



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:17 AM UTC

PDB ID : 6ULY / pdb_00006uly
Title : Adenylation domain of a keto acid-selecting NRPS module bound to keto acyl
adenylate space group P212121
Authors : Alonzo, D.A.; Chiche-Lapierre, C.; Schmeing, T.M.
Deposited on : 2019-10-08
Resolution : 2.30 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

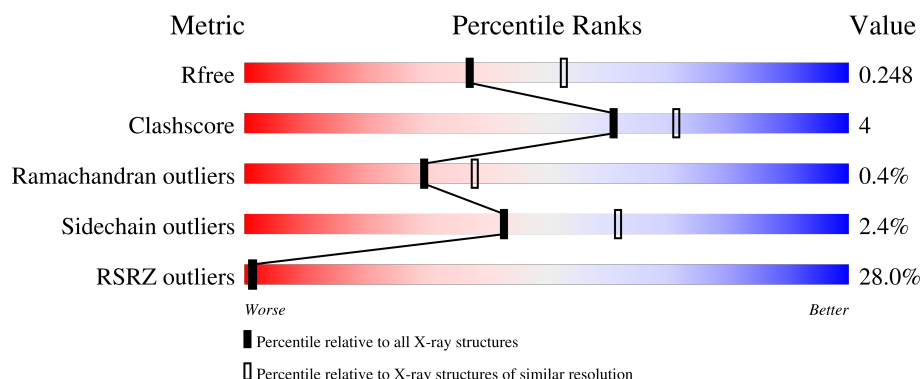
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	576	24% 84% 10% 5%
1	B	576	29% 82% 9% 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16777 atoms, of which 8101 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.

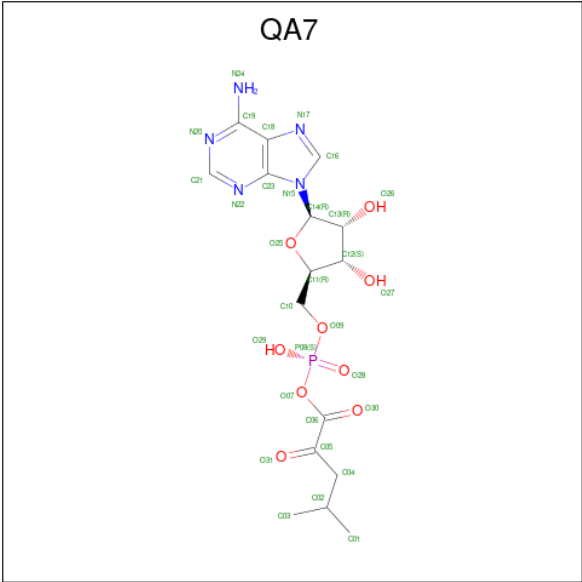
- Molecule 1 is a protein called Amino acid adenylation domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	545	Total	C	H	N	O	S	0	0	0
			8312	2696	4072	730	794	20			
1	B	531	Total	C	H	N	O	S	0	1	0
			8122	2640	3979	708	775	20			

There are 18 discrepancies between the modelled and reference sequences:

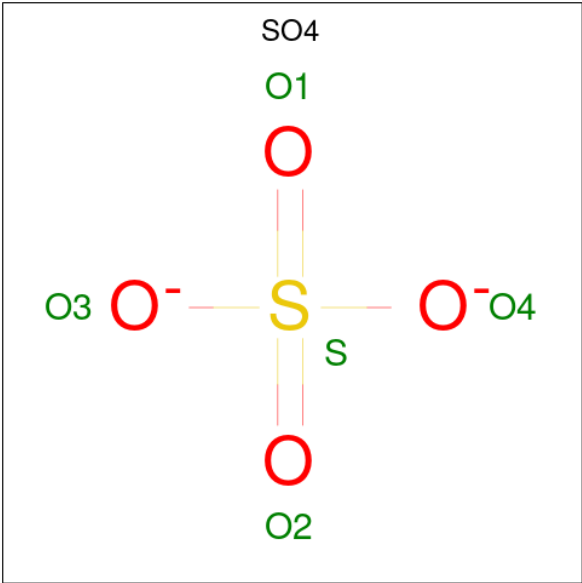
Chain	Residue	Modelled	Actual	Comment	Reference
A	650	ALA	-	expression tag	UNP M5R382
A	651	ALA	-	expression tag	UNP M5R382
A	652	ALA	-	expression tag	UNP M5R382
A	653	GLU	-	expression tag	UNP M5R382
A	654	ASN	-	expression tag	UNP M5R382
A	655	LEU	-	expression tag	UNP M5R382
A	656	TYR	-	expression tag	UNP M5R382
A	657	PHE	-	expression tag	UNP M5R382
A	658	GLN	-	expression tag	UNP M5R382
B	650	ALA	-	expression tag	UNP M5R382
B	651	ALA	-	expression tag	UNP M5R382
B	652	ALA	-	expression tag	UNP M5R382
B	653	GLU	-	expression tag	UNP M5R382
B	654	ASN	-	expression tag	UNP M5R382
B	655	LEU	-	expression tag	UNP M5R382
B	656	TYR	-	expression tag	UNP M5R382
B	657	PHE	-	expression tag	UNP M5R382
B	658	GLN	-	expression tag	UNP M5R382

- Molecule 2 is 5'-O-{(S)-hydroxy[(4-methyl-2-oxopentanoyl)oxy]phosphoryl}adenosine (CCD ID: QA7) (formula: C₁₆H₂₂N₅O₉P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	H	N	O	P	0	0
			52	16	21	5	9	1		
2	B	1	Total	C	H	N	O	P	0	0
			52	16	21	5	9	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



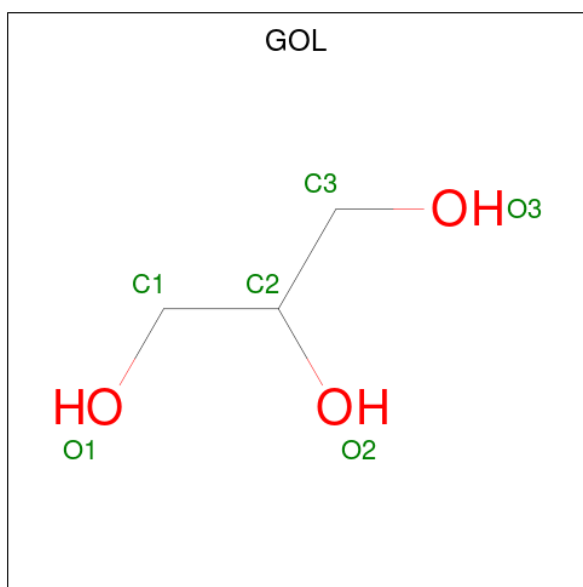
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	55	Total	O	0	0
			55	55		
5	B	65	Total	O	0	0
			65	65		

S619	R620	T621	T622	P623	V624	Q625	LYS	HIS	ALA	PHE	PRO	LYS	THR	SER	GLY	LYS	ILE	GLU	ARG	ALA	GLN	LEU	LYS	THR	ARG	TRP	GLN	GLU	GLY	ALA	ALA	GLU	ASN	LEU	TYR	PHE	GLN
------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.91Å 107.03Å 168.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.98 – 2.30 66.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (66.98-2.30) 99.3 (66.98-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.15.2 _3472	Depositor
R, R_{free}	0.228 , 0.247 0.233 , 0.248	Depositor DCC
R_{free} test set	1220 reflections (1.51%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.932	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16777	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: SO4, GOL, QA7

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	0.36	0/4337	0.50	0/5891
1	B	0.40	1/4242 (0.0%)	0.56	1/5768 (0.0%)
All	All	0.38	1/8579 (0.0%)	0.53	1/11659 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	588	PHE	C-O	-6.95	1.15	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	588	PHE	CA-C-O	-5.25	114.55	120.43

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	A	4240	4072	4146	31	0
1	B	4143	3979	4054	39	0
2	A	31	21	0	0	0
2	B	31	21	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	65	0	0	1	0
3	B	40	0	0	0	0
4	B	6	8	8	1	0
5	A	55	0	0	1	0
5	B	65	0	0	1	0
All	All	8676	8101	8208	70	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 4.

All (70) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:545:ILE:HB	1:B:616:LEU:HD21	1.47	0.96
1:B:545:ILE:HD13	1:B:616:LEU:HD21	1.48	0.94
1:B:342:MET:HE3	1:B:377:MET:HE3	1.50	0.90
1:B:367:ILE:HD13	1:B:398:LEU:HD21	1.60	0.82
1:B:545:ILE:CD1	1:B:616:LEU:HD21	2.10	0.82
1:B:545:ILE:HB	1:B:616:LEU:CD2	2.11	0.80
1:B:364:GLU:OE1	1:B:394:ARG:NH2	2.22	0.73
1:B:545:ILE:HD13	1:B:616:LEU:CD2	2.23	0.69
1:B:367:ILE:CD1	1:B:398:LEU:HD21	2.22	0.69
1:B:543:ILE:HD13	1:B:555:ILE:CD1	2.24	0.68
1:A:516:ALA:HB2	4:B:701:GOL:H12	1.75	0.68
1:B:545:ILE:CB	1:B:616:LEU:HD21	2.24	0.62
1:A:208:ILE:HD12	1:A:230:LEU:HD11	1.83	0.60
1:B:367:ILE:HD13	1:B:398:LEU:CD2	2.31	0.59
1:A:115:THR:HG23	1:A:125:THR:HG22	1.84	0.58
1:B:603:SER:OG	1:B:623:PRO:CG	2.53	0.56
1:A:584:GLU:CD	1:A:620:ARG:HA	2.30	0.56
1:A:617:SER:OG	1:A:620:ARG:NE	2.39	0.55
1:A:309:ILE:HG23	1:A:310:VAL:HG23	1.89	0.54
1:B:309:ILE:HG23	1:B:310:VAL:HG23	1.90	0.53
1:A:103:VAL:HG12	1:A:317:VAL:HG12	1.91	0.53
1:A:163:MET:HE3	1:A:303:LEU:HB2	1.91	0.52
1:A:210:THR:OG1	1:A:211:ASP:N	2.43	0.52
1:A:584:GLU:OE1	1:A:620:ARG:HA	2.10	0.52
1:B:551:HIS:HB3	1:B:553:TYR:CE2	2.43	0.52
1:B:84:ALA:C	1:B:528:LEU:HD12	2.35	0.52
1:A:603:SER:HB3	1:A:623:PRO:CG	2.39	0.51
1:A:521:HIS:NE2	1:A:539:GLU:OE2	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:MET:HE3	1:A:377:MET:HE3	1.92	0.50
1:B:342:MET:CE	1:B:377:MET:HE3	2.32	0.50
1:A:335:PRO:HG3	1:A:359:MET:HE2	1.94	0.50
1:A:383:GLY:O	1:A:384:ALA:CB	2.60	0.49
1:B:543:ILE:HG13	1:B:572:ALA:HB2	1.95	0.48
1:B:367:ILE:HG21	1:B:398:LEU:HD21	1.94	0.48
1:B:193:VAL:HG11	1:B:224:LEU:HD23	1.95	0.47
1:B:383:GLY:O	1:B:384:ALA:HB3	2.14	0.47
1:B:367:ILE:HG21	1:B:398:LEU:CD2	2.44	0.47
3:A:709:SO4:O2	1:B:194:LYS:NZ	2.48	0.46
1:B:236:GLU:HB2	1:B:237:PRO:HD3	1.96	0.46
1:B:383:GLY:O	1:B:384:ALA:CB	2.63	0.46
1:B:545:ILE:CG1	1:B:616:LEU:HD21	2.46	0.46
1:B:445:LEU:HB2	1:B:553:TYR:CD1	2.50	0.46
1:A:97:ALA:HB1	1:A:102:ASP:HB2	1.97	0.45
1:B:445:LEU:HD23	1:B:449:LEU:CD2	2.46	0.45
1:B:349:LYS:HA	1:B:379:CYS:O	2.17	0.45
1:A:603:SER:HB3	1:A:623:PRO:HG3	1.98	0.44
1:B:552:ASN:O	1:B:556:GLU:HG3	2.16	0.44
1:A:270:CYS:HB3	1:A:504:TYR:HB3	1.99	0.43
1:B:322:GLU:HG3	5:B:806:HOH:O	2.17	0.43
1:A:419:SER:O	1:A:420:SER:CB	2.66	0.43
1:A:287:ALA:HB2	5:A:825:HOH:O	2.19	0.42
1:B:562:VAL:HG21	1:B:606:ILE:HA	2.01	0.42
1:A:180:VAL:HB	1:A:260:LEU:HD22	2.00	0.42
1:B:419:SER:O	1:B:420:SER:CB	2.68	0.42
1:A:313:HIS:O	1:A:317:VAL:HG23	2.20	0.42
1:B:113:GLY:HA3	1:B:127:SER:HA	2.02	0.41
1:B:412:ALA:O	2:B:702:QA7:N24	2.53	0.41
1:A:163:MET:HE3	1:A:303:LEU:HD12	2.01	0.41
1:A:100:LEU:HD12	1:A:256:VAL:HG21	2.02	0.41
1:A:342:MET:HE2	1:A:374:LEU:HD22	2.02	0.41
1:A:383:GLY:O	1:A:384:ALA:HB3	2.20	0.41
1:B:413:PHE:HB2	1:B:465:LEU:HD13	2.03	0.41
1:A:142:LEU:HB3	1:A:147:LEU:HD22	2.03	0.41
1:A:445:LEU:HD21	1:A:460:VAL:HG21	2.03	0.41
1:A:413:PHE:HB2	1:A:465:LEU:HD13	2.02	0.41
1:B:591:PRO:HG3	1:B:599:ILE:HG12	2.02	0.41
1:B:552:ASN:OD1	1:B:553:TYR:N	2.54	0.41
1:A:113:GLY:HA3	1:A:127:SER:HA	2.03	0.40
1:A:177:PRO:HD2	1:A:256:VAL:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:VAL:HG12	1:B:317:VAL:HG12	2.03	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	535/576 (93%)	520 (97%)	13 (2%)	2 (0%)	30	38
1	B	526/576 (91%)	513 (98%)	11 (2%)	2 (0%)	30	38
All	All	1061/1152 (92%)	1033 (97%)	24 (2%)	4 (0%)	30	38

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	SER
1	B	420	SER
1	A	384	ALA
1	B	384	ALA

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	447/478 (94%)	435 (97%)	12 (3%)	39	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	441/478 (92%)	432 (98%)	9 (2%)	48 67
All	All	888/956 (93%)	867 (98%)	21 (2%)	43 62

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	THR
1	A	188	GLU
1	A	242	GLU
1	A	366	GLU
1	A	543	ILE
1	A	573	CYS
1	A	586	ILE
1	A	587	LEU
1	A	622	ILE
1	A	637	ILE
1	A	639	ARG
1	A	644	THR
1	B	121	LYS
1	B	212	ASP
1	B	213	SER
1	B	359	MET
1	B	517	ASP
1	B	560	GLU
1	B	566	GLU
1	B	570	VAL
1	B	573	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	248	HIS
1	A	488	HIS
1	B	480	GLN
1	B	515	GLN

5.3.3 RNA ⓘ

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](#)

24 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	GOL	B	701	-	5,5,5	0.29	0	5,5,5	0.44	0
3	SO4	B	708	-	4,4,4	1.17	0	6,6,6	0.27	0
3	SO4	B	706	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	B	707	-	4,4,4	0.28	0	6,6,6	0.14	0
3	SO4	A	703	-	4,4,4	0.40	0	6,6,6	0.07	0
3	SO4	A	712	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	A	706	-	4,4,4	0.35	0	6,6,6	0.27	0
3	SO4	A	709	-	4,4,4	0.36	0	6,6,6	0.14	0
3	SO4	B	704	-	4,4,4	0.27	0	6,6,6	0.23	0
3	SO4	A	707	-	4,4,4	0.30	0	6,6,6	0.14	0
3	SO4	B	709	-	4,4,4	0.60	0	6,6,6	0.32	0
3	SO4	A	708	-	4,4,4	0.26	0	6,6,6	0.13	0
3	SO4	A	713	-	4,4,4	0.38	0	6,6,6	0.07	0
3	SO4	A	704	-	4,4,4	0.39	0	6,6,6	0.07	0
2	QA7	B	702	-	33,33,33	3.39	21 (63%)	48,49,49	1.84	9 (18%)
3	SO4	A	711	-	4,4,4	0.39	0	6,6,6	0.09	0
3	SO4	A	714	-	4,4,4	0.68	0	6,6,6	0.22	0
2	QA7	A	701	-	33,33,33	3.35	19 (57%)	48,49,49	2.21	16 (33%)
3	SO4	A	710	-	4,4,4	0.61	0	6,6,6	0.14	0
3	SO4	B	705	-	4,4,4	0.33	0	6,6,6	0.10	0
3	SO4	B	710	-	4,4,4	0.87	0	6,6,6	0.39	0
3	SO4	A	702	-	4,4,4	0.40	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	B	703	-	4,4,4	0.29	0	6,6,6	0.15	0
3	SO4	A	705	-	4,4,4	0.29	0	6,6,6	0.29	0

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	QA7	B	702	-	-	3/23/39/39	0/3/3/3
4	GOL	B	701	-	-	2/4/4/4	-
2	QA7	A	701	-	-	3/23/39/39	0/3/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	QA7	C13-C12	-11.27	1.22	1.53
2	B	702	QA7	C13-C12	-11.22	1.23	1.53
2	B	702	QA7	O25-C14	-7.24	1.25	1.42
2	A	701	QA7	O25-C14	-6.94	1.26	1.42
2	B	702	QA7	C10-C11	-4.76	1.37	1.51
2	A	701	QA7	O31-C05	-4.55	1.13	1.23
2	A	701	QA7	C10-C11	-4.52	1.38	1.51
2	B	702	QA7	C13-C14	4.41	1.67	1.53
2	A	701	QA7	C16-N15	-4.30	1.30	1.37
2	A	701	QA7	O30-C06	-4.18	1.13	1.21
2	B	702	QA7	O27-C12	3.99	1.52	1.43
2	B	702	QA7	C16-N15	-3.97	1.30	1.37
2	B	702	QA7	O31-C05	-3.95	1.15	1.23
2	A	701	QA7	C13-C14	3.70	1.65	1.53
2	B	702	QA7	C18-N17	-3.46	1.32	1.39
2	B	702	QA7	O30-C06	-3.27	1.15	1.21
2	A	701	QA7	P08-O29	-3.24	1.40	1.55
2	A	701	QA7	O27-C12	3.19	1.50	1.43
2	A	701	QA7	C18-C23	-3.18	1.33	1.39
2	B	702	QA7	P08-O29	-3.04	1.41	1.55
2	A	701	QA7	C18-N17	-3.03	1.33	1.39
2	B	702	QA7	C21-N22	-2.99	1.28	1.33
2	B	702	QA7	C18-C23	-2.97	1.33	1.39
2	B	702	QA7	C19-N24	2.90	1.41	1.34
2	A	701	QA7	C21-N20	-2.89	1.28	1.33
2	A	701	QA7	C21-N22	-2.87	1.28	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	QA7	C12-C11	2.72	1.59	1.53
2	B	702	QA7	C05-C06	-2.69	1.49	1.53
2	A	701	QA7	P08-O28	-2.57	1.41	1.50
2	B	702	QA7	C21-N20	-2.42	1.29	1.33
2	A	701	QA7	C19-N24	2.41	1.40	1.34
2	A	701	QA7	C12-C11	2.40	1.59	1.53
2	A	701	QA7	C19-N20	-2.33	1.29	1.35
2	A	701	QA7	C05-C06	-2.28	1.49	1.53
2	A	701	QA7	O25-C11	2.27	1.50	1.45
2	B	702	QA7	C23-N15	-2.21	1.33	1.37
2	B	702	QA7	O07-C06	-2.18	1.34	1.37
2	B	702	QA7	C14-N15	-2.16	1.40	1.46
2	B	702	QA7	C19-N20	-2.11	1.29	1.35
2	B	702	QA7	P08-O07	-2.03	1.56	1.60

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	QA7	C18-C23-N22	-6.03	118.41	126.72
2	B	702	QA7	C18-C23-N22	-5.34	119.36	126.72
2	A	701	QA7	N22-C23-N15	4.78	135.29	127.17
2	A	701	QA7	O07-P08-O09	4.39	116.19	103.00
2	A	701	QA7	N22-C21-N20	-4.15	122.29	128.58
2	B	702	QA7	N22-C21-N20	-4.15	122.30	128.58
2	B	702	QA7	N22-C23-N15	4.01	134.00	127.17
2	B	702	QA7	O07-P08-O09	3.96	114.92	103.00
2	A	701	QA7	C21-N22-C23	3.72	120.91	111.83
2	B	702	QA7	C21-N22-C23	3.65	120.74	111.83
2	A	701	QA7	N15-C16-N17	-3.60	108.83	113.94
2	A	701	QA7	O30-C06-C05	-3.51	118.02	122.05
2	B	702	QA7	N15-C16-N17	-3.43	109.07	113.94
2	A	701	QA7	C12-C13-C14	3.08	107.29	101.46
2	A	701	QA7	C18-N17-C16	3.02	108.20	103.45
2	A	701	QA7	C23-N15-C16	2.95	108.84	105.74
2	B	702	QA7	C18-N17-C16	2.76	107.79	103.45
2	B	702	QA7	C23-N15-C16	2.60	108.47	105.74
2	A	701	QA7	C23-C18-N17	-2.40	107.84	110.58
2	A	701	QA7	P08-O07-C06	2.34	128.11	123.01
2	B	702	QA7	C23-C18-N17	-2.24	108.02	110.58
2	A	701	QA7	O07-C06-O30	-2.15	119.61	122.76
2	A	701	QA7	O26-C13-C14	-2.12	102.79	110.10
2	A	701	QA7	C13-C14-N15	-2.12	108.05	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	QA7	O25-C14-N15	2.03	111.98	108.09

There are no chirality outliers.

All (8) torsion outliers are listed below:

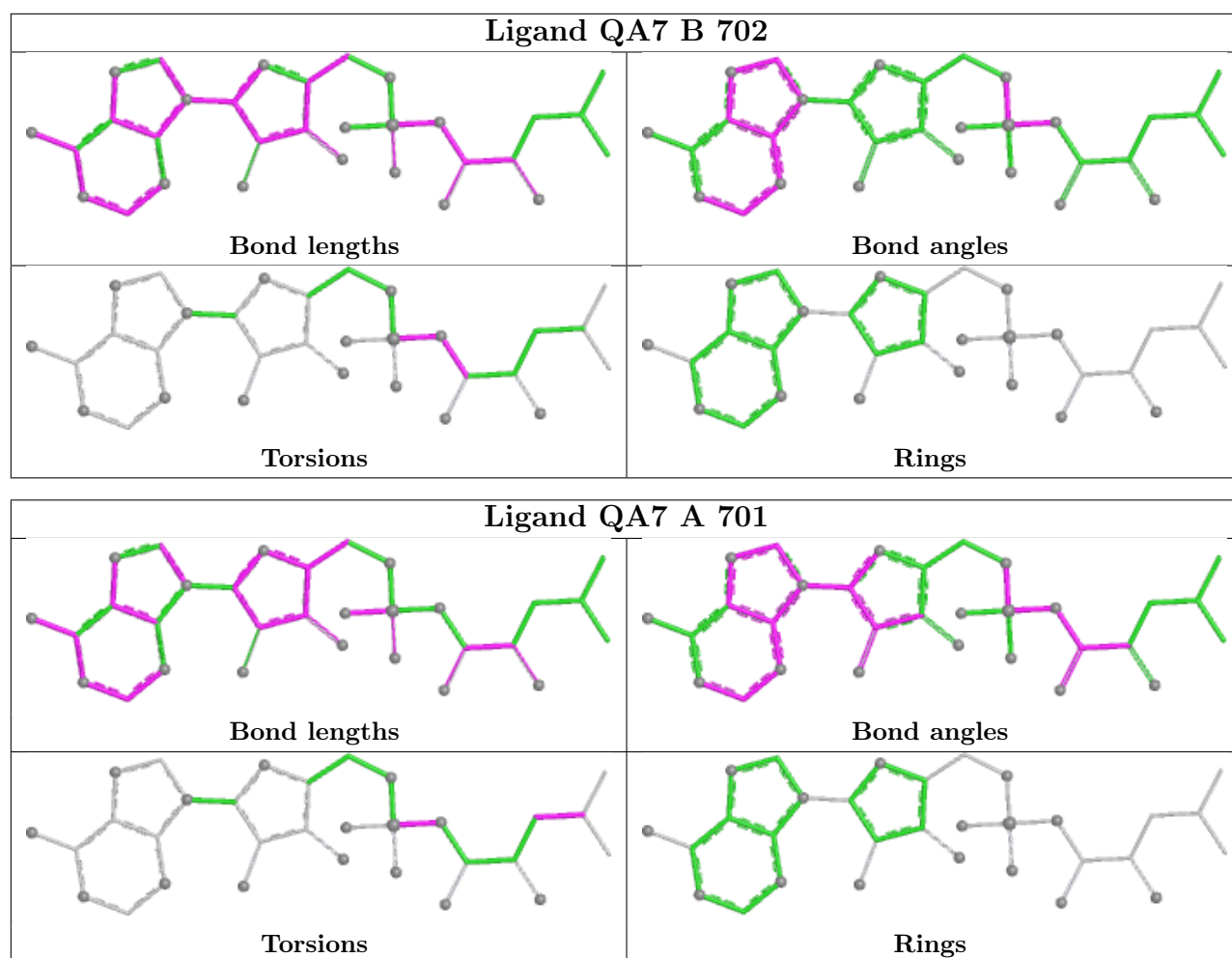
Mol	Chain	Res	Type	Atoms
2	B	702	QA7	C05-C06-O07-P08
2	B	702	QA7	O30-C06-O07-P08
4	B	701	GOL	C1-C2-C3-O3
2	A	701	QA7	C01-C02-C04-C05
2	A	701	QA7	C03-C02-C04-C05
2	B	702	QA7	C06-O07-P08-O09
4	B	701	GOL	O2-C2-C3-O3
2	A	701	QA7	C06-O07-P08-O09

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	701	GOL	1	0
3	A	709	SO4	1	0
2	B	702	QA7	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	545/576 (94%)	1.52	136 (24%)	2 2	37, 55, 129, 164	23 (4%)
1	B	531/576 (92%)	1.86	165 (31%)	1 1	33, 57, 148, 168	17 (3%)
All	All	1076/1152 (93%)	1.69	301 (27%)	1 1	33, 56, 137, 168	40 (3%)

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	575	VAL	11.0
1	B	620	ARG	10.8
1	B	594	TYR	10.3
1	B	585	LEU	10.1
1	B	593	LEU	10.1
1	B	599	ILE	9.8
1	B	572	ALA	9.6
1	B	602	ALA	9.3
1	B	597	ALA	9.0
1	B	600	MET	9.0
1	A	553	TYR	8.9
1	A	588	PHE	8.8
1	A	543	ILE	8.8
1	B	571	ALA	8.5
1	B	570	VAL	8.4
1	A	574	SER	8.3
1	B	223	PHE	8.1
1	B	606	ILE	7.7
1	B	616	LEU	7.7
1	B	610	ILE	7.4
1	A	569	PHE	7.4
1	B	589	PHE	7.2
1	B	622	ILE	7.1
1	A	611	ALA	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	614	MET	7.0
1	A	610	ILE	7.0
1	B	598	TYR	7.0
1	B	618	ALA	6.9
1	B	553	TYR	6.9
1	B	624	VAL	6.8
1	A	586	ILE	6.8
1	B	545	ILE	6.7
1	B	623	PRO	6.7
1	A	623	PRO	6.7
1	B	596	PRO	6.7
1	B	603	SER	6.5
1	B	619	SER	6.5
1	A	594	TYR	6.5
1	B	588	PHE	6.3
1	A	585	LEU	6.3
1	B	621	ILE	6.2
1	A	622	ILE	6.2
1	B	569	PHE	6.1
1	A	555	ILE	6.1
1	B	587	LEU	6.1
1	A	567	THR	6.1
1	B	397[A]	HIS	6.0
1	A	624	VAL	6.0
1	A	566	GLU	6.0
1	B	443	THR	6.0
1	B	452	ALA	5.9
1	B	573	CYS	5.9
1	A	618	ALA	5.8
1	A	573	CYS	5.8
1	B	543	ILE	5.8
1	B	586	ILE	5.8
1	A	626	LYS	5.7
1	B	567	THR	5.6
1	B	554	GLU	5.6
1	A	570	VAL	5.6
1	A	616	LEU	5.5
1	B	591	PRO	5.5
1	B	121	LYS	5.5
1	B	607	LYS	5.5
1	A	597	ALA	5.4
1	B	517	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	595	GLU	5.4
1	A	571	ALA	5.3
1	B	563	PRO	5.3
1	A	551	HIS	5.3
1	A	599	ILE	5.3
1	A	572	ALA	5.3
1	B	625	GLN	5.3
1	B	608	SER	5.3
1	B	439	THR	5.3
1	B	557	ALA	5.3
1	B	555	ILE	5.2
1	A	581	ALA	5.2
1	A	646	TRP	5.2
1	B	544	ILE	5.1
1	B	558	ILE	5.1
1	A	562	VAL	5.1
1	A	563	PRO	5.0
1	A	621	ILE	5.0
1	A	590	THR	5.0
1	A	587	LEU	5.0
1	A	558	ILE	5.0
1	B	479	HIS	5.0
1	B	460	VAL	4.9
1	B	565	VAL	4.9
1	B	550	TYR	4.9
1	B	552	ASN	4.9
1	B	266	GLY	4.9
1	A	653	GLU	4.8
1	B	188	GLU	4.8
1	B	559	ALA	4.8
1	A	637	ILE	4.8
1	B	441	GLU	4.8
1	B	547	GLY	4.8
1	A	593	LEU	4.8
1	B	605	HIS	4.8
1	B	450	ARG	4.7
1	B	440	PHE	4.7
1	A	640	ALA	4.7
1	B	568	SER	4.7
1	B	446	THR	4.7
1	B	445	LEU	4.6
1	B	612	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	604	GLN	4.5
1	B	564	GLY	4.5
1	A	582	SER	4.5
1	A	619	SER	4.5
1	B	365	LYS	4.5
1	B	542	MET	4.5
1	B	548	LYS	4.5
1	A	612	THR	4.5
1	A	642	LEU	4.5
1	A	636	LYS	4.4
1	A	583	ASP	4.4
1	A	650	ALA	4.4
1	A	457	THR	4.4
1	B	549	ASN	4.4
1	A	565	VAL	4.3
1	A	600	MET	4.3
1	A	559	ALA	4.3
1	A	552	ASN	4.3
1	A	615	GLY	4.3
1	A	223	PHE	4.2
1	A	644	THR	4.2
1	B	262	SER	4.2
1	A	557	ALA	4.2
1	B	457	THR	4.2
1	A	595	GLU	4.2
1	A	613	LYS	4.2
1	B	461	SER	4.1
1	B	611	ALA	4.1
1	A	643	LYS	4.1
1	B	562	VAL	4.0
1	B	609	HIS	4.0
1	B	454	ALA	4.0
1	B	601	ARG	4.0
1	A	603	SER	4.0
1	B	183	ALA	4.0
1	A	589	PHE	4.0
1	B	212	ASP	4.0
1	A	620	ARG	3.9
1	B	551	HIS	3.9
1	A	560	GLU	3.9
1	B	615	GLY	3.9
1	A	541	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	596	PRO	3.8
1	B	459	THR	3.8
1	A	609	HIS	3.8
1	B	458	GLY	3.8
1	B	230	LEU	3.7
1	B	449	LEU	3.7
1	B	614	MET	3.7
1	B	456	GLU	3.7
1	B	590	THR	3.7
1	B	222	ALA	3.7
1	A	568	SER	3.7
1	A	556	GLU	3.6
1	A	652	ALA	3.6
1	A	564	GLY	3.6
1	A	617	SER	3.6
1	B	617	SER	3.6
1	B	185	THR	3.6
1	A	598	TYR	3.5
1	B	398	LEU	3.5
1	A	605	HIS	3.4
1	B	220	GLY	3.4
1	A	625	GLN	3.4
1	A	332	ILE	3.4
1	B	613	LYS	3.4
1	B	186	TYR	3.4
1	B	451	PRO	3.4
1	A	561	GLU	3.4
1	B	442	GLU	3.4
1	B	94	THR	3.3
1	B	218	VAL	3.3
1	A	584	GLU	3.3
1	A	592	LYS	3.3
1	B	438	LEU	3.3
1	B	184	PRO	3.3
1	B	187	ARG	3.2
1	A	346	ARG	3.2
1	B	531	GLY	3.2
1	A	607	LYS	3.2
1	A	638	GLU	3.2
1	A	608	SER	3.2
1	B	485	PRO	3.2
1	B	556	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	228	ASP	3.1
1	A	606	ILE	3.1
1	B	540	LYS	3.1
1	A	456	GLU	3.1
1	B	95	GLN	3.0
1	A	517	ASP	3.0
1	B	189	MET	3.0
1	A	554	GLU	3.0
1	A	479	HIS	3.0
1	B	242	GLU	3.0
1	A	467	LYS	3.0
1	B	515	GLN	3.0
1	B	124	LEU	2.9
1	A	511	GLN	2.9
1	A	542	MET	2.9
1	B	216	GLU	2.9
1	B	234	ALA	2.9
1	A	447	GLU	2.9
1	A	329	ASP	2.9
1	A	442	GLU	2.9
1	B	560	GLU	2.9
1	A	124	LEU	2.9
1	B	191	ALA	2.8
1	A	460	VAL	2.8
1	A	601	ARG	2.8
1	B	489	ILE	2.8
1	B	546	ASN	2.8
1	A	641	GLN	2.8
1	A	242	GLU	2.8
1	B	332	ILE	2.7
1	B	229	GLN	2.7
1	B	224	LEU	2.7
1	B	267	MET	2.7
1	B	227	THR	2.7
1	A	453	GLU	2.7
1	B	539	GLU	2.7
1	B	215	ILE	2.7
1	B	592	LYS	2.7
1	A	649	GLY	2.7
1	B	455	ARG	2.6
1	B	433	GLU	2.6
1	B	566	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	116	TYR	2.6
1	B	488	HIS	2.6
1	A	229	GLN	2.6
1	A	211	ASP	2.6
1	A	591	PRO	2.6
1	A	121	LYS	2.6
1	B	434	ASN	2.5
1	A	141	GLY	2.5
1	A	194	LYS	2.5
1	B	444	SER	2.5
1	B	448	GLN	2.5
1	A	645	ARG	2.5
1	B	231	ARG	2.5
1	B	516	ALA	2.5
1	A	213	SER	2.5
1	B	561	GLU	2.5
1	B	241	LEU	2.5
1	B	211	ASP	2.4
1	B	226	HIS	2.4
1	B	574	SER	2.4
1	B	232	VAL	2.4
1	A	651	ALA	2.4
1	A	446	THR	2.4
1	A	540	LYS	2.4
1	A	445	LEU	2.4
1	B	334	GLN	2.4
1	B	453	GLU	2.4
1	A	401	PRO	2.4
1	A	117	ILE	2.4
1	A	95	GLN	2.4
1	A	429	GLU	2.4
1	A	433	GLU	2.4
1	B	447	GLU	2.4
1	A	602	ALA	2.3
1	B	214	LEU	2.3
1	B	221	LEU	2.3
1	A	648	GLU	2.3
1	A	455	ARG	2.3
1	B	528	LEU	2.3
1	B	333	ALA	2.3
1	A	439	THR	2.3
1	A	459	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	450	ARG	2.3
1	A	345	TYR	2.3
1	A	118	VAL	2.3
1	A	115	THR	2.2
1	B	536	THR	2.2
1	A	393	HIS	2.2
1	B	435	SER	2.2
1	B	235	VAL	2.2
1	B	462	PHE	2.2
1	A	443	THR	2.2
1	A	639	ARG	2.1
1	B	432	ASP	2.1
1	A	180	VAL	2.1
1	B	268	PRO	2.1
1	A	320	GLY	2.1
1	A	458	GLY	2.1
1	B	366	GLU	2.1
1	A	181	SER	2.1
1	B	360	ILE	2.1
1	A	235	VAL	2.1
1	A	187	ARG	2.1
1	B	194	LYS	2.0
1	B	480	GLN	2.0
1	A	294	GLU	2.0
1	B	541	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

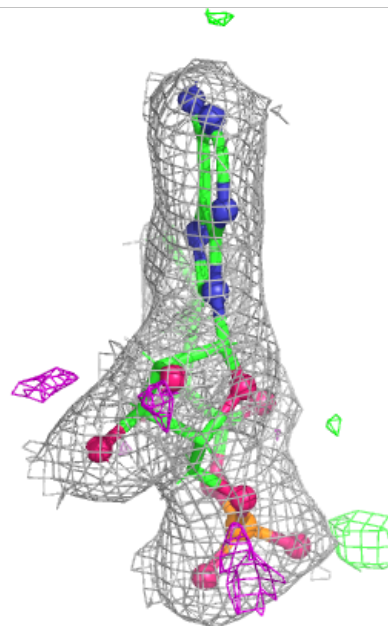
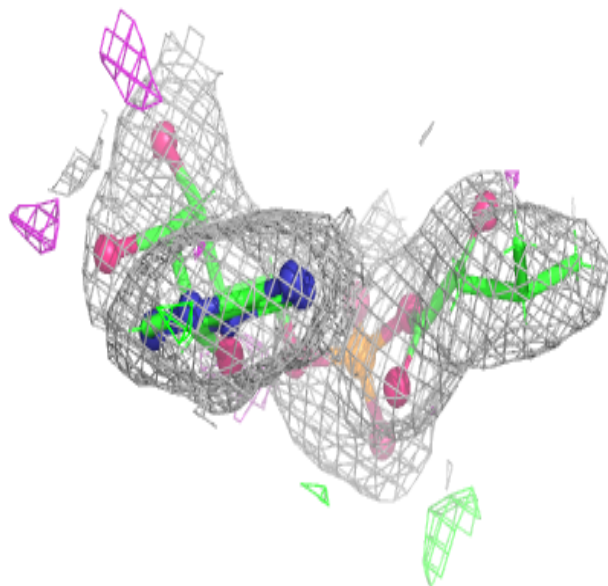
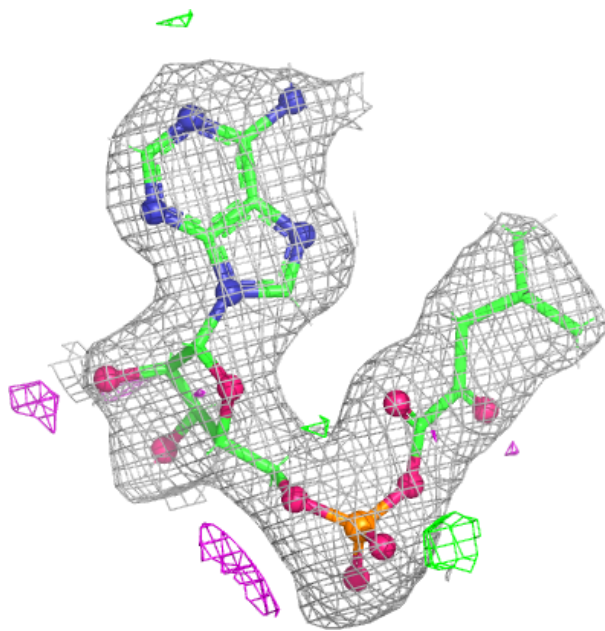
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	SO4	B	710	5/5	0.53	0.17	97,122,139,145	0
3	SO4	B	707	5/5	0.64	0.18	83,94,101,123	0
3	SO4	A	710	5/5	0.67	0.13	95,99,112,112	0
3	SO4	B	709	5/5	0.69	0.12	74,81,95,101	0
3	SO4	A	709	5/5	0.69	0.16	83,89,101,113	0
3	SO4	A	712	5/5	0.71	0.14	82,86,99,101	0
3	SO4	B	706	5/5	0.76	0.14	78,86,91,99	0
3	SO4	A	708	5/5	0.76	0.18	73,89,91,101	0
3	SO4	A	714	5/5	0.77	0.14	60,79,100,149	0
3	SO4	B	708	5/5	0.79	0.13	77,79,86,99	0
3	SO4	A	704	5/5	0.81	0.15	69,79,86,93	0
3	SO4	A	713	5/5	0.81	0.12	86,95,96,110	0
4	GOL	B	701	6/6	0.84	0.21	63,75,89,89	0
3	SO4	A	706	5/5	0.85	0.16	59,63,79,82	0
3	SO4	B	705	5/5	0.85	0.16	62,72,77,77	0
3	SO4	A	703	5/5	0.86	0.12	70,74,78,81	0
3	SO4	A	705	5/5	0.86	0.15	56,57,62,66	0
3	SO4	A	707	5/5	0.88	0.10	68,69,78,84	0
3	SO4	B	703	5/5	0.90	0.10	63,67,70,80	0
3	SO4	A	711	5/5	0.92	0.16	57,63,76,78	0
3	SO4	A	702	5/5	0.93	0.15	50,64,66,71	0
2	QA7	A	701	31/31	0.93	0.09	39,49,59,61	0
2	QA7	B	702	31/31	0.93	0.10	35,51,63,70	0
3	SO4	B	704	5/5	0.97	0.10	51,55,57,67	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.

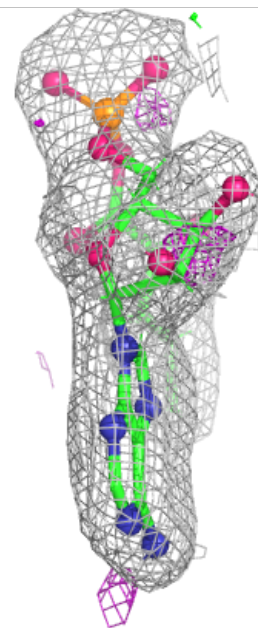
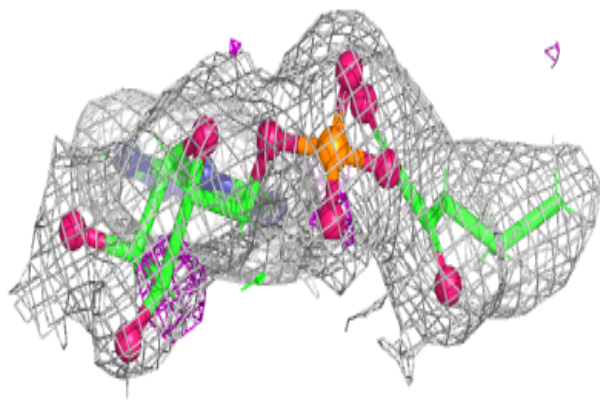
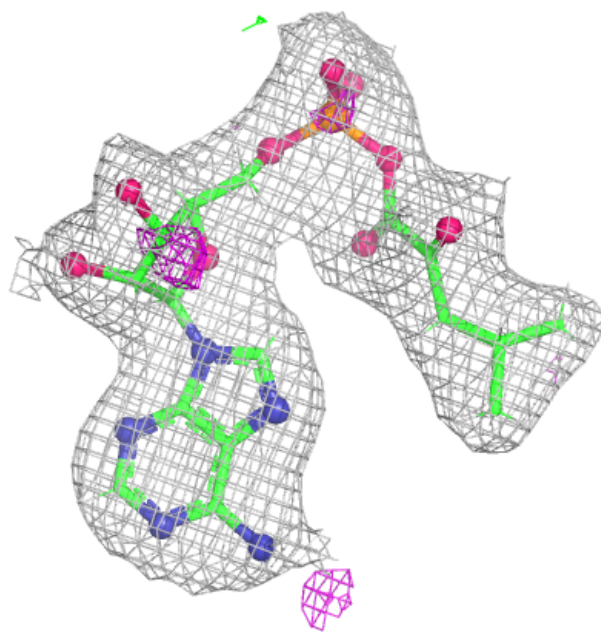
Electron density around QA7 A 701:

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



Electron density around QA7 B 702:

$2mF_o-DF_c$ (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.