



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:19 AM UTC

PDB ID : 5XG3 / pdb_00005xg3
Title : Crystal structure of the ATPgS-engaged Smc head domain with an extended coiled coil bound to the C-terminal domain of ScpA derived from *Bacillus subtilis*
Authors : Shin, H.-C.; Lee, H.; Oh, B.-H.
Deposited on : 2017-04-11
Resolution : 3.50 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

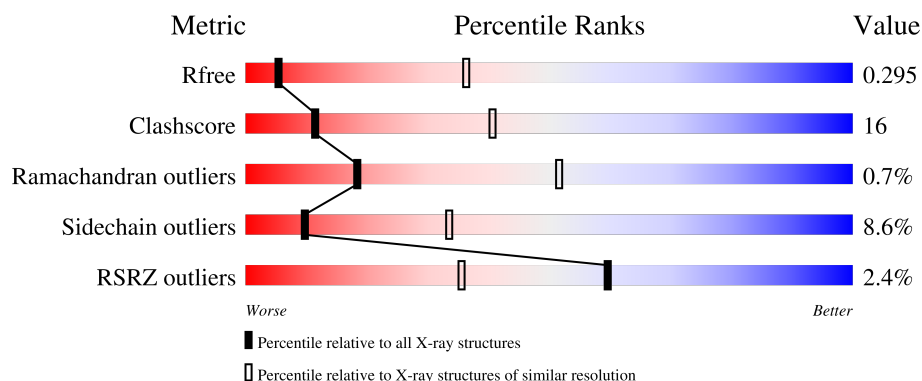
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	435	 2% 61% 22% 15%
1	B	435	 % 62% 20% 14%
2	C	89	 % 60% 17% 24%
2	D	89	 4% 52% 7% 40%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5698 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 Chromosome partition protein Smc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2400	1492	429	475	4			
1	B	374	Total	C	N	O	S	0	0	0
			2459	1546	426	482	5			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	971	SER	-	linker	UNP P51834
A	972	GLY	-	linker	UNP P51834
A	973	GLY	-	linker	UNP P51834
A	974	SER	-	linker	UNP P51834
A	1118	GLN	GLU	engineered mutation	UNP P51834
B	971	SER	-	linker	UNP P51834
B	972	GLY	-	linker	UNP P51834
B	973	GLY	-	linker	UNP P51834
B	974	SER	-	linker	UNP P51834
B	1118	GLN	GLU	engineered mutation	UNP P51834

- Molecule 2 is a protein called Segregation and condensation protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	68	Total	C	N	O	S	0	0	0
			453	282	80	89	2			
2	D	53	Total	C	N	O	S	0	0	0
			318	195	60	62	1			

There are 8 discrepancies between the modelled and reference sequences:

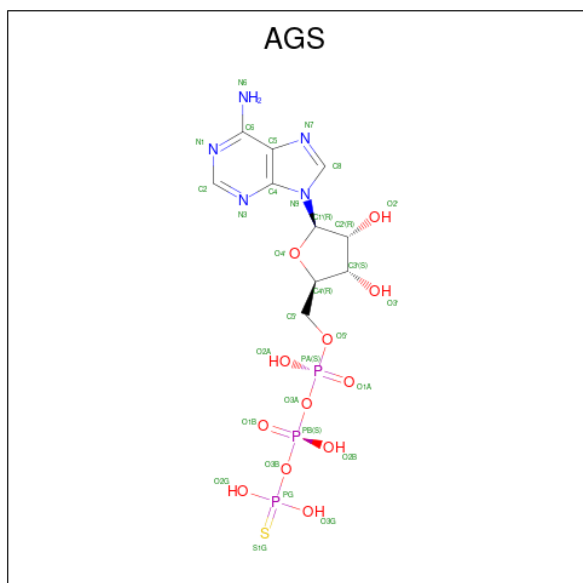
Chain	Residue	Modelled	Actual	Comment	Reference
C	252	VAL	-	expression tag	UNP A0A1N6WAJ8
C	253	ASP	-	expression tag	UNP A0A1N6WAJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	254	LYS	-	expression tag	UNP A0A1N6WAJ8
C	255	LEU	-	expression tag	UNP A0A1N6WAJ8
D	252	VAL	-	expression tag	UNP A0A1N6WAJ8
D	253	ASP	-	expression tag	UNP A0A1N6WAJ8
D	254	LYS	-	expression tag	UNP A0A1N6WAJ8
D	255	LEU	-	expression tag	UNP A0A1N6WAJ8

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Co 1	0	0

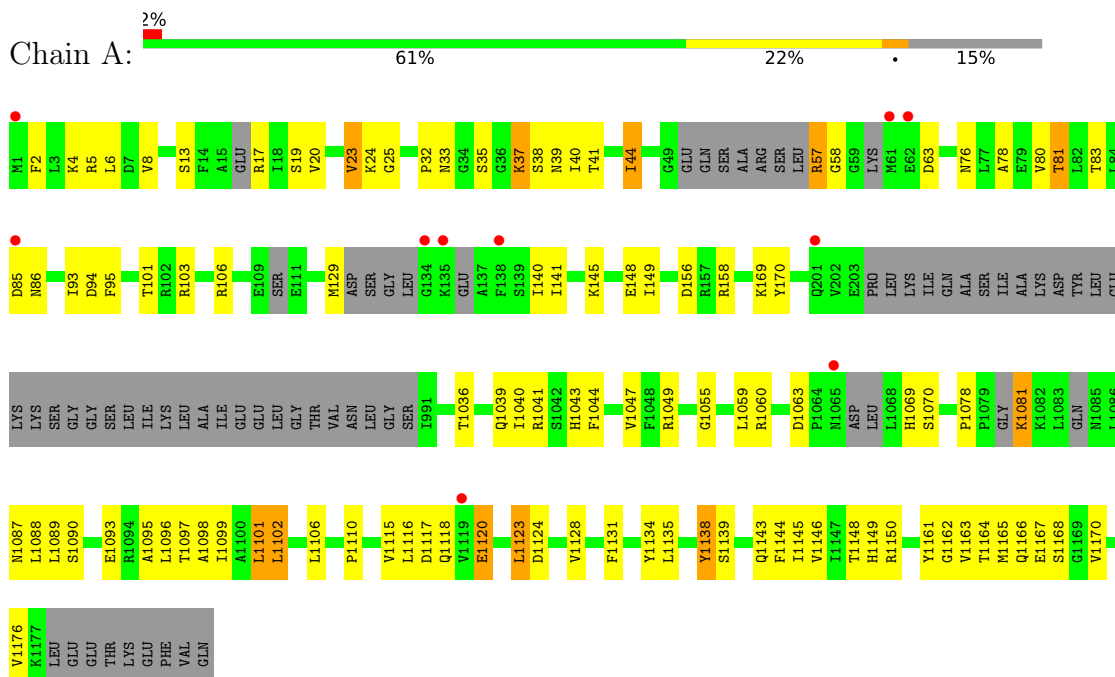
- Molecule 6 is water.

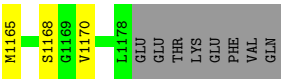
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total 3	O 3	0	0

3 Residue-property plots [i](#)

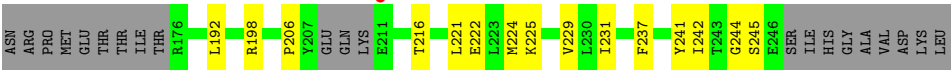
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

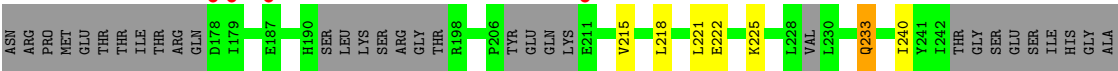




● Molecule 2: Segregation and condensation protein A



● Molecule 2: Segregation and condensation protein A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.10Å 104.78Å 185.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.99 – 3.50 40.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	84.1 (40.99-3.50) 83.5 (40.99-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.261 , 0.296 0.261 , 0.295	Depositor DCC
R_{free} test set	2000 reflections (6.79%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.640	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.30$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	5698	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.77% 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: AGS, MG, CO

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	0.52	0/2417	0.88	9/3296 (0.3%)
1	B	0.56	0/2486	0.89	7/3398 (0.2%)
2	C	0.41	0/458	0.68	0/627
2	D	0.49	0/317	0.75	0/435
All	All	0.53	0/5678	0.86	16/7756 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1064	PRO	N-CA-CB	8.57	112.25	103.25
1	A	57	ARG	CA-C-N	-6.82	111.58	121.26
1	A	57	ARG	C-N-CA	-6.82	111.58	121.26
1	A	1095	ALA	CA-C-N	-6.11	112.99	122.16
1	A	1095	ALA	C-N-CA	-6.11	112.99	122.16
1	B	1063	ASP	CA-C-N	6.06	127.41	119.84
1	B	1063	ASP	C-N-CA	6.06	127.41	119.84
1	A	1131	PHE	CA-C-O	-5.62	109.92	118.91
1	A	1081	LYS	CA-C-N	-5.48	115.13	122.42
1	A	1081	LYS	C-N-CA	-5.48	115.13	122.42
1	A	1131	PHE	O-C-N	5.29	130.87	122.41
1	A	44	ILE	N-CA-C	-5.23	106.44	112.98
1	B	1164	THR	CA-C-N	-5.23	115.42	122.95
1	B	1164	THR	C-N-CA	-5.23	115.42	122.95
1	B	1081	LYS	CA-C-N	5.18	131.44	121.54
1	B	1081	LYS	C-N-CA	5.18	131.44	121.54

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	2400	0	1954	86	0
1	B	2459	0	2006	74	0
2	C	453	0	366	16	0
2	D	318	0	221	5	0
3	A	31	0	12	5	0
3	B	31	0	12	3	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
6	B	3	0	0	2	0
All	All	5698	0	4571	165	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 16.

All (165) 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)
3:B:1201:AGS:S1G	6:B:1302:HOH:O	2.22	0.96
1:B:12:LYS:HD2	1:B:39:ASN:HD21	1.36	0.87
1:B:30:VAL:HG12	1:B:31:GLY:H	1.42	0.83
1:B:28:ALA:HB3	1:B:1160:LEU:HD22	1.63	0.80
1:B:1116:LEU:HB2	1:B:1146:VAL:HA	1.65	0.79
2:C:206:PRO:HG3	2:C:216:THR:HG21	1.66	0.77
1:A:1115:VAL:HG22	1:A:1145:ILE:HB	1.67	0.76
1:B:92:PRO:O	1:B:93:ILE:HD12	1.89	0.73
3:A:1201:AGS:H8	3:A:1201:AGS:O5'	1.89	0.72
1:A:57:ARG:NH1	3:A:1201:AGS:O2A	2.21	0.72
1:A:1123:LEU:HA	1:B:33:ASN:HD21	1.53	0.72
1:A:8:VAL:O	1:A:17:ARG:HA	1.90	0.71
1:B:152:SER:O	1:B:157:ARG:NH2	2.26	0.68
1:A:1041:ARG:HA	1:A:1044:PHE:HD2	1.59	0.67
1:A:33:ASN:ND2	1:B:1092:GLY:HA3	2.10	0.66
1:A:1106:LEU:O	1:A:1110:PRO:HB3	1.96	0.65
1:A:1164:THR:HG21	2:C:224:MET:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:PRO:C	2:C:225:LYS:HZ1	2.04	0.64
1:A:41:THR:HG22	1:A:1115:VAL:HG11	1.80	0.64
1:A:1123:LEU:O	1:A:1150:ARG:NH1	2.30	0.64
1:A:5:ARG:HA	1:A:20:VAL:O	1.96	0.64
1:B:30:VAL:HG11	2:D:218:LEU:HD22	1.79	0.62
1:B:66:PHE:CZ	1:B:68:GLY:HA2	2.34	0.62
1:A:1096:LEU:HD23	1:A:1099:ILE:HD12	1.82	0.61
1:B:1116:LEU:HD22	1:B:1119:VAL:HG21	1.82	0.61
1:A:1138:TYR:HB2	1:A:1144:PHE:HE2	1.65	0.61
2:D:222:GLU:O	2:D:225:LYS:N	2.34	0.60
1:B:93:ILE:HG23	1:B:95:PHE:H	1.66	0.60
1:A:33:ASN:O	2:C:225:LYS:NZ	2.30	0.60
1:B:1090:SER:OG	1:B:1091:GLY:N	2.35	0.59
1:A:145:LYS:O	1:A:148:GLU:CB	2.50	0.59
1:B:112:PHE:HB3	1:B:124:ILE:HD11	1.84	0.59
1:B:112:PHE:HB2	1:B:119:CYS:HB2	1.84	0.58
1:B:12:LYS:HD2	1:B:39:ASN:ND2	2.15	0.58
1:A:33:ASN:HD21	1:B:1092:GLY:HA3	1.67	0.58
1:A:149:ILE:HG21	1:A:1101:LEU:HD21	1.84	0.58
1:B:1165:MET:HG2	1:B:1168:SER:O	2.03	0.57
1:A:1165:MET:HG3	1:A:1170:VAL:O	2.04	0.57
2:C:231:ILE:HG12	2:C:242:ILE:HA	1.86	0.57
1:A:1041:ARG:HA	1:A:1044:PHE:CD2	2.40	0.57
1:B:140:ILE:HG23	1:B:1115:VAL:HB	1.87	0.57
1:A:1049:ARG:HG2	1:A:1055:GLY:O	2.05	0.57
1:A:1089:LEU:HD22	1:A:1093:GLU:HB3	1.87	0.56
1:A:140:ILE:HG23	1:A:1115:VAL:HB	1.87	0.56
1:B:1036:THR:O	1:B:1040:ILE:HG13	2.06	0.56
1:A:86:ASN:HB3	1:A:95:PHE:O	2.05	0.56
1:B:30:VAL:HG13	1:B:1154:MET:HE1	1.88	0.56
1:B:1151:LYS:HA	1:B:1154:MET:HG3	1.88	0.56
1:B:1103:PHE:CZ	1:B:1134:TYR:HB3	2.42	0.55
1:A:149:ILE:HD12	1:A:1098:ALA:HB1	1.89	0.55
1:B:143:GLN:HB2	1:B:1117:ASP:HB3	1.88	0.55
1:A:1036:THR:O	1:A:1040:ILE:HG13	2.07	0.54
1:A:1146:VAL:HG12	1:A:1148:THR:HG23	1.90	0.54
1:A:1047:VAL:HG13	1:A:1134:TYR:CZ	2.42	0.54
1:A:58:GLY:HA2	1:A:63:ASP:HB2	1.89	0.54
1:B:86:ASN:HB3	1:B:95:PHE:O	2.06	0.54
1:A:1118:GLN:HA	1:A:1148:THR:HG22	1.89	0.54
1:A:1166:GLN:O	1:A:1167:GLU:C	2.51	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:CB	1:A:83:THR:O	2.55	0.54
1:A:20:VAL:HG13	1:A:1161:TYR:CE2	2.43	0.54
1:A:1123:LEU:HD13	1:A:1128:VAL:HG22	1.89	0.53
1:A:76:ASN:O	1:A:106:ARG:N	2.40	0.53
1:A:156:ASP:OD1	1:A:156:ASP:N	2.39	0.53
1:A:13:SER:OG	1:A:39:ASN:ND2	2.42	0.53
1:B:1059:LEU:HD11	1:B:1074:ILE:HG12	1.91	0.53
1:B:1120:GLU:OE2	1:B:1148:THR:HG23	2.08	0.53
1:A:35:SER:HB3	1:A:1163:VAL:HG12	1.90	0.53
1:A:1098:ALA:HA	1:A:1101:LEU:HD23	1.90	0.53
1:A:1081:LYS:NZ	3:B:1201:AGS:O3'	2.42	0.52
1:A:1165:MET:O	2:C:225:LYS:HA	2.09	0.52
1:B:1045:ASP:N	1:B:1045:ASP:OD1	2.41	0.52
1:B:1118:GLN:NE2	6:B:1301:HOH:O	2.11	0.52
1:A:141:ILE:O	1:A:1117:ASP:N	2.34	0.52
2:C:229:VAL:HA	2:C:244:GLY:HA2	1.91	0.51
1:A:57:ARG:NH2	3:A:1201:AGS:O1A	2.43	0.51
1:B:23:VAL:HG12	1:B:24:LYS:H	1.75	0.51
1:B:1059:LEU:HD21	1:B:1074:ILE:HG23	1.92	0.51
2:D:215:VAL:HA	2:D:218:LEU:HG	1.93	0.51
1:A:1078:PRO:HG2	1:A:1081:LYS:NZ	2.25	0.51
1:B:1012:THR:O	1:B:1015:LYS:N	2.42	0.51
1:A:1165:MET:H	2:C:225:LYS:HG2	1.76	0.50
1:B:1099:ILE:HD11	1:B:1119:VAL:HG12	1.94	0.50
1:A:2:PHE:HB3	1:A:85:ASP:HB2	1.93	0.50
1:B:11:PHE:CE2	1:B:43:ALA:HB2	2.47	0.50
1:B:1048:PHE:CE1	1:B:1052:PHE:HD2	2.29	0.50
2:C:192:LEU:HD21	2:C:198:ARG:HA	1.93	0.50
1:A:1164:THR:HG22	2:C:221:LEU:O	2.10	0.50
1:B:66:PHE:CE2	1:B:68:GLY:HA2	2.46	0.49
1:A:39:ASN:OD1	1:A:57:ARG:NH1	2.46	0.49
1:B:1000:ARG:O	1:B:1004:LEU:N	2.45	0.49
1:A:1165:MET:HG3	1:A:1170:VAL:C	2.38	0.49
1:B:1038:VAL:O	1:B:1041:ARG:HB2	2.11	0.49
1:A:23:VAL:HG12	1:A:24:LYS:H	1.78	0.49
1:B:1124:ASP:N	1:B:1124:ASP:OD1	2.46	0.48
1:B:153:LYS:HE2	1:B:155:GLU:HB2	1.95	0.48
1:A:25:GLY:HA2	1:A:1139:SER:HB2	1.95	0.48
1:A:1081:LYS:NZ	3:B:1201:AGS:O2'	2.29	0.48
1:B:1165:MET:HG3	1:B:1170:VAL:O	2.13	0.48
1:B:1103:PHE:CE1	1:B:1134:TYR:HB3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1048:PHE:HE2	1:B:1097:THR:HG22	1.79	0.48
1:A:37:LYS:HG3	3:A:1201:AGS:O3G	2.14	0.47
1:A:1090:SER:N	1:A:1093:GLU:HB2	2.28	0.47
1:A:1059:LEU:HD22	1:A:1060:ARG:N	2.30	0.47
1:A:1123:LEU:CD1	1:A:1128:VAL:HG22	2.45	0.47
1:A:1165:MET:HG2	1:A:1168:SER:O	2.14	0.47
1:B:1113:PHE:HA	1:B:1143:GLN:O	2.15	0.47
1:A:35:SER:OG	2:C:225:LYS:NZ	2.43	0.47
1:A:6:LEU:O	1:A:19:SER:HA	2.15	0.47
1:A:40:ILE:O	1:A:44:ILE:HG13	2.15	0.47
1:A:1059:LEU:C	1:A:1059:LEU:HD13	2.40	0.47
1:A:1162:GLY:HA3	2:C:221:LEU:HD13	1.97	0.47
1:A:1124:ASP:O	1:A:1128:VAL:HG23	2.15	0.46
1:B:1055:GLY:HA2	1:B:1079:PRO:HD3	1.97	0.46
1:B:1048:PHE:CZ	1:B:1052:PHE:CD2	3.03	0.46
2:D:233:GLN:HG3	2:D:240:ILE:HA	1.98	0.46
1:A:33:ASN:OD1	1:B:1090:SER:OG	2.33	0.46
1:A:1039:GLN:O	1:A:1043:HIS:ND1	2.49	0.46
1:B:1048:PHE:HE2	1:B:1097:THR:CG2	2.29	0.46
2:C:244:GLY:O	2:C:245:SER:HB2	2.14	0.46
1:A:129:MET:HG2	1:A:169:LYS:HG2	1.98	0.46
1:A:1120:GLU:H	1:A:1120:GLU:HG3	1.62	0.46
1:A:78:ALA:O	1:A:103:ARG:HA	2.17	0.45
1:B:1047:VAL:HG13	1:B:1134:TYR:HE2	1.81	0.45
1:A:1047:VAL:HA	1:A:1134:TYR:OH	2.16	0.45
1:A:1116:LEU:HB2	1:A:1146:VAL:HG13	1.98	0.44
1:B:1117:ASP:OD1	1:B:1147:ILE:HD12	2.16	0.44
1:B:1154:MET:H	1:B:1154:MET:HG2	1.55	0.44
1:B:1128:VAL:HG21	1:B:1150:ARG:HH11	1.83	0.44
1:B:142:SER:C	1:B:1117:ASP:HB2	2.42	0.44
1:A:32:PRO:HG2	2:C:222:GLU:HA	1.99	0.43
1:B:8:VAL:HG13	1:B:80:VAL:HG13	2.01	0.43
1:A:158:ARG:NH1	1:A:1070:SER:H	2.17	0.43
1:B:151:SER:HB3	1:B:1094:ARG:NH1	2.33	0.43
1:B:1148:THR:HG22	1:B:1150:ARG:H	1.83	0.43
1:A:58:GLY:CA	1:A:63:ASP:HB2	2.49	0.42
1:A:1093:GLU:CD	1:B:34:GLY:HA2	2.44	0.42
1:B:1111:VAL:O	1:B:1142:THR:HB	2.19	0.42
1:A:93:ILE:HG22	1:A:94:ASP:H	1.83	0.42
1:A:1102:LEU:HA	1:A:1102:LEU:HD23	1.68	0.42
1:B:83:THR:HA	1:B:98:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:VAL:HG12	1:A:80:VAL:HG22	2.00	0.42
1:B:1059:LEU:HA	1:B:1059:LEU:HD13	1.83	0.42
1:A:1047:VAL:HG13	1:A:1134:TYR:CE1	2.55	0.42
1:A:1069:HIS:ND1	1:A:1069:HIS:N	2.68	0.42
1:B:5:ARG:O	1:B:6:LEU:HD23	2.19	0.42
1:A:81:THR:HB	1:A:101:THR:HG22	2.02	0.42
1:A:32:PRO:HD2	2:C:225:LYS:HE3	2.00	0.41
1:B:41:THR:HB	1:B:1115:VAL:HG11	2.01	0.41
1:B:11:PHE:O	1:B:14:PHE:N	2.48	0.41
1:A:33:ASN:ND2	1:B:1124:ASP:OD1	2.46	0.41
1:B:1005:SER:O	1:B:1009:GLU:N	2.51	0.41
1:B:1048:PHE:CZ	1:B:1052:PHE:HD2	2.39	0.41
1:B:1129:PHE:O	1:B:1133:GLN:HG2	2.20	0.41
1:B:1048:PHE:CD1	1:B:1055:GLY:HA3	2.56	0.41
1:A:1115:VAL:HA	1:A:1145:ILE:O	2.20	0.41
1:A:38:SER:HB3	1:A:57:ARG:HH22	1.85	0.41
1:B:154:ALA:HA	1:B:157:ARG:HG2	2.03	0.41
1:B:157:ARG:O	1:B:160:ILE:HG22	2.21	0.41
1:B:1164:THR:HG22	2:D:221:LEU:HA	2.02	0.41
1:B:140:ILE:HG21	1:B:140:ILE:HD13	1.71	0.40
1:B:1116:LEU:N	1:B:1145:ILE:O	2.55	0.40
1:B:1118:GLN:OE1	1:B:1148:THR:HA	2.21	0.40
1:A:1135:LEU:HD23	1:A:1135:LEU:HA	1.93	0.40
1:A:57:ARG:CZ	3:A:1201:AGS:O1A	2.69	0.40
2:C:231:ILE:HG23	2:C:241:TYR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	349/435 (80%)	326 (93%)	23 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	358/435 (82%)	322 (90%)	30 (8%)	6 (2%)	7	35
2	C	64/89 (72%)	59 (92%)	5 (8%)	0	100	100
2	D	45/89 (51%)	41 (91%)	4 (9%)	0	100	100
All	All	816/1048 (78%)	748 (92%)	62 (8%)	6 (1%)	18	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1063	ASP
1	B	1064	PRO
1	B	1082	LYS
1	B	117	GLN
1	B	1044	PHE
1	B	30	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	182/381 (48%)	166 (91%)	16 (9%)	9	32
1	B	192/381 (50%)	173 (90%)	19 (10%)	7	29
2	C	38/83 (46%)	37 (97%)	1 (3%)	40	62
2	D	19/83 (23%)	18 (95%)	1 (5%)	20	47
All	All	431/928 (46%)	394 (91%)	37 (9%)	10	33

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	37	LYS
1	A	81	THR
1	A	170	TYR
1	A	1063	ASP

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Mol	Chain	Res	Type
1	A	1087	ASN
1	A	1088	LEU
1	A	1097	THR
1	A	1101	LEU
1	A	1102	LEU
1	A	1120	GLU
1	A	1123	LEU
1	A	1138	TYR
1	A	1143	GLN
1	A	1149	HIS
1	A	1176	VAL
1	B	8	VAL
1	B	23	VAL
1	B	29	VAL
1	B	30	VAL
1	B	46	TRP
1	B	48	LEU
1	B	77	LEU
1	B	93	ILE
1	B	142	SER
1	B	1018	LEU
1	B	1026	ASP
1	B	1036	THR
1	B	1090	SER
1	B	1096	LEU
1	B	1097	THR
1	B	1120	GLU
1	B	1124	ASP
1	B	1142	THR
1	B	1154	MET
2	C	237	PHE
2	D	233	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1077	GLN
1	B	33	ASN
1	B	39	ASN
1	B	1016	ASN
1	B	1034	ASN
1	B	1084	GLN

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Mol	Chain	Res	Type
2	D	186	ASN
2	D	200	ASN
2	D	233	GLN

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](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGS	A	1201	4	32,33,33	0.99	2 (6%)	45,52,52	0.98	3 (6%)
3	AGS	B	1201	4	32,33,33	0.92	1 (3%)	45,52,52	1.27	6 (13%)

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
3	AGS	A	1201	4	-	2/21/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AGS	B	1201	4	-	2/21/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	AGS	PA-O3A	3.05	1.62	1.59
3	B	1201	AGS	PB-O3B	-2.89	1.56	1.59
3	A	1201	AGS	PB-O3A	2.05	1.61	1.59

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1201	AGS	O5'-PA-O1A	3.53	122.92	108.94
3	B	1201	AGS	O2A-PA-O3A	3.06	115.53	107.27
3	A	1201	AGS	O2G-PG-O3B	2.96	114.53	104.64
3	B	1201	AGS	O2G-PG-O3B	2.88	114.25	104.64
3	A	1201	AGS	PB-O3B-PG	-2.82	122.87	133.17
3	B	1201	AGS	PB-O3B-PG	-2.81	122.90	133.17
3	A	1201	AGS	O3B-PB-O1B	2.48	118.17	110.70
3	B	1201	AGS	O3A-PA-O1A	-2.38	103.55	110.70
3	B	1201	AGS	O3B-PB-O1B	2.14	117.15	110.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	AGS	O4'-C4'-C5'-O5'
3	A	1201	AGS	C3'-C4'-C5'-O5'
3	B	1201	AGS	O4'-C4'-C5'-O5'
3	B	1201	AGS	C3'-C4'-C5'-O5'

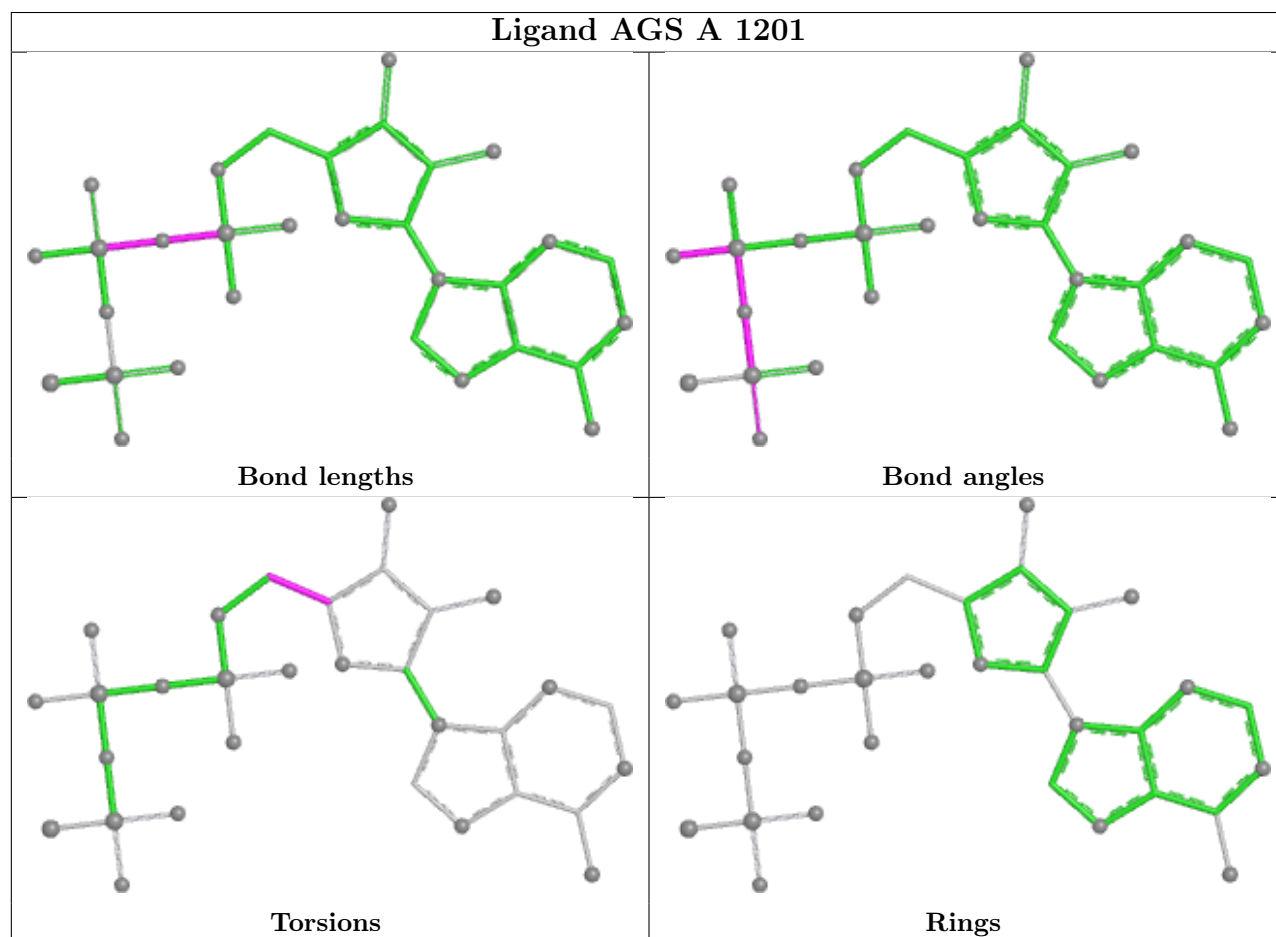
There are no ring outliers.

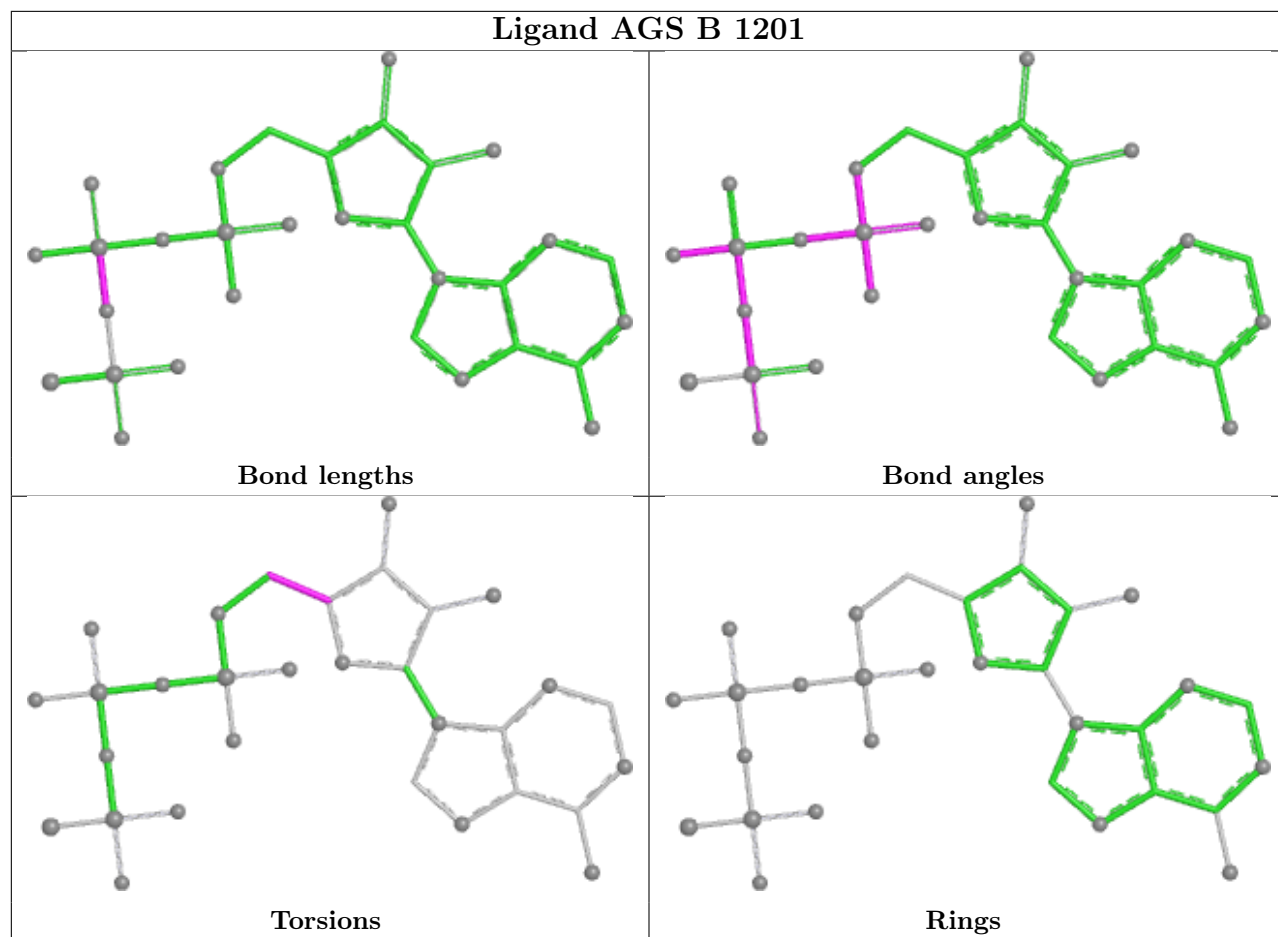
2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1201	AGS	5	0
3	B	1201	AGS	3	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.





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	371/435 (85%)	0.06	10 (2%) 56 33	16, 49, 91, 115	0
1	B	374/435 (85%)	0.01	6 (1%) 70 45	17, 49, 84, 107	0
2	C	68/89 (76%)	0.47	1 (1%) 72 47	52, 89, 130, 137	0
2	D	53/89 (59%)	0.63	4 (7%) 20 13	28, 78, 114, 118	0
All	All	866/1048 (82%)	0.10	21 (2%) 59 35	16, 51, 100, 137	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.4
2	D	179	ILE	4.1
2	D	178	ASP	3.7
1	A	135	LYS	3.7
1	A	134	GLY	3.2
1	A	201	GLN	2.9
1	B	1141	ASP	2.9
2	D	211	GLU	2.8
1	A	1065	ASN	2.7
1	A	85	ASP	2.5
2	C	211	GLU	2.5
1	A	61	MET	2.5
1	A	138	PHE	2.4
1	B	7	ASP	2.4
1	A	62	GLU	2.3
2	D	187	GLU	2.3
1	A	1119	VAL	2.1
1	B	68	GLY	2.1
1	B	19	SER	2.1
1	B	1147	ILE	2.1
1	B	1	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

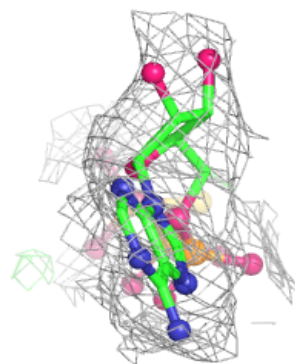
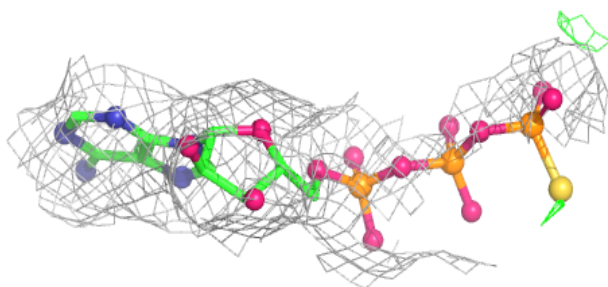
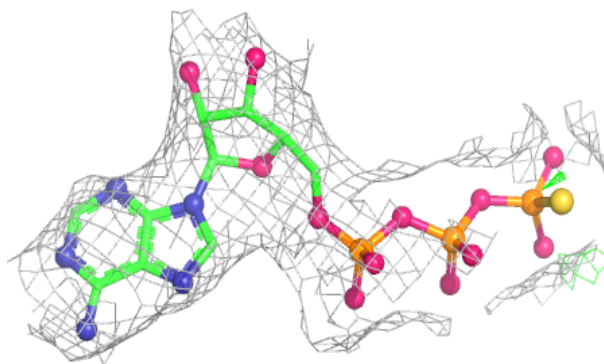
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	B	1202	1/1	0.93	0.19	37,37,37,37	0
3	AGS	B	1201	31/31	0.96	0.10	23,44,67,80	0
3	AGS	A	1201	31/31	0.97	0.10	19,37,65,77	0
5	CO	A	1203	1/1	0.97	0.05	59,59,59,59	0
4	MG	A	1202	1/1	0.98	0.11	17,17,17,17	0

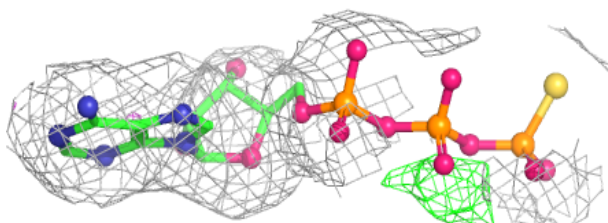
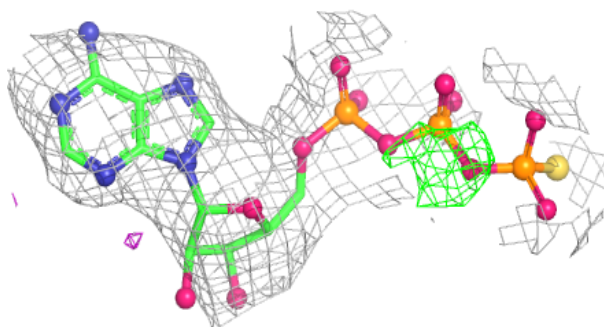
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS B 1201:

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

**Electron density around AGS A 1201:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.