



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:50 PM GMT

PDB ID : 4MW6
Title : Trypanosoma brucei methionyl-tRNA synthetase in complex with inhibitor 1-(3-{[2-(benzyloxy)-5-chloro-3-(prop-2-en-1-yl)benzyl]amino}propyl)-3-thiophen-3-ylurea (Chem 1476)
Authors : Koh, C.Y.; Kim, J.E.; Wetzel, A.B.; de van der Schueren, W.J.; Shibata, S.; Liu, J.; Zhang, Z.; Fan, E.; Verlinde, C.L.M.J.; Hol, W.G.J.
Deposited on : 2013-09-24
Resolution : 2.56 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

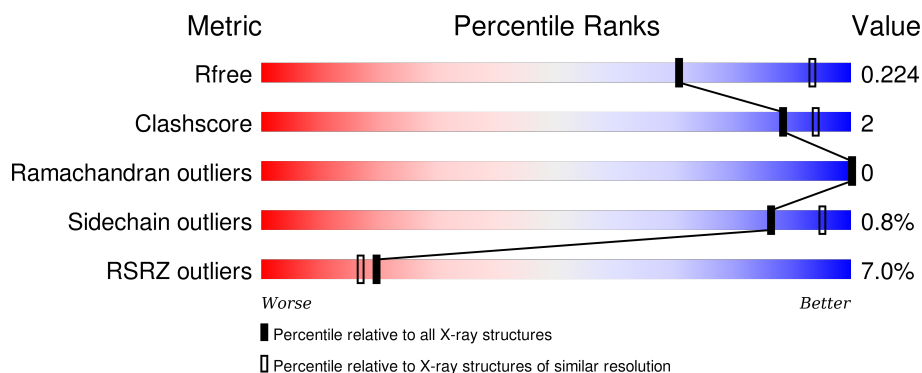
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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}	91344	3324 (2.60-2.52)
Clashscore	102246	3729 (2.60-2.52)
Ramachandran outliers	100387	3673 (2.60-2.52)
Sidechain outliers	100360	3673 (2.60-2.52)
RSRZ outliers	91569	3333 (2.60-2.52)

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. 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>8%</div> <div>92%</div> <div>6% •</div> </div>
1	B	542	<div> <div>6%</div> <div>92%</div> <div>6% •</div> </div>

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	801	-	-	-	X
2	GOL	A	803	-	-	-	X
2	GOL	B	801	-	-	-	X
2	GOL	B	803	-	-	-	X
3	DMS	A	807	-	-	-	X
3	DMS	A	808	-	-	-	X
3	DMS	A	809	-	-	-	X
5	2EE	B	806	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8978 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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	531	Total	As	C	N	O	S	0	1	0
			4263	2	2745	720	785	11			
1	B	527	Total	As	C	N	O	S	0	4	0
			4260	2	2749	720	778	11			

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).



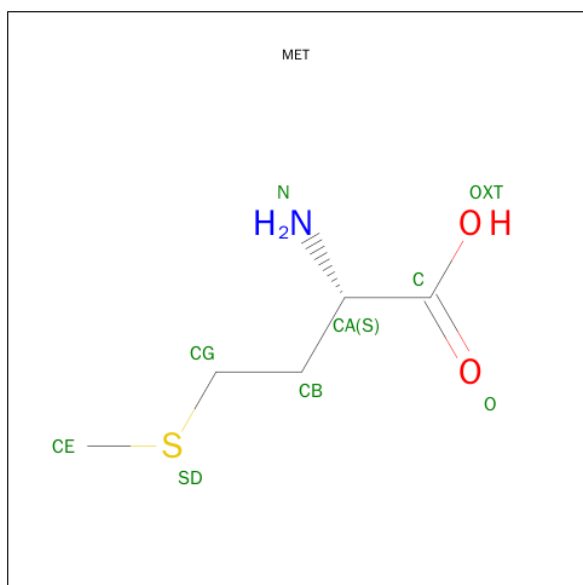
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



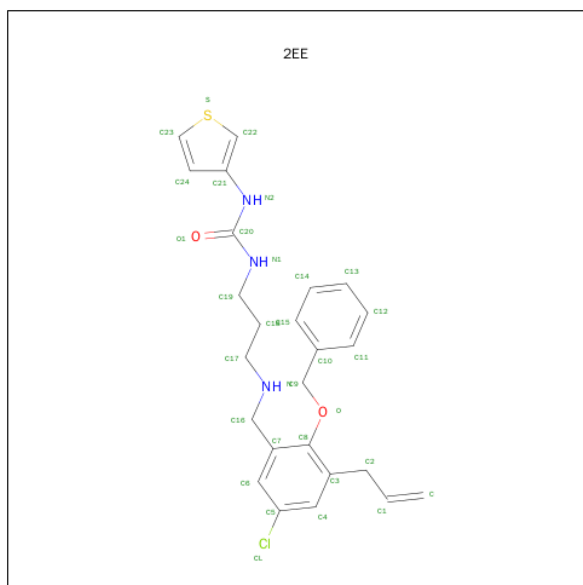
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- 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 1-(3-{[2-(BENZYLOXY)-5-CHLORO-3-(PROP-2-EN-1-YL)BENZYL]AMINO}PROPYL)-3-THIOPHEN-3-YLUREA (three-letter code: 2EE) (formula: C₂₅H₂₈ClN₃O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	Cl	N	O	S	0
			32	25	1	3	2	1	0

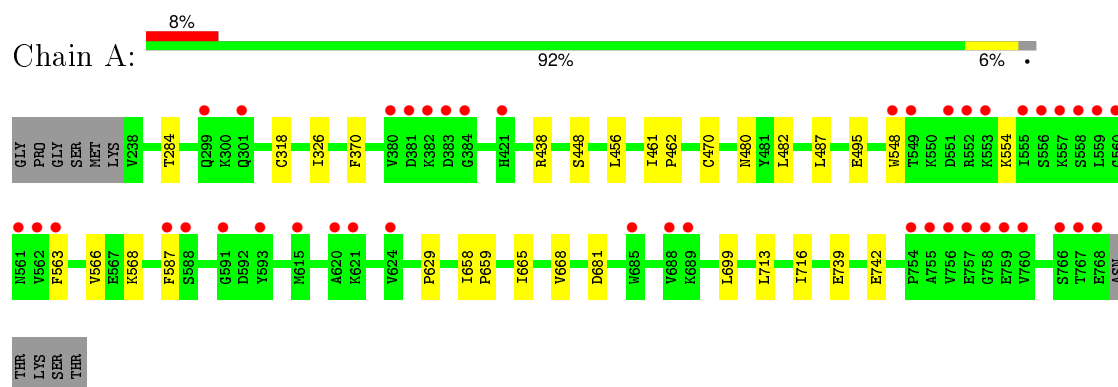
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	159	Total	O	0	0
			159	159		
6	B	179	Total	O	0	0
			179	179		

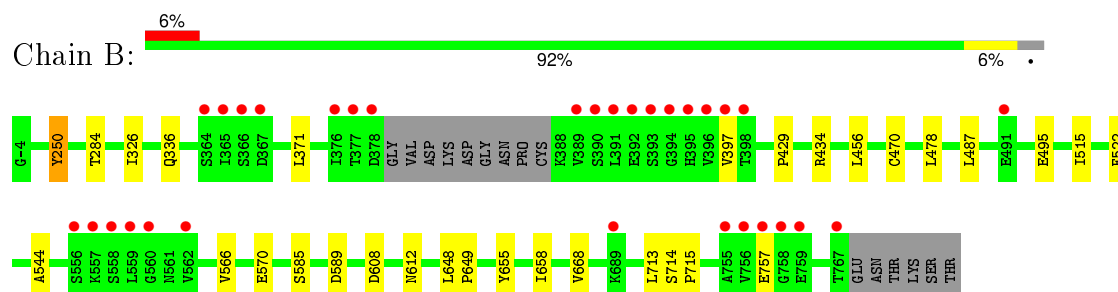
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



• Molecule 1: Methionyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.28Å 106.14Å 207.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.56 48.23 – 2.56	Depositor EDS
% Data completeness (in resolution range)	98.9 (30.00-2.56) 98.9 (48.23-2.56)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.201 , 0.241 0.188 , 0.224	Depositor DCC
R_{free} test set	3174 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 62431 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8978	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CAS, GOL, DMS, 2EE

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	0.41	0/4357	0.58	0/5919
1	B	0.41	0/4364	0.59	0/5925
All	All	0.41	0/8721	0.58	0/11844

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4263	0	4212	18	0
1	B	4260	0	4229	20	0
2	A	36	0	48	1	0
2	B	24	0	32	0	0
3	A	12	0	18	0	0
3	B	4	0	6	0	0
4	A	9	0	8	0	0
5	B	32	0	28	11	0
6	A	159	0	0	3	0
6	B	179	0	0	0	0
All	All	8978	0	8581	43	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 2.

All (43) 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)
5:B:806:2EE:H11	5:B:806:2EE:H3	1.53	0.90
5:B:806:2EE:H11	5:B:806:2EE:C9	2.02	0.89
1:A:462:PRO:HA	1:A:470:CAS:CE2	2.05	0.86
1:A:462:PRO:CA	1:A:470:CAS:CE2	2.59	0.81
1:A:462:PRO:N	1:A:470:CAS:CE2	2.48	0.77
1:A:487:LEU:HD22	1:A:495:GLU:HG3	1.69	0.74
1:A:548:TRP:CZ3	6:A:1029:HOH:O	2.43	0.71
1:B:284:THR:HG22	1:B:326:ILE:HG21	1.79	0.65
1:B:371:LEU:HD12	1:B:397:VAL:HG11	1.79	0.63
6:A:1036:HOH:O	1:B:434:ARG:HD3	1.99	0.61
1:A:461:ILE:C	1:A:470:CAS:CE2	2.70	0.59
5:B:806:2EE:H4	5:B:806:2EE:H11	1.83	0.58
1:A:284:THR:HG22	1:A:326:ILE:HG21	1.86	0.57
1:A:668:VAL:HG11	1:A:713:LEU:HG	1.86	0.57
5:B:806:2EE:C9	5:B:806:2EE:C2	2.75	0.54
1:B:522:PHE:HB3	5:B:806:2EE:C	2.38	0.54
1:A:370:PHE:CZ	1:A:448:SER:HB3	2.45	0.52
1:B:608:ASP:O	1:B:612:ASN:HB3	2.09	0.52
1:B:487:LEU:HD22	1:B:495:GLU:HG3	1.90	0.52
1:B:456:LEU:HD12	1:B:470:CAS:HB3	1.92	0.51
1:B:668:VAL:HG11	1:B:713:LEU:HG	1.93	0.50
1:A:482:LEU:HD21	2:A:801:GOL:H12	1.93	0.50
1:A:665:ILE:HG12	1:A:716:ILE:HD13	1.92	0.49
1:A:563:PHE:CE1	1:A:568:LYS:HG3	2.48	0.49
1:B:585:SER:OG	1:B:589:ASP:HB2	2.12	0.49
1:B:655:TYR:HA	1:B:658:ILE:HD12	1.97	0.47
1:B:522:PHE:CB	5:B:806:2EE:H13	2.46	0.46
1:B:478:LEU:HG	5:B:806:2EE:H12	1.98	0.44
1:A:456:LEU:HD12	1:A:470:CAS:HB3	1.98	0.44
1:B:336:GLN:HG3	1:B:495:GLU:OE2	2.18	0.44
1:A:658:ILE:N	1:A:659:PRO:HA	2.32	0.44
1:A:438:ARG:NH1	6:A:924:HOH:O	2.51	0.44
1:B:714:SER:N	1:B:715:PRO:CD	2.81	0.43
1:B:522:PHE:CB	5:B:806:2EE:C	2.96	0.42
1:B:566:VAL:O	1:B:570:GLU:HG2	2.19	0.42
1:B:250:TYR:HB2	5:B:806:2EE:H19	2.01	0.42
1:A:629:PRO:HG3	1:A:699:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:CAS:AS	1:A:566:VAL:HG23	2.80	0.41
1:B:522:PHE:HB2	5:B:806:2EE:H13	2.03	0.41
1:B:515:ILE:O	1:B:544:ALA:HA	2.21	0.41
1:B:648:LEU:HB3	1:B:649:PRO:HD3	2.03	0.40
5:B:806:2EE:H4	5:B:806:2EE:C2	2.47	0.40
1:A:739:GLU:O	1:A:742:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	528/542 (97%)	515 (98%)	13 (2%)	0	100	100
1	B	525/542 (97%)	513 (98%)	12 (2%)	0	100	100
All	All	1053/1084 (97%)	1028 (98%)	25 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	458/467 (98%)	454 (99%)	4 (1%)	84	94
1	B	458/467 (98%)	455 (99%)	3 (1%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	916/934 (98%)	909 (99%)	7 (1%)	86	95

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	480	ASN
1	A	554	LYS
1	A	587	PHE
1	A	681	ASP
1	B	250	TYR
1	B	429	PRO
1	B	757	GLU

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	A	318	1	5,8,9	0.99	0	2,9,11	1.42	0
1	CAS	A	470	1	5,8,9	1.09	0	2,9,11	1.17	0
1	CAS	B	318	1	5,8,9	1.02	0	2,9,11	1.33	0
1	CAS	B	470	1	5,8,9	0.97	0	2,9,11	1.22	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	A	318	1	-	0/0/7/9	0/0/0/0
1	CAS	A	470	1	-	0/0/7/9	0/0/0/0
1	CAS	B	318	1	-	0/0/7/9	0/0/0/0
1	CAS	B	470	1	-	0/0/7/9	0/0/0/0

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 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	318	CAS	1	0
1	A	470	CAS	5	0
1	B	470	CAS	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 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	A	801	-	5,5,5	0.44	0	5,5,5	1.38	1 (20%)
2	GOL	A	802	-	5,5,5	0.45	0	5,5,5	0.42	0
2	GOL	A	803	-	5,5,5	0.32	0	5,5,5	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	804	-	5,5,5	0.38	0	5,5,5	0.52	0
2	GOL	A	805	-	5,5,5	0.32	0	5,5,5	0.56	0
2	GOL	A	806	-	5,5,5	0.26	0	5,5,5	0.11	0
3	DMS	A	807	-	3,3,3	0.55	0	3,3,3	0.48	0
3	DMS	A	808	-	3,3,3	0.53	0	3,3,3	0.35	0
3	DMS	A	809	-	3,3,3	0.44	0	3,3,3	0.76	0
4	MET	A	810	-	5,8,8	0.28	0	3,9,9	0.30	0
2	GOL	B	801	-	5,5,5	0.39	0	5,5,5	1.14	1 (20%)
2	GOL	B	802	-	5,5,5	0.18	0	5,5,5	0.42	0
2	GOL	B	803	-	5,5,5	0.50	0	5,5,5	0.57	0
2	GOL	B	804	-	5,5,5	0.22	0	5,5,5	0.32	0
3	DMS	B	805	-	3,3,3	0.44	0	3,3,3	0.57	0
5	2EE	B	806	-	32,34,34	0.99	1 (3%)	37,43,43	1.33	2 (5%)

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	801	-	-	0/4/4/4	0/0/0/0
2	GOL	A	802	-	-	0/4/4/4	0/0/0/0
2	GOL	A	803	-	-	0/4/4/4	0/0/0/0
2	GOL	A	804	-	-	0/4/4/4	0/0/0/0
2	GOL	A	805	-	-	0/4/4/4	0/0/0/0
2	GOL	A	806	-	-	0/4/4/4	0/0/0/0
3	DMS	A	807	-	-	0/0/0/0	0/0/0/0
3	DMS	A	808	-	-	0/0/0/0	0/0/0/0
3	DMS	A	809	-	-	0/0/0/0	0/0/0/0
4	MET	A	810	-	-	0/4/8/8	0/0/0/0
2	GOL	B	801	-	-	0/4/4/4	0/0/0/0
2	GOL	B	802	-	-	0/4/4/4	0/0/0/0
2	GOL	B	803	-	-	0/4/4/4	0/0/0/0
2	GOL	B	804	-	-	0/4/4/4	0/0/0/0
3	DMS	B	805	-	-	0/0/0/0	0/0/0/0
5	2EE	B	806	-	-	0/19/21/21	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	806	2EE	C24-C21	4.68	1.43	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	806	2EE	C2-C3-C4	-3.81	112.05	120.47
2	A	801	GOL	O1-C1-C2	-2.51	97.99	110.18
2	B	801	GOL	O1-C1-C2	-2.00	100.46	110.18
5	B	806	2EE	C2-C3-C8	6.24	129.37	119.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GOL	1	0
5	B	806	2EE	11	0

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	529/542 (97%)	0.20	43 (8%)	15 13	25, 38, 89, 131	0
1	B	525/542 (96%)	0.12	31 (5%)	26 23	26, 40, 100, 125	0
All	All	1054/1084 (97%)	0.16	74 (7%)	19 17	25, 39, 96, 131	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	558	SER	7.2
1	A	557	LYS	7.0
1	A	383	ASP	6.8
1	A	551	ASP	6.3
1	A	767	THR	6.1
1	A	552	ARG	6.0
1	B	757	GLU	5.7
1	A	768	GLU	5.5
1	A	556	SER	5.5
1	B	377	THR	5.5
1	A	758	GLY	5.4
1	B	394	GLY	5.3
1	A	757	GLU	5.2
1	B	397	VAL	5.2
1	B	756	VAL	4.8
1	B	758	GLY	4.8
1	A	756	VAL	4.7
1	A	559	LEU	4.5
1	B	395	HIS	4.4
1	B	396	VAL	4.1
1	A	766	SER	3.9
1	A	593	TYR	3.9
1	A	560	GLY	3.8
1	A	553	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	560	GLY	3.6
1	B	559	LEU	3.6
1	A	555	ILE	3.6
1	B	364	SER	3.5
1	A	299	GLN	3.4
1	B	391	LEU	3.4
1	A	384	GLY	3.4
1	B	558	SER	3.4
1	A	755	ALA	3.4
1	A	685	TRP	3.3
1	A	620	ALA	3.3
1	A	587	PHE	3.2
1	B	689	LYS	3.2
1	B	755	ALA	3.2
1	B	491	GLU	3.2
1	A	548	TRP	3.2
1	B	389	VAL	3.1
1	A	561	ASN	3.0
1	B	366	SER	2.9
1	A	549	THR	2.9
1	A	588	SER	2.8
1	A	624	VAL	2.8
1	B	390	SER	2.8
1	A	760	VAL	2.7
1	A	562	VAL	2.7
1	B	392	GLU	2.6
1	A	754	PRO	2.6
1	B	365	ILE	2.6
1	B	376	ILE	2.6
1	B	767	THR	2.6
1	A	759	GLU	2.5
1	A	382	LYS	2.5
1	A	380	VAL	2.4
1	A	591	GLY	2.4
1	A	563	PHE	2.4
1	A	381	ASP	2.3
1	B	759	GLU	2.3
1	B	393	SER	2.3
1	B	378	ASP	2.3
1	B	562	VAL	2.3
1	A	301	GLN	2.2
1	A	689	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	557	LYS	2.1
1	B	398	THR	2.1
1	A	621	LYS	2.1
1	B	367	ASP	2.1
1	A	615	MET	2.1
1	A	688	VAL	2.1
1	A	421[A]	HIS	2.1
1	B	556	SER	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	CAS	A	318	9/10	0.96	0.13	-	41,43,45,45	3
1	CAS	A	470	9/10	0.98	0.11	-	32,35,45,45	3
1	CAS	B	470	9/10	0.99	0.10	-	36,37,43,43	3
1	CAS	B	318	9/10	0.96	0.15	-	37,39,41,42	3

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	A	803	6/6	0.91	0.29	6.26	49,60,64,65	0
3	DMS	A	808	4/4	0.95	0.25	5.09	75,78,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	B	803	6/6	0.89	0.24	4.27	46,49,50,52	0
3	DMS	A	809	4/4	0.83	0.17	3.98	81,81,83,88	0
2	GOL	A	801	6/6	0.84	0.24	3.74	38,40,41,41	0
2	GOL	B	801	6/6	0.93	0.23	2.93	45,46,48,48	0
3	DMS	A	807	4/4	0.95	0.18	2.51	64,70,71,72	0
5	2EE	B	806	32/32	0.91	0.20	2.08	46,60,72,73	0
2	GOL	A	804	6/6	0.90	0.26	1.35	48,50,51,53	0
4	MET	A	810	9/9	0.97	0.14	-0.11	29,30,31,32	0
2	GOL	A	805	6/6	0.91	0.28	-	58,61,62,65	0
2	GOL	A	806	6/6	0.80	0.25	-	76,78,78,79	0
2	GOL	A	802	6/6	0.91	0.12	-	48,51,51,52	0
2	GOL	B	802	6/6	0.94	0.22	-	53,58,60,62	0
3	DMS	B	805	4/4	0.93	0.18	-	70,76,79,80	0
2	GOL	B	804	6/6	0.86	0.27	-	81,86,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.