



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 04:08 PM BST

PDB ID : 4EGA
Title : Trypanosoma brucei methionyl-tRNA synthetase in complex with inhibitor Chem 1320
Authors : Koh, C.Y.; Kim, J.E.; Shibata, S.; Fan, E.; Verlinde, C.L.M.J.; Hol, W.G.J.
Deposited on : 2012-03-30
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4.dev1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

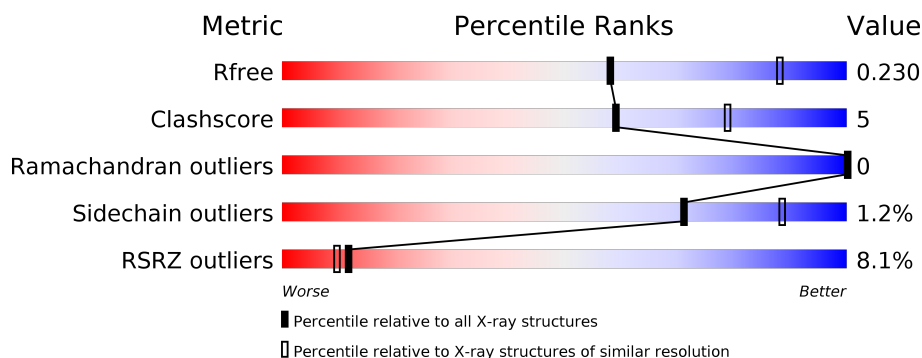
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 on 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	542	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>9%</div> <div></div> </div> </div>
1	B	542	<div> <div>10%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div></div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8936 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 Methionyl-tRNA synthetase, putative.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	524	Total	As	C	N	O	S	0	1	0
			4210	2	2710	711	776	11			
1	B	528	Total	As	C	N	O	S	0	4	0
			4253	2	2741	718	780	12			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q38C91
A	-3	PRO	-	EXPRESSION TAG	UNP Q38C91
A	-2	GLY	-	EXPRESSION TAG	UNP Q38C91
A	-1	SER	-	EXPRESSION TAG	UNP Q38C91
A	0	MET	-	EXPRESSION TAG	UNP Q38C91
A	309	THR	ALA	CONFLICT	UNP Q38C91
A	452	ALA	LYS	ENGINEERED MUTATION	UNP Q38C91
A	453	ARG	LYS	ENGINEERED MUTATION	UNP Q38C91
A	454	ALA	GLU	ENGINEERED MUTATION	UNP Q38C91
A	499	VAL	ALA	CONFLICT	UNP Q38C91
A	503	ASN	SER	CONFLICT	UNP Q38C91
B	-4	GLY	-	EXPRESSION TAG	UNP Q38C91
B	-3	PRO	-	EXPRESSION TAG	UNP Q38C91
B	-2	GLY	-	EXPRESSION TAG	UNP Q38C91
B	-1	SER	-	EXPRESSION TAG	UNP Q38C91
B	0	MET	-	EXPRESSION TAG	UNP Q38C91
B	309	THR	ALA	CONFLICT	UNP Q38C91
B	452	ALA	LYS	ENGINEERED MUTATION	UNP Q38C91
B	453	ARG	LYS	ENGINEERED MUTATION	UNP Q38C91
B	454	ALA	GLU	ENGINEERED MUTATION	UNP Q38C91
B	499	VAL	ALA	CONFLICT	UNP Q38C91
B	503	ASN	SER	CONFLICT	UNP Q38C91

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



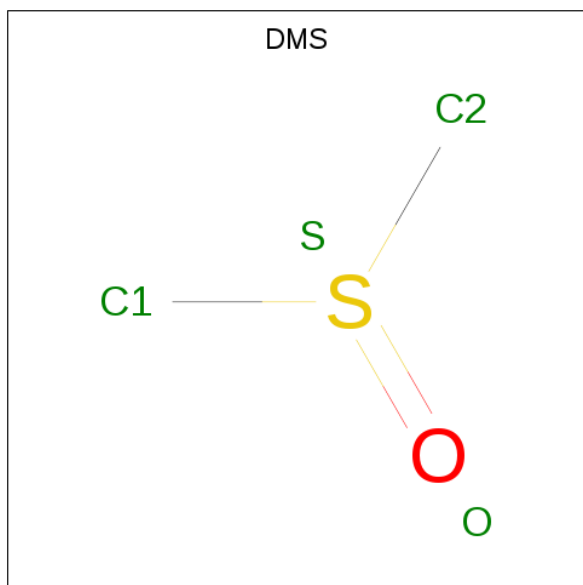
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total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

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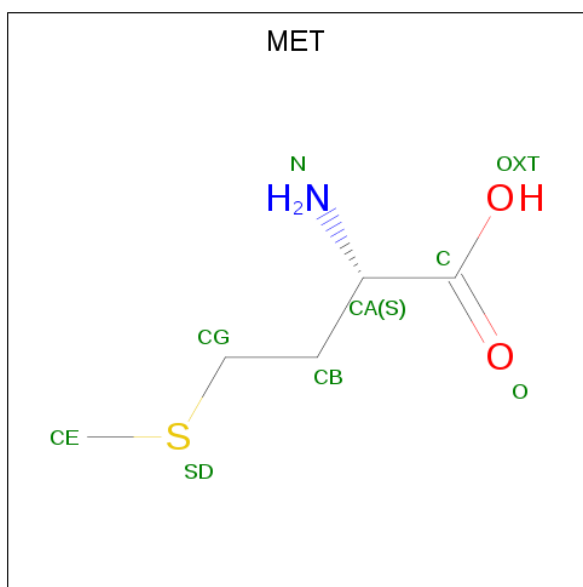
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



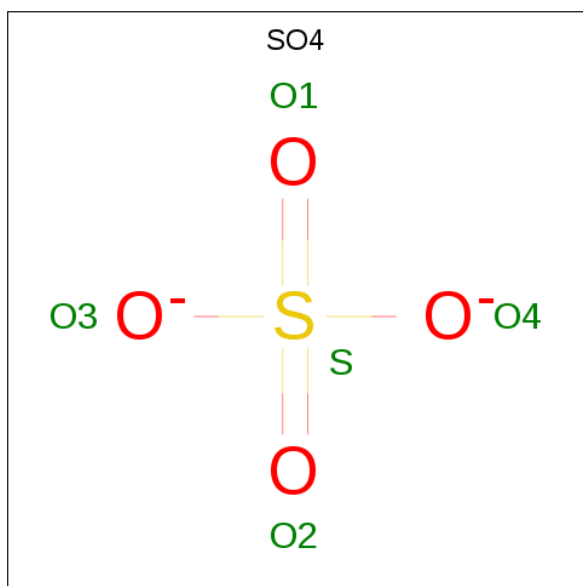
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is METHIONINE (three-letter code: MET) (formula: $C_5H_{11}NO_2S$).



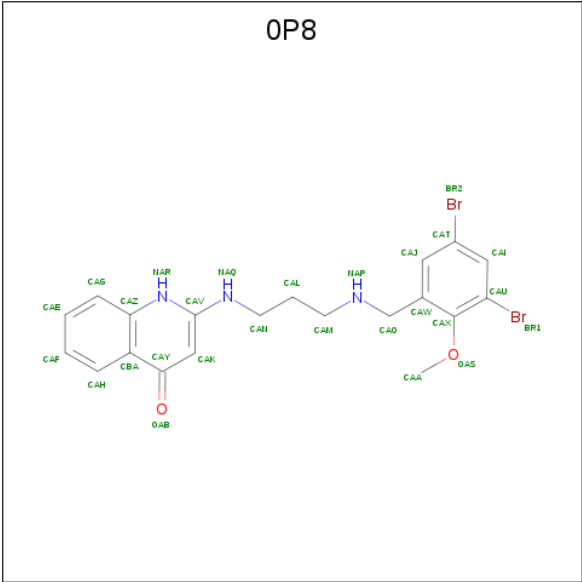
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			9	5	1	2	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is 2-({3-[(3,5-dibromo-2-methoxybenzyl)amino]propyl}amino)quinolin-4(1H)-one (three-letter code: 0P8) (formula: C₂₀H₂₁Br₂N₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
6	B	1	27	2	20	3	2	0	0

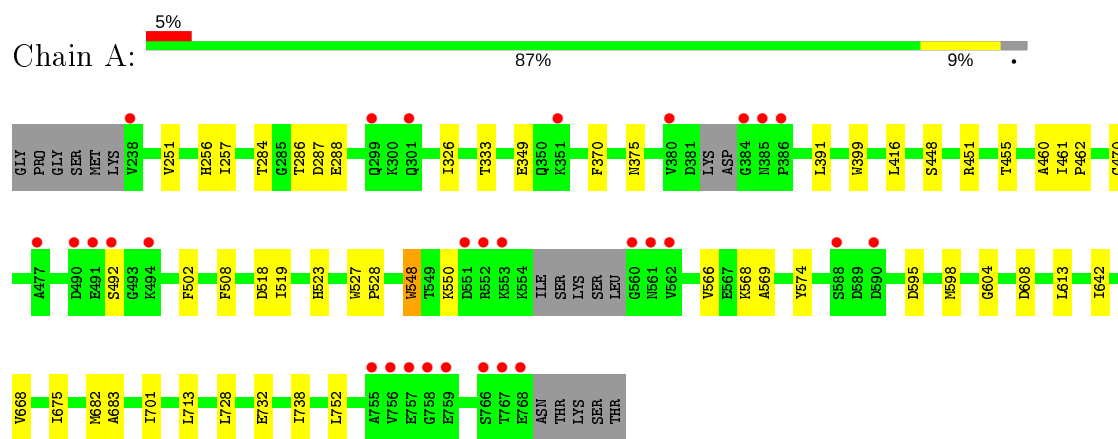
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	159	Total	O	0	0
			159	159		
7	B	143	Total	O	0	0
			143	143		

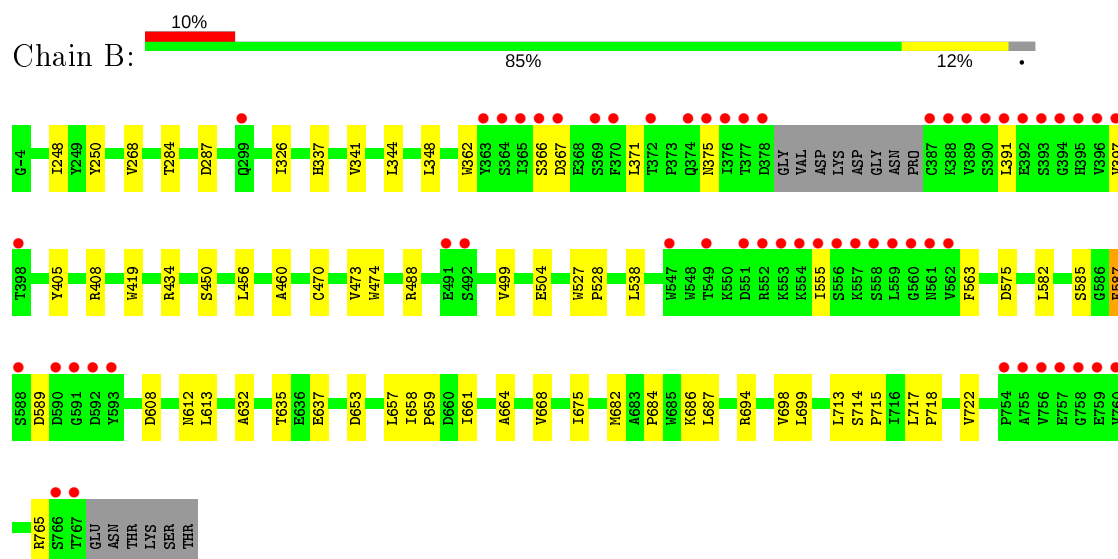
3 Residue-property plots

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: Methionyl-tRNA synthetase, putative



- Molecule 1: Methionyl-tRNA synthetase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.54Å 105.92Å 207.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 31.45 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-2.70) 98.8 (31.45-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.68Å)	Xtriage
Refinement program	REFMAC refmac_5.6.0117	Depositor
R, R_{free}	0.188 , 0.228 0.192 , 0.230	Depositor DCC
R_{free} test set	2675 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.547	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	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	8936	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: CAS, GOL, DMS, SO4, OP8

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	0.55	2/4301 (0.0%)	0.63	0/5842
1	B	0.55	2/4355 (0.0%)	0.60	0/5913
All	All	0.55	4/8656 (0.0%)	0.61	0/11755

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	399	TRP	CD2-CE2	5.33	1.47	1.41
1	B	362	TRP	CD2-CE2	5.26	1.47	1.41
1	B	419	TRP	CD2-CE2	5.23	1.47	1.41
1	A	548	TRP	CD2-CE2	5.05	1.47	1.41

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	A	4210	0	4147	34	0
1	B	4253	0	4213	41	0
2	A	54	0	72	5	0
2	B	48	0	64	2	0
3	A	16	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	18	1	0
4	A	9	0	8	1	0
5	B	5	0	0	0	0
6	B	27	0	21	6	0
7	A	159	0	0	0	0
7	B	143	0	0	4	0
All	All	8936	0	8567	80	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 5.

All (80) 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)
6:B:813:OP8:H7	6:B:813:OP8:H2	1.49	0.94
1:B:460:ALA:O	1:B:470:CAS:CE2	2.23	0.87
6:B:813:OP8:H7	6:B:813:OP8:CAA	2.14	0.77
1:B:284:THR:HG22	1:B:326:ILE:HG21	1.67	0.77
6:B:813:OP8:CAO	6:B:813:OP8:H2	2.16	0.75
1:A:460:ALA:O	1:A:470:CAS:CE2	2.38	0.71
1:B:668:VAL:HG11	1:B:713:LEU:HG	1.77	0.66
1:B:632:ALA:HB1	2:B:806:GOL:H31	1.78	0.65
1:B:635:THR:OG1	1:B:637[B]:GLU:HG2	1.97	0.64
1:B:488:ARG:NH2	1:B:504:GLU:OE2	2.32	0.62
1:A:416:LEU:HD21	1:A:528:PRO:HB2	1.81	0.62
1:A:256:HIS:ND1	1:A:257:ILE:O	2.29	0.61
1:B:371:LEU:HD12	1:B:397:VAL:HG11	1.84	0.59
1:B:653:ASP:O	1:B:657:LEU:HD13	2.02	0.59
1:A:460:ALA:C	1:A:470:CAS:CE2	2.72	0.58
1:A:461:ILE:C	1:A:470:CAS:CE2	2.71	0.58
6:B:813:OP8:CAO	6:B:813:OP8:CAA	2.80	0.57
6:B:813:OP8:H11	6:B:813:OP8:H2	1.88	0.55
1:B:585:SER:OG	1:B:589:ASP:HB2	2.06	0.55
1:B:765:ARG:NE	7:B:977:HOH:O	2.37	0.55
1:B:408:ARG:NH2	2:B:804:GOL:O2	2.39	0.55
3:A:811:DMS:H23	3:A:812:DMS:S	2.47	0.54
1:A:668:VAL:HG11	1:A:713:LEU:HG	1.89	0.54
1:A:550:LYS:O	2:A:809:GOL:C3	2.56	0.54
1:B:658:ILE:N	1:B:659:PRO:HA	2.22	0.53
1:A:451:ARG:NH2	1:A:455:THR:HG21	2.23	0.53
1:B:268:VAL:HG11	1:B:661:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:ALA:C	1:B:470:CAS:CE2	2.79	0.51
1:B:686:LYS:NZ	7:B:986:HOH:O	2.42	0.51
1:B:613:LEU:HD11	1:B:675:ILE:HG22	1.93	0.51
1:B:575:ASP:H	3:B:811:DMS:H21	1.76	0.51
1:A:518:ASP:HB3	1:A:548:TRP:CE3	2.47	0.50
1:A:462:PRO:N	1:A:470:CAS:CE2	2.74	0.50
1:B:268:VAL:HG21	1:B:582:LEU:HD11	1.92	0.49
1:A:519:ILE:HD12	1:A:523:HIS:CE1	2.47	0.49
1:B:714:SER:N	1:B:715:PRO:CD	2.76	0.49
1:B:555:ILE:HD13	1:B:563:PHE:HB3	1.95	0.49
1:A:251:VAL:HG13	1:A:286:THR:HB	1.95	0.48
1:A:284:THR:HG22	1:A:326:ILE:HG21	1.95	0.48
1:A:288:GLU:HB2	1:A:333:THR:HG23	1.94	0.48
1:A:349:GLU:HG3	2:A:807:GOL:C1	2.44	0.48
1:A:287:ASP:OD2	4:A:814:MET:N	2.47	0.47
1:B:344:LEU:O	1:B:348:LEU:HD13	2.14	0.47
1:A:732:GLU:HB2	2:A:804:GOL:H2	1.96	0.47
1:B:405:TYR:HB2	1:B:450:SER:HB3	1.98	0.47
1:B:473:VAL:HG23	6:B:813:OP8:NAR	2.31	0.46
1:B:613:LEU:HD21	1:B:675:ILE:CG2	2.46	0.46
1:A:568:LYS:NZ	1:A:595:ASP:OD1	2.39	0.46
1:A:349:GLU:HG3	2:A:807:GOL:H11	1.98	0.46
1:A:527:TRP:HB3	1:A:528:PRO:HD3	1.97	0.45
1:B:682:MET:HE1	7:B:903:HOH:O	2.16	0.45
1:B:456:LEU:HD22	7:B:995:HOH:O	2.15	0.45
1:A:502:PHE:CD1	1:A:508:PHE:HB3	2.52	0.45
1:B:248:ILE:HD12	1:B:287:ASP:HB2	1.99	0.45
1:A:683:ALA:HB3	1:B:434[B]:ARG:NH1	2.32	0.44
1:A:598:MET:HB2	1:A:598:MET:HE3	1.75	0.44
1:B:694:ARG:O	1:B:698:VAL:HG23	2.17	0.44
1:A:550:LYS:O	2:A:809:GOL:H31	2.17	0.44
1:B:608:ASP:O	1:B:612:ASN:HB3	2.18	0.44
1:B:718:PRO:O	1:B:722:VAL:HG23	2.17	0.44
1:A:569:ALA:HB1	1:A:574:TYR:CD2	2.52	0.44
1:B:587:PHE:HE2	1:B:659:PRO:O	2.01	0.44
1:B:613:LEU:HD21	1:B:675:ILE:HG21	1.99	0.43
1:A:519:ILE:HD12	1:A:523:HIS:HE1	1.84	0.43
1:B:684:PRO:HA	1:B:687:LEU:HD12	2.01	0.43
1:A:642:ILE:HD11	1:A:701:ILE:HD11	2.00	0.42
1:A:728:LEU:HA	1:A:752:LEU:HD22	2.00	0.42
1:A:613:LEU:HD21	1:A:675:ILE:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:PHE:CZ	1:A:448:SER:HB3	2.56	0.41
1:A:523:HIS:O	1:A:528:PRO:HD3	2.21	0.41
1:A:682:MET:O	1:B:434[B]:ARG:NH2	2.49	0.41
3:A:811:DMS:C2	3:A:812:DMS:S	3.08	0.41
1:B:456:LEU:HD12	1:B:470:CAS:HB3	2.02	0.41
1:B:375:ASN:HA	1:B:391:LEU:HD12	2.01	0.41
1:B:527:TRP:HB3	1:B:528:PRO:HD3	2.01	0.41
1:B:473:VAL:HG13	1:B:474:TRP:N	2.36	0.41
1:B:664:ALA:O	1:B:668:VAL:HG23	2.21	0.41
1:A:375:ASN:HA	1:A:391:LEU:HD12	2.03	0.40
1:A:604:GLY:O	1:A:608:ASP:HB2	2.21	0.40
1:B:337:HIS:O	1:B:341:VAL:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	517/542 (95%)	499 (96%)	18 (4%)	0	100	100
1	B	526/542 (97%)	509 (97%)	17 (3%)	0	100	100
All	All	1043/1084 (96%)	1008 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	451/467 (97%)	448 (99%)	3 (1%)	84	94
1	B	457/467 (98%)	449 (98%)	8 (2%)	59	83
All	All	908/934 (97%)	897 (99%)	11 (1%)	71	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	492	SER
1	A	566	VAL
1	A	738	ILE
1	B	250	TYR
1	B	366	SER
1	B	367	ASP
1	B	499	VAL
1	B	538	LEU
1	B	587	PHE
1	B	699	LEU
1	B	717	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	CAS	B	318	1	5,8,9	1.02	0	1,9,11	0.42	0
1	CAS	B	470	1	5,8,9	0.89	0	1,9,11	0.33	0
1	CAS	A	470	1	5,8,9	0.84	0	1,9,11	0.65	0
1	CAS	A	318	1	5,8,9	1.00	0	1,9,11	0.57	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
1	CAS	B	318	1	-	0/0/7/9	-
1	CAS	B	470	1	-	0/0/7/9	-
1	CAS	A	470	1	-	0/0/7/9	-
1	CAS	A	318	1	-	0/0/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	470	CAS	3	0
1	A	470	CAS	4	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

27 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	803	-	5,5,5	0.27	0	5,5,5	0.36	0
4	MET	A	814	-	4,8,8	0.16	0	2,9,9	0.54	0
3	DMS	B	810	-	3,3,3	0.53	0	3,3,3	0.57	0
3	DMS	A	813	-	3,3,3	0.50	0	3,3,3	0.55	0
2	GOL	A	803	-	5,5,5	0.30	0	5,5,5	0.15	0
2	GOL	B	801	-	5,5,5	0.34	0	5,5,5	0.30	0
2	GOL	A	806	-	5,5,5	0.21	0	5,5,5	0.67	0
3	DMS	A	811	-	3,3,3	0.55	0	3,3,3	0.53	0
3	DMS	A	812	-	3,3,3	0.57	0	3,3,3	0.57	0
2	GOL	A	801	-	5,5,5	0.24	0	5,5,5	0.26	0
2	GOL	B	804	-	5,5,5	0.42	0	5,5,5	0.60	0
2	GOL	A	808	-	5,5,5	0.31	0	5,5,5	0.31	0
2	GOL	A	804	-	5,5,5	0.47	0	5,5,5	0.28	0
3	DMS	A	810	-	3,3,3	0.50	0	3,3,3	0.67	0
2	GOL	B	806	-	5,5,5	0.31	0	5,5,5	0.37	0
2	GOL	A	809	-	5,5,5	0.51	0	5,5,5	0.35	0
2	GOL	A	802	-	5,5,5	0.36	0	5,5,5	0.55	0
5	SO4	B	812	-	4,4,4	0.43	0	6,6,6	0.23	0
2	GOL	A	807	-	5,5,5	0.32	0	5,5,5	0.33	0
2	GOL	B	805	-	5,5,5	0.52	0	5,5,5	0.56	0
6	OP8	B	813	-	28,29,29	0.97	2 (7%)	35,39,39	2.06	7 (20%)
3	DMS	B	811	-	3,3,3	0.50	0	3,3,3	0.56	0
3	DMS	B	809	-	3,3,3	0.46	0	3,3,3	0.61	0
2	GOL	A	805	-	5,5,5	0.37	0	5,5,5	0.42	0
2	GOL	B	802	-	5,5,5	0.40	0	5,5,5	0.22	0
2	GOL	B	807	-	5,5,5	0.44	0	5,5,5	0.21	0
2	GOL	B	808	-	5,5,5	0.35	0	5,5,5	0.27	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	GOL	A	804	-	-	4/4/4/4	-
2	GOL	B	803	-	-	2/4/4/4	-
2	GOL	A	807	-	-	2/4/4/4	-
2	GOL	B	805	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	803	-	-	2/4/4/4	-
6	0P8	B	813	-	-	5/11/11/11	0/3/3/3
2	GOL	B	801	-	-	2/4/4/4	-
2	GOL	B	806	-	-	0/4/4/4	-
2	GOL	A	806	-	-	2/4/4/4	-
2	GOL	A	809	-	-	4/4/4/4	-
2	GOL	A	802	-	-	2/4/4/4	-
4	MET	A	814	-	-	1/4/8/8	-
2	GOL	A	805	-	-	2/4/4/4	-
2	GOL	B	802	-	-	4/4/4/4	-
2	GOL	B	807	-	-	4/4/4/4	-
2	GOL	A	801	-	-	2/4/4/4	-
2	GOL	B	808	-	-	2/4/4/4	-
2	GOL	B	804	-	-	2/4/4/4	-
2	GOL	A	808	-	-	1/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	813	0P8	CAV-NAQ	-2.21	1.33	1.36
6	B	813	0P8	CAV-NAR	2.20	1.39	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	813	0P8	CBA-CAZ-NAR	-6.78	119.92	123.60
6	B	813	0P8	OAS-CAX-CAW	4.95	126.24	119.08
6	B	813	0P8	BR2-CAT-CAJ	4.00	124.82	119.27
6	B	813	0P8	CAK-CAY-CBA	-3.62	119.04	123.05
6	B	813	0P8	OAS-CAX-CAU	-2.72	115.51	120.74
6	B	813	0P8	CAJ-CAT-CAI	-2.43	117.92	121.51
6	B	813	0P8	CAV-NAR-CAZ	2.14	119.89	117.13

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	803	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	B	801	GOL	O1-C1-C2-C3
2	A	806	GOL	C1-C2-C3-O3
2	A	806	GOL	O2-C2-C3-O3
2	B	804	GOL	C1-C2-C3-O3
2	A	804	GOL	C1-C2-C3-O3
2	A	804	GOL	O2-C2-C3-O3
2	A	809	GOL	C1-C2-C3-O3
2	A	809	GOL	O2-C2-C3-O3
2	A	802	GOL	C1-C2-C3-O3
2	A	802	GOL	O2-C2-C3-O3
2	B	805	GOL	O1-C1-C2-C3
2	B	805	GOL	C1-C2-C3-O3
2	A	805	GOL	C1-C2-C3-O3
2	B	802	GOL	O1-C1-C2-C3
2	B	807	GOL	O1-C1-C2-C3
2	B	807	GOL	C1-C2-C3-O3
2	B	808	GOL	O1-C1-C2-O2
2	B	808	GOL	O1-C1-C2-C3
6	B	813	0P8	CAM-CAL-CAN-NAQ
6	B	813	0P8	CAW-CAO-NAP-CAM
6	B	813	0P8	CAW-CAX-OAS-CAA
2	A	803	GOL	O1-C1-C2-O2
2	B	807	GOL	O1-C1-C2-O2
2	A	801	GOL	C1-C2-C3-O3
2	A	804	GOL	O1-C1-C2-C3
2	A	809	GOL	O1-C1-C2-C3
2	A	807	GOL	C1-C2-C3-O3
2	B	805	GOL	O1-C1-C2-O2
2	A	805	GOL	O2-C2-C3-O3
2	B	802	GOL	O1-C1-C2-O2
6	B	813	0P8	CAU-CAX-OAS-CAA
2	B	801	GOL	O1-C1-C2-O2
2	A	801	GOL	O2-C2-C3-O3
2	B	804	GOL	O2-C2-C3-O3
2	A	809	GOL	O1-C1-C2-O2
2	B	805	GOL	O2-C2-C3-O3
2	B	807	GOL	O2-C2-C3-O3
6	B	813	0P8	CAN-CAL-CAM-NAP
2	A	807	GOL	O2-C2-C3-O3
2	B	802	GOL	O2-C2-C3-O3
2	B	803	GOL	O2-C2-C3-O3
2	A	804	GOL	O1-C1-C2-O2

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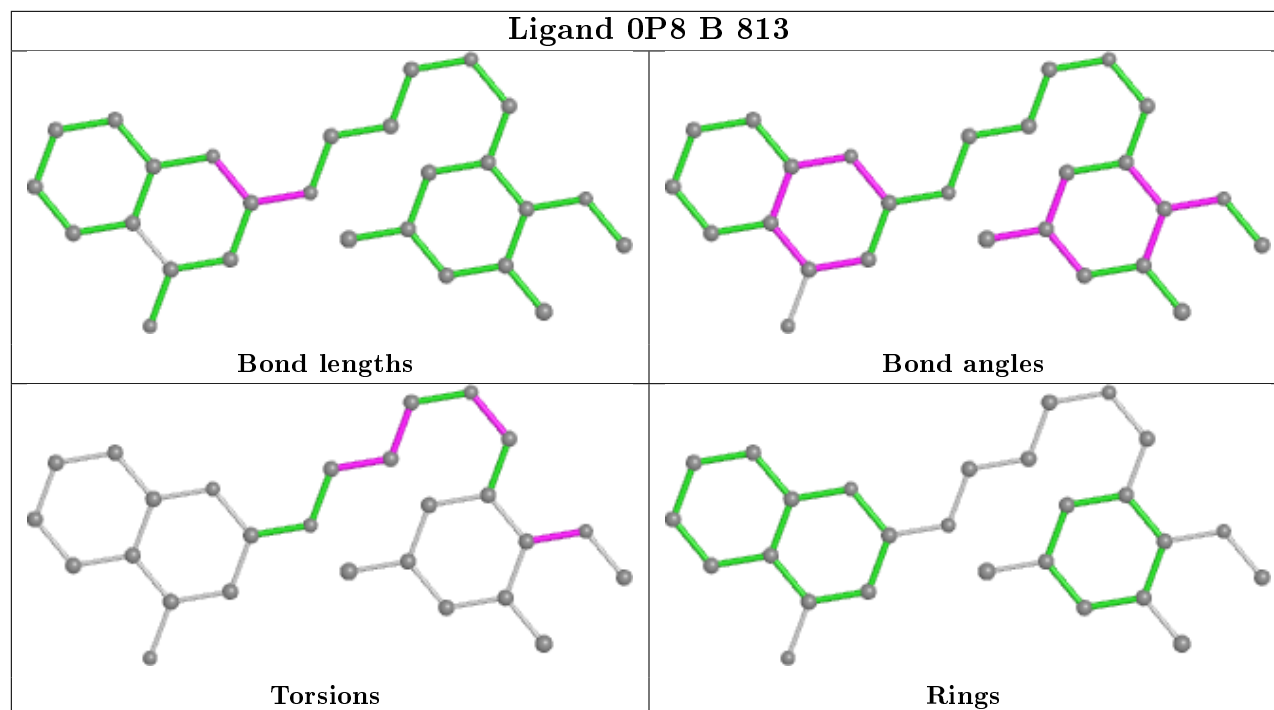
Mol	Chain	Res	Type	Atoms
2	A	808	GOL	O1-C1-C2-C3
2	B	803	GOL	C1-C2-C3-O3
2	B	802	GOL	C1-C2-C3-O3
4	A	814	MET	N-CA-CB-CG

There are no ring outliers.

10 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	814	MET	1	0
3	A	811	DMS	2	0
3	A	812	DMS	2	0
2	B	804	GOL	1	0
2	A	804	GOL	1	0
2	B	806	GOL	1	0
2	A	809	GOL	2	0
2	A	807	GOL	2	0
6	B	813	0P8	6	0
3	B	811	DMS	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	522/542 (96%)	-0.07	29 (5%) 24 23	32, 46, 89, 135	0
1	B	526/542 (97%)	0.20	56 (10%) 6 4	34, 49, 119, 144	0
All	All	1048/1084 (96%)	0.06	85 (8%) 12 10	32, 47, 108, 144	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	559	LEU	9.5
1	B	756	VAL	7.1
1	B	758	GLY	7.0
1	B	556	SER	6.6
1	B	391	LEU	6.4
1	B	757	GLU	6.1
1	B	560	GLY	5.9
1	A	758	GLY	5.8
1	B	547	TRP	5.8
1	B	365	ILE	5.8
1	B	558	SER	5.7
1	A	756	VAL	5.6
1	B	395	HIS	5.4
1	B	397	VAL	5.3
1	A	757	GLU	5.3
1	B	396	VAL	5.2
1	A	238	VAL	5.1
1	A	766	SER	5.1
1	B	392	GLU	5.0
1	B	390	SER	4.9
1	A	767	THR	4.8
1	B	393	SER	4.4
1	B	755	ALA	4.4
1	B	590	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	366	SER	4.3
1	B	394	GLY	4.3
1	A	491	GLU	4.3
1	B	767	THR	4.1
1	A	755	ALA	4.1
1	B	387	CYS	4.0
1	B	377	THR	4.0
1	B	375	ASN	3.9
1	B	369	SER	3.9
1	B	389	VAL	3.8
1	B	766	SER	3.8
1	B	549	THR	3.7
1	B	378	ASP	3.6
1	B	491	GLU	3.6
1	B	759	GLU	3.6
1	A	768	GLU	3.5
1	A	561	ASN	3.5
1	B	561	ASN	3.4
1	B	557	LYS	3.4
1	A	492	SER	3.4
1	B	552	ARG	3.4
1	B	370	PHE	3.3
1	B	364	SER	3.3
1	B	554	LYS	3.3
1	B	388	LYS	3.2
1	B	555	ILE	3.2
1	B	372	THR	3.2
1	A	560	GLY	3.1
1	B	376	ILE	3.1
1	B	551	ASP	3.1
1	B	591	GLY	3.1
1	B	588	SER	3.1
1	B	592	ASP	3.0
1	A	588	SER	3.0
1	B	367	ASP	3.0
1	A	301	GLN	3.0
1	B	593	TYR	3.0
1	B	760	VAL	2.9
1	A	299	GLN	2.9
1	B	363	TYR	2.9
1	B	299	GLN	2.9
1	B	553	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	492	SER	2.7
1	A	590	ASP	2.7
1	B	374	GLN	2.7
1	B	398	THR	2.7
1	A	562	VAL	2.6
1	A	552	ARG	2.5
1	A	384	GLY	2.4
1	A	351	LYS	2.3
1	A	490	ASP	2.3
1	A	759	GLU	2.3
1	A	551	ASP	2.2
1	A	553	LYS	2.2
1	B	562	VAL	2.2
1	A	380	VAL	2.1
1	A	477	ALA	2.1
1	A	385	ASN	2.1
1	A	386	PRO	2.1
1	A	494	LYS	2.1
1	B	754	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CAS	A	318	9/10	0.95	0.15	50,51,58,59	3
1	CAS	B	318	9/10	0.96	0.12	46,47,48,49	3
1	CAS	A	470	9/10	0.99	0.11	40,42,49,50	3
1	CAS	B	470	9/10	0.99	0.12	43,47,54,55	3

6.3 Carbohydrates [i](#)

There are no monosaccharides 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,

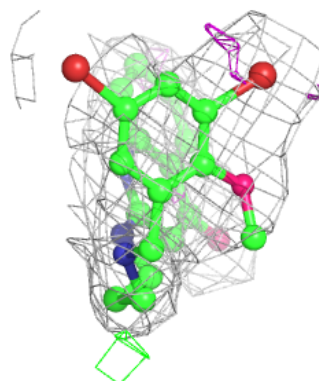
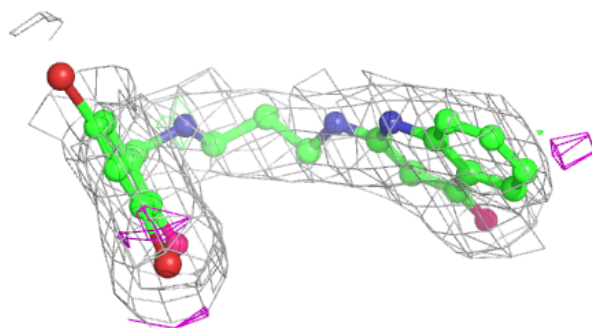
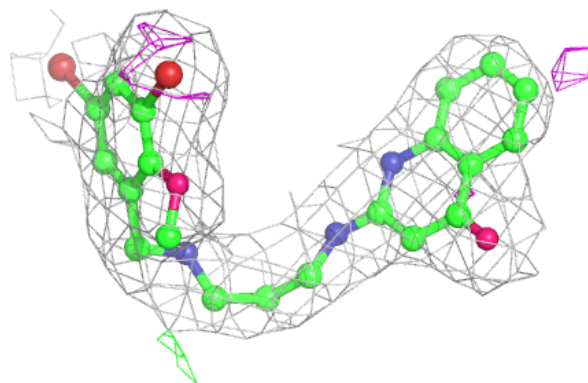
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	B	805	6/6	0.74	0.33	56,67,69,73	0
2	GOL	A	805	6/6	0.79	0.28	65,74,81,87	0
2	GOL	A	803	6/6	0.84	0.34	63,71,78,82	0
2	GOL	A	808	6/6	0.85	0.23	58,68,71,72	0
2	GOL	A	807	6/6	0.85	0.26	63,71,74,80	0
2	GOL	B	802	6/6	0.87	0.18	66,70,71,71	0
3	DMS	B	809	4/4	0.88	0.34	84,86,92,95	0
2	GOL	A	809	6/6	0.88	0.19	69,75,80,86	0
2	GOL	B	804	6/6	0.88	0.28	58,60,68,69	0
2	GOL	B	806	6/6	0.90	0.39	63,63,67,74	0
2	GOL	B	808	6/6	0.90	0.24	71,80,81,83	0
3	DMS	A	810	4/4	0.91	0.21	94,96,99,103	0
2	GOL	A	804	6/6	0.91	0.23	52,55,59,60	0
2	GOL	A	802	6/6	0.92	0.33	62,63,71,72	0
2	GOL	A	806	6/6	0.92	0.24	56,61,67,68	0
2	GOL	B	807	6/6	0.93	0.23	55,62,64,66	0
5	SO4	B	812	5/5	0.93	0.28	67,72,76,76	0
2	GOL	B	803	6/6	0.94	0.14	57,59,64,66	0
2	GOL	A	801	6/6	0.94	0.17	64,68,70,73	0
3	DMS	A	813	4/4	0.94	0.18	74,78,80,83	0
3	DMS	B	811	4/4	0.95	0.15	73,81,87,88	0
2	GOL	B	801	6/6	0.95	0.19	58,62,64,67	0
3	DMS	B	810	4/4	0.95	0.21	83,85,91,95	0
3	DMS	A	811	4/4	0.96	0.21	78,80,83,84	0
3	DMS	A	812	4/4	0.96	0.16	68,74,75,77	0
6	OP8	B	813	27/27	0.97	0.13	40,47,57,80	0
4	MET	A	814	9/9	0.97	0.24	37,39,39,41	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 0P8 B 813:

$2mF_o-DF_c$ (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.