



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:14 PM UTC

PDB ID : 6CVL / pdb_00006cvl
Title : Crystal structure of the Escherichia coli ATPgS-bound MetNI methionine ABC transporter in complex with its MetQ binding protein
Authors : Nguyen, P.T.; Kaiser, J.T.; Rees, D.C.
Deposited on : 2018-03-28
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

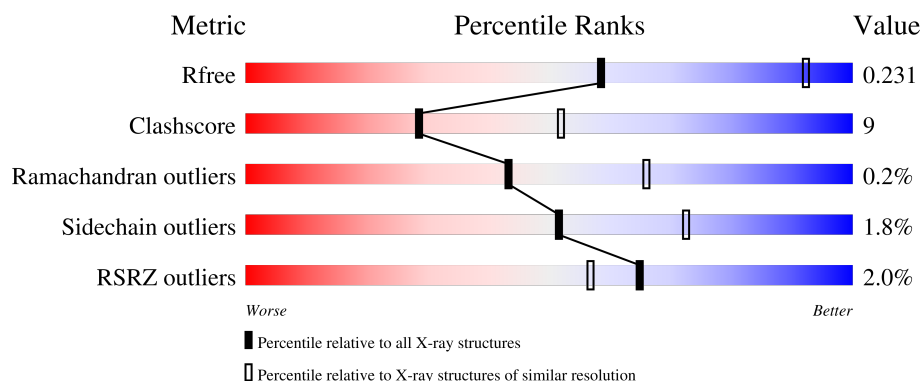
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	C	344	
1	D	344	
2	A	215	
2	B	215	
3	E	226	

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
6	IOD	D	403	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21046 atoms, of which 10688 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 MetN nucleotide-binding subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	344	Total	C	H	N	O	S	0	0	0
			5367	1668	2709	470	508	12			
1	D	344	Total	C	H	N	O	S	0	0	0
			5367	1668	2709	470	508	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP P30750
C	166	GLN	GLU	engineered mutation	UNP P30750
C	295	ALA	ASN	engineered mutation	UNP P30750
D	0	HIS	-	expression tag	UNP P30750
D	166	GLN	GLU	engineered mutation	UNP P30750
D	295	ALA	ASN	engineered mutation	UNP P30750

- Molecule 2 is a protein called MetI transmembrane subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	215	Total	C	H	N	O	S	0	0	0
			3349	1073	1733	262	271	10			
2	B	215	Total	C	H	N	O	S	0	0	0
			3349	1073	1733	262	271	10			

- Molecule 3 is a protein called MetQ periplasmic binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	226	Total	C	H	N	O	0	0	0
			3522	1113	1779	286	344			

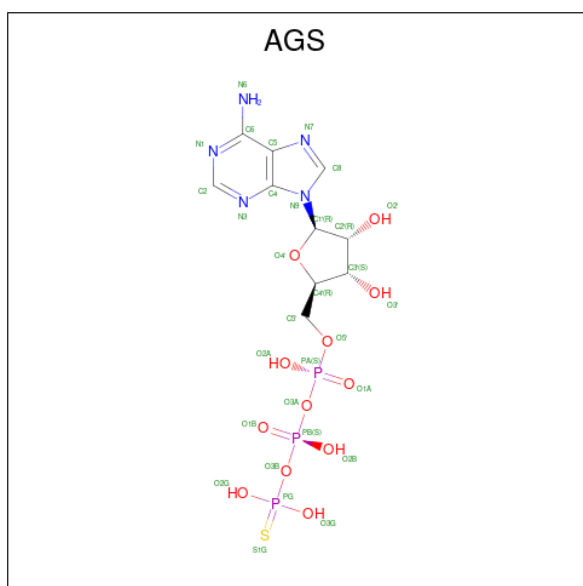
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	229	ALA	ASN	engineered mutation	UNP P28635

- Molecule 4 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	2	Total Hg 2 2	0	0
4	D	1	Total Hg 1 1	0	0

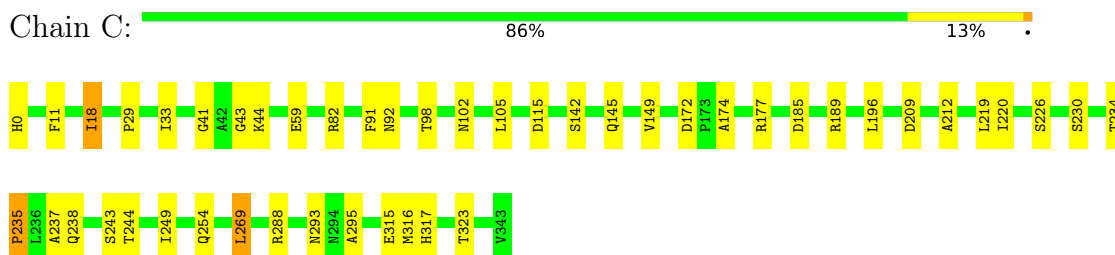
- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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.

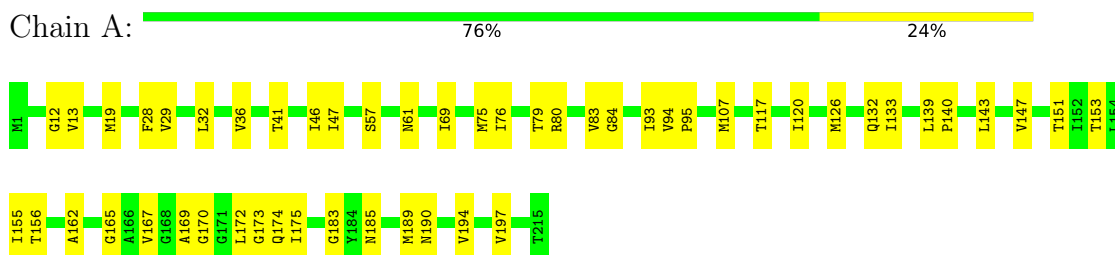
- Molecule 1: MetN nucleotide-binding subunit



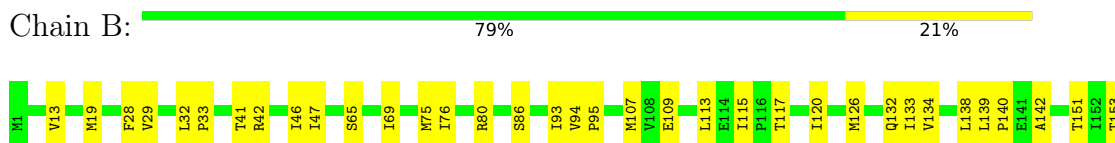
- Molecule 1: MetN nucleotide-binding subunit



- Molecule 2: MetI transmembrane subunit

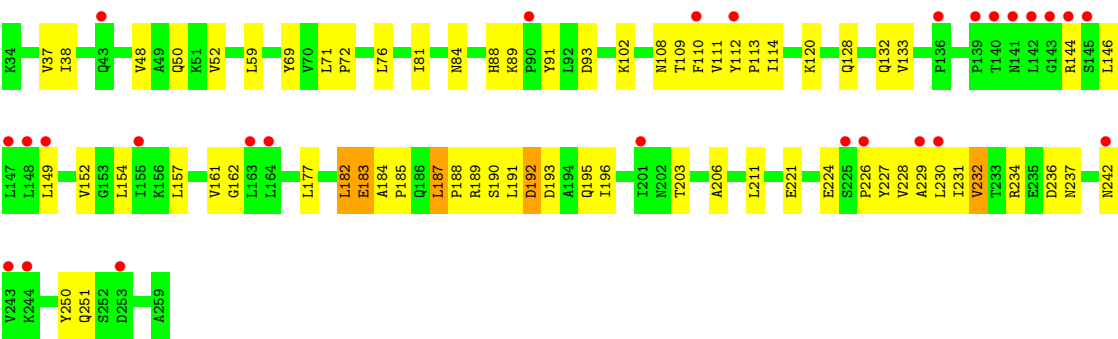


- Molecule 2: MetI transmembrane subunit





● Molecule 3: MetQ periplasmic binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.96Å 107.96Å 354.52Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.85 – 2.95 39.85 – 2.95	Depositor EDS
% Data completeness (in resolution range)	83.5 (39.85-2.95) 83.6 (39.85-2.95)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.208 , 0.226 0.205 , 0.231	Depositor DCC
R_{free} test set	2174 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	92.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.276 for -h,-k,l	Xtriage
Reported twinning fraction	0.330 for -h,-k,l	Depositor
Outliers	0 of 42969 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21046	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, AGS, HG

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	C	0.18	0/2696	0.37	0/3651
1	D	0.18	0/2698	0.39	0/3656
2	A	0.20	0/1649	0.36	0/2253
2	B	0.20	0/1649	0.35	0/2253
3	E	0.15	0/1769	0.41	0/2403
All	All	0.18	0/10461	0.38	0/14216

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	C	2658	2709	2708	40	0
1	D	2658	2709	2709	54	0
2	A	1616	1733	1733	32	0
2	B	1616	1733	1733	31	0
3	E	1743	1779	1779	48	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	C	31	13	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	31	12	12	5	0
6	D	2	0	0	5	0
All	All	10358	10688	10686	185	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 9.

All (185) 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:E:185:PRO:O	3:E:189:ARG:NH2	2.03	0.92
1:C:288:ARG:NH2	1:D:293:ASN:OD1	2.14	0.80
1:C:220:ILE:HG23	1:C:234:THR:HG21	1.66	0.78
1:D:44:LYS:N	5:D:404:AGS:O2B	2.20	0.74
3:E:69:TYR:O	3:E:91:TYR:OH	2.06	0.73
2:A:107:MET:HE1	2:B:107:MET:HE1	1.71	0.72
1:C:43:GLY:N	5:C:403:AGS:O1B	2.22	0.72
1:D:183:LEU:HD11	6:D:403:IOD:I	2.60	0.72
1:C:177:ARG:NH2	1:D:243:SER:O	2.27	0.67
3:E:120:LYS:NZ	3:E:193:ASP:O	2.28	0.67
1:C:44:LYS:N	5:C:403:AGS:O1B	2.28	0.67
3:E:111:VAL:HG23	3:E:113:PRO:HD3	1.77	0.67
1:C:244:THR:HG22	1:D:173:PRO:HG2	1.80	0.64
2:B:69:ILE:H	2:B:69:ILE:HD12	1.63	0.64
3:E:133:VAL:HG21	3:E:177:LEU:HD13	1.79	0.64
1:C:185:ASP:OD1	1:C:189:ARG:NH2	2.30	0.63
5:C:403:AGS:O2'	1:D:140:ASN:O	2.10	0.63
3:E:81:ILE:O	3:E:234:ARG:NH1	2.31	0.63
2:A:41:THR:HA	2:A:47:ILE:O	1.99	0.63
3:E:183:GLU:N	3:E:183:GLU:OE1	2.32	0.63
2:A:69:ILE:HD12	2:A:69:ILE:H	1.64	0.62
2:B:167:VAL:HG23	2:B:167:VAL:O	1.99	0.62
1:C:105:LEU:HD21	2:A:126:MET:HE1	1.82	0.62
2:A:167:VAL:O	2:A:167:VAL:HG23	2.00	0.61
1:C:105:LEU:CD2	2:A:126:MET:HE1	2.31	0.61
1:D:234:THR:O	1:D:237:ALA:N	2.33	0.61
3:E:144:ARG:NH2	3:E:221:GLU:OE1	2.34	0.61
1:D:220:ILE:HG23	1:D:234:THR:HG21	1.83	0.61
1:C:316:MET:HG3	1:C:323:THR:HG22	1.82	0.60
2:A:80:ARG:NH1	3:E:193:ASP:OD1	2.35	0.60
3:E:187:LEU:O	3:E:190:SER:N	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:GLN:OE1	1:D:82:ARG:NH2	2.35	0.59
1:D:41:GLY:N	5:D:404:AGS:O3G	2.34	0.59
2:A:13:VAL:HG22	2:A:172:LEU:HD11	1.85	0.59
2:A:162:ALA:HB1	2:A:173:GLY:HA3	1.85	0.58
3:E:187:LEU:O	3:E:190:SER:OG	2.18	0.58
2:B:41:THR:HA	2:B:47:ILE:O	2.03	0.58
5:C:403:AGS:O2G	1:D:142:SER:OG	2.18	0.57
1:C:234:THR:O	1:C:237:ALA:N	2.37	0.57
1:C:142:SER:OG	5:D:404:AGS:O3G	2.23	0.56
1:D:110:ASP:HB2	1:D:112:THR:HG23	1.88	0.56
1:D:185:ASP:OD1	1:D:189:ARG:NH2	2.39	0.55
1:D:164:CYS:SG	6:D:403:IOD:I	3.28	0.55
1:D:220:ILE:HG21	1:D:237:ALA:HB2	1.88	0.55
3:E:192:ASP:N	3:E:192:ASP:OD1	2.41	0.54
1:C:249:ILE:O	1:C:254:GLN:NE2	2.40	0.54
3:E:108:ASN:N	3:E:251:GLN:OE1	2.35	0.54
3:E:187:LEU:HD22	3:E:188:PRO:HD3	1.89	0.53
1:C:315:GLU:OE1	1:C:317:HIS:NE2	2.38	0.53
2:A:19:MET:HA	2:A:93:ILE:HG12	1.91	0.52
2:B:46:ILE:HD11	2:B:133:ILE:HG21	1.90	0.52
2:B:115:ILE:HD11	2:B:142:ALA:HB2	1.90	0.52
1:C:98:THR:O	1:C:102:ASN:ND2	2.39	0.52
1:D:212:ALA:HB1	1:D:219:LEU:HD11	1.92	0.52
1:C:220:ILE:HG21	1:C:237:ALA:HB2	1.92	0.52
2:B:13:VAL:HG23	2:B:172:LEU:HD21	1.90	0.52
1:D:220:ILE:CG2	1:D:237:ALA:HB2	2.39	0.52
1:C:0:HIS:HA	1:C:29:PRO:HA	1.91	0.51
1:C:243:SER:O	1:D:177:ARG:NH2	2.44	0.51
1:D:293:ASN:HB2	1:D:317:HIS:HB2	1.93	0.51
2:A:189:MET:HE3	2:A:189:MET:HA	1.92	0.51
3:E:230:LEU:O	3:E:232:VAL:HG22	2.11	0.51
1:D:167:ALA:HB3	6:D:403:IOD:I	2.82	0.50
1:D:226:SER:O	1:D:230:SER:N	2.44	0.50
2:A:183:GLY:O	2:A:185:ASN:N	2.45	0.50
2:A:94:VAL:HB	2:A:95:PRO:HD3	1.93	0.49
3:E:193:ASP:OD2	3:E:195:GLN:HG2	2.12	0.49
1:D:183:LEU:CD1	6:D:403:IOD:I	3.30	0.49
3:E:182:LEU:HD12	3:E:182:LEU:N	2.27	0.49
2:B:165:GLY:CA	2:B:169:ALA:O	2.61	0.49
1:D:316:MET:HG3	1:D:323:THR:HG22	1.93	0.49
2:A:165:GLY:O	2:A:169:ALA:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:VAL:HG22	2:B:172:LEU:HD11	1.96	0.48
3:E:161:VAL:HG23	3:E:162:GLY:N	2.29	0.48
1:C:235:PRO:HA	1:C:238:GLN:HG3	1.95	0.48
1:C:243:SER:HB2	1:D:174:ALA:HB2	1.94	0.48
2:B:126:MET:HE1	1:D:105:LEU:HD21	1.95	0.48
2:B:134:VAL:HG22	2:B:138:LEU:HD12	1.95	0.48
1:C:293:ASN:OD1	1:D:288:ARG:NH2	2.45	0.48
1:D:235:PRO:HA	1:D:238:GLN:HG3	1.94	0.48
2:A:153:THR:O	2:A:156:THR:OG1	2.30	0.48
1:D:11:PHE:HB2	1:D:18:ILE:HG23	1.96	0.48
3:E:224:GLU:O	3:E:227:TYR:CD2	2.67	0.48
3:E:234:ARG:N	3:E:237:ASN:OD1	2.47	0.48
2:B:165:GLY:HA3	2:B:169:ALA:O	2.15	0.47
3:E:161:VAL:HG23	3:E:162:GLY:H	1.79	0.47
1:C:174:ALA:HB2	1:D:243:SER:HB2	1.97	0.47
2:A:151:THR:O	2:A:155:ILE:HG12	2.14	0.47
2:B:94:VAL:HB	2:B:95:PRO:HD3	1.97	0.47
3:E:184:ALA:HA	3:E:187:LEU:HD11	1.96	0.47
1:C:234:THR:O	1:C:235:PRO:C	2.58	0.47
2:A:13:VAL:HG23	2:A:172:LEU:HD21	1.95	0.47
2:A:32:LEU:O	2:A:36:VAL:HG23	2.14	0.47
2:B:189:MET:HE3	2:B:189:MET:HA	1.97	0.47
1:D:91:PHE:O	1:D:92:ASN:C	2.58	0.47
1:D:145:GLN:O	1:D:149:VAL:HG23	2.15	0.47
3:E:236:ASP:OD1	3:E:237:ASN:N	2.48	0.47
1:C:212:ALA:HB1	1:C:219:LEU:HD11	1.97	0.47
2:B:151:THR:O	2:B:155:ILE:HG12	2.15	0.47
1:C:91:PHE:O	1:C:92:ASN:C	2.58	0.47
2:A:139:LEU:HB2	2:A:140:PRO:HD3	1.97	0.46
1:D:42:ALA:N	5:D:404:AGS:O1B	2.48	0.46
3:E:112:TYR:CE2	3:E:229:ALA:HB2	2.51	0.46
2:B:170:GLY:HA3	2:B:174:GLN:CB	2.46	0.46
3:E:149:LEU:HA	3:E:152:VAL:HG22	1.97	0.46
1:C:82:ARG:NH2	2:A:132:GLN:OE1	2.49	0.46
3:E:190:SER:O	3:E:193:ASP:HB3	2.16	0.46
1:D:234:THR:O	1:D:235:PRO:C	2.58	0.45
2:B:126:MET:HE1	1:D:105:LEU:CD2	2.46	0.45
2:B:162:ALA:HB1	2:B:173:GLY:HA3	1.98	0.45
3:E:113:PRO:HG2	3:E:203:THR:OG1	2.17	0.45
2:A:75:MET:O	2:A:76:ILE:C	2.60	0.45
3:E:89:LYS:NZ	3:E:93:ASP:OD2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:109:THR:HG21	3:E:228:VAL:HB	1.97	0.45
1:D:226:SER:HB3	1:D:304:ALA:HB3	1.99	0.45
1:C:33:ILE:O	1:C:209:ASP:N	2.49	0.45
1:C:293:ASN:HB2	1:C:317:HIS:HB2	1.99	0.45
1:D:45:SER:O	1:D:48:ILE:HG22	2.17	0.44
1:D:199:HIS:NE2	5:D:404:AGS:S1G	2.90	0.44
1:D:249:ILE:O	1:D:254:GLN:NE2	2.50	0.44
2:A:197:VAL:HG22	2:B:65:SER:OG	2.18	0.44
3:E:76:LEU:O	3:E:234:ARG:HD3	2.17	0.44
1:C:226:SER:O	1:C:230:SER:N	2.50	0.44
3:E:109:THR:HG21	3:E:229:ALA:N	2.33	0.44
3:E:132:GLN:HB2	3:E:196:ILE:HD13	1.98	0.44
2:B:153:THR:O	2:B:156:THR:OG1	2.30	0.44
2:A:170:GLY:HA3	2:A:174:GLN:HB2	1.98	0.43
2:B:28:PHE:O	2:B:29:VAL:C	2.61	0.43
2:B:75:MET:O	2:B:76:ILE:C	2.60	0.43
3:E:146:LEU:HB3	3:E:157:LEU:HD11	2.00	0.43
3:E:187:LEU:N	3:E:188:PRO:CD	2.81	0.43
1:D:247:LEU:O	1:D:247:LEU:HG	2.19	0.43
2:B:139:LEU:HB2	2:B:140:PRO:HD3	1.99	0.43
1:D:269:LEU:N	1:D:269:LEU:HD23	2.34	0.43
3:E:71:LEU:N	3:E:72:PRO:CD	2.82	0.43
3:E:187:LEU:N	3:E:188:PRO:HD2	2.34	0.43
2:A:28:PHE:O	2:A:29:VAL:C	2.62	0.43
2:A:190:ASN:O	2:A:194:VAL:HG23	2.19	0.43
1:D:261:PRO:HB3	1:D:342:TYR:CZ	2.54	0.43
2:B:42:ARG:NH1	2:B:109:GLU:OE2	2.52	0.43
1:D:329:TRP:O	1:D:332:GLU:HB2	2.19	0.43
3:E:206:ALA:HB1	3:E:211:LEU:O	2.19	0.42
3:E:120:LYS:NZ	3:E:191:LEU:O	2.49	0.42
1:C:172:ASP:OD2	1:D:40:SER:N	2.47	0.42
2:A:143:LEU:O	2:A:147:VAL:HG23	2.19	0.42
1:D:234:THR:O	1:D:236:LEU:N	2.53	0.42
3:E:37:VAL:HG12	3:E:38:ILE:N	2.34	0.42
1:C:196:LEU:HD12	1:C:196:LEU:C	2.44	0.42
2:A:107:MET:CE	2:B:107:MET:HE1	2.46	0.42
1:C:243:SER:CB	1:D:174:ALA:HB2	2.50	0.42
3:E:152:VAL:HG23	3:E:154:LEU:HG	2.02	0.42
2:B:109:GLU:O	2:B:113:LEU:HG	2.20	0.42
1:D:201:MET:O	1:D:205:LYS:HG2	2.20	0.42
1:C:11:PHE:HB2	1:C:18:ILE:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:88:HIS:HA	3:E:228:VAL:O	2.19	0.42
1:D:278:VAL:HG13	1:D:279:ASP:N	2.35	0.41
3:E:110:PHE:CG	3:E:111:VAL:N	2.88	0.41
5:C:403:AGS:S1G	5:C:403:AGS:O2B	2.78	0.41
2:B:80:ARG:NH2	2:B:86:SER:OG	2.53	0.41
1:C:220:ILE:CG2	1:C:237:ALA:HB2	2.50	0.41
1:D:265:CYS:SG	1:D:320:GLN:OE1	2.78	0.41
1:C:172:ASP:HA	1:D:199:HIS:ND1	2.36	0.41
1:C:269:LEU:HD23	1:C:269:LEU:N	2.35	0.41
2:A:79:THR:O	2:A:83:VAL:HG22	2.21	0.41
2:B:32:LEU:HB3	2:B:33:PRO:HD3	2.02	0.41
3:E:59:LEU:HD21	3:E:242:ASN:HB3	2.02	0.41
3:E:88:HIS:HB2	3:E:226:PRO:O	2.21	0.41
2:A:12:GLY:HA3	2:A:175:ILE:HD12	2.02	0.41
3:E:84:ASN:OD1	3:E:232:VAL:HB	2.21	0.41
1:C:41:GLY:H	5:C:403:AGS:PG	2.44	0.41
2:A:57:SER:O	2:A:61:ASN:ND2	2.54	0.41
3:E:231:ILE:HD11	3:E:250:TYR:CD1	2.55	0.41
1:D:166:GLN:HA	6:D:402:IOD:I	2.91	0.41
3:E:48:VAL:O	3:E:52:VAL:HG23	2.21	0.41
1:D:115:ASP:OD1	1:D:115:ASP:N	2.54	0.41
1:D:10:VAL:HA	1:D:18:ILE:O	2.20	0.40
1:D:117:VAL:O	1:D:121:VAL:HG23	2.21	0.40
1:C:145:GLN:O	1:C:149:VAL:HG23	2.22	0.40
1:C:142:SER:N	1:C:145:GLN:OE1	2.45	0.40
1:C:295:ALA:HB1	1:D:278:VAL:O	2.22	0.40
2:A:46:ILE:HD11	2:A:133:ILE:HG21	2.03	0.40
2:B:19:MET:HA	2:B:93:ILE:HG12	2.03	0.40
3:E:114:ILE:HG22	3:E:144:ARG:CZ	2.51	0.40
2:A:80:ARG:O	2:A:84:GLY:N	2.42	0.40
2:B:69:ILE:HD12	2:B:69:ILE:N	2.34	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	C	341/344 (99%)	322 (94%)	18 (5%)	1 (0%)	36	59
1	D	342/344 (99%)	320 (94%)	21 (6%)	1 (0%)	36	59
2	A	213/215 (99%)	198 (93%)	15 (7%)	0	100	100
2	B	213/215 (99%)	198 (93%)	15 (7%)	0	100	100
3	E	224/226 (99%)	211 (94%)	13 (6%)	0	100	100
All	All	1333/1344 (99%)	1249 (94%)	82 (6%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	235	PRO
1	D	235	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	297/298 (100%)	293 (99%)	4 (1%)	61	78
1	D	298/298 (100%)	294 (99%)	4 (1%)	61	78
2	A	170/170 (100%)	168 (99%)	2 (1%)	63	79
2	B	170/170 (100%)	168 (99%)	2 (1%)	63	79
3	E	191/191 (100%)	183 (96%)	8 (4%)	26	53
All	All	1126/1127 (100%)	1106 (98%)	20 (2%)	51	72

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	18	ILE
1	C	59	GLU
1	C	115	ASP

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Mol	Chain	Res	Type
1	C	269	LEU
2	A	117	THR
2	A	120	ILE
2	B	117	THR
2	B	120	ILE
1	D	18	ILE
1	D	91	PHE
1	D	115	ASP
1	D	269	LEU
3	E	50	GLN
3	E	102	LYS
3	E	128	GLN
3	E	182	LEU
3	E	183	GLU
3	E	187	LEU
3	E	192	ASP
3	E	232	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	27	HIS
3	E	73	ASN
3	E	202	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 5 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
5	AGS	D	404	-	32,33,33	1.83	5 (15%)	45,52,52	1.92	11 (24%)
5	AGS	C	403	-	32,33,33	1.98	5 (15%)	45,52,52	1.88	11 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AGS	D	404	-	-	2/21/38/38	0/3/3/3
5	AGS	C	403	-	-	2/21/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	403	AGS	PG-S1G	7.86	2.07	1.90
5	D	404	AGS	PG-S1G	6.89	2.05	1.90
5	D	404	AGS	C5-C4	4.59	1.47	1.39
5	C	403	AGS	C5-C4	4.41	1.47	1.39
5	D	404	AGS	C5-C6	2.86	1.49	1.41
5	C	403	AGS	C5-C6	2.63	1.48	1.41
5	C	403	AGS	C8-N7	2.37	1.36	1.31
5	D	404	AGS	C8-N7	2.34	1.36	1.31
5	C	403	AGS	C5-N7	-2.28	1.34	1.39
5	D	404	AGS	C5-N7	-2.10	1.35	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	404	AGS	C5-C4-N3	-6.02	118.43	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	403	AGS	C5-C4-N3	-5.75	118.81	126.72
5	D	404	AGS	N3-C4-N9	4.85	135.41	127.17
5	C	403	AGS	N3-C4-N9	4.68	135.12	127.17
5	C	403	AGS	C2-N3-C4	3.88	121.30	111.83
5	D	404	AGS	C2-N3-C4	3.84	121.21	111.83
5	D	404	AGS	C4-C5-N7	-3.81	106.23	110.58
5	C	403	AGS	N3-C2-N1	-3.77	122.87	128.58
5	C	403	AGS	C4-C5-N7	-3.48	106.60	110.58
5	D	404	AGS	N3-C2-N1	-3.47	123.33	128.58
5	C	403	AGS	PB-O3B-PG	-3.31	121.06	133.17
5	D	404	AGS	C4-N9-C8	3.30	109.20	105.74
5	C	403	AGS	C4-N9-C8	3.24	109.14	105.74
5	D	404	AGS	PB-O3B-PG	-3.11	121.80	133.17
5	D	404	AGS	C5-N7-C8	2.96	108.10	103.45
5	C	403	AGS	C5-N7-C8	2.77	107.81	103.45
5	D	404	AGS	N9-C8-N7	-2.55	110.32	113.94
5	C	403	AGS	N9-C8-N7	-2.51	110.38	113.94
5	D	404	AGS	O3G-PG-O3B	2.31	112.35	104.64
5	D	404	AGS	C6-C5-N7	2.23	136.39	132.09
5	C	403	AGS	C6-C5-N7	2.20	136.34	132.09
5	C	403	AGS	C2-N1-C6	2.03	122.06	118.73

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	403	AGS	C5'-O5'-PA-O1A
5	D	404	AGS	C5'-O5'-PA-O2A
5	D	404	AGS	C5'-O5'-PA-O3A
5	C	403	AGS	PB-O3B-PG-O3G

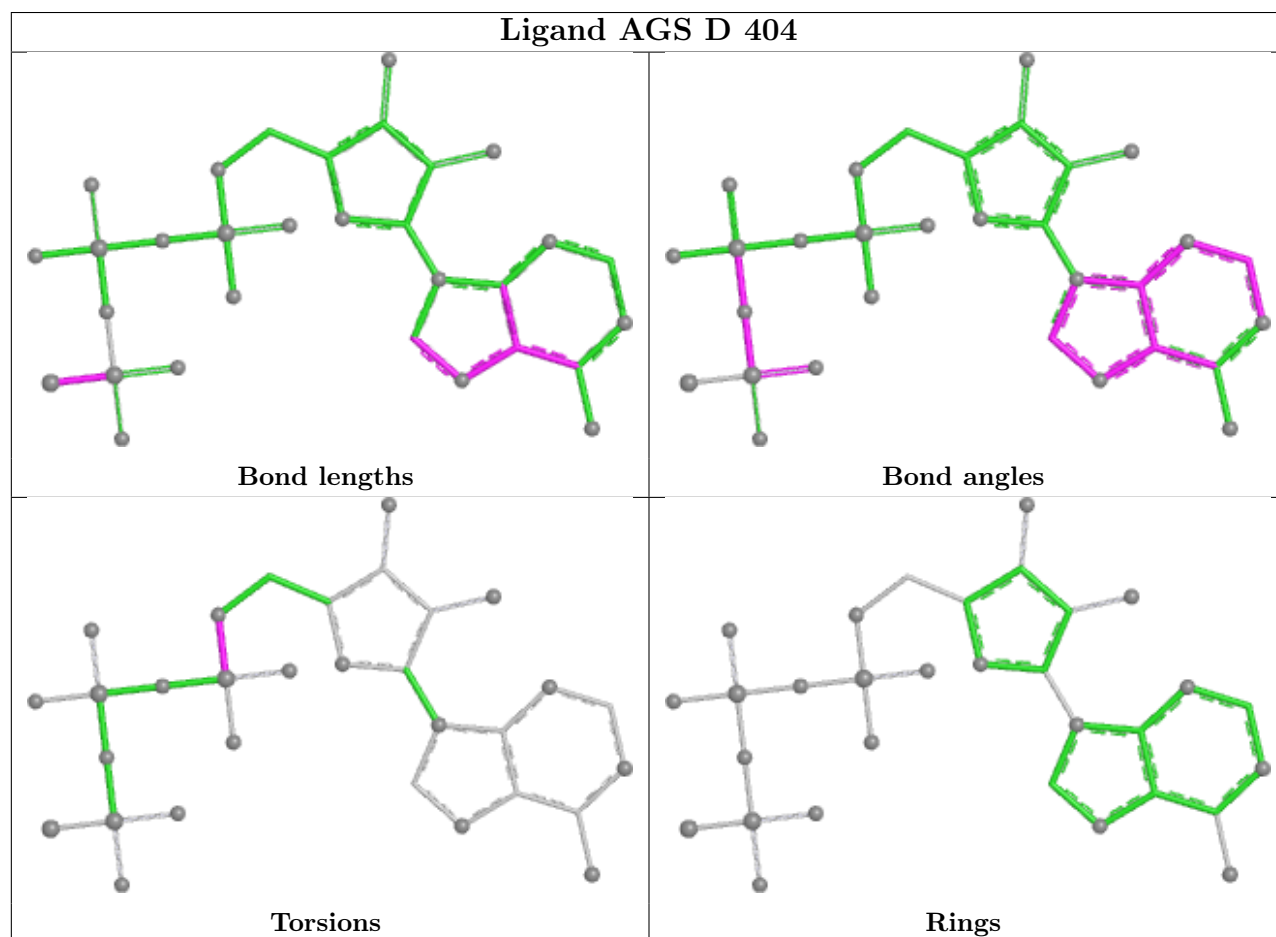
There are no ring outliers.

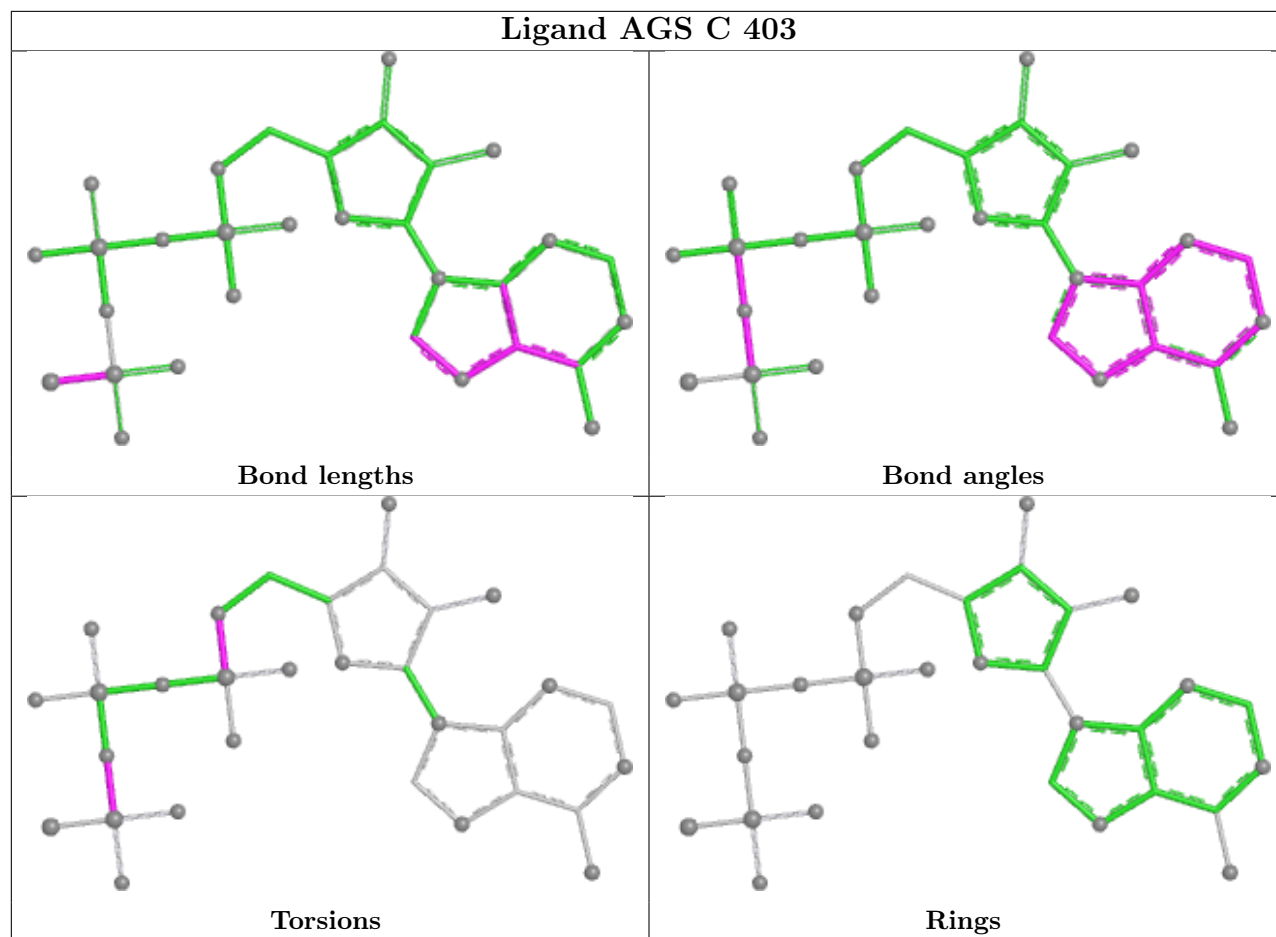
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	404	AGS	5	0
5	C	403	AGS	6	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	C	344/344 (100%)	-0.94	0 100 100	67, 101, 176, 205	0
1	D	344/344 (100%)	-1.02	0 100 100	65, 95, 154, 192	0
2	A	215/215 (100%)	-1.11	0 100 100	63, 91, 131, 153	0
2	B	215/215 (100%)	-1.09	0 100 100	65, 88, 120, 146	0
3	E	226/226 (100%)	0.56	27 (11%) 9 8	129, 166, 205, 228	0
All	All	1344/1344 (100%)	-0.76	27 (2%) 65 57	63, 101, 179, 228	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	225	SER	5.1
3	E	110	PHE	5.0
3	E	141	ASN	3.7
3	E	140	THR	3.7
3	E	229	ALA	3.6
3	E	43	GLN	3.3
3	E	136	PRO	3.2
3	E	112	TYR	3.1
3	E	148	LEU	3.0
3	E	139	PRO	2.7
3	E	226	PRO	2.7
3	E	230	LEU	2.7
3	E	144	ARG	2.6
3	E	201	ILE	2.5
3	E	155	ILE	2.5
3	E	142	LEU	2.4
3	E	243	VAL	2.4
3	E	163	LEU	2.4
3	E	147	LEU	2.3
3	E	145	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	244	LYS	2.2
3	E	253	ASP	2.2
3	E	143	GLY	2.2
3	E	242	ASN	2.1
3	E	90	PRO	2.1
3	E	149	LEU	2.0
3	E	164	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

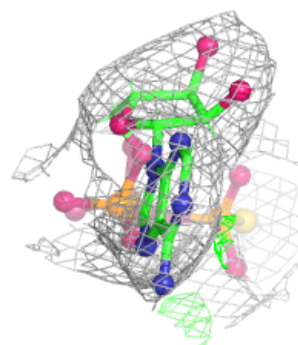
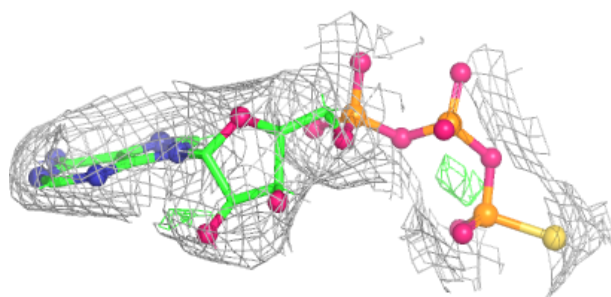
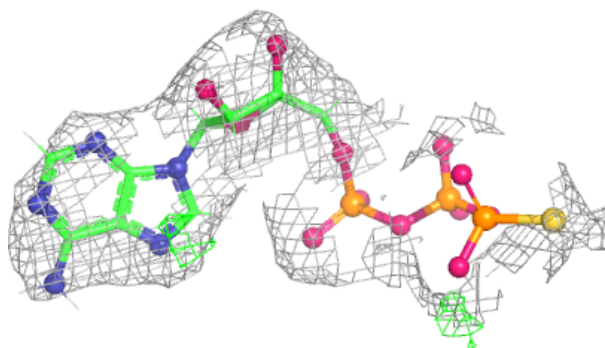
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	HG	C	402	1/1	0.99	0.05	130,130,130,130	0
5	AGS	D	404	31/31	0.99	0.03	56,65,79,81	0
6	IOD	D	403	1/1	0.99	0.03	124,124,124,124	0
5	AGS	C	403	31/31	1.00	0.03	59,70,89,97	0
4	HG	C	401	1/1	1.00	0.01	147,147,147,147	0
6	IOD	D	402	1/1	1.00	0.03	135,135,135,135	0
4	HG	D	401	1/1	1.00	0.02	151,151,151,151	0

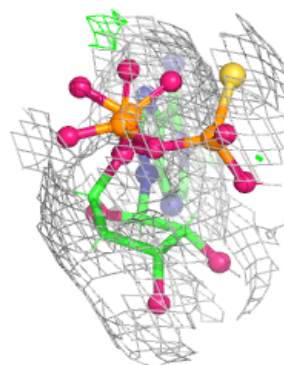
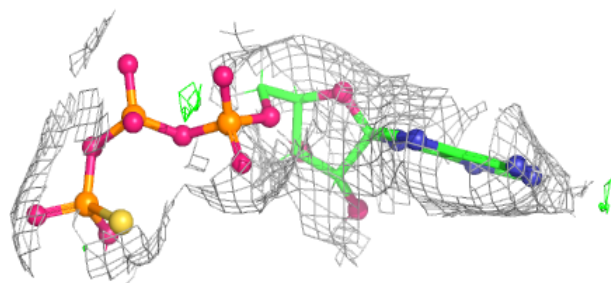
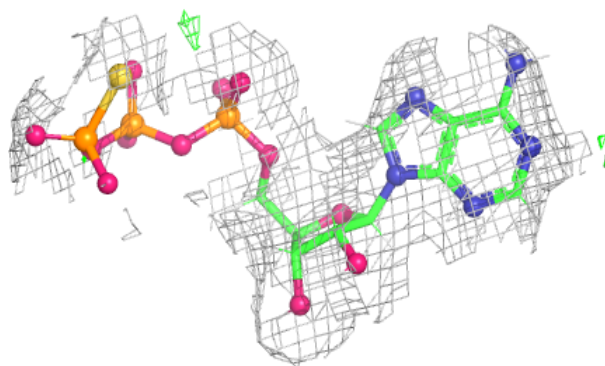
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS D 404:

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

**Electron density around AGS C 403:**

$2mF_o-DF_c$ (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.