



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 11:10 PM EDT

PDB ID : 4EG4
Title : Trypanosoma brucei methionyl-tRNA synthetase in complex with inhibitor Chem 1289
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 : 3.15 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

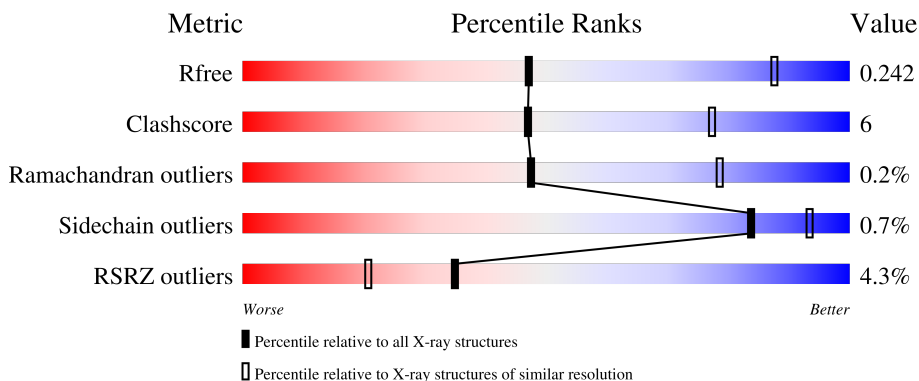
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	542	
1	B	542	

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
3	DMS	A	814	-	-	X	-
3	DMS	A	815	-	-	X	-
3	DMS	B	801	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8612 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
			Total	As	C	N	O	S			
1	A	522	4172	2	2689	700	770	11	0	0	0
1	B	511	4085	2	2636	688	748	11	0	1	0

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).



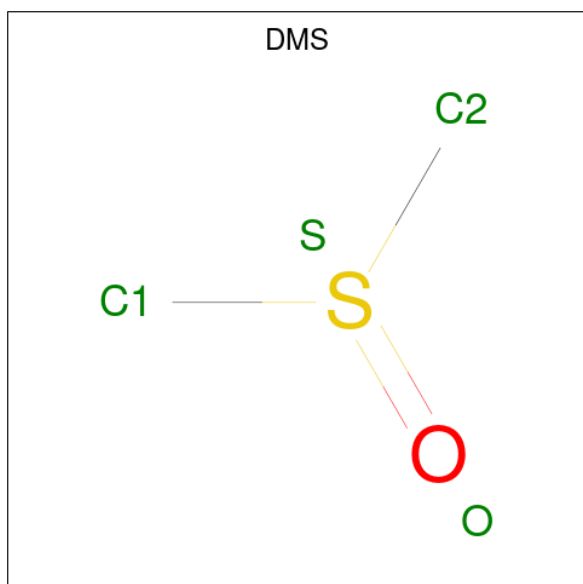
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0
2	A	1	Total C O 6 3 3	0	0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

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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		
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: C₂H₆OS).



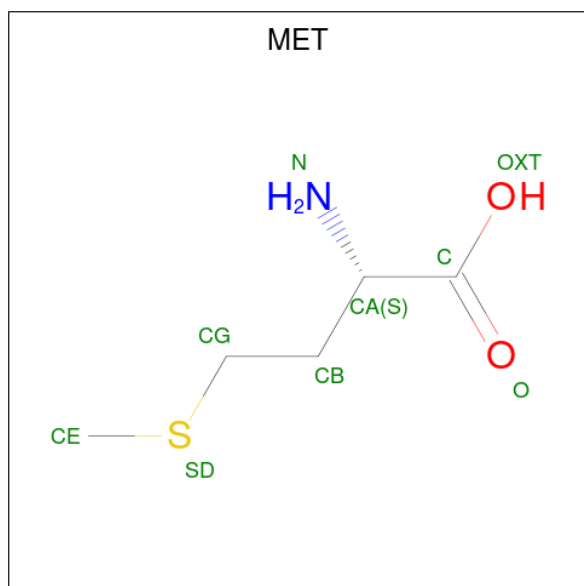
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

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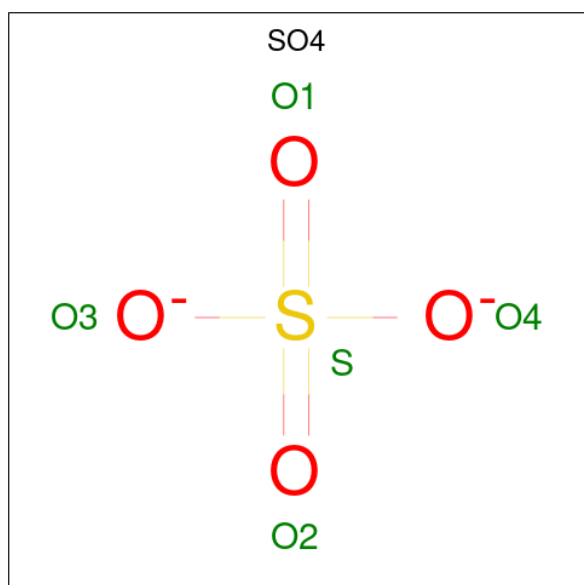
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
3	B	1	4	2	1	1	0	0

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



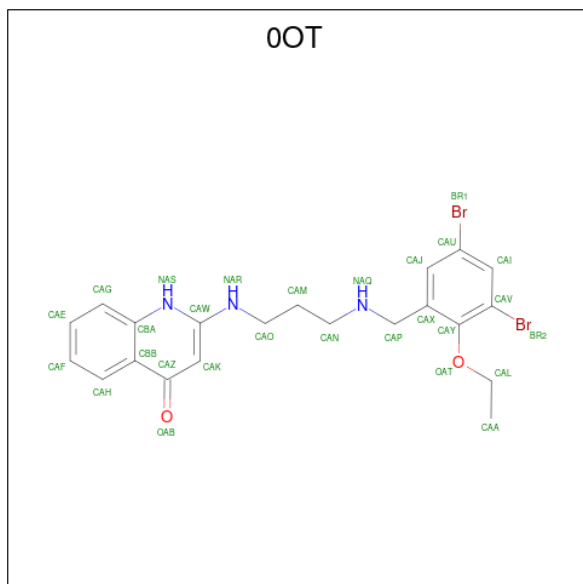
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	9	5	1	2	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO₄) (formula: O_4S).



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-ethoxybenzyl)amino]propyl}amino)quinolin-4(1H)-one (three-letter code: 0OT) (formula: C₂₁H₂₃Br₂N₃O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	Br	C	N	O	0	0
			28	2	21	3	2		

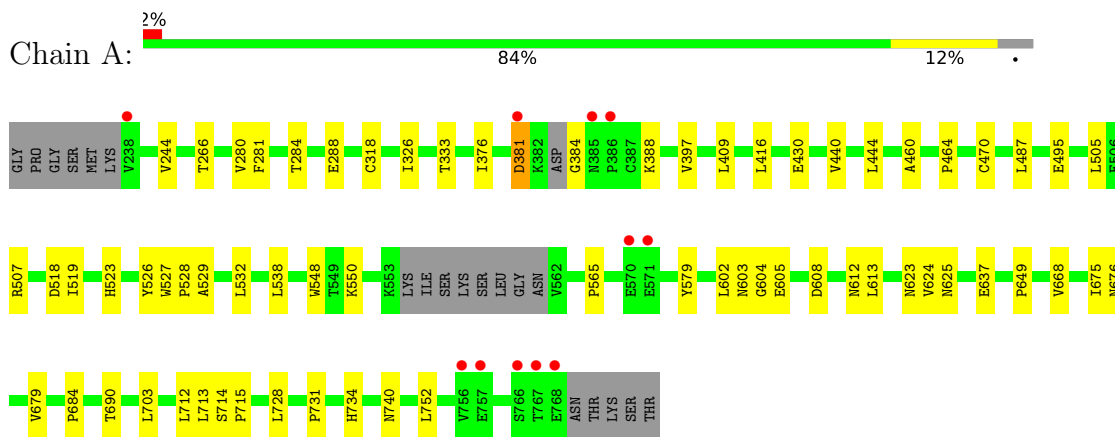
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	92	Total	O	0	0
			92	92		
7	B	77	Total	O	0	0
			77	77		

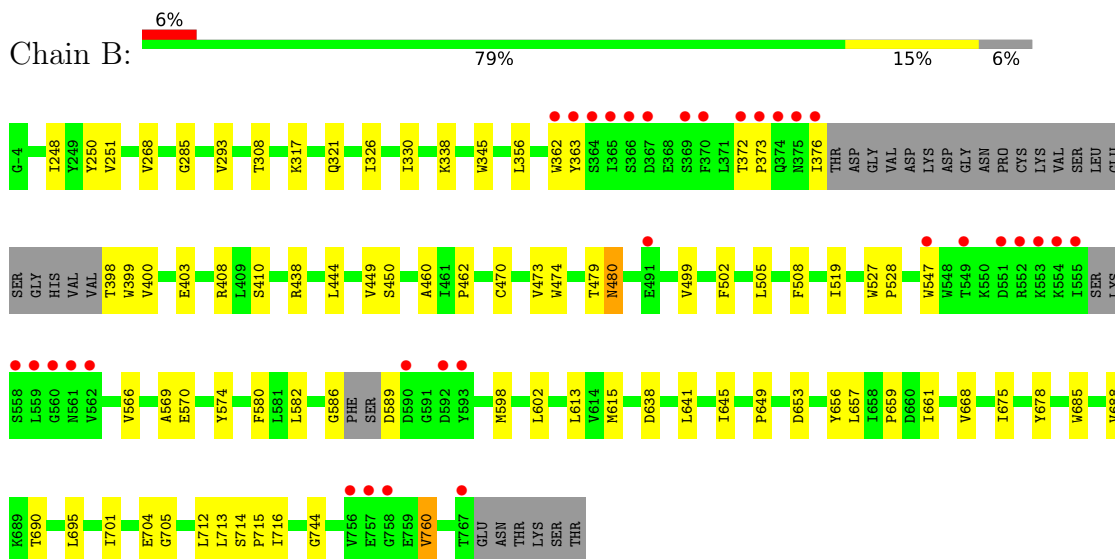
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 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	87.48Å 105.89Å 207.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.15 37.90 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-3.15) 99.1 (37.90-3.15)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.12Å)	Xtrriage
Refinement program	REFMAC refmac_5.6.0117	Depositor
R, R_{free}	0.191 , 0.240 0.194 , 0.242	Depositor DCC
R_{free} test set	1721 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtrriage
Anisotropy	0.508	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8612	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% 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: GOL, SO4, OOT, CAS, DMS

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	0/4260	0.60	0/5791
1	B	0.55	3/4174 (0.1%)	0.60	0/5673
All	All	0.55	3/8434 (0.0%)	0.60	0/11464

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	399	TRP	CD2-CE2	5.34	1.47	1.41
1	B	547	TRP	CD2-CE2	5.29	1.47	1.41
1	B	474	TRP	CD2-CE2	5.08	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	4172	0	4093	46	0
1	B	4085	0	4013	53	0
2	A	72	0	96	4	0
2	B	48	0	64	2	0
3	A	16	0	24	7	0
3	B	8	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	9	0	8	0	0
5	B	5	0	0	1	0
6	B	28	0	23	3	0
7	A	92	0	0	2	0
7	B	77	0	0	0	0
All	All	8612	0	8333	104	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 6.

All (104) 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:A:460:ALA:O	1:A:470:CAS:CE2	2.29	0.80
1:B:326:ILE:HB	3:B:801:DMS:H22	1.67	0.75
3:A:814:DMS:H21	3:A:815:DMS:H22	1.72	0.72
3:A:814:DMS:H21	3:A:815:DMS:C2	2.23	0.69
1:A:690:THR:HG21	1:B:438:ARG:HH22	1.61	0.66
1:A:284:THR:HG22	1:A:326:ILE:HG21	1.78	0.64
6:B:812:OOT:CAL	6:B:812:OOT:BR2	3.02	0.63
1:B:668:VAL:HG11	1:B:713:LEU:HG	1.83	0.61
1:A:416:LEU:HD21	1:A:528:PRO:HB2	1.81	0.61
1:A:731:PRO:HA	2:A:803:GOL:H2	1.83	0.61
3:A:814:DMS:H21	3:A:815:DMS:C1	2.31	0.60
1:A:649:PRO:HA	1:A:712:LEU:HD11	1.83	0.60
6:B:812:OOT:BR2	6:B:812:OOT:H5	2.57	0.60
1:A:519:ILE:HD12	1:A:523:HIS:CE1	2.37	0.59
1:A:244:VAL:HG22	1:A:266:THR:HG23	1.86	0.57
1:A:579:TYR:OH	1:A:605:GLU:OE2	2.22	0.57
1:B:685:TRP:O	1:B:688:VAL:HG22	2.05	0.57
1:A:487:LEU:HD22	1:A:495:GLU:HG3	1.87	0.56
1:B:569:ALA:HB1	1:B:574:TYR:CD1	2.41	0.55
1:A:518:ASP:HB3	1:A:548:TRP:CE3	2.42	0.55
1:B:372:THR:CG2	1:B:373:PRO:HD2	2.37	0.55
1:A:416:LEU:CD2	1:A:528:PRO:HB2	2.37	0.55
1:A:440:VAL:HG22	1:A:444:LEU:HD21	1.88	0.54
1:B:345:TRP:CH2	1:B:449:VAL:HG23	2.42	0.54
1:A:624:VAL:HG23	1:A:625:ASN:OD1	2.08	0.53
1:A:690:THR:HG21	1:B:438:ARG:NH2	2.23	0.53
1:B:613:LEU:HD21	1:B:675:ILE:HG21	1.92	0.52
1:B:462:PRO:HA	1:B:470:CAS:CE1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ILE:HG22	1:B:285:GLY:CA	2.42	0.50
1:B:645:ILE:HD13	1:B:705:GLY:CA	2.42	0.50
1:A:679:VAL:HG13	1:A:684:PRO:HG3	1.93	0.50
1:A:519:ILE:HD12	1:A:523:HIS:HE1	1.77	0.49
1:A:637:GLU:HB3	7:A:921:HOH:O	2.12	0.49
1:A:602:LEU:C	1:A:602:LEU:HD23	2.33	0.49
1:A:495:GLU:HB3	7:A:944:HOH:O	2.11	0.49
1:A:613:LEU:HD13	1:A:676:ASN:ND2	2.27	0.49
1:B:251:VAL:HG21	1:B:308:THR:HG22	1.95	0.48
1:B:479:THR:HG22	1:B:479:THR:O	2.13	0.48
1:B:372:THR:HG23	1:B:373:PRO:HD2	1.94	0.48
1:B:268:VAL:HG11	1:B:661:ILE:HD13	1.95	0.48
1:B:499:VAL:HG21	1:B:505:LEU:HD21	1.96	0.48
1:B:649:PRO:HA	1:B:712:LEU:HD11	1.96	0.48
1:B:615:MET:CE	1:B:760:VAL:HA	2.44	0.47
1:A:703:LEU:CD2	1:A:728:LEU:HD22	2.45	0.47
1:A:550:LYS:O	2:A:810:GOL:H32	2.14	0.47
1:B:363:TYR:HB3	1:B:400:VAL:HG21	1.97	0.47
1:A:714:SER:N	1:A:715:PRO:CD	2.79	0.46
1:A:734:HIS:HA	1:A:740:ASN:ND2	2.30	0.46
1:A:532:LEU:HG	1:A:538:LEU:HD21	1.98	0.46
1:B:268:VAL:HG21	1:B:582:LEU:HD11	1.97	0.46
1:B:602:LEU:C	1:B:602:LEU:HD23	2.37	0.45
1:A:526:TYR:OH	3:A:814:DMS:C2	2.64	0.45
1:B:714:SER:N	1:B:715:PRO:CD	2.80	0.45
1:B:330:ILE:HD13	1:B:480:ASN:HB2	1.99	0.45
1:B:519:ILE:HG21	6:B:812:OOT:H9	1.99	0.45
1:B:688:VAL:HG12	1:B:695:LEU:HD22	1.99	0.45
1:A:604:GLY:O	1:A:608:ASP:HB2	2.17	0.45
1:B:613:LEU:HD21	1:B:675:ILE:CG2	2.46	0.45
1:B:704:GLU:CD	1:B:744:GLY:H	2.20	0.45
1:B:586:GLY:H	1:B:589:ASP:HB2	1.82	0.45
1:B:653:ASP:O	1:B:657:LEU:HD13	2.16	0.44
1:B:580:PHE:CE1	1:B:598:MET:HA	2.52	0.44
1:B:250:TYR:N	5:B:811:SO4:O2	2.36	0.44
1:B:248:ILE:HG22	1:B:285:GLY:C	2.37	0.44
1:A:409:LEU:CD1	1:A:529:ALA:CB	2.96	0.44
1:A:487:LEU:HD22	1:A:495:GLU:CG	2.48	0.44
1:B:645:ILE:HD13	1:B:705:GLY:HA2	1.99	0.44
1:A:608:ASP:O	1:A:612:ASN:HB3	2.19	0.43
1:A:376:ILE:HD12	1:A:388:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:PRO:O	2:A:801:GOL:O2	2.36	0.43
1:A:526:TYR:OH	3:A:814:DMS:H22	2.19	0.43
1:B:317:LYS:HE2	1:B:321:GLN:HE22	1.83	0.42
1:A:527:TRP:HB3	1:A:528:PRO:HD3	2.00	0.42
1:B:460:ALA:O	1:B:470:CAS:CE2	2.67	0.42
1:B:613:LEU:HD11	1:B:675:ILE:HG22	2.01	0.42
1:A:613:LEU:HD21	1:A:675:ILE:HB	2.01	0.42
3:A:814:DMS:C2	3:A:815:DMS:H13	2.48	0.42
1:A:381:ASP:O	1:A:384:GLY:HA2	2.20	0.42
1:A:602:LEU:HD22	1:A:603:ASN:OD1	2.20	0.42
3:A:814:DMS:C2	3:A:815:DMS:C1	2.96	0.42
1:B:574:TYR:N	2:B:807:GOL:H2	2.34	0.42
1:B:688:VAL:HG12	1:B:695:LEU:CD2	2.50	0.42
1:A:318:CAS:CE2	1:A:565:PRO:HG2	2.49	0.42
1:A:668:VAL:HG11	1:A:713:LEU:HG	2.02	0.42
1:B:582:LEU:HD12	1:B:716:ILE:HG23	2.01	0.42
1:A:288:GLU:HB2	1:A:333:THR:HG23	2.02	0.42
1:B:362:TRP:CD1	1:B:376:ILE:HD13	2.54	0.41
1:B:566:VAL:O	1:B:570:GLU:HG2	2.19	0.41
1:A:388:LYS:O	1:A:397:VAL:HG22	2.19	0.41
1:B:410:SER:HB3	1:B:444:LEU:O	2.21	0.41
1:A:430:GLU:H	2:A:816:GOL:H11	1.85	0.41
1:B:638:ASP:HB3	1:B:701:ILE:CD1	2.50	0.41
1:B:656:TYR:O	1:B:659:PRO:HB3	2.21	0.41
1:B:248:ILE:HG22	1:B:285:GLY:HA3	2.03	0.41
1:B:356:LEU:HD11	1:B:403:GLU:HB3	2.03	0.41
1:B:527:TRP:HB3	1:B:528:PRO:HD3	2.03	0.41
1:B:250:TYR:CZ	1:B:293:VAL:HG23	2.56	0.41
1:B:641:LEU:HD22	1:B:678:TYR:CB	2.51	0.41
1:A:623:ASN:ND2	1:A:752:LEU:HD11	2.36	0.41
1:A:280:VAL:HG12	1:A:281:PHE:N	2.35	0.40
1:A:505:LEU:HD13	1:A:507:ARG:CZ	2.51	0.40
1:B:338:LYS:NZ	2:B:806:GOL:H32	2.36	0.40
1:B:502:PHE:CD1	1:B:508:PHE:HB3	2.57	0.40
1:B:363:TYR:CB	1:B:400:VAL:HG21	2.52	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	514/542 (95%)	496 (96%)	18 (4%)	0	100	100
1	B	502/542 (93%)	482 (96%)	18 (4%)	2 (0%)	34	68
All	All	1016/1084 (94%)	978 (96%)	36 (4%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	408	ARG
1	B	473	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/467 (95%)	444 (100%)	1 (0%)	93	98
1	B	433/467 (93%)	428 (99%)	5 (1%)	71	87
All	All	878/934 (94%)	872 (99%)	6 (1%)	84	93

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	ASP
1	B	398	THR
1	B	450	SER
1	B	480	ASN

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Mol	Chain	Res	Type
1	B	690	THR
1	B	760	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	423	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	0.94	0	1,9,11	0.49	0
1	CAS	A	470	1	5,8,9	0.90	0	1,9,11	0.16	0
1	CAS	A	318	1	5,8,9	1.00	0	1,9,11	0.69	0
1	CAS	B	470	1	5,8,9	0.92	0	1,9,11	0.60	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	A	470	1	-	0/0/7/9	-
1	CAS	A	318	1	-	0/0/7/9	-
1	CAS	B	470	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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	470	CAS	1	0
1	A	318	CAS	1	0
1	B	470	CAS	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

29 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	$\# Z > 2$
3	DMS	B	810	-	3,3,3	0.44	0	3,3,3	0.78	0
2	GOL	A	811	-	5,5,5	0.22	0	5,5,5	0.33	0
2	GOL	A	803	-	5,5,5	0.72	0	5,5,5	0.50	0
2	GOL	A	810	-	5,5,5	0.54	0	5,5,5	0.63	0
2	GOL	A	808	-	5,5,5	0.30	0	5,5,5	0.49	0
2	GOL	A	804	-	5,5,5	0.35	0	5,5,5	0.46	0
2	GOL	B	804	-	5,5,5	0.18	0	5,5,5	0.51	0
4	MET	A	817	-	7,8,8	0.92	1 (14%)	7,9,9	1.35	1 (14%)
3	DMS	A	815	-	3,3,3	0.45	0	3,3,3	0.83	0
2	GOL	A	802	-	5,5,5	0.33	0	5,5,5	0.47	0
5	SO4	B	811	-	4,4,4	0.38	0	6,6,6	0.28	0
2	GOL	B	805	-	5,5,5	0.40	0	5,5,5	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	801	-	5,5,5	0.27	0	5,5,5	0.19	0
2	GOL	B	803	-	5,5,5	0.33	0	5,5,5	0.66	0
2	GOL	A	807	-	5,5,5	0.36	0	5,5,5	0.43	0
2	GOL	B	806	-	5,5,5	0.48	0	5,5,5	0.39	0
2	GOL	B	809	-	5,5,5	0.31	0	5,5,5	0.28	0
2	GOL	B	808	-	5,5,5	0.41	0	5,5,5	0.12	0
2	GOL	A	805	-	5,5,5	0.32	0	5,5,5	0.39	0
6	OOT	B	812	-	29,30,30	1.01	1 (3%)	36,40,40	1.79	6 (16%)
2	GOL	B	802	-	5,5,5	0.50	0	5,5,5	0.26	0
2	GOL	A	806	-	5,5,5	0.55	0	5,5,5	0.50	0
3	DMS	A	813	-	3,3,3	0.45	0	3,3,3	0.72	0
2	GOL	A	809	-	5,5,5	0.18	0	5,5,5	0.33	0
3	DMS	A	812	-	3,3,3	0.52	0	3,3,3	0.59	0
2	GOL	A	816	-	5,5,5	0.35	0	5,5,5	0.44	0
2	GOL	B	807	-	5,5,5	0.37	0	5,5,5	0.38	0
3	DMS	A	814	-	3,3,3	0.51	0	3,3,3	0.71	0
3	DMS	B	801	-	3,3,3	0.45	0	3,3,3	0.88	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	811	-	-	2/4/4/4	-
2	GOL	A	803	-	-	0/4/4/4	-
2	GOL	A	810	-	-	0/4/4/4	-
2	GOL	A	808	-	-	4/4/4/4	-
2	GOL	A	804	-	-	0/4/4/4	-
2	GOL	B	804	-	-	0/4/4/4	-
4	MET	A	817	-	-	0/8/8/8	-
2	GOL	A	802	-	-	2/4/4/4	-
2	GOL	B	805	-	-	2/4/4/4	-
2	GOL	A	801	-	-	2/4/4/4	-
2	GOL	B	803	-	-	0/4/4/4	-
2	GOL	A	807	-	-	0/4/4/4	-
2	GOL	B	806	-	-	2/4/4/4	-
2	GOL	B	809	-	-	2/4/4/4	-
2	GOL	B	808	-	-	2/4/4/4	-
2	GOL	A	805	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	00T	B	812	-	-	5/11/12/12	0/3/3/3
2	GOL	B	802	-	-	4/4/4/4	-
2	GOL	A	806	-	-	2/4/4/4	-
2	GOL	A	809	-	-	1/4/4/4	-
2	GOL	A	816	-	-	2/4/4/4	-
2	GOL	B	807	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	812	00T	CBB-CAZ	-4.13	1.41	1.48
4	A	817	MET	OXT-C	-2.10	1.23	1.30

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	812	00T	BR2-CAV-CAY	6.42	127.87	118.51
6	B	812	00T	BR2-CAV-CAI	-3.18	112.97	118.39
6	B	812	00T	CAP-CAX-CAJ	-3.11	114.42	120.41
6	B	812	00T	OAT-CAY-CAX	-3.09	114.20	119.08
4	A	817	MET	OXT-C-O	-2.87	117.56	124.09
6	B	812	00T	CAP-CAX-CAY	2.82	125.98	120.47
6	B	812	00T	BR1-CAU-CAJ	2.20	122.32	119.27

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	C1-C2-C3-O3
2	A	806	GOL	O1-C1-C2-C3
2	A	808	GOL	C1-C2-C3-O3
2	A	816	GOL	C1-C2-C3-O3
2	B	805	GOL	O1-C1-C2-C3
2	B	806	GOL	O1-C1-C2-C3
2	B	808	GOL	O1-C1-C2-C3
6	B	812	00T	CAV-CAY-OAT-CAL
6	B	812	00T	NAS-CAW-NAR-CAO
6	B	812	00T	CAX-CAY-OAT-CAL
6	B	812	00T	CAX-CAP-NAQ-CAN
6	B	812	00T	CAO-CAM-CAN-NAQ

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Mol	Chain	Res	Type	Atoms
2	B	805	GOL	O1-C1-C2-O2
2	B	806	GOL	O1-C1-C2-O2
2	A	802	GOL	O1-C1-C2-C3
2	A	808	GOL	O1-C1-C2-C3
2	A	809	GOL	O1-C1-C2-C3
2	A	811	GOL	O1-C1-C2-C3
2	B	802	GOL	O1-C1-C2-C3
2	B	802	GOL	C1-C2-C3-O3
2	B	807	GOL	O1-C1-C2-C3
2	A	801	GOL	O2-C2-C3-O3
2	A	806	GOL	O1-C1-C2-O2
2	A	811	GOL	O1-C1-C2-O2
2	A	816	GOL	O2-C2-C3-O3
2	B	802	GOL	O2-C2-C3-O3
2	B	807	GOL	O1-C1-C2-O2
2	A	802	GOL	O1-C1-C2-O2
2	B	802	GOL	O1-C1-C2-O2
2	A	808	GOL	O2-C2-C3-O3
2	B	809	GOL	O2-C2-C3-O3
2	B	809	GOL	C1-C2-C3-O3
2	B	808	GOL	O1-C1-C2-O2
2	A	808	GOL	O1-C1-C2-O2

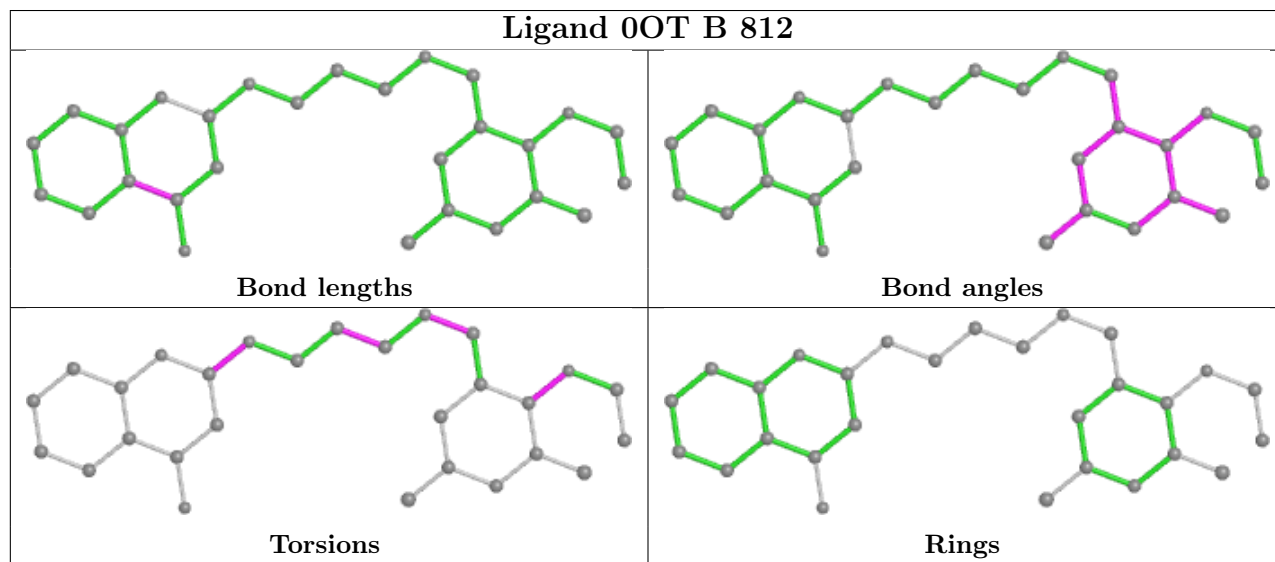
There are no ring outliers.

11 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	803	GOL	1	0
2	A	810	GOL	1	0
3	A	815	DMS	5	0
5	B	811	SO4	1	0
2	A	801	GOL	1	0
2	B	806	GOL	1	0
6	B	812	OOT	3	0
2	A	816	GOL	1	0
2	B	807	GOL	1	0
3	A	814	DMS	7	0
3	B	801	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	520/542 (95%)	-0.29	11 (2%) 63 49	25, 38, 79, 125	0
1	B	509/542 (93%)	-0.11	33 (6%) 18 10	24, 41, 106, 129	0
All	All	1029/1084 (94%)	-0.20	44 (4%) 35 21	24, 39, 90, 129	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	551	ASP	5.7
1	B	549	THR	5.6
1	B	375	ASN	5.0
1	B	559	LEU	4.8
1	B	558	SER	4.7
1	B	561	ASN	4.5
1	B	758	GLY	4.3
1	B	366	SER	4.0
1	B	767	THR	4.0
1	B	376	ILE	4.0
1	A	767	THR	3.8
1	A	766	SER	3.8
1	B	560	GLY	3.7
1	B	555	ILE	3.3
1	B	756	VAL	3.3
1	A	238	VAL	3.1
1	B	757	GLU	3.0
1	B	374	GLN	3.0
1	B	365	ILE	2.9
1	B	364	SER	2.8
1	B	369	SER	2.8
1	B	547	TRP	2.8
1	B	362	TRP	2.7
1	A	756	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	593	TYR	2.6
1	B	554	LYS	2.6
1	B	553	LYS	2.6
1	A	385	ASN	2.6
1	B	373	PRO	2.5
1	B	592	ASP	2.5
1	B	372	THR	2.5
1	B	491	GLU	2.4
1	A	768	GLU	2.4
1	B	552	ARG	2.4
1	B	367	ASP	2.4
1	B	370	PHE	2.3
1	B	562	VAL	2.3
1	A	757	GLU	2.3
1	B	363	TYR	2.3
1	A	571	GLU	2.2
1	A	386	PRO	2.2
1	A	381	ASP	2.1
1	A	570	GLU	2.1
1	B	590	ASP	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	0.97	0.16	43,44,46,48	3
1	CAS	B	318	9/10	0.97	0.13	41,42,45,45	3
1	CAS	A	470	9/10	0.99	0.12	35,36,41,41	3
1	CAS	B	470	9/10	0.99	0.13	36,38,39,40	3

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

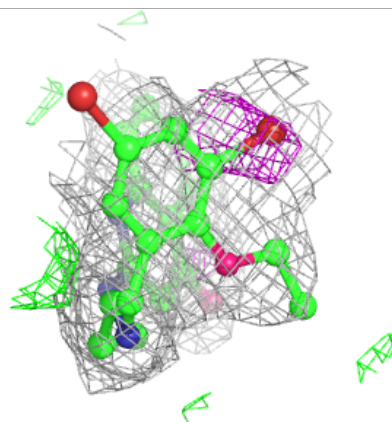
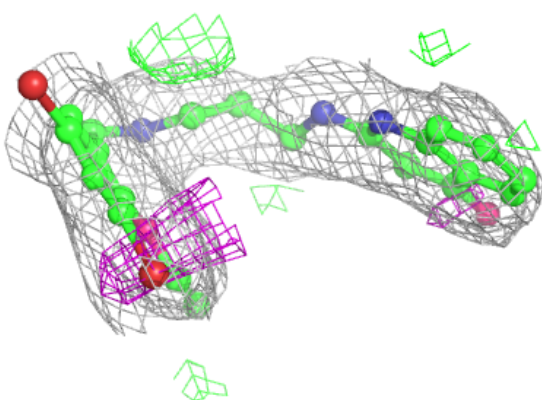
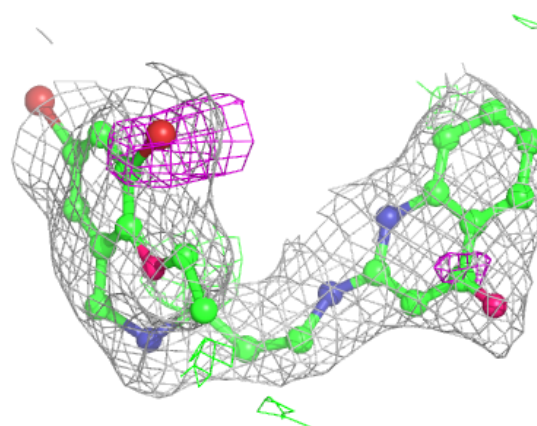
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	A	803	6/6	0.65	0.30	39,43,45,48	0
2	GOL	B	805	6/6	0.75	0.32	59,63,65,65	0
2	GOL	B	802	6/6	0.76	0.34	47,48,50,52	0
3	DMS	B	801	4/4	0.76	0.43	76,78,84,94	0
2	GOL	B	809	6/6	0.78	0.30	59,62,68,69	0
3	DMS	A	815	4/4	0.80	0.29	77,79,91,91	0
2	GOL	A	810	6/6	0.82	0.23	48,54,55,58	0
2	GOL	A	811	6/6	0.84	0.43	52,52,53,55	0
3	DMS	B	810	4/4	0.86	0.30	70,72,77,79	0
2	GOL	A	805	6/6	0.87	0.23	50,54,55,56	0
2	GOL	B	803	6/6	0.88	0.26	64,66,67,69	0
2	GOL	B	808	6/6	0.88	0.35	54,57,58,59	0
2	GOL	B	804	6/6	0.91	0.17	43,45,49,52	0
2	GOL	B	807	6/6	0.91	0.19	53,55,58,58	0
3	DMS	A	812	4/4	0.91	0.23	77,78,78,81	0
2	GOL	A	807	6/6	0.92	0.52	51,56,58,59	0
2	GOL	A	808	6/6	0.93	0.20	46,47,49,52	0
5	SO4	B	811	5/5	0.93	0.22	76,80,83,83	0
2	GOL	B	806	6/6	0.94	0.19	46,48,51,55	0
3	DMS	A	813	4/4	0.94	0.17	62,63,64,68	0
2	GOL	A	804	6/6	0.94	0.14	39,40,41,41	0
2	GOL	A	816	6/6	0.95	0.13	38,38,39,39	0
3	DMS	A	814	4/4	0.95	0.15	49,50,52,53	0
2	GOL	A	801	6/6	0.95	0.30	37,37,37,39	0
2	GOL	A	809	6/6	0.95	0.26	49,51,55,57	0
2	GOL	A	806	6/6	0.95	0.32	52,55,57,57	0
2	GOL	A	802	6/6	0.95	0.19	39,42,45,47	0
6	OOT	B	812	28/28	0.96	0.16	35,43,52,75	0
4	MET	A	817	9/9	0.97	0.23	26,27,28,29	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 0OT B 812:

$2mF_o-DF_c$ (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.