN:ND2	1:A:206:LYS:H	1.88	0.66
1:A:142:VAL:O	1:A:145:PRO:HG2	1.95	0.66
1:A:94:LYS:HG2	1:B:293:ILE:HD12	1.78	0.65
1:B:167:LEU:HD21	1:B:174:PRO:HB3	1.80	0.62
1:A:94:LYS:HG2	1:B:293:ILE:CD1	2.31	0.61
1:A:198:LEU:HD13	1:A:260:CYS:SG	2.40	0.61
1:B:198:LEU:HD13	1:B:260:CYS:SG	2.42	0.60
1:B:215:ASN:H	1:B:215:ASN:HD22	1.50	0.60
1:A:321:LEU:HD13	1:A:349:GLY:HA3	1.83	0.60
1:B:57:PRO:HG2	3:B:1431:HOH:O	2.02	0.59
1:A:390:GLN:HG2	1:A:401:PRO:HB2	1.84	0.59
1:B:424:ASP:HA	1:B:433:LYS:HZ3	1.68	0.58
1:A:192:GLU:HG2	1:A:459:HIS:ND1	2.19	0.58
1:B:440:THR:H	1:B:443:ASN:ND2	2.02	0.58
1:B:423:ILE:HD13	1:B:436:LEU:HB3	1.86	0.57
1:B:63:ALA:HB1	1:B:110:LEU:HD11	1.87	0.57
1:A:192:GLU:HG2	1:A:459:HIS:CG	2.40	0.56
1:A:109:GLU:HB2	3:A:549:HOH:O	2.05	0.56
1:A:440:THR:H	1:A:443:ASN:ND2	2.03	0.56
1:B:213:ASN:HB2	1:B:215:ASN:HD21	1.70	0.56
1:A:213:ASN:HB2	1:A:215:ASN:ND2	2.21	0.56
1:A:335:ARG:C	1:A:335:ARG:HD3	2.30	0.56
1:B:327:LYS:HD3	1:B:327:LYS:C	2.31	0.55
1:A:214:TYR:OH	1:A:227:HIS:HD2	1.89	0.55
1:A:447:ARG:HH12	1:A:451:MET:HE3	1.70	0.55
1:B:131:HIS:HD2	3:B:1312:HOH:O	1.89	0.55
1:A:447:ARG:HH11	1:A:451:MET:HE3	1.70	0.55
1:A:57:PRO:HG2	3:A:640:HOH:O	2.05	0.55
1:A:390:GLN:NE2	1:A:394:ARG:HH21	2.05	0.54
1:B:447:ARG:O	1:B:451:MET:HG2	2.07	0.54
1:B:144:LEU:N	1:B:145:PRO:HD2	2.23	0.54
1:B:447:ARG:HH12	1:B:451:MET:HE3	1.72	0.54
1:A:334:GLN:O	1:A:335:ARG:HB3	2.07	0.53
1:A:283:HIS:CD2	1:A:373:HIS:HD2	2.25	0.53
1:B:108:PRO:HG2	3:B:1324:HOH:O	2.08	0.53
1:B:387:GLU:O	1:B:390:GLN:HG3	2.08	0.53
1:A:362:LYS:HE2	1:A:366:LYS:NZ	2.24	0.53
1:B:334:GLN:O	1:B:335:ARG:HB3	2.08	0.52
1:A:337:LEU:HD13	1:B:305:ILE:HG22	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ASP:HA	1:B:433:LYS:NZ	2.24	0.52
1:A:215:ASN:H	1:A:215:ASN:ND2	2.06	0.52
1:A:208:ASN:CG	1:A:212:GLY:HA2	2.35	0.51
1:B:416:ALA:O	1:B:420:LYS:HG3	2.11	0.51
1:B:447:ARG:HH11	1:B:451:MET:HE3	1.73	0.50
1:B:81:ARG:HG2	1:B:99:PHE:HD2	1.77	0.50
1:A:443:ASN:C	1:A:443:ASN:ND2	2.65	0.50
1:A:50:HIS:CD2	1:A:52:ALA:HB3	2.47	0.50
1:B:194:GLN:NE2	1:B:263:ARG:HE	2.04	0.50
1:B:73:SER:O	1:B:74:PHE:C	2.55	0.49
1:B:192:GLU:HG2	1:B:459:HIS:CG	2.47	0.49
1:A:142:VAL:C	1:A:145:PRO:HD2	2.38	0.49
1:B:63:ALA:HB1	1:B:110:LEU:CD1	2.42	0.49
1:A:194:GLN:NE2	1:A:263:ARG:HE	2.03	0.49
1:A:217:HIS:HB3	1:A:226:TRP:CE2	2.48	0.49
1:A:443:ASN:HD22	1:A:444:TYR:N	2.10	0.48
1:B:424:ASP:OD2	1:B:437:LYS:HD3	2.12	0.48
1:A:401:PRO:HG2	1:A:402:TYR:H	1.78	0.48
1:B:196:ARG:CG	1:B:200:GLN:NE2	2.77	0.48
1:B:163:ASP:O	1:B:165:PRO:HD3	2.13	0.48
1:B:443:ASN:C	1:B:443:ASN:ND2	2.66	0.48
1:A:450:THR:O	1:A:454:GLU:HG3	2.13	0.48
1:B:207:ILE:HG23	1:B:207:ILE:O	2.12	0.48
1:B:443:ASN:HD22	1:B:444:TYR:N	2.12	0.48
1:B:59:PHE:HA	1:B:109:GLU:OE1	2.14	0.48
1:A:107:ILE:HD12	1:A:107:ILE:N	2.29	0.47
1:B:196:ARG:HG3	1:B:200:GLN:NE2	2.29	0.47
1:B:394:ARG:HG2	1:B:401:PRO:HG3	1.97	0.47
1:B:215:ASN:H	1:B:215:ASN:ND2	2.11	0.47
1:A:35:PHE:CD2	1:A:134:MET:HG3	2.50	0.46
1:A:206:LYS:HD2	1:A:206:LYS:C	2.41	0.46
1:B:196:ARG:HG3	1:B:200:GLN:HE21	1.81	0.46
1:B:48:ALA:HA	1:B:56:VAL:O	2.16	0.46
1:B:335:ARG:C	1:B:335:ARG:HD3	2.40	0.46
1:A:144:LEU:N	1:A:145:PRO:HD2	2.31	0.45
1:A:334:GLN:O	1:A:335:ARG:CB	2.64	0.45
1:A:432:GLU:HA	1:A:432:GLU:OE2	2.16	0.45
1:B:98:TYR:O	1:B:102:GLU:HG3	2.16	0.45
1:B:83:LYS:NZ	3:B:1426:HOH:O	2.50	0.45
1:B:214:TYR:OH	1:B:227:HIS:HD2	2.00	0.45
1:B:451:MET:HE3	1:B:451:MET:HA	1.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:TYR:CD1	1:B:402:TYR:C	2.95	0.45
1:B:370:ASN:C	1:B:370:ASN:HD22	2.25	0.45
1:A:400:LYS:O	1:A:404:LYS:HG3	2.17	0.44
1:B:192:GLU:HG2	1:B:459:HIS:CD2	2.52	0.44
1:A:208:ASN:OD1	1:A:212:GLY:HA2	2.17	0.44
1:A:293:ILE:HG13	1:B:94:LYS:HG2	1.98	0.44
1:B:128:ASN:ND2	1:B:206:LYS:H	1.99	0.44
1:B:459:HIS:HD2	3:B:1447:HOH:O	2.00	0.44
1:A:105:ALA:HA	1:A:111:HIS:CD2	2.52	0.43
1:B:148:ARG:NH2	3:B:1492:HOH:O	2.51	0.43
1:B:81:ARG:HD3	1:B:102:GLU:OE1	2.18	0.43
1:A:131:HIS:HD2	3:A:589:HOH:O	2.01	0.43
1:B:154:LEU:HD11	1:B:271:PHE:CE1	2.53	0.43
1:B:217:HIS:HB3	1:B:226:TRP:CE2	2.54	0.43
1:A:87:ARG:NH1	3:A:620:HOH:O	2.51	0.43
1:B:213:ASN:HB2	1:B:215:ASN:ND2	2.31	0.42
1:B:440:THR:H	1:B:443:ASN:HD21	1.64	0.42
1:A:440:THR:H	1:A:443:ASN:HD21	1.65	0.42
1:B:50:HIS:CD2	1:B:52:ALA:HB3	2.54	0.42
1:B:334:GLN:O	1:B:335:ARG:CB	2.66	0.42
1:A:337:LEU:CD1	1:B:305:ILE:HG22	2.50	0.42
1:A:207:ILE:O	1:A:207:ILE:HG23	2.19	0.42
1:B:206:LYS:C	1:B:206:LYS:HD2	2.45	0.42
1:A:154:LEU:HD11	1:A:271:PHE:CE1	2.54	0.42
1:B:13:ASP:HB2	3:B:1293:HOH:O	2.19	0.41
1:B:208:ASN:CG	1:B:212:GLY:HA2	2.45	0.41
1:A:327:LYS:HD3	1:A:327:LYS:C	2.45	0.41
1:A:228:GLN:O	1:A:232:GLU:HG3	2.20	0.41
1:B:38:GLN:O	1:B:42:ARG:HG2	2.21	0.41
1:B:124:GLU:HG3	1:B:248:ILE:HG22	2.03	0.41
1:B:447:ARG:NH1	1:B:451:MET:CE	2.79	0.41
1:A:423:ILE:HD13	1:A:436:LEU:HB3	2.02	0.41
1:A:170:THR:O	1:A:171:ALA:HB3	2.21	0.41
1:A:447:ARG:O	1:A:451:MET:HG2	2.20	0.41
1:B:107:ILE:HG21	1:B:110:LEU:HD22	2.02	0.41
1:B:398:ILE:O	1:B:401:PRO:HD3	2.21	0.41
1:A:217:HIS:HB3	1:A:226:TRP:CD2	2.56	0.40
1:A:370:ASN:C	1:A:370:ASN:HD22	2.29	0.40
1:A:283:HIS:CD2	1:A:373:HIS:CD2	3.07	0.40
1:A:392:VAL:HG21	1:A:436:LEU:HD21	2.02	0.40
1:B:208:ASN:OD1	1:B:212:GLY:HA2	2.22	0.40

There are no symmetry-related clashes.

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	450/462 (97%)	436 (97%)	11 (2%)	3 (1%)	18	8
1	B	452/462 (98%)	437 (97%)	13 (3%)	2 (0%)	30	17
All	All	902/924 (98%)	873 (97%)	24 (3%)	5 (1%)	21	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	335	ARG
1	B	335	ARG
1	A	458	HIS
1	B	207	ILE
1	A	207	ILE

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	370/392 (94%)	365 (99%)	5 (1%)	59	49
1	B	382/392 (97%)	375 (98%)	7 (2%)	51	40
All	All	752/784 (96%)	740 (98%)	12 (2%)	55	44

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	ASN
1	A	321	LEU
1	A	335	ARG
1	A	443	ASN
1	A	451	MET
1	B	81	ARG
1	B	104	VAL
1	B	110	LEU
1	B	287	LYS
1	B	301	LYS
1	B	443	ASN
1	B	451	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	50	HIS
1	A	90	ASN
1	A	111	HIS
1	A	128	ASN
1	A	131	HIS
1	A	149	GLN
1	A	194	GLN
1	A	197	GLN
1	A	215	ASN
1	A	227	HIS
1	A	228	GLN
1	A	240	GLN
1	A	242	ASN
1	A	283	HIS
1	A	334	GLN
1	A	358	GLN
1	A	370	ASN
1	A	373	HIS
1	A	443	ASN
1	A	458	HIS
1	B	128	ASN
1	B	131	HIS
1	B	149	GLN
1	B	194	GLN
1	B	200	GLN
1	B	215	ASN

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Mol	Chain	Res	Type
1	B	227	HIS
1	B	242	ASN
1	B	282	ASN
1	B	322	GLN
1	B	334	GLN
1	B	358	GLN
1	B	370	ASN
1	B	443	ASN
1	B	459	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
2	2SA	B	1100	-	33,33,33	1.85	6 (18%)	47,49,49	1.82	8 (17%)
2	2SA	B	1200	-	33,33,33	2.53	3 (9%)	47,49,49	1.53	4 (8%)

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	2SA	B	1100	-	-	10/22/38/38	0/3/3/3
2	2SA	B	1200	-	-	12/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1200	2SA	C6-N6	12.33	1.55	1.35
2	B	1100	2SA	O5'-C5'	-6.23	1.21	1.44
2	B	1200	2SA	C61-N6	-5.36	1.32	1.46
2	B	1100	2SA	C6-N6	4.45	1.42	1.35
2	B	1100	2SA	C63-C61	3.94	1.61	1.53
2	B	1200	2SA	C6-N1	2.50	1.38	1.35
2	B	1100	2SA	C6-N1	2.26	1.38	1.35
2	B	1100	2SA	O65-C62	2.19	1.28	1.22
2	B	1100	2SA	PA-O5'	2.04	1.66	1.60

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1200	2SA	C62-C61-N6	-6.96	94.37	110.56
2	B	1100	2SA	C61-C63-C64	5.96	129.51	112.75
2	B	1100	2SA	O5'-C5'-C4'	5.80	128.76	108.99
2	B	1200	2SA	N6-C6-N1	5.01	125.12	118.00
2	B	1100	2SA	C62-C61-N6	-4.50	100.10	110.56
2	B	1100	2SA	C63-C61-C62	4.30	119.38	110.79
2	B	1100	2SA	C4'-O4'-C1'	-2.62	103.67	109.47
2	B	1100	2SA	O68-C64-C63	-2.62	114.81	122.84
2	B	1200	2SA	O66-C62-C61	2.40	121.62	113.51
2	B	1100	2SA	O67-C64-C63	2.23	120.92	114.00
2	B	1100	2SA	C3'-C2'-C1'	-2.20	97.29	101.46
2	B	1200	2SA	O4'-C1'-N9	2.13	112.18	108.09

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1100	2SA	N1-C6-N6-C61
2	B	1100	2SA	C5-C6-N6-C61

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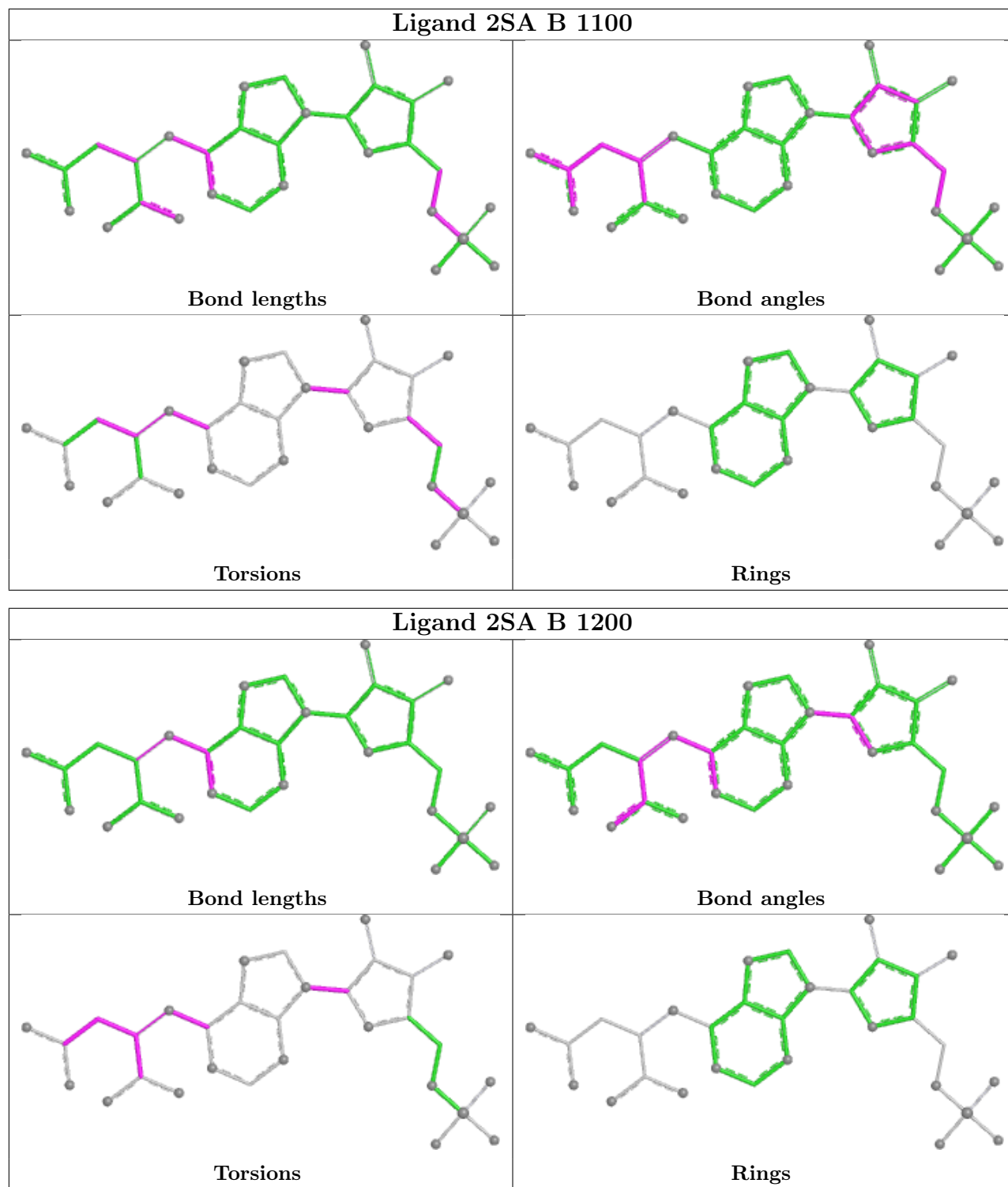
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Mol	Chain	Res	Type	Atoms
2	B	1200	2SA	N1-C6-N6-C61
2	B	1200	2SA	C5-C6-N6-C61
2	B	1200	2SA	C63-C61-N6-C6
2	B	1200	2SA	N6-C61-C62-O65
2	B	1200	2SA	N6-C61-C62-O66
2	B	1100	2SA	C5'-O5'-PA-O3A
2	B	1100	2SA	C2'-C1'-N9-C8
2	B	1200	2SA	C2'-C1'-N9-C8
2	B	1100	2SA	C62-C61-C63-C64
2	B	1200	2SA	N6-C61-C63-C64
2	B	1100	2SA	C2'-C1'-N9-C4
2	B	1200	2SA	C2'-C1'-N9-C4
2	B	1200	2SA	C61-C63-C64-O68
2	B	1100	2SA	O4'-C1'-N9-C8
2	B	1100	2SA	O4'-C1'-N9-C4
2	B	1200	2SA	O4'-C1'-N9-C8
2	B	1200	2SA	C61-C63-C64-O67
2	B	1200	2SA	O4'-C1'-N9-C4
2	B	1100	2SA	O4'-C4'-C5'-O5'
2	B	1100	2SA	C63-C61-N6-C6

There are no ring outliers.

No monomer is involved in short contacts.

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.



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, 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	454/462 (98%)	-0.20	15 (3%) 49 53	12, 20, 45, 61	0
1	B	456/462 (98%)	-0.25	12 (2%) 57 61	11, 20, 41, 51	0
All	All	910/924 (98%)	-0.22	27 (2%) 52 56	11, 20, 42, 61	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	408	LEU	6.6
1	B	289	ILE	4.3
1	A	290	ALA	3.9
1	A	402	TYR	3.7
1	A	414	VAL	3.7
1	A	417	GLU	3.4
1	A	406	LYS	3.2
1	B	104	VAL	3.1
1	A	418	GLY	3.0
1	A	419	MET	2.8
1	B	294	GLY	2.8
1	A	459	HIS	2.8
1	A	416	ALA	2.7
1	B	293	ILE	2.6
1	A	405	LEU	2.5
1	B	417	GLU	2.4
1	B	290	ALA	2.3
1	B	288	THR	2.3
1	A	107	ILE	2.2
1	B	291	GLY	2.2
1	B	300	HIS	2.2
1	A	425	GLY	2.1
1	B	459	HIS	2.1
1	A	87	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	260	CYS	2.1
1	B	298	MET	2.0
1	B	145	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](#)

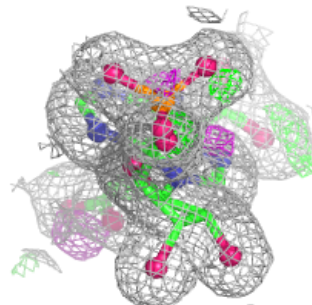
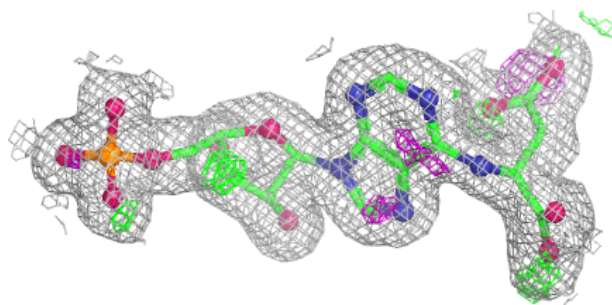
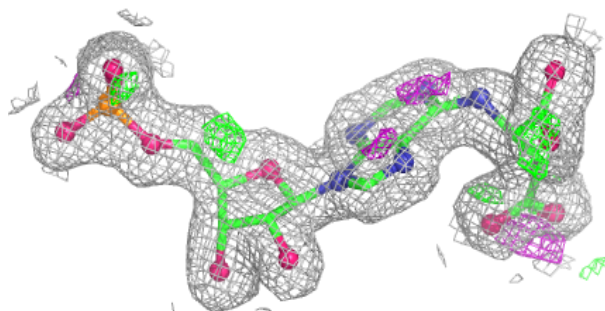
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	2SA	B	1100	31/31	0.95	0.07	12,17,22,27	0
2	2SA	B	1200	31/31	0.96	0.07	13,21,32,35	0

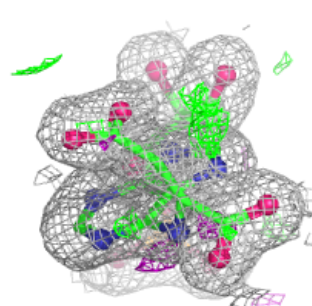
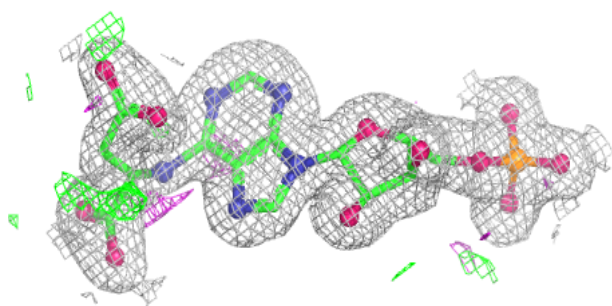
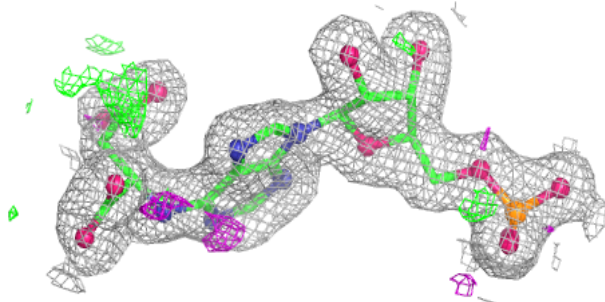
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2SA B 1100:

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

**Electron density around 2SA B 1200:**

$2mF_o-DF_c$ (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.