



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 03:54 PM UTC

PDB ID : 3ZWA / pdb_00003zwa
Title : CRYSTAL STRUCTURE OF RAT PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE 1 (RPMFE1) COMPLEXED WITH 3S-HYDROXY-HEXA NOYL-COA
Authors : Kasaragod, P.; Schmitz, W.; Hiltunen, J.K.; Wierenga, R.K.
Deposited on : 2011-07-28
Resolution : 2.47 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

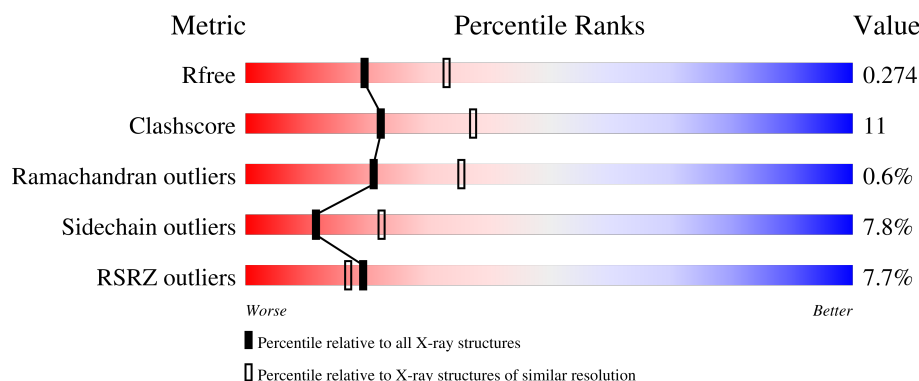
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.47 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	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (2.50-2.46)

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	742	
1	B	742	

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
2	GOL	A	1722	-	-	X	-
2	GOL	B	1719	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11617 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 PEROXISOMAL BIFUNCTIONAL ENZYME.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5578	3564	979	1012	23			
1	B	721	Total	C	N	O	S	0	0	0
			5534	3537	969	1005	23			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P07896
A	-18	GLY	-	expression tag	UNP P07896
A	-17	SER	-	expression tag	UNP P07896
A	-16	SER	-	expression tag	UNP P07896
A	-15	HIS	-	expression tag	UNP P07896
A	-14	HIS	-	expression tag	UNP P07896
A	-13	HIS	-	expression tag	UNP P07896
A	-12	HIS	-	expression tag	UNP P07896
A	-11	HIS	-	expression tag	UNP P07896
A	-10	HIS	-	expression tag	UNP P07896
A	-9	SER	-	expression tag	UNP P07896
A	-8	SER	-	expression tag	UNP P07896
A	-7	GLY	-	expression tag	UNP P07896
A	-6	LEU	-	expression tag	UNP P07896
A	-5	VAL	-	expression tag	UNP P07896
A	-4	PRO	-	expression tag	UNP P07896
A	-3	ARG	-	expression tag	UNP P07896
A	-2	GLY	-	expression tag	UNP P07896
A	-1	SER	-	expression tag	UNP P07896
A	0	HIS	-	expression tag	UNP P07896
B	-19	MET	-	expression tag	UNP P07896
B	-18	GLY	-	expression tag	UNP P07896
B	-17	SER	-	expression tag	UNP P07896
B	-16	SER	-	expression tag	UNP P07896
B	-15	HIS	-	expression tag	UNP P07896

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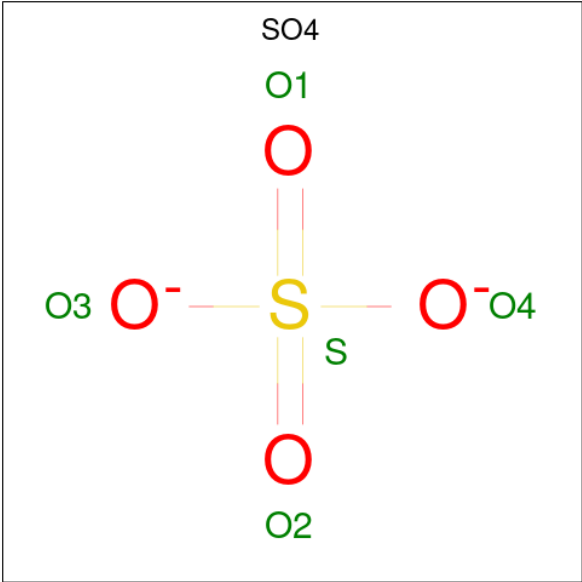
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP P07896
B	-13	HIS	-	expression tag	UNP P07896
B	-12	HIS	-	expression tag	UNP P07896
B	-11	HIS	-	expression tag	UNP P07896
B	-10	HIS	-	expression tag	UNP P07896
B	-9	SER	-	expression tag	UNP P07896
B	-8	SER	-	expression tag	UNP P07896
B	-7	GLY	-	expression tag	UNP P07896
B	-6	LEU	-	expression tag	UNP P07896
B	-5	VAL	-	expression tag	UNP P07896
B	-4	PRO	-	expression tag	UNP P07896
B	-3	ARG	-	expression tag	UNP P07896
B	-2	GLY	-	expression tag	UNP P07896
B	-1	SER	-	expression tag	UNP P07896
B	0	HIS	-	expression tag	UNP P07896

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



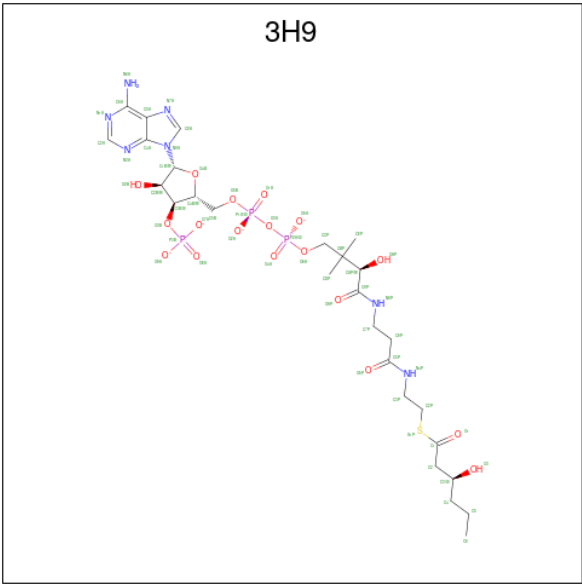
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



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	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is (S)-3-Hydroxyhexanoyl-CoA (CCD ID: 3H9) (formula: C₂₇H₄₂N₇O₁₈P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			56	27	7	18	3	1		
4	B	1	Total	C	N	O	P	S	0	0
			56	27	7	18	3	1		

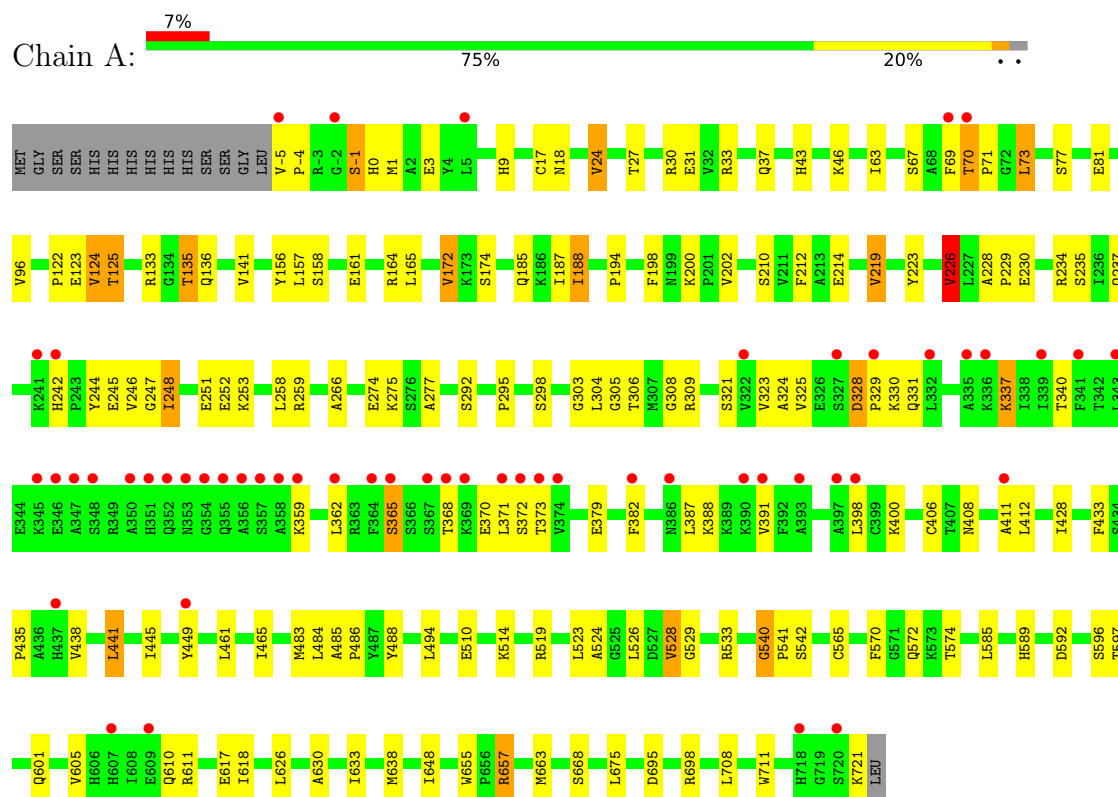
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	182	Total	O	0	0
			182	182		
5	A	1	Total	O	0	0
			1	1		
5	B	176	Total	O	0	0
			176	176		
5	B	2	Total	O	0	0
			2	2		

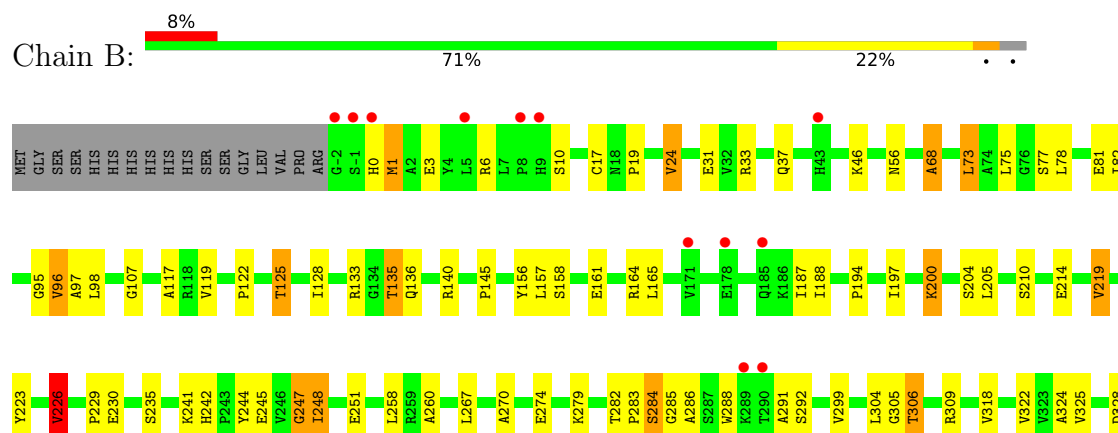
3 Residue-property plots

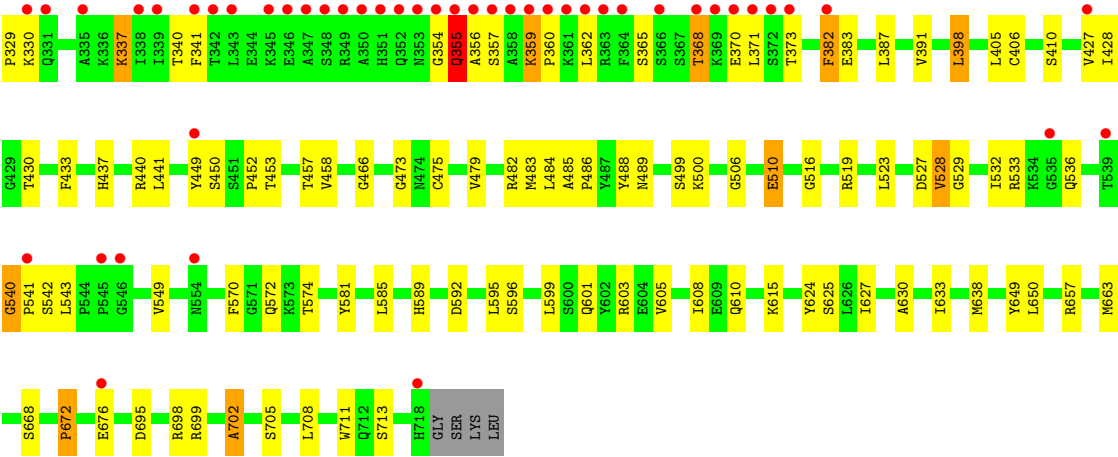
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: PEROXISOMAL BIFUNCTIONAL ENZYME





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.35Å 125.76Å 225.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.90 – 2.47 112.90 – 2.47	Depositor EDS
% Data completeness (in resolution range)	94.9 (112.90-2.47) 94.9 (112.90-2.47)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.55 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.218 , 0.279 0.215 , 0.274	Depositor DCC
R_{free} test set	3247 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	34.1	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11617	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: SO4, 3H9, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.01	4/5707 (0.1%)	1.13	24/7731 (0.3%)
1	B	0.98	2/5662 (0.0%)	1.12	19/7671 (0.2%)
All	All	1.00	6/11369 (0.1%)	1.12	43/15402 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	528	VAL	CA-CB	6.94	1.63	1.54
1	A	528	VAL	CA-CB	5.29	1.61	1.54
1	A	124	VAL	CA-C	5.29	1.59	1.52
1	B	242	HIS	C-O	-5.26	1.18	1.24
1	A	655	TRP	CA-C	5.21	1.59	1.53
1	A	648	ILE	CA-CB	5.06	1.60	1.54

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	THR	CA-C-N	-10.59	107.70	119.98
1	A	70	THR	C-N-CA	-10.59	107.70	119.98
1	B	540	GLY	CA-C-N	-7.76	111.51	120.12
1	B	540	GLY	C-N-CA	-7.76	111.51	120.12
1	A	540	GLY	CA-C-N	-7.39	111.92	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	540	GLY	C-N-CA	-7.39	111.92	120.12
1	A	226	VAL	CB-CA-C	7.22	120.42	111.25
1	B	541	PRO	N-CA-C	-6.85	105.98	114.20
1	A	445	ILE	N-CA-C	6.74	114.83	108.15
1	B	702	ALA	N-CA-C	-6.38	104.33	111.28
1	B	698	ARG	N-CA-C	-6.31	104.48	111.36
1	A	325	VAL	N-CA-C	6.30	116.94	107.75
1	A	541	PRO	N-CA-C	-6.21	106.75	114.20
1	A	266	ALA	N-CA-C	5.82	117.63	111.28
1	B	528	VAL	N-CA-C	5.73	116.51	110.72
1	A	202	VAL	CA-C-N	5.67	125.95	119.83
1	A	202	VAL	C-N-CA	5.67	125.95	119.83
1	A	277	ALA	CA-C-N	5.51	128.22	120.28
1	A	277	ALA	C-N-CA	5.51	128.22	120.28
1	B	24	VAL	CB-CA-C	-5.51	104.08	110.91
1	A	188	ILE	N-CA-C	5.50	116.88	110.62
1	B	516	GLY	CA-C-N	5.44	124.90	119.24
1	B	516	GLY	C-N-CA	5.44	124.90	119.24
1	A	592	ASP	CA-C-N	5.37	125.70	119.47
1	A	592	ASP	C-N-CA	5.37	125.70	119.47
1	B	649	TYR	CA-CB-CG	-5.37	104.24	113.90
1	A	141	VAL	CB-CA-C	-5.36	105.18	111.94
1	A	-4	PRO	N-CA-C	5.34	119.60	110.95
1	B	226	VAL	N-CA-C	5.32	115.75	107.99
1	B	325	VAL	N-CA-C	5.28	115.67	107.28
1	B	241	LYS	N-CA-C	5.21	117.87	111.82
1	B	247	GLY	CA-C-N	5.20	127.59	120.46
1	B	247	GLY	C-N-CA	5.20	127.59	120.46
1	A	328	ASP	CA-C-N	5.16	124.66	119.19
1	A	328	ASP	C-N-CA	5.16	124.66	119.19
1	A	18	ASN	CA-C-N	5.16	125.69	120.38
1	A	18	ASN	C-N-CA	5.16	125.69	120.38
1	A	24	VAL	CB-CA-C	5.15	117.19	110.96
1	B	200	LYS	CA-C-N	-5.14	115.06	120.66
1	B	200	LYS	C-N-CA	-5.14	115.06	120.66
1	B	107	GLY	N-CA-C	-5.06	108.38	114.66
1	A	657	ARG	NE-CZ-NH2	5.06	123.75	119.20
1	B	676	GLU	CB-CA-C	-5.05	102.72	110.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	69	PHE	Peptide

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	5578	0	5689	111	0
1	B	5534	0	5639	131	0
2	A	6	0	8	8	0
2	B	6	0	8	4	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0
4	A	56	0	42	2	0
4	B	56	0	42	4	0
5	A	183	0	0	17	1
5	B	178	0	0	31	1
All	All	11617	0	11428	240	1

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 11.

All (240) 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:603:ARG:HG2	5:B:2112:HOH:O	1.56	1.04
1:A:3:GLU:HB2	2:A:1722:GOL:H32	1.30	1.04
1:A:0:HIS:O	2:A:1722:GOL:H31	1.58	1.02
1:A:3:GLU:HB2	2:A:1722:GOL:C3	1.91	1.00
1:B:19:PRO:HD2	5:B:2007:HOH:O	1.58	1.00
1:A:67:SER:HB2	1:A:70:THR:OG1	1.63	0.99
1:B:592:ASP:HB3	5:B:2137:HOH:O	1.61	0.96
1:A:438:VAL:HB	5:A:2098:HOH:O	1.65	0.94
1:B:713:SER:HA	5:B:2174:HOH:O	1.68	0.91
1:B:713:SER:CA	5:B:2174:HOH:O	2.22	0.87
1:B:608:ILE:HB	5:B:2112:HOH:O	1.75	0.87
1:A:387:LEU:O	1:A:391:VAL:HG23	1.77	0.84
1:B:615:LYS:HD3	5:B:2147:HOH:O	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:CYS:SG	2:A:1722:GOL:H11	2.18	0.83
1:B:136:GLN:HG3	1:B:248:ILE:HD12	1.60	0.82
1:A:122:PRO:O	1:A:125:THR:HB	1.78	0.82
1:A:589:HIS:HD2	5:A:2136:HOH:O	1.62	0.82
1:B:267:LEU:HD23	1:B:657:ARG:HG2	1.61	0.82
1:B:595:LEU:HB2	5:B:2137:HOH:O	1.79	0.81
1:A:433:PHE:CE1	1:A:441:LEU:HD13	2.18	0.77
1:B:387:LEU:O	1:B:391:VAL:HG23	1.84	0.77
1:B:33:ARG:NH2	5:B:2011:HOH:O	2.18	0.76
1:A:411:ALA:HA	5:A:2091:HOH:O	1.87	0.73
1:B:702:ALA:HB2	2:B:1719:GOL:H12	1.71	0.73
1:B:663:MET:HA	1:B:663:MET:HE2	1.73	0.71
1:A:135:THR:HG21	1:A:235:SER:OG	1.91	0.71
1:A:449:TYR:HD2	5:A:2093:HOH:O	1.72	0.71
1:B:33:ARG:CD	5:B:2010:HOH:O	2.37	0.71
1:B:122:PRO:O	1:B:125:THR:HB	1.90	0.70
1:A:71:PRO:HD2	1:A:259:ARG:HD2	1.73	0.70
1:A:304:LEU:HD11	1:A:324:ALA:HB1	1.72	0.70
1:A:17:CYS:CB	2:A:1722:GOL:H11	2.22	0.69
1:A:657:ARG:NH1	5:A:2032:HOH:O	2.09	0.69
1:B:657:ARG:HD3	5:B:2039:HOH:O	1.92	0.69
1:A:136:GLN:HG3	1:A:248:ILE:HD12	1.74	0.69
1:B:603:ARG:HA	5:B:2112:HOH:O	1.93	0.69
1:B:135:THR:HG21	1:B:235:SER:OG	1.92	0.68
1:B:244:TYR:CE1	1:B:248:ILE:HD11	2.29	0.68
1:B:73:LEU:HD13	4:B:1720:3H9:H6	1.77	0.67
1:B:33:ARG:HD2	5:B:2010:HOH:O	1.94	0.67
1:B:519:ARG:HD2	5:B:2123:HOH:O	1.94	0.66
1:B:33:ARG:NH1	1:B:81:GLU:OE1	2.23	0.66
1:A:67:SER:CB	1:A:70:THR:OG1	2.42	0.66
1:B:135:THR:HG22	1:B:251:GLU:OE2	1.96	0.66
1:A:589:HIS:CD2	5:A:2136:HOH:O	2.42	0.66
1:A:33:ARG:NH1	1:A:81:GLU:OE1	2.23	0.65
1:A:-1:SER:N	1:A:31:GLU:OE2	2.30	0.65
1:A:0:HIS:O	2:A:1722:GOL:C3	2.39	0.64
1:B:473:GLY:HA3	1:B:638:MET:SD	2.37	0.64
1:A:601:GLN:O	1:A:605:VAL:HG23	1.97	0.64
1:A:9:HIS:HB3	1:A:185:GLN:HE22	1.63	0.64
1:A:194:PRO:O	1:A:200:LYS:NZ	2.23	0.64
1:B:194:PRO:O	1:B:200:LYS:NZ	2.29	0.63
1:A:3:GLU:CB	2:A:1722:GOL:H32	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:SER:OG	1:A:161:GLU:HG3	1.98	0.62
1:B:304:LEU:HD11	1:B:324:ALA:HB1	1.79	0.62
1:A:461:LEU:O	1:A:465:ILE:HG12	2.00	0.62
1:A:708:LEU:HA	1:A:711:TRP:CE2	2.36	0.61
1:A:274:GLU:CD	1:A:657:ARG:HH21	2.07	0.61
1:B:540:GLY:HA3	5:B:2129:HOH:O	1.99	0.61
1:B:699:ARG:HG2	2:B:1719:GOL:O2	2.00	0.60
1:B:37:GLN:HB3	5:B:2012:HOH:O	2.02	0.60
1:B:68:ALA:HB2	1:B:260:ALA:HA	1.84	0.59
1:B:305:GLY:O	1:B:309:ARG:HG3	2.02	0.59
1:B:483:MET:HE3	1:B:630:ALA:HB2	1.85	0.59
1:A:136:GLN:NE2	1:A:247:GLY:HA3	2.19	0.58
1:B:0:HIS:O	1:B:17:CYS:HB3	2.04	0.58
1:A:135:THR:HB	1:A:251:GLU:OE2	2.03	0.58
1:B:245:GLU:CD	1:B:245:GLU:H	2.12	0.58
1:A:226:VAL:HG22	1:A:229:PRO:CD	2.34	0.58
1:B:33:ARG:HD3	5:B:2010:HOH:O	2.00	0.58
1:B:279:LYS:NZ	4:B:1720:3H9:O9A	2.35	0.57
1:B:226:VAL:HG22	1:B:229:PRO:CD	2.35	0.57
1:B:708:LEU:HA	1:B:711:TRP:CE2	2.38	0.57
1:B:267:LEU:CD2	1:B:657:ARG:HG2	2.33	0.57
1:B:359:LYS:HE3	1:B:360:PRO:HD2	1.86	0.57
1:B:226:VAL:O	1:B:229:PRO:HD2	2.04	0.57
1:B:145:PRO:O	5:B:2047:HOH:O	2.17	0.57
1:A:365:SER:CB	1:A:370:GLU:HG3	2.34	0.57
1:B:244:TYR:CZ	1:B:248:ILE:HD11	2.38	0.57
1:B:500:LYS:HE2	5:B:2113:HOH:O	2.05	0.57
1:A:435:PRO:HB2	5:A:2098:HOH:O	2.04	0.56
1:B:713:SER:N	5:B:2174:HOH:O	2.36	0.56
1:B:484:LEU:HD21	1:B:488:TYR:HE2	1.71	0.56
1:B:540:GLY:C	1:B:542:SER:H	2.13	0.56
1:A:242:HIS:HB3	1:A:246:VAL:HB	1.88	0.56
1:B:383:GLU:OE1	1:B:410:SER:HB2	2.06	0.55
1:B:437:HIS:HD2	5:B:2096:HOH:O	1.88	0.55
1:B:282:THR:OG1	1:B:286:ALA:HB3	2.07	0.55
1:A:274:GLU:OE1	1:A:657:ARG:NH2	2.40	0.55
1:B:354:GLY:O	1:B:355:GLN:HG2	2.07	0.55
1:A:570:PHE:HB2	1:A:574:THR:HG23	1.89	0.54
1:B:95:GLY:O	1:B:117:ALA:HA	2.07	0.54
1:A:435:PRO:HG2	5:A:2098:HOH:O	2.08	0.54
1:B:158:SER:OG	1:B:161:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:GLY:C	1:B:542:SER:N	2.63	0.54
1:B:97:ALA:HB3	1:B:119:VAL:HG12	1.90	0.53
1:A:33:ARG:HD3	1:A:81:GLU:OE1	2.09	0.53
1:A:540:GLY:C	1:A:542:SER:N	2.66	0.53
1:B:77:SER:HB2	5:B:2026:HOH:O	2.08	0.53
1:A:244:TYR:CZ	1:A:248:ILE:HD11	2.45	0.52
1:B:306:THR:OG1	5:B:2093:HOH:O	2.14	0.52
1:B:453:THR:O	1:B:457:THR:OG1	2.18	0.52
1:A:245:GLU:CD	1:A:245:GLU:H	2.16	0.52
1:B:529:GLY:O	1:B:533:ARG:HG3	2.09	0.52
1:A:133:ARG:HD2	1:A:248:ILE:CG1	2.40	0.51
1:A:212:PHE:CZ	1:A:237:GLN:HA	2.45	0.51
1:B:365:SER:CB	1:B:370:GLU:HG3	2.40	0.51
1:B:219:VAL:HG11	1:B:230:GLU:HA	1.93	0.51
1:B:46:LYS:HB2	1:B:188:ILE:HD11	1.93	0.51
1:B:96:VAL:HG21	4:B:1720:3H9:HDP	1.93	0.50
1:B:133:ARG:HD2	1:B:248:ILE:HG13	1.93	0.50
1:A:219:VAL:HG11	1:A:230:GLU:HA	1.94	0.50
1:B:56:ASN:HB2	5:B:2008:HOH:O	2.12	0.50
1:A:331:GLN:HB2	5:A:2085:HOH:O	2.11	0.50
1:A:570:PHE:HB2	1:A:574:THR:CG2	2.42	0.50
1:B:135:THR:CG2	1:B:251:GLU:OE2	2.59	0.50
1:B:405:LEU:O	1:B:427:VAL:HA	2.11	0.50
1:B:532:ILE:O	1:B:536:GLN:HG3	2.11	0.50
1:B:205:LEU:O	5:B:2054:HOH:O	2.20	0.49
1:B:244:TYR:CE1	1:B:248:ILE:CD1	2.95	0.49
1:B:291:ALA:HB2	1:B:452:PRO:HB3	1.93	0.49
1:A:529:GLY:O	1:A:533:ARG:HG3	2.12	0.49
1:B:135:THR:HB	1:B:251:GLU:OE2	2.13	0.49
1:B:187:ILE:HD12	1:B:187:ILE:C	2.38	0.49
1:A:135:THR:CG2	1:A:136:GLN:OE1	2.61	0.48
1:B:136:GLN:NE2	1:B:247:GLY:HA3	2.27	0.48
1:A:485:ALA:HB3	1:A:486:PRO:HD3	1.95	0.48
1:A:519:ARG:HD3	1:A:589:HIS:CE1	2.48	0.48
1:A:30:ARG:CZ	5:A:2007:HOH:O	2.62	0.48
1:A:305:GLY:O	1:A:309:ARG:HG3	2.13	0.48
1:A:519:ARG:HD2	5:A:2119:HOH:O	2.14	0.48
1:B:440:ARG:HD2	1:B:466:GLY:O	2.13	0.48
1:A:540:GLY:C	1:A:542:SER:H	2.20	0.48
1:A:228:ALA:N	1:A:229:PRO:CD	2.76	0.48
1:B:633:ILE:HG23	1:B:638:MET:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:TYR:O	1:A:226:VAL:HG13	2.14	0.47
1:A:337:LYS:NZ	5:A:2086:HOH:O	2.47	0.47
1:A:133:ARG:HD2	1:A:248:ILE:HD11	1.96	0.47
1:B:274:GLU:CD	1:B:657:ARG:HH21	2.23	0.47
1:B:519:ARG:HD3	1:B:589:HIS:CE1	2.49	0.47
1:A:226:VAL:HG22	1:A:229:PRO:HD2	1.96	0.47
1:A:435:PRO:CB	5:A:2098:HOH:O	2.62	0.47
1:B:136:GLN:CG	1:B:248:ILE:HD12	2.38	0.47
1:B:479:VAL:HG22	1:B:633:ILE:HG21	1.95	0.47
1:A:135:THR:HG22	1:A:251:GLU:OE2	2.14	0.47
1:A:708:LEU:HA	1:A:711:TRP:CD2	2.50	0.47
1:B:368:THR:O	1:B:398:LEU:HD21	2.15	0.47
1:B:485:ALA:HB3	1:B:486:PRO:HD3	1.95	0.47
1:A:133:ARG:CD	1:A:248:ILE:HG13	2.45	0.47
1:B:223:TYR:O	1:B:226:VAL:HG13	2.15	0.47
1:B:672:PRO:HD3	1:B:705:SER:OG	2.15	0.47
1:B:708:LEU:C	1:B:708:LEU:HD23	2.40	0.46
1:B:475:CYS:SG	1:B:638:MET:HG3	2.56	0.46
1:B:601:GLN:O	1:B:605:VAL:HG23	2.15	0.46
1:A:187:ILE:C	1:A:187:ILE:HD12	2.40	0.46
1:B:288:TRP:NE1	5:B:2092:HOH:O	2.08	0.46
1:B:527:ASP:HB3	1:B:570:PHE:CD1	2.50	0.46
1:B:337:LYS:HD2	1:B:337:LYS:HA	1.60	0.46
1:B:283:PRO:C	1:B:285:GLY:H	2.24	0.46
1:B:133:ARG:CD	1:B:248:ILE:HG13	2.46	0.46
1:A:337:LYS:HD2	1:A:337:LYS:HA	1.67	0.46
1:A:483:MET:HE3	1:A:630:ALA:HB2	1.98	0.45
1:B:24:VAL:HG11	1:B:75:LEU:HD13	1.98	0.45
1:A:435:PRO:CG	5:A:2098:HOH:O	2.63	0.45
1:B:428:ILE:HG21	1:B:458:VAL:HG21	1.99	0.45
1:B:1:MET:HB2	1:B:31:GLU:OE1	2.16	0.45
1:A:611:ARG:NH2	1:A:617:GLU:OE1	2.50	0.45
1:B:581:TYR:N	1:B:581:TYR:CD1	2.85	0.45
1:B:650:LEU:HD22	1:B:657:ARG:HA	1.99	0.44
1:B:699:ARG:HG2	2:B:1719:GOL:C2	2.47	0.44
1:A:136:GLN:HE21	1:A:247:GLY:HA3	1.80	0.44
1:A:406:CYS:HA	1:A:428:ILE:O	2.17	0.44
1:B:270:ALA:O	1:B:274:GLU:HG3	2.17	0.44
4:A:1725:3H9:O9P	4:A:1725:3H9:HDP	2.18	0.44
1:B:433:PHE:CE1	1:B:441:LEU:HD23	2.52	0.44
1:A:133:ARG:HD2	1:A:248:ILE:HG13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:SER:HB3	1:B:46:LYS:HG3	1.99	0.44
1:B:624:TYR:O	1:B:625:SER:C	2.56	0.44
1:B:713:SER:HB3	5:B:2174:HOH:O	2.18	0.43
1:A:3:GLU:HB2	2:A:1722:GOL:O3	2.15	0.43
1:B:78:LEU:O	1:B:82:ILE:HG13	2.17	0.43
1:A:223:TYR:HB3	1:A:226:VAL:HG13	1.98	0.43
1:A:400:LYS:N	5:A:2088:HOH:O	2.47	0.43
1:A:663:MET:HE2	1:A:663:MET:HA	1.99	0.43
1:A:698:ARG:HH11	1:A:698:ARG:HG2	1.84	0.43
1:B:6:ARG:HG3	1:B:6:ARG:HH11	1.82	0.43
1:A:244:TYR:CZ	1:A:248:ILE:CD1	3.02	0.43
1:A:484:LEU:HD21	1:A:488:TYR:HE2	1.83	0.43
1:B:406:CYS:HA	1:B:428:ILE:O	2.17	0.43
1:B:156:TYR:N	1:B:156:TYR:CD1	2.87	0.43
1:A:70:THR:O	1:A:71:PRO:C	2.58	0.43
1:A:123:GLU:O	1:A:124:VAL:C	2.61	0.43
1:A:411:ALA:O	1:A:412:LEU:HD23	2.19	0.43
1:A:485:ALA:N	1:A:486:PRO:HD2	2.33	0.43
1:A:494:LEU:HD13	1:A:618:ILE:HG12	2.00	0.43
1:A:43:HIS:O	1:A:46:LYS:NZ	2.52	0.43
1:B:328:ASP:HA	1:B:329:PRO:HD3	1.76	0.43
1:A:303:GLY:O	1:A:308:GLY:HA3	2.18	0.42
1:A:597:THR:CG2	1:B:382:PHE:HD2	2.32	0.42
1:B:337:LYS:HE3	1:B:341:PHE:HB2	2.00	0.42
1:A:135:THR:CB	1:A:251:GLU:OE2	2.67	0.42
1:A:524:ALA:HB2	5:A:2121:HOH:O	2.18	0.42
1:B:449:TYR:O	1:B:450:SER:C	2.63	0.42
1:B:499:SER:OG	1:B:500:LYS:N	2.52	0.42
1:A:156:TYR:N	1:A:156:TYR:CD1	2.88	0.42
1:B:133:ARG:HD2	1:B:248:ILE:CG1	2.50	0.42
1:B:699:ARG:HA	2:B:1719:GOL:H2	2.00	0.42
1:A:485:ALA:N	1:A:486:PRO:CD	2.82	0.42
1:B:3:GLU:HB2	5:B:2004:HOH:O	2.19	0.42
1:B:570:PHE:HB2	1:B:574:THR:HG23	2.02	0.42
1:A:565:CYS:O	1:B:570:PHE:CE2	2.73	0.42
1:A:330:LYS:H	1:A:330:LYS:HG2	1.71	0.42
1:A:253:LYS:CE	5:A:2053:HOH:O	2.67	0.42
1:A:9:HIS:HB3	1:A:185:GLN:NE2	2.31	0.41
1:A:596:SER:OG	1:B:330:LYS:HD2	2.19	0.41
1:A:626:LEU:HD23	1:A:626:LEU:C	2.45	0.41
1:B:98:LEU:CD1	4:B:1720:3H9:HDP	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:713:SER:CB	5:B:2174:HOH:O	2.62	0.41
1:B:73:LEU:N	1:B:73:LEU:HD12	2.35	0.41
1:B:406:CYS:HB3	1:B:430:THR:HG23	2.02	0.41
1:A:298:SER:HA	1:A:321:SER:HB2	2.01	0.41
1:A:408:ASN:O	1:A:408:ASN:CG	2.62	0.41
1:B:482:ARG:HD3	1:B:633:ILE:HD11	2.03	0.41
1:B:603:ARG:CB	5:B:2112:HOH:O	2.68	0.41
1:B:299:VAL:O	1:B:322:VAL:HA	2.20	0.41
1:A:379:GLU:OE2	1:A:388:LYS:NZ	2.51	0.41
1:B:506:GLY:O	1:B:510:GLU:HB2	2.21	0.41
1:A:244:TYR:CE1	1:A:248:ILE:CD1	3.04	0.41
1:B:140:ARG:HD3	1:B:197:ILE:O	2.21	0.41
1:B:430:THR:O	1:B:430:THR:OG1	2.31	0.41
1:B:489:ASN:ND2	5:B:2109:HOH:O	2.51	0.41
1:A:328:ASP:HA	1:A:329:PRO:HD3	1.77	0.40
1:A:27:THR:O	1:A:31:GLU:HG3	2.21	0.40
1:A:633:ILE:HG23	1:A:638:MET:HB2	2.04	0.40
1:A:73:LEU:HD21	1:A:252:GLU:HG3	2.04	0.40
1:A:123:GLU:HG3	4:A:1725:3H9:S1P	2.61	0.40
1:A:172:VAL:HG13	1:A:174:SER:H	1.87	0.40
1:A:244:TYR:CE1	1:A:248:ILE:HD11	2.56	0.40
1:A:323:VAL:HG11	1:A:370:GLU:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2010:HOH:O	5:B:2051:HOH:O[2_254]	2.08	0.12

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	725/742 (98%)	687 (95%)	36 (5%)	2 (0%)	36	53
1	B	719/742 (97%)	678 (94%)	35 (5%)	6 (1%)	16	28
All	All	1444/1484 (97%)	1365 (94%)	71 (5%)	8 (1%)	21	35

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-1	SER
1	B	284	SER
1	B	355	GLN
1	A	365	SER
1	B	356	ALA
1	B	68	ALA
1	B	318	VAL
1	B	128	ILE

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	596/609 (98%)	546 (92%)	50 (8%)	10	20
1	B	591/609 (97%)	548 (93%)	43 (7%)	13	25
All	All	1187/1218 (98%)	1094 (92%)	93 (8%)	11	22

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-5	VAL
1	A	1	MET
1	A	24	VAL
1	A	37	GLN
1	A	63	ILE
1	A	73	LEU
1	A	77	SER
1	A	96	VAL

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Mol	Chain	Res	Type
1	A	125	THR
1	A	135	THR
1	A	157	LEU
1	A	164	ARG
1	A	165	LEU
1	A	172	VAL
1	A	188	ILE
1	A	198	PHE
1	A	210	SER
1	A	214	GLU
1	A	219	VAL
1	A	226	VAL
1	A	234	ARG
1	A	248	ILE
1	A	258	LEU
1	A	275	LYS
1	A	292	SER
1	A	295	PRO
1	A	306	THR
1	A	337	LYS
1	A	340	THR
1	A	359	LYS
1	A	362	LEU
1	A	368	THR
1	A	371	LEU
1	A	372	SER
1	A	373	THR
1	A	382	PHE
1	A	398	LEU
1	A	441	LEU
1	A	510	GLU
1	A	514	LYS
1	A	523	LEU
1	A	526	LEU
1	A	528	VAL
1	A	572	GLN
1	A	585	LEU
1	A	610	GLN
1	A	668	SER
1	A	675	LEU
1	A	695	ASP
1	A	721	LYS

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Mol	Chain	Res	Type
1	B	1	MET
1	B	73	LEU
1	B	96	VAL
1	B	125	THR
1	B	135	THR
1	B	157	LEU
1	B	164	ARG
1	B	165	LEU
1	B	204	SER
1	B	210	SER
1	B	214	GLU
1	B	219	VAL
1	B	226	VAL
1	B	248	ILE
1	B	258	LEU
1	B	284	SER
1	B	292	SER
1	B	306	THR
1	B	337	LYS
1	B	340	THR
1	B	355	GLN
1	B	357	SER
1	B	359	LYS
1	B	362	LEU
1	B	368	THR
1	B	371	LEU
1	B	373	THR
1	B	382	PHE
1	B	398	LEU
1	B	510	GLU
1	B	523	LEU
1	B	528	VAL
1	B	543	LEU
1	B	549	VAL
1	B	572	GLN
1	B	585	LEU
1	B	596	SER
1	B	599	LEU
1	B	610	GLN
1	B	627	ILE
1	B	668	SER
1	B	672	PRO

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Mol	Chain	Res	Type
1	B	695	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	HIS
1	A	56	ASN
1	A	64	HIS
1	A	185	GLN
1	A	352	GLN
1	A	572	GLN
1	A	589	HIS
1	A	610	GLN
1	A	679	GLN
1	B	0	HIS
1	B	37	GLN
1	B	94	GLN
1	B	185	GLN
1	B	353	ASN
1	B	489	ASN
1	B	554	ASN
1	B	572	GLN
1	B	610	GLN
1	B	679	GLN
1	B	718	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

8 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	GOL	B	1719	-	5,5,5	0.37	0	5,5,5	0.45	0
3	SO4	B	1721	-	4,4,4	0.35	0	6,6,6	0.30	0
4	3H9	B	1720	-	56,58,58	1.43	6 (10%)	79,85,85	1.67	16 (20%)
3	SO4	A	1723	-	4,4,4	0.44	0	6,6,6	0.51	0
3	SO4	A	1724	-	4,4,4	0.40	0	6,6,6	0.28	0
2	GOL	A	1722	-	5,5,5	0.83	0	5,5,5	1.67	1 (20%)
3	SO4	A	1726	-	4,4,4	0.49	0	6,6,6	0.83	0
4	3H9	A	1725	-	56,58,58	1.98	13 (23%)	79,85,85	1.72	14 (17%)

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	GOL	B	1719	-	-	2/4/4/4	-
2	GOL	A	1722	-	-	4/4/4/4	-
4	3H9	B	1720	-	-	11/58/74/74	0/3/3/3
4	3H9	A	1725	-	-	13/58/74/74	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1725	3H9	P2A-O3A	8.40	1.68	1.59
4	B	1720	3H9	P2A-O3A	5.83	1.65	1.59
4	A	1725	3H9	P3B-O8A	5.14	1.66	1.50
4	A	1725	3H9	P3B-O3B	5.05	1.68	1.59
4	B	1720	3H9	P1A-O3A	4.16	1.64	1.59
4	A	1725	3H9	C5A-N7A	-4.04	1.31	1.39
4	B	1720	3H9	P3B-O9A	-3.11	1.43	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1725	3H9	P1A-O3A	2.93	1.62	1.59
4	A	1725	3H9	O4B-C4B	2.65	1.50	1.45
4	A	1725	3H9	C8A-N9A	-2.58	1.33	1.37
4	B	1720	3H9	C4A-N9A	-2.56	1.32	1.37
4	B	1720	3H9	P3B-O8A	2.55	1.58	1.50
4	A	1725	3H9	OAP-CAP	2.49	1.46	1.42
4	B	1720	3H9	C5A-N7A	-2.45	1.34	1.39
4	A	1725	3H9	C5B-C4B	2.37	1.58	1.51
4	A	1725	3H9	C1B-N9A	2.31	1.52	1.46
4	A	1725	3H9	P2A-O6A	2.21	1.68	1.59
4	A	1725	3H9	O4B-C1B	2.15	1.47	1.42
4	A	1725	3H9	CCP-CBP	2.05	1.56	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1725	3H9	C5A-C4A-N3A	-5.84	118.67	126.72
4	A	1725	3H9	N3A-C2A-N1A	-4.94	121.10	128.58
4	B	1720	3H9	C5A-C4A-N3A	-4.84	120.06	126.72
4	B	1720	3H9	N3A-C2A-N1A	-4.77	121.36	128.58
4	A	1725	3H9	N3A-C4A-N9A	3.89	133.78	127.17
4	A	1725	3H9	C2A-N3A-C4A	3.77	121.04	111.83
4	B	1720	3H9	C2A-N3A-C4A	3.75	120.98	111.83
4	B	1720	3H9	C2-C1-S1P	3.73	118.27	113.56
4	B	1720	3H9	O9A-P3B-O7A	3.72	121.76	107.80
4	A	1725	3H9	C4-C3-C2	-3.54	100.99	112.88
4	B	1720	3H9	C2P-C3P-N4P	-3.25	105.62	112.41
4	B	1720	3H9	O1-C1-S1P	-3.08	118.76	122.68
4	A	1725	3H9	C5A-N7A-C8A	3.03	108.22	103.45
4	B	1720	3H9	C4A-C5A-N7A	-3.02	107.13	110.58
4	A	1725	3H9	C6P-C7P-N8P	-3.01	105.58	112.00
2	A	1722	GOL	O2-C2-C1	3.00	121.60	109.18
4	B	1720	3H9	N9A-C8A-N7A	-2.98	109.71	113.94
4	B	1720	3H9	O3A-P1A-O1A	2.95	119.58	110.70
4	B	1720	3H9	N3A-C4A-N9A	2.92	132.13	127.17
4	A	1725	3H9	C4A-C5A-N7A	-2.87	107.30	110.58
4	A	1725	3H9	N9A-C8A-N7A	-2.73	110.06	113.94
4	A	1725	3H9	O4B-C4B-C5B	2.61	117.70	109.33
4	A	1725	3H9	O2A-P1A-O3A	2.45	113.91	107.27
4	B	1720	3H9	C5A-N7A-C8A	2.44	107.28	103.45
4	B	1720	3H9	O5A-P2A-O4A	2.27	122.99	112.44
4	B	1720	3H9	CDP-CBP-CAP	2.23	112.57	108.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1720	3H9	C4A-N9A-C8A	2.20	108.05	105.74
4	B	1720	3H9	O2B-C2B-C1B	-2.20	102.53	110.10
4	A	1725	3H9	O3-C3-C2	2.11	115.12	109.64
4	A	1725	3H9	C3-C2-C1	2.11	118.55	113.86
4	A	1725	3H9	O9A-P3B-O3B	2.09	113.98	105.85

There are no chirality outliers.

All (30) torsion outliers are listed below:

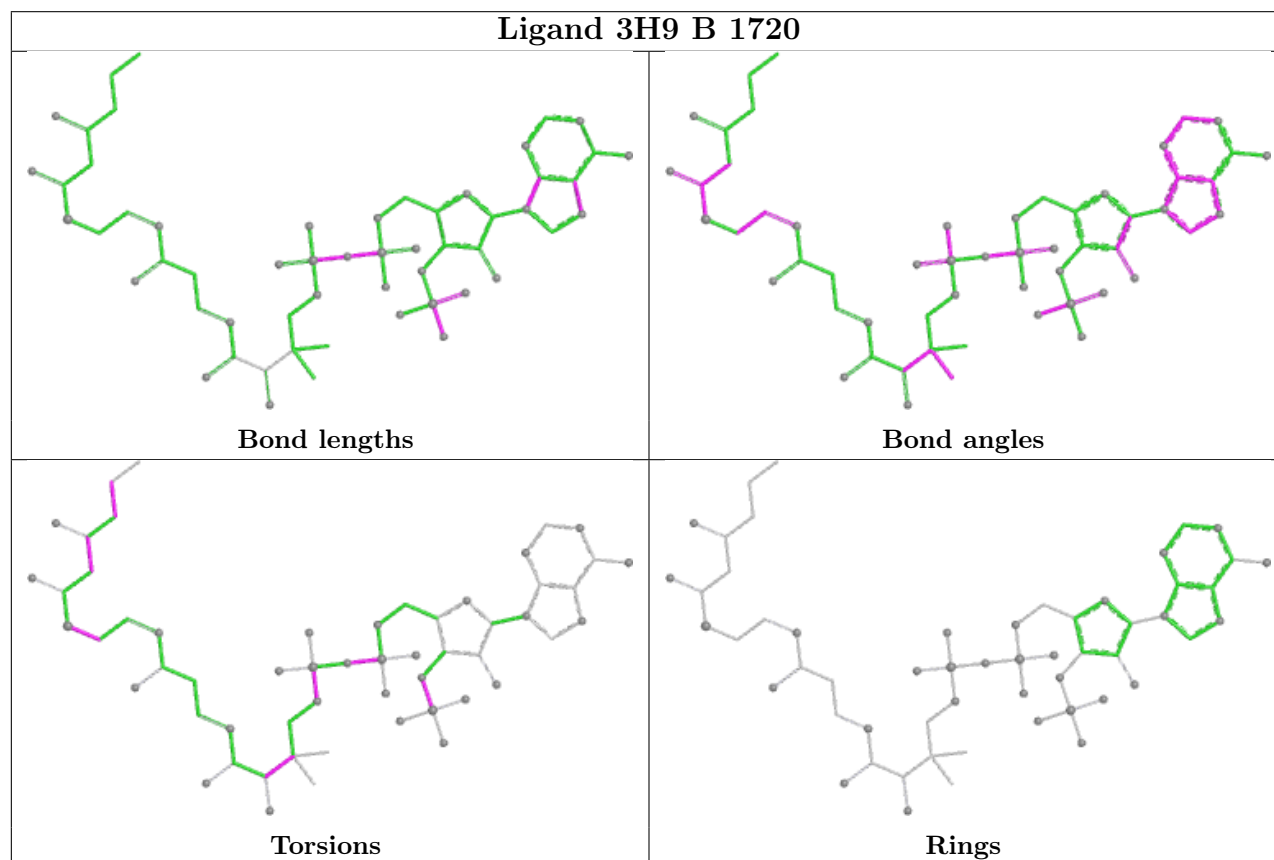
Mol	Chain	Res	Type	Atoms
2	A	1722	GOL	O1-C1-C2-C3
4	A	1725	3H9	C1-C2-C3-O3
4	A	1725	3H9	C1-C2-C3-C4
4	A	1725	3H9	P1A-O3A-P2A-O6A
4	A	1725	3H9	CCP-O6A-P2A-O3A
4	A	1725	3H9	CCP-O6A-P2A-O4A
4	A	1725	3H9	CCP-O6A-P2A-O5A
4	A	1725	3H9	CAP-CBP-CCP-O6A
4	A	1725	3H9	CDP-CBP-CCP-O6A
4	A	1725	3H9	CEP-CBP-CCP-O6A
4	B	1720	3H9	C3P-C2P-S1P-C1
4	B	1720	3H9	CCP-O6A-P2A-O3A
4	B	1720	3H9	CCP-O6A-P2A-O5A
4	B	1720	3H9	C9P-CAP-CBP-CCP
2	A	1722	GOL	C1-C2-C3-O3
2	B	1719	GOL	C1-C2-C3-O3
4	A	1725	3H9	O3-C3-C4-C5
2	A	1722	GOL	O2-C2-C3-O3
4	A	1725	3H9	C2-C3-C4-C5
2	A	1722	GOL	O1-C1-C2-O2
2	B	1719	GOL	O2-C2-C3-O3
4	B	1720	3H9	C3-C4-C5-C6
4	A	1725	3H9	N8P-C9P-CAP-CBP
4	B	1720	3H9	C1-C2-C3-O3
4	A	1725	3H9	C3B-O3B-P3B-O8A
4	B	1720	3H9	C3B-O3B-P3B-O8A
4	B	1720	3H9	C9P-CAP-CBP-CDP
4	B	1720	3H9	C9P-CAP-CBP-CEP
4	B	1720	3H9	OAP-CAP-CBP-CEP
4	B	1720	3H9	P2A-O3A-P1A-O2A

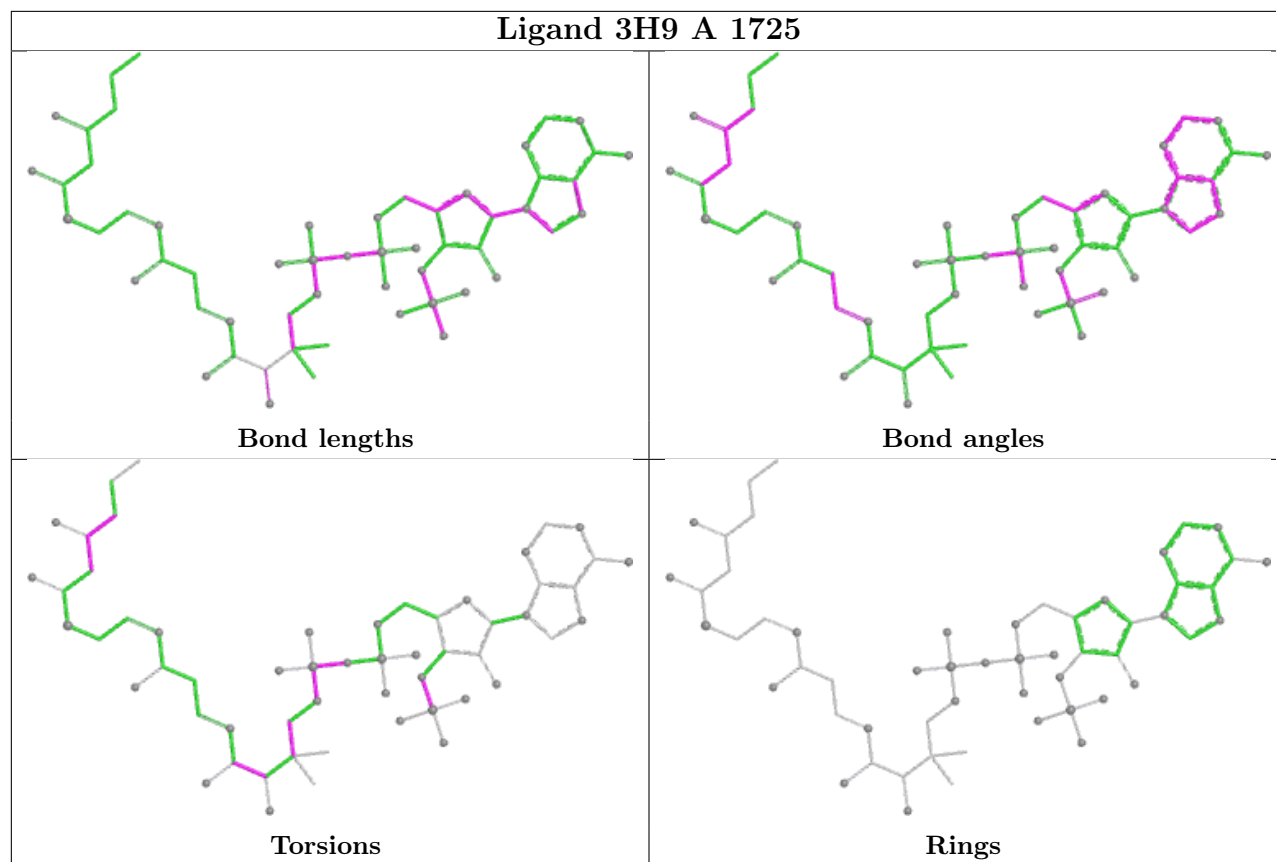
There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1719	GOL	4	0
4	B	1720	3H9	4	0
2	A	1722	GOL	8	0
4	A	1725	3H9	2	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	727/742 (97%)	0.31	54 (7%)	20	18	9, 33, 72, 112	0
1	B	721/742 (97%)	0.32	58 (8%)	18	16	11, 34, 72, 112	0
All	All	1448/1484 (97%)	0.31	112 (7%)	19	17	9, 34, 73, 112	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	411	ALA	6.1
1	A	355	GLN	6.0
1	A	-5	VAL	5.2
1	A	350	ALA	5.0
1	B	355	GLN	4.9
1	A	351	HIS	4.6
1	B	449	TYR	4.5
1	A	382	PHE	4.5
1	B	356	ALA	4.5
1	B	347	ALA	4.4
1	B	354	GLY	4.3
1	A	356	ALA	4.2
1	B	348	SER	3.9
1	B	43	HIS	3.9
1	B	358	ALA	3.8
1	A	364	PHE	3.8
1	A	358	ALA	3.6
1	B	382	PHE	3.6
1	B	343	LEU	3.4
1	A	357	SER	3.4
1	B	535	GLY	3.4
1	A	348	SER	3.3
1	A	329	PRO	3.3
1	A	352	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	365	SER	3.2
1	A	70	THR	3.1
1	A	346	GLU	3.1
1	A	359	LYS	3.1
1	A	343	LEU	3.1
1	A	242	HIS	3.1
1	A	354	GLY	3.0
1	A	327	SER	3.0
1	A	362	LEU	3.0
1	B	372	SER	2.9
1	B	351	HIS	2.9
1	B	718	HIS	2.9
1	B	330	LYS	2.9
1	B	364	PHE	2.9
1	A	345	LYS	2.8
1	B	359	LYS	2.8
1	B	0	HIS	2.8
1	A	69	PHE	2.8
1	B	339	ILE	2.8
1	A	347	ALA	2.8
1	B	346	GLU	2.8
1	B	353	ASN	2.7
1	A	353	ASN	2.7
1	B	350	ALA	2.7
1	B	373	THR	2.7
1	B	9	HIS	2.7
1	A	374	VAL	2.7
1	B	335	ALA	2.7
1	B	360	PRO	2.6
1	B	-2	GLY	2.6
1	B	5	LEU	2.6
1	B	371	LEU	2.6
1	A	336	LYS	2.6
1	A	339	ILE	2.5
1	A	5	LEU	2.5
1	A	391	VAL	2.5
1	A	397	ALA	2.5
1	B	541	PRO	2.5
1	B	545	PRO	2.5
1	A	437	HIS	2.5
1	A	367	SER	2.5
1	B	345	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	554	ASN	2.5
1	B	185	GLN	2.5
1	A	449	TYR	2.4
1	A	332	LEU	2.4
1	B	349	ARG	2.4
1	A	390	LYS	2.4
1	A	373	THR	2.3
1	A	398	LEU	2.3
1	A	341	PHE	2.3
1	A	369	LYS	2.3
1	B	361	LYS	2.3
1	A	393	ALA	2.3
1	B	290	THR	2.3
1	B	342	THR	2.3
1	B	357	SER	2.3
1	A	-2	GLY	2.3
1	B	341	PHE	2.3
1	A	718	HIS	2.3
1	A	371	LEU	2.3
1	A	372	SER	2.2
1	B	676	GLU	2.2
1	B	370	GLU	2.2
1	B	289	LYS	2.2
1	A	368	THR	2.2
1	B	-1	SER	2.2
1	B	8	PRO	2.2
1	A	607	HIS	2.1
1	B	539	THR	2.1
1	B	331	GLN	2.1
1	B	368	THR	2.1
1	A	609	GLU	2.1
1	B	178	GLU	2.1
1	B	366	SER	2.1
1	B	427	VAL	2.1
1	A	241	LYS	2.1
1	A	322	VAL	2.1
1	B	171	VAL	2.1
1	B	362	LEU	2.1
1	B	363	ARG	2.1
1	A	720	SER	2.1
1	A	335	ALA	2.0
1	A	386	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	352	GLN	2.0
1	B	369	LYS	2.0
1	B	546	GLY	2.0
1	B	338	ILE	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](#)

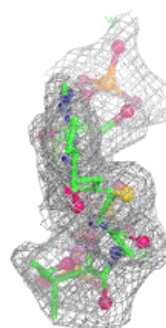
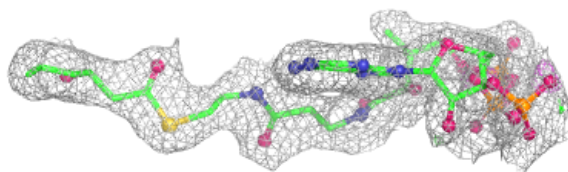
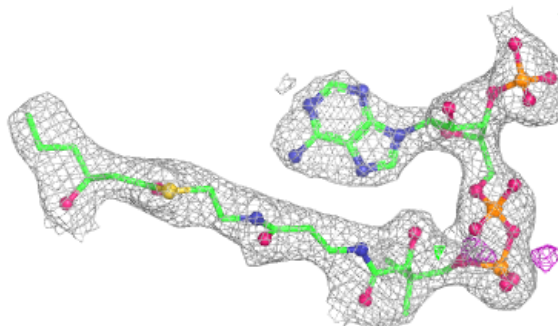
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	1722	6/6	0.78	0.32	36,37,38,39	0
3	SO4	A	1724	5/5	0.78	0.19	71,73,74,74	0
2	GOL	B	1719	6/6	0.80	0.19	51,52,54,56	0
3	SO4	A	1723	5/5	0.87	0.17	50,54,56,57	0
3	SO4	B	1721	5/5	0.91	0.11	59,61,63,63	0
4	3H9	A	1725	56/56	0.92	0.10	21,50,55,59	0
4	3H9	B	1720	56/56	0.97	0.07	21,31,38,40	0
3	SO4	A	1726	5/5	0.98	0.07	29,29,32,34	0

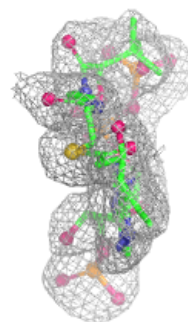
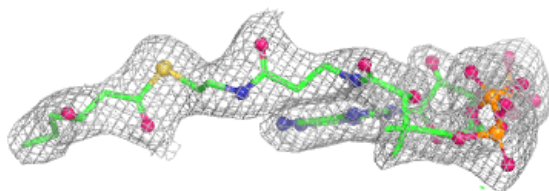
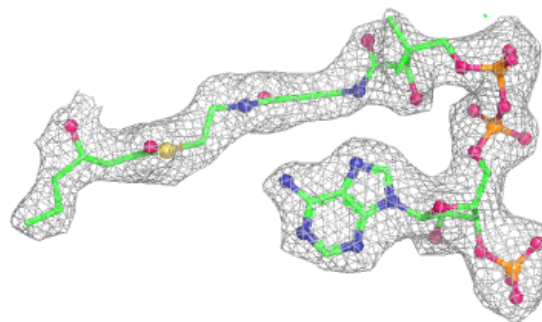
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3H9 A 1725:

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

**Electron density around 3H9 B 1720:**

$2mF_o-DF_c$ (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.