



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 04:06 PM BST

PDB ID : 4EG8
Title : Trypanosoma brucei methionyl-tRNA synthetase in complex with compound Chem 89
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 : 2.60 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
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

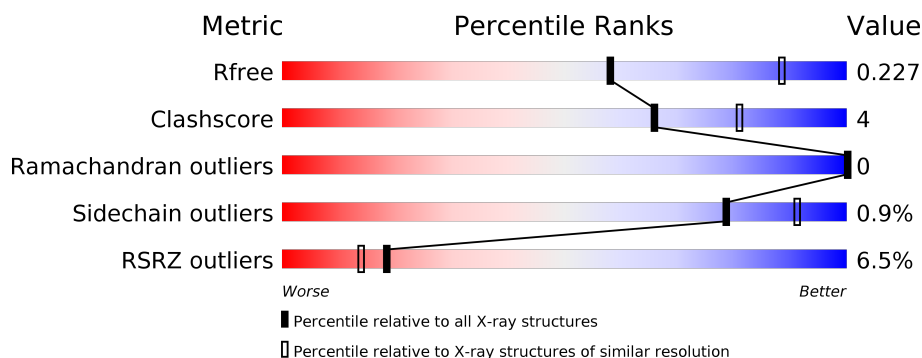
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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>6%</div> <div>89%</div> <div>9%</div> </div>
1	B	542	<div> <div>6%</div> <div>89%</div> <div>9%</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
1	CAS	A	470	-	-	X	-
3	DMS	A	813	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9164 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	531	Total	As	C	N	O	S	0	1	0
			4261	1	2743	721	785	11			
1	B	533	Total	As	C	N	O	S	0	3	0
			4281	1	2762	724	782	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).



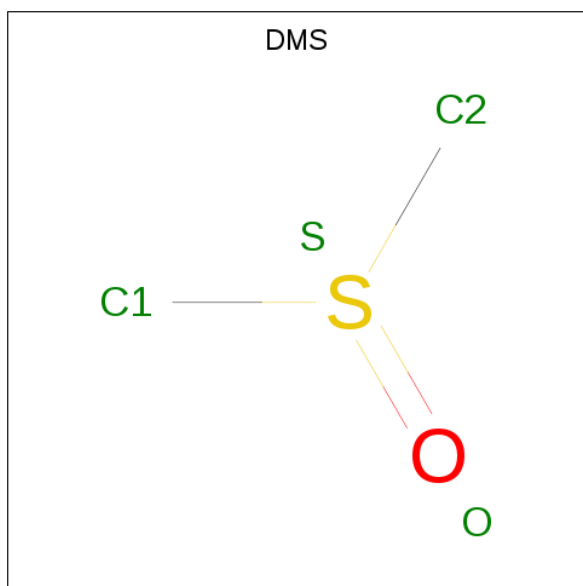
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total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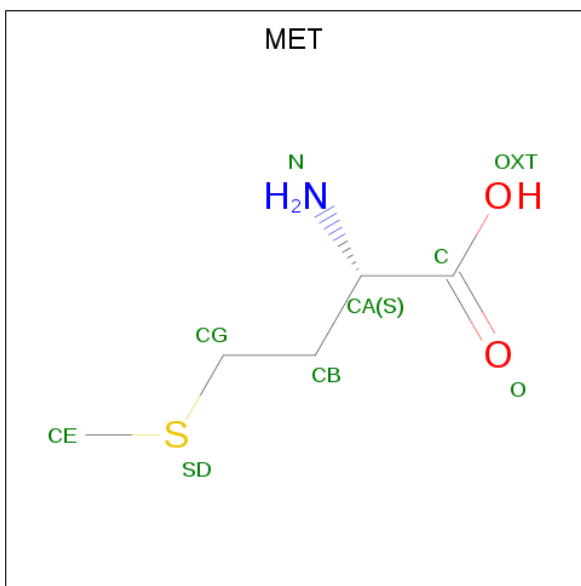
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

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



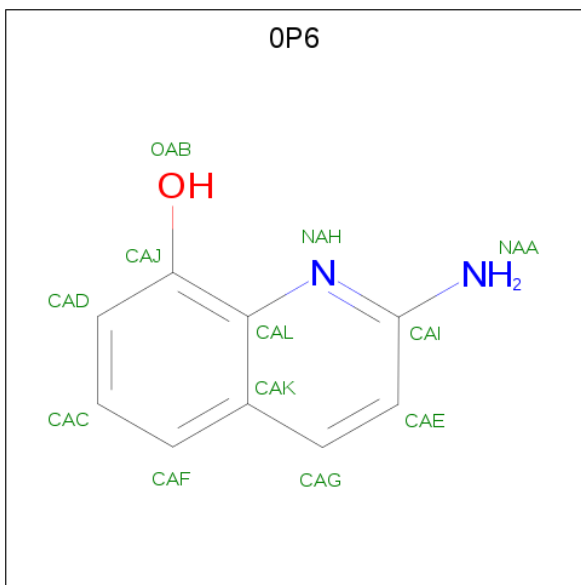
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	A	1	Total	C	O	S	0	0
			4	2	1	1		
3	B	1	Total	C	O	S	0	0
			4	2	1	1		

- 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 2-aminoquinolin-8-ol (three-letter code: OP6) (formula: $C_9H_8N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			12	9	2	1		

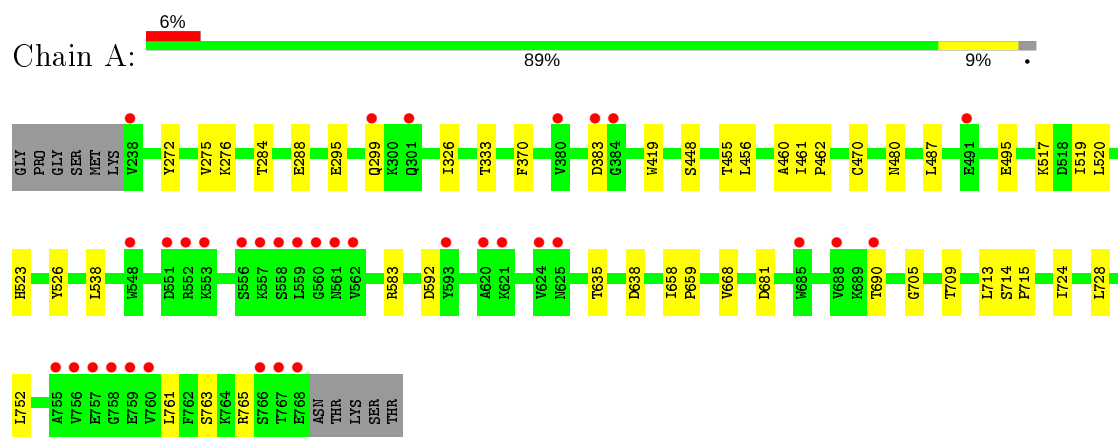
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	224	Total 224	O 224	0	0
6	B	237	Total 237	O 237	0	0

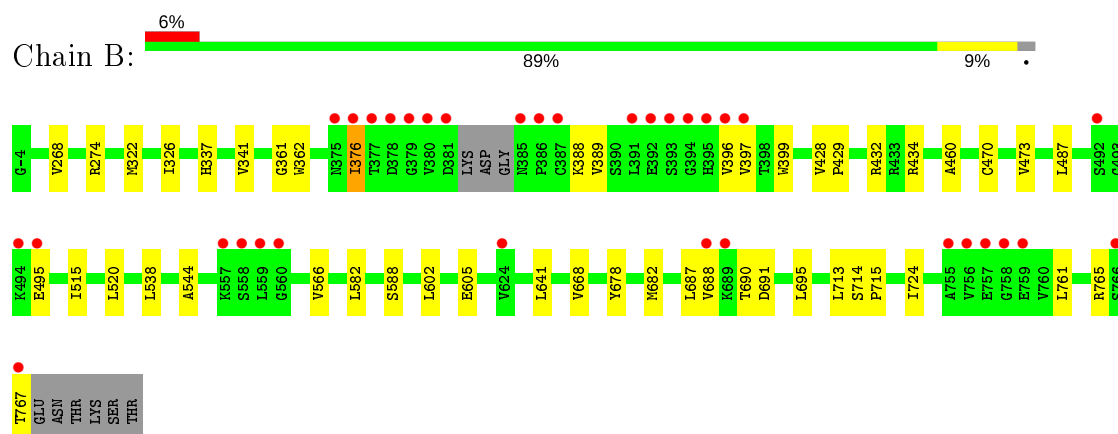
3 Residue-property plots [i](#)

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	87.86Å 105.73Å 206.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 45.30 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.60) 99.4 (45.30-2.60)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.61Å)	Xtriage
Refinement program	REFMAC refmac_5.6.0117	Depositor
R, R_{free}	0.177 , 0.224 0.183 , 0.227	Depositor DCC
R_{free} test set	3031 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9164	wwPDB-VP
Average B, all atoms (Å ²)	43.0	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, 0.333 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, 0P6

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	0.53	0/4364	0.59	0/5929
1	B	0.55	1/4393 (0.0%)	0.60	0/5968
All	All	0.54	1/8757 (0.0%)	0.60	0/11897

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	362	TRP	CD2-CE2	5.37	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	4261	0	4219	36	0
1	B	4281	0	4248	34	0
2	A	60	0	80	1	0
2	B	60	0	80	0	0
3	A	16	0	24	7	0
3	B	4	0	6	3	0
4	A	9	0	8	0	0
5	B	12	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	224	0	0	5	0
6	B	237	0	0	1	0
All	All	9164	0	8673	70	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1072:HOH:O	1:B:434:ARG:HD3	1.76	0.84
1:A:461:ILE:C	1:A:470:CAS:CE1	2.46	0.83
1:A:526:TYR:OH	3:A:813:DMS:H23	1.81	0.81
1:A:462:PRO:N	1:A:470:CAS:CE1	2.43	0.81
1:A:526:TYR:OH	3:A:813:DMS:C2	2.32	0.78
1:B:376:ILE:HD11	1:B:397:VAL:HG21	1.70	0.74
1:B:460:ALA:O	1:B:470:CAS:CE2	2.36	0.73
1:B:487:LEU:HD22	1:B:495:GLU:HG3	1.77	0.66
1:B:602:LEU:HD21	1:B:765:ARG:NH1	2.13	0.63
1:A:460:ALA:O	1:A:470:CAS:CE1	2.46	0.63
1:B:688:VAL:HG12	1:B:695:LEU:CD2	2.30	0.61
1:A:668:VAL:HG11	1:A:713:LEU:HG	1.85	0.58
1:A:370:PHE:O	3:A:813:DMS:H21	2.06	0.56
1:A:724:ILE:HG12	1:A:761:LEU:HD11	1.87	0.56
1:A:460:ALA:C	1:A:470:CAS:CE1	2.74	0.55
1:A:526:TYR:OH	3:A:813:DMS:H22	2.07	0.54
1:A:284:THR:HG22	1:A:326:ILE:HG21	1.90	0.53
1:B:432:ARG:HG2	1:B:520:LEU:HD22	1.90	0.53
1:B:487:LEU:HD22	1:B:495:GLU:CG	2.38	0.53
1:B:389:VAL:HG12	1:B:396:VAL:HA	1.91	0.53
6:A:908:HOH:O	1:B:682:MET:HE1	2.09	0.53
1:A:517:LYS:O	3:A:811:DMS:H13	2.08	0.52
1:B:326:ILE:H	3:B:801:DMS:H22	1.74	0.51
1:B:668:VAL:HG11	1:B:713:LEU:HG	1.94	0.50
1:B:376:ILE:HD11	1:B:397:VAL:HG11	1.93	0.50
1:B:688:VAL:HG12	1:B:695:LEU:HD22	1.93	0.50
1:B:326:ILE:N	3:B:801:DMS:H11	2.26	0.49
1:B:690:THR:HG22	1:B:691:ASP:HB2	1.95	0.48
1:A:690:THR:HG21	6:A:1123:HOH:O	2.14	0.48
1:B:473:VAL:HG23	5:B:812:OP6:NAH	2.29	0.48
1:B:322:MET:CE	1:B:566:VAL:HG22	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:SER:N	1:A:715:PRO:CD	2.78	0.47
1:B:515:ILE:O	1:B:544:ALA:HA	2.16	0.46
1:B:688:VAL:HG12	1:B:695:LEU:HD21	1.96	0.46
1:A:272:TYR:O	1:A:275:VAL:HG22	2.15	0.46
1:A:592:ASP:N	6:A:930:HOH:O	2.50	0.45
1:A:635:THR:O	1:A:638:ASP:HB2	2.17	0.45
1:A:763:SER:O	1:A:765[A]:ARG:NH1	2.50	0.45
1:B:326:ILE:HB	3:B:801:DMS:H23	1.98	0.45
1:A:658:ILE:N	1:A:659:PRO:HA	2.31	0.45
1:B:767:THR:O	1:B:767:THR:HG23	2.16	0.45
1:A:370:PHE:CZ	1:A:448:SER:HB3	2.52	0.45
1:A:462:PRO:CA	1:A:470:CAS:CE1	2.95	0.45
1:A:462:PRO:CD	1:A:470:CAS:CE1	2.94	0.45
1:A:419:TRP:CD1	1:A:538:LEU:HD12	2.52	0.44
1:B:428:VAL:HG13	1:B:429:PRO:HA	1.99	0.44
1:B:388:LYS:O	1:B:397:VAL:HG22	2.16	0.44
1:A:487:LEU:HD22	1:A:495:GLU:HG3	2.00	0.44
1:A:705:GLY:O	1:A:709:THR:HG23	2.17	0.44
1:A:520:LEU:HB3	3:A:811:DMS:H12	2.00	0.43
1:A:728:LEU:HA	1:A:752:LEU:HD22	1.99	0.43
1:B:322:MET:HE2	1:B:566:VAL:HG22	2.00	0.42
1:A:288:GLU:HB2	1:A:333:THR:HG23	2.01	0.42
1:B:268:VAL:HG21	1:B:582:LEU:HD11	2.01	0.42
1:B:724:ILE:HD11	1:B:761:LEU:HD21	2.01	0.42
1:B:361:GLY:HA2	1:B:399:TRP:CZ3	2.54	0.42
1:A:272:TYR:CE2	1:A:276:LYS:HD2	2.54	0.42
1:A:519:ILE:HD12	1:A:523:HIS:HE1	1.84	0.42
1:A:520:LEU:HD23	3:A:810:DMS:H13	2.02	0.42
1:B:515:ILE:CD1	1:B:520:LEU:HA	2.50	0.41
1:A:295:GLU:O	1:A:299:GLN:HG3	2.20	0.41
1:B:687:LEU:HD22	1:B:691:ASP:HB3	2.02	0.41
1:B:274:ARG:NH2	6:B:985:HOH:O	2.53	0.41
1:A:456:LEU:HD22	1:A:470:CAS:HB3	2.02	0.41
1:B:337:HIS:O	1:B:341:VAL:HG23	2.21	0.41
1:B:714:SER:N	1:B:715:PRO:CD	2.84	0.41
1:B:641:LEU:HD22	1:B:678:TYR:CG	2.56	0.41
1:A:690:THR:CG2	6:A:1123:HOH:O	2.70	0.40
1:A:583:ARG:HH22	2:A:802:GOL:H11	1.86	0.40
1:A:761:LEU:HD23	1:A:761:LEU:HA	1.94	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	529/542 (98%)	515 (97%)	14 (3%)	0	100	100
1	B	531/542 (98%)	516 (97%)	15 (3%)	0	100	100
All	All	1060/1084 (98%)	1031 (97%)	29 (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	459/468 (98%)	455 (99%)	4 (1%)	78	91
1	B	461/468 (98%)	457 (99%)	4 (1%)	78	91
All	All	920/936 (98%)	912 (99%)	8 (1%)	78	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	383	ASP
1	A	455	THR
1	A	480	ASN
1	A	681	ASP
1	B	376	ILE
1	B	538	LEU
1	B	588	SER
1	B	605	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 ⓘ

2 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	470	1	5,8,9	0.98	0	1,9,11	0.09	0
1	CAS	B	470	1	5,8,9	1.10	0	1,9,11	0.17	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	470	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.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	470	CAS	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	470	CAS	1	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	$\# Z > 2$
3	DMS	B	801	-	3,3,3	0.47	0	3,3,3	0.73	0
2	GOL	A	809	-	5,5,5	0.47	0	5,5,5	0.56	0
2	GOL	A	804	-	5,5,5	0.32	0	5,5,5	0.17	0
2	GOL	B	804	-	5,5,5	0.58	0	5,5,5	0.73	0
2	GOL	B	808	-	5,5,5	0.39	0	5,5,5	0.23	0
2	GOL	B	811	-	5,5,5	0.26	0	5,5,5	0.24	0
2	GOL	B	806	-	5,5,5	0.37	0	5,5,5	0.20	0
2	GOL	A	808	-	5,5,5	0.46	0	5,5,5	0.82	0
2	GOL	A	814	-	5,5,5	0.53	0	5,5,5	0.49	0
3	DMS	A	813	-	3,3,3	0.52	0	3,3,3	0.80	0
2	GOL	B	803	-	5,5,5	0.26	0	5,5,5	0.29	0
2	GOL	B	807	-	5,5,5	0.31	0	5,5,5	0.20	0
3	DMS	A	811	-	3,3,3	0.60	0	3,3,3	0.52	0
2	GOL	A	803	-	5,5,5	0.63	0	5,5,5	0.43	0
2	GOL	B	805	-	5,5,5	0.26	0	5,5,5	0.32	0
2	GOL	B	809	-	5,5,5	0.68	0	5,5,5	1.11	0
4	MET	A	815	-	4,8,8	0.48	0	2,9,9	0.42	0
2	GOL	A	801	-	5,5,5	0.26	0	5,5,5	0.62	0
2	GOL	A	805	-	5,5,5	0.40	0	5,5,5	0.31	0
2	GOL	B	802	-	5,5,5	0.24	0	5,5,5	0.55	0
3	DMS	A	810	-	3,3,3	0.50	0	3,3,3	0.60	0
2	GOL	A	807	-	5,5,5	0.44	0	5,5,5	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	B	810	-	5,5,5	0.39	0	5,5,5	0.39	0
5	0P6	B	812	-	13,13,13	1.09	0	17,18,18	1.49	2 (11%)
3	DMS	A	812	-	3,3,3	0.47	0	3,3,3	0.77	0
2	GOL	A	802	-	5,5,5	0.25	0	5,5,5	0.48	0
2	GOL	A	806	-	5,5,5	0.28	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	809	-	-	3/4/4/4	-
2	GOL	A	804	-	-	2/4/4/4	-
2	GOL	B	804	-	-	2/4/4/4	-
2	GOL	B	808	-	-	2/4/4/4	-
2	GOL	B	811	-	-	2/4/4/4	-
2	GOL	B	806	-	-	2/4/4/4	-
2	GOL	A	808	-	-	0/4/4/4	-
2	GOL	A	814	-	-	4/4/4/4	-
2	GOL	B	803	-	-	2/4/4/4	-
2	GOL	B	807	-	-	2/4/4/4	-
2	GOL	A	803	-	-	2/4/4/4	-
2	GOL	B	805	-	-	2/4/4/4	-
2	GOL	B	809	-	-	4/4/4/4	-
4	MET	A	815	-	-	0/4/8/8	-
2	GOL	A	801	-	-	0/4/4/4	-
2	GOL	A	805	-	-	2/4/4/4	-
2	GOL	B	802	-	-	0/4/4/4	-
2	GOL	A	807	-	-	2/4/4/4	-
2	GOL	B	810	-	-	4/4/4/4	-
5	0P6	B	812	-	-	-	0/2/2/2
2	GOL	A	802	-	-	0/4/4/4	-
2	GOL	A	806	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	812	OP6	CAJ-CAL-NAH	3.85	121.20	117.33
5	B	812	OP6	NAA-CAI-NAH	2.82	120.59	118.26

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	809	GOL	C1-C2-C3-O3
2	A	804	GOL	C1-C2-C3-O3
2	B	804	GOL	O1-C1-C2-C3
2	B	808	GOL	O1-C1-C2-C3
2	B	811	GOL	O1-C1-C2-C3
2	A	814	GOL	O1-C1-C2-C3
2	A	814	GOL	C1-C2-C3-O3
2	B	803	GOL	O1-C1-C2-C3
2	B	807	GOL	C1-C2-C3-O3
2	A	803	GOL	O1-C1-C2-C3
2	B	809	GOL	C1-C2-C3-O3
2	A	805	GOL	C1-C2-C3-O3
2	A	807	GOL	O1-C1-C2-C3
2	B	810	GOL	C1-C2-C3-O3
2	A	804	GOL	O2-C2-C3-O3
2	B	804	GOL	O1-C1-C2-O2
2	B	806	GOL	O2-C2-C3-O3
2	B	803	GOL	O1-C1-C2-O2
2	B	806	GOL	C1-C2-C3-O3
2	B	810	GOL	O1-C1-C2-C3
2	A	809	GOL	O2-C2-C3-O3
2	B	808	GOL	O1-C1-C2-O2
2	B	811	GOL	O1-C1-C2-O2
2	A	814	GOL	O1-C1-C2-O2
2	A	803	GOL	O1-C1-C2-O2
2	A	807	GOL	O1-C1-C2-O2
2	B	810	GOL	O1-C1-C2-O2
2	B	810	GOL	O2-C2-C3-O3
2	B	807	GOL	O2-C2-C3-O3
2	B	809	GOL	O2-C2-C3-O3
2	A	805	GOL	O2-C2-C3-O3
2	A	809	GOL	O1-C1-C2-C3
2	A	814	GOL	O2-C2-C3-O3
2	B	809	GOL	O1-C1-C2-O2
2	B	805	GOL	C1-C2-C3-O3
2	B	805	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	B	809	GOL	O1-C1-C2-C3

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	DMS	3	0
3	A	813	DMS	4	0
3	A	811	DMS	2	0
3	A	810	DMS	1	0
5	B	812	0P6	1	0
2	A	802	GOL	1	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	530/542 (97%)	-0.00	35 (6%)	18 13	24, 37, 84, 131	0
1	B	532/542 (98%)	0.00	34 (6%)	19 14	23, 37, 93, 134	0
All	All	1062/1084 (97%)	0.00	69 (6%)	18 14	23, 37, 89, 134	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	757	GLU	7.6
1	B	380	VAL	7.0
1	B	756	VAL	7.0
1	B	755	ALA	6.8
1	A	756	VAL	6.4
1	B	386	PRO	5.5
1	B	757	GLU	5.1
1	B	758	GLY	4.7
1	B	381	ASP	4.6
1	A	559	LEU	4.4
1	A	767	THR	4.4
1	B	767	THR	4.2
1	A	383	ASP	4.1
1	B	391	LEU	4.0
1	A	755	ALA	4.0
1	B	377	THR	3.9
1	B	385	ASN	3.9
1	A	624	VAL	3.8
1	A	556	SER	3.7
1	B	379	GLY	3.7
1	A	766	SER	3.6
1	B	558	SER	3.6
1	B	559	LEU	3.6
1	A	558	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	768	GLU	3.5
1	A	685	TRP	3.5
1	A	557	LYS	3.4
1	B	387	CYS	3.3
1	B	397	VAL	3.3
1	A	552	ARG	3.2
1	B	378	ASP	3.2
1	A	384	GLY	3.2
1	B	688	VAL	3.1
1	A	301	GLN	3.1
1	B	395	HIS	3.1
1	B	759	GLU	3.0
1	A	759	GLU	3.0
1	A	758	GLY	3.0
1	A	620	ALA	2.9
1	A	621	LYS	2.9
1	B	557	LYS	2.9
1	A	553	LYS	2.9
1	B	689	LYS	2.9
1	A	560	GLY	2.8
1	A	562	VAL	2.7
1	B	560	GLY	2.6
1	B	376	ILE	2.6
1	B	394	GLY	2.4
1	A	625	ASN	2.4
1	A	551	ASP	2.4
1	B	492	SER	2.4
1	A	561	ASN	2.4
1	B	495	GLU	2.4
1	A	688	VAL	2.3
1	B	393	SER	2.3
1	A	491	GLU	2.3
1	A	760	VAL	2.3
1	B	494	LYS	2.3
1	A	690	THR	2.2
1	A	299	GLN	2.2
1	B	375	ASN	2.2
1	B	624	VAL	2.2
1	A	238	VAL	2.2
1	B	396	VAL	2.2
1	B	766	SER	2.2
1	A	548	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	392	GLU	2.1
1	A	593	TYR	2.1
1	A	380	VAL	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	470	9/10	0.97	0.10	34,35,43,44	3
1	CAS	B	470	9/10	0.98	0.12	34,37,48,50	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	808	6/6	0.72	0.37	78,82,83,87	0
2	GOL	A	803	6/6	0.72	0.32	51,57,58,59	0
2	GOL	A	801	6/6	0.75	0.28	59,61,64,71	0
2	GOL	B	806	6/6	0.80	0.31	78,83,86,87	0
2	GOL	A	807	6/6	0.80	0.29	78,82,83,83	0
3	DMS	A	812	4/4	0.80	0.32	84,90,93,102	0
2	GOL	A	814	6/6	0.81	0.38	64,66,68,70	0
2	GOL	A	805	6/6	0.81	0.29	73,78,82,83	0
2	GOL	A	806	6/6	0.82	0.24	62,67,72,77	0
2	GOL	B	809	6/6	0.84	0.29	53,53,56,57	0
3	DMS	A	813	4/4	0.85	0.26	66,69,71,79	0
2	GOL	A	804	6/6	0.85	0.21	61,68,71,72	0
2	GOL	A	808	6/6	0.87	0.23	57,58,60,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	B	807	6/6	0.88	0.23	75,82,84,86	0
2	GOL	A	809	6/6	0.89	0.25	52,57,59,60	0
2	GOL	B	810	6/6	0.89	0.21	61,65,66,73	0
2	GOL	B	803	6/6	0.90	0.24	52,52,56,63	0
2	GOL	B	811	6/6	0.90	0.23	61,62,63,64	0
2	GOL	B	804	6/6	0.91	0.23	50,55,56,58	0
2	GOL	B	805	6/6	0.93	0.19	47,53,56,61	0
3	DMS	B	801	4/4	0.93	0.20	59,61,73,78	0
3	DMS	A	811	4/4	0.95	0.31	60,73,79,79	0
2	GOL	A	802	6/6	0.95	0.13	44,45,47,48	0
2	GOL	B	802	6/6	0.95	0.25	60,62,64,65	0
3	DMS	A	810	4/4	0.97	0.14	77,78,81,82	0
4	MET	A	815	9/9	0.97	0.14	28,31,35,35	0
5	0P6	B	812	12/12	0.98	0.12	29,31,31,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.