



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:50 PM GMT

PDB ID : 4MWD
Title : Trypanosoma brucei methionyl-tRNA synthetase in complex with inhibitor 1-{3-[(3,5-dichlorobenzyl)amino]propyl}-3-thiophen-3-ylurea (Chem 1433) and ATP analog AMPPCP
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 : 2.25 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

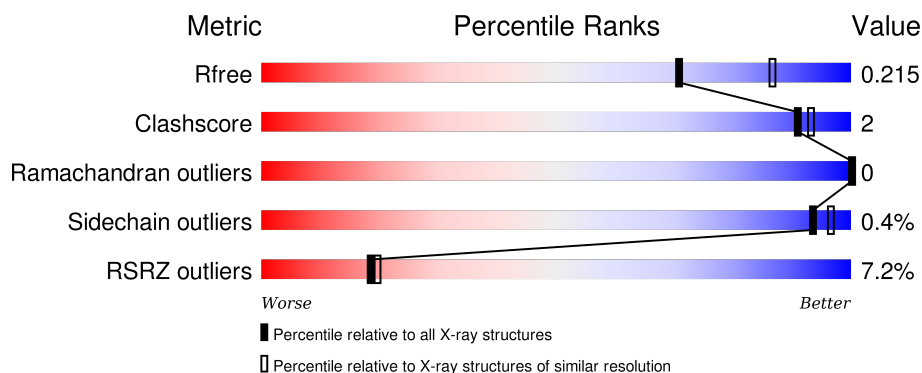
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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>6%</div> <div>94%</div> <div>• •</div> </div>
1	B	542	<div> <div>8%</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
1	CAS	B	470	-	-	X	-
2	GOL	A	901	-	-	-	X
2	GOL	B	804	-	-	-	X
2	GOL	B	805	-	-	-	X
3	DMS	A	905	-	-	-	X
3	DMS	A	906	-	-	-	X
4	SO4	A	907	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9178 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
			4256	2	2739	719	785	11			
1	B	533	Total	As	C	N	O	S	0	1	0
			4267	2	2749	722	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).



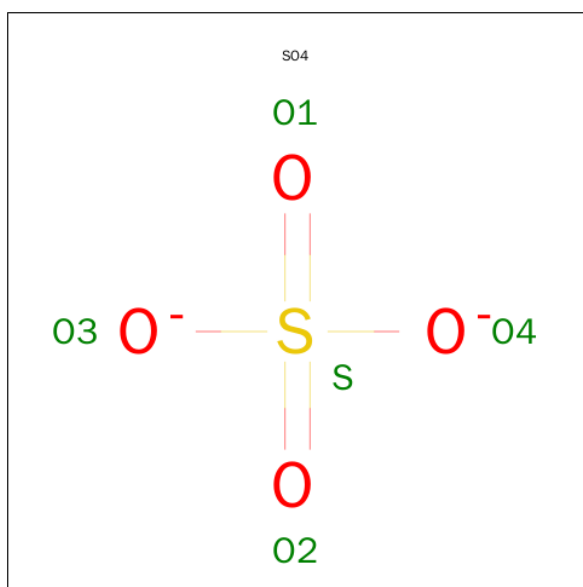
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- 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	B	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



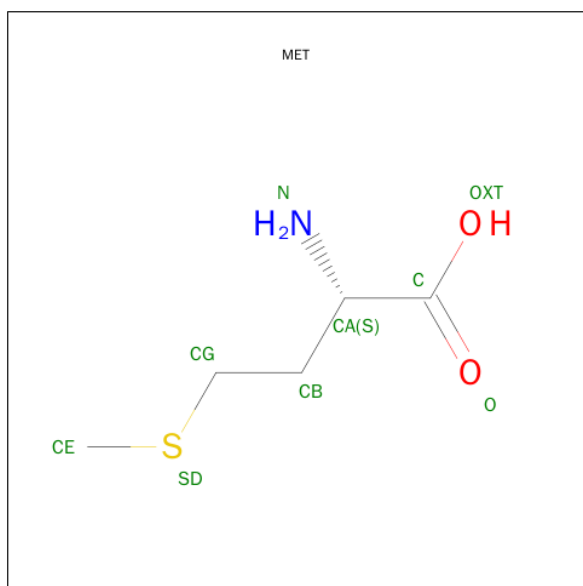
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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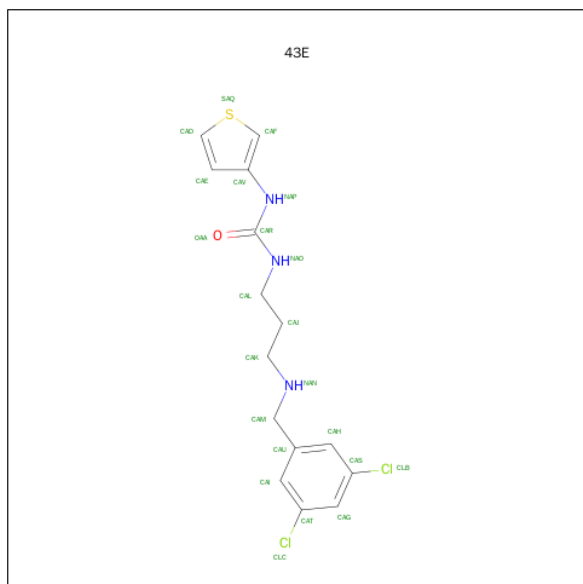
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



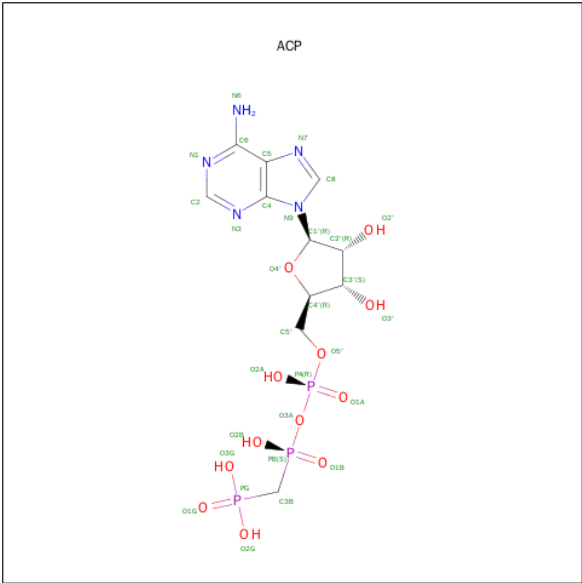
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0
			9	5	1	2	1	0

- Molecule 6 is 1-{3-[(3,5-DICHLOROBENZYL)AMINO]PROPYL}-3-THIOPHEN-3-YLUREA (three-letter code: 43E) (formula: C₁₅H₁₇Cl₂N₃OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	Cl	N	O	0	0
			22	15	2	3	1		

- Molecule 7 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

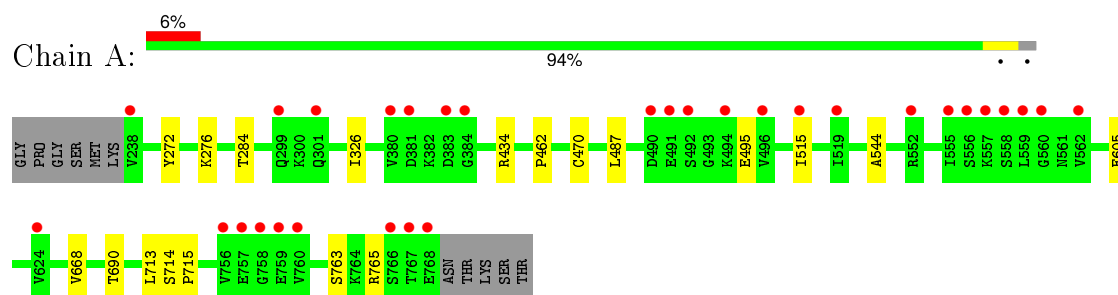
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	254	Total O	0	0
			254 254		
8	B	263	Total O	0	0
			263 263		

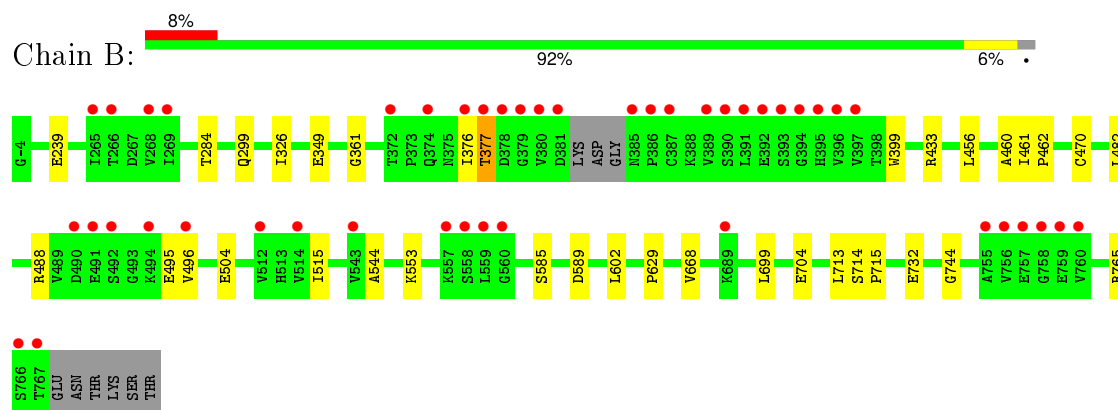
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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	88.27Å 105.88Å 206.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.25 39.97 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.25) 99.7 (39.97-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.24Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.182 , 0.211 0.188 , 0.215	Depositor DCC
R_{free} test set	4605 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 91918 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9178	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CAS, 43E, DMS, SO4, ACP

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	0.38	0/4349	0.58	0/5910
1	B	0.39	0/4361	0.59	1/5923 (0.0%)
All	All	0.38	0/8710	0.58	1/11833 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	ARG	NE-CZ-NH2	-5.42	117.59	120.30

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	4256	0	4196	11	0
1	B	4267	0	4224	26	0
2	A	24	0	32	0	0
2	B	30	0	40	2	0
3	A	8	0	12	0	0
3	B	4	0	6	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	9	0	8	0	0
6	B	22	0	17	0	0
7	B	31	0	14	0	0
8	A	254	0	0	2	0
8	B	263	0	0	5	0
All	All	9178	0	8549	37	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 (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:ILE:C	1:B:470:CAS:CE1	2.27	1.02
1:B:462:PRO:N	1:B:470:CAS:CE1	2.37	0.86
1:B:482:LEU:HD21	2:B:801:GOL:H32	1.75	0.68
1:A:487:LEU:HD22	1:A:495:GLU:HG3	1.75	0.67
1:B:299:GLN:HB3	8:B:1060:HOH:O	1.95	0.66
1:B:284:THR:HG22	1:B:326:ILE:HG21	1.79	0.64
1:A:668:VAL:HG11	1:A:713:LEU:HG	1.81	0.61
1:B:602:LEU:HD21	1:B:765:ARG:NH1	2.20	0.56
1:B:460:ALA:O	1:B:470:CAS:CE1	2.56	0.54
1:B:732:GLU:HG2	8:B:978:HOH:O	2.08	0.52
1:A:272:TYR:CE2	1:A:276:LYS:HD2	2.45	0.51
1:B:668:VAL:HG11	1:B:713:LEU:HG	1.92	0.51
1:B:460:ALA:C	1:B:470:CAS:CE1	2.79	0.50
1:A:763:SER:O	1:A:765[A]:ARG:NH1	2.44	0.50
1:A:284:THR:HG22	1:A:326:ILE:HG21	1.93	0.50
1:B:585:SER:OG	1:B:589:ASP:HB2	2.13	0.48
1:A:487:LEU:HD22	1:A:495:GLU:CG	2.43	0.48
1:B:461:ILE:O	1:B:470:CAS:CE1	2.62	0.47
1:B:462:PRO:CA	1:B:470:CAS:CE1	2.94	0.46
1:B:461:ILE:CA	1:B:470:CAS:CE1	2.94	0.46
1:B:376:ILE:O	1:B:377:THR:HG23	2.16	0.45
1:A:690:THR:CG2	8:A:1222:HOH:O	2.63	0.45
1:B:349:GLU:HG3	8:B:962:HOH:O	2.16	0.44
1:B:361:GLY:HA2	1:B:399:TRP:CZ3	2.52	0.44
1:B:482:LEU:HD21	2:B:801:GOL:C3	2.44	0.44
1:B:515:ILE:O	1:B:544:ALA:HA	2.17	0.44
1:B:239:GLU:HG3	8:B:996:HOH:O	2.18	0.44
1:B:488:ARG:NH2	1:B:504:GLU:OE2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ILE:O	1:A:544:ALA:HA	2.19	0.42
1:B:496:VAL:HG22	8:B:1063:HOH:O	2.17	0.42
1:B:456:LEU:HD12	1:B:470:CAS:HB3	2.01	0.42
1:A:462:PRO:HA	1:A:470:CAS:CE1	2.49	0.42
1:A:434:ARG:HD3	8:A:1223:HOH:O	2.19	0.42
1:B:629:PRO:HG2	1:B:699:LEU:HB3	2.02	0.41
1:A:714:SER:N	1:A:715:PRO:CD	2.85	0.40
1:B:714:SER:N	1:B:715:PRO:CD	2.84	0.40
1:B:704:GLU:OE2	1:B:744:GLY:N	2.46	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%)	514 (97%)	14 (3%)	0	100	100
1	B	528/542 (97%)	513 (97%)	15 (3%)	0	100	100
All	All	1056/1084 (97%)	1027 (97%)	29 (3%)	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	456/467 (98%)	455 (100%)	1 (0%)	95	98
1	B	458/467 (98%)	455 (99%)	3 (1%)	88	93
All	All	914/934 (98%)	910 (100%)	4 (0%)	93	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	605	GLU
1	B	377	THR
1	B	495	GLU
1	B	553	LYS

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	1.17	0	2,9,11	1.55	1 (50%)
1	CAS	A	470	1	5,8,9	0.82	0	2,9,11	1.27	0
1	CAS	B	318	1	5,8,9	1.20	0	2,9,11	1.30	0
1	CAS	B	470	1	5,8,9	1.48	1 (20%)	2,9,11	1.04	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	470	CAS	AS-CE1	-2.46	1.89	1.96

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	CAS	O-C-CA	-2.12	119.97	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	470	CAS	1	0
1	B	470	CAS	8	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

17 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	901	-	5,5,5	0.21	0	5,5,5	0.35	0
2	GOL	A	902	-	5,5,5	0.23	0	5,5,5	0.65	0
2	GOL	A	903	-	5,5,5	0.25	0	5,5,5	0.24	0
2	GOL	A	904	-	5,5,5	0.24	0	5,5,5	0.13	0
3	DMS	A	905	-	3,3,3	0.48	0	3,3,3	0.55	0
3	DMS	A	906	-	3,3,3	0.49	0	3,3,3	0.72	0
4	SO4	A	907	-	4,4,4	0.41	0	6,6,6	0.13	0
5	MET	A	908	-	5,8,8	0.23	0	3,9,9	0.36	0
2	GOL	B	801	-	5,5,5	0.38	0	5,5,5	0.69	0
2	GOL	B	802	-	5,5,5	0.37	0	5,5,5	0.93	0
2	GOL	B	803	-	5,5,5	0.21	0	5,5,5	0.32	0
2	GOL	B	804	-	5,5,5	0.27	0	5,5,5	0.44	0
2	GOL	B	805	-	5,5,5	0.07	0	5,5,5	0.59	0
3	DMS	B	806	-	3,3,3	0.41	0	3,3,3	0.65	0
4	SO4	B	807	-	4,4,4	0.37	0	6,6,6	0.33	0
6	43E	B	808	-	21,23,23	1.02	1 (4%)	23,29,29	0.57	0
7	ACP	B	809	-	25,33,33	2.03	7 (28%)	31,52,52	1.93	5 (16%)

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	901	-	-	0/4/4/4	0/0/0/0
2	GOL	A	902	-	-	0/4/4/4	0/0/0/0
2	GOL	A	903	-	-	0/4/4/4	0/0/0/0
2	GOL	A	904	-	-	0/4/4/4	0/0/0/0
3	DMS	A	905	-	-	0/0/0/0	0/0/0/0
3	DMS	A	906	-	-	0/0/0/0	0/0/0/0
4	SO4	A	907	-	-	0/0/0/0	0/0/0/0
5	MET	A	908	-	-	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
2	GOL	B	805	-	-	0/4/4/4	0/0/0/0
3	DMS	B	806	-	-	0/0/0/0	0/0/0/0
4	SO4	B	807	-	-	0/0/0/0	0/0/0/0
6	43E	B	808	-	-	0/11/13/13	0/2/2/2
7	ACP	B	809	-	-	0/15/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	809	ACP	PB-O2B	-3.27	1.48	1.56
7	B	809	ACP	PG-O2G	-2.40	1.49	1.54
7	B	809	ACP	PG-O3G	2.76	1.61	1.54
7	B	809	ACP	C5-C4	3.16	1.47	1.40
7	B	809	ACP	PB-O1B	3.44	1.60	1.51
7	B	809	ACP	PB-O3A	4.40	1.63	1.58
6	B	808	43E	CAE-CAV	4.49	1.43	1.39
7	B	809	ACP	PG-O1G	5.03	1.61	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	809	ACP	N3-C2-N1	-8.20	122.62	128.89
7	B	809	ACP	C4-C5-N7	-2.83	106.87	109.48
7	B	809	ACP	C1'-N9-C4	-2.75	122.80	126.94
7	B	809	ACP	C2-N1-C6	2.28	122.84	118.77
7	B	809	ACP	O3G-PG-C3B	2.33	112.05	106.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	GOL	2	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%)	-0.04	31 (5%) 26 28	23, 34, 69, 114	0
1	B	531/542 (97%)	0.08	45 (8%) 13 14	23, 33, 74, 109	0
All	All	1060/1084 (97%)	0.02	76 (7%) 18 20	23, 34, 73, 114	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	380	VAL	7.9
1	B	385	ASN	6.9
1	A	768	GLU	6.8
1	A	767	THR	6.1
1	A	766	SER	5.5
1	A	383	ASP	5.4
1	B	767	THR	5.2
1	B	757	GLU	5.0
1	B	756	VAL	4.9
1	A	559	LEU	4.8
1	B	386	PRO	4.8
1	A	757	GLU	4.5
1	B	391	LEU	4.5
1	B	387	CYS	4.5
1	B	396	VAL	4.3
1	B	377	THR	4.2
1	A	238	VAL	4.0
1	B	394	GLY	4.0
1	B	758	GLY	4.0
1	A	491	GLU	3.9
1	B	381	ASP	3.9
1	A	384	GLY	3.9
1	A	758	GLY	3.8
1	A	492	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	380	VAL	3.7
1	B	560	GLY	3.6
1	A	756	VAL	3.4
1	A	556	SER	3.4
1	B	378	ASP	3.3
1	A	557	LYS	3.2
1	B	514	VAL	3.2
1	A	552	ARG	3.2
1	B	393	SER	3.2
1	B	496	VAL	3.2
1	B	491	GLU	3.1
1	B	766	SER	3.0
1	B	755	ALA	3.0
1	A	558	SER	3.0
1	B	395	HIS	2.9
1	B	492	SER	2.9
1	B	559	LEU	2.9
1	B	557	LYS	2.8
1	B	759	GLU	2.8
1	B	397	VAL	2.8
1	B	269	ILE	2.8
1	B	689	LYS	2.8
1	B	374	GLN	2.7
1	B	376	ILE	2.7
1	A	560	GLY	2.7
1	B	558	SER	2.7
1	A	381	ASP	2.7
1	A	562	VAL	2.6
1	B	389	VAL	2.6
1	A	555	ILE	2.6
1	A	301	GLN	2.5
1	A	299	GLN	2.4
1	A	759	GLU	2.4
1	B	379	GLY	2.4
1	B	390	SER	2.4
1	B	265	ILE	2.3
1	A	494	LYS	2.3
1	B	392	GLU	2.3
1	B	268	VAL	2.3
1	B	760	VAL	2.3
1	A	496	VAL	2.2
1	B	372	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	494	LYS	2.2
1	A	490	ASP	2.1
1	B	543	VAL	2.1
1	A	519	ILE	2.1
1	A	760	VAL	2.1
1	B	512	VAL	2.1
1	B	266	THR	2.0
1	B	490	ASP	2.0
1	A	515	ILE	2.0
1	A	624	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. 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	B	470	9/10	0.99	0.10	-	26,28,30,31	3
1	CAS	B	318	9/10	0.97	0.10	-	35,37,42,44	3
1	CAS	A	318	9/10	0.96	0.10	-	36,41,50,51	3
1	CAS	A	470	9/10	0.99	0.07	-	28,30,35,35	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
4	SO4	A	907	5/5	0.94	0.21	7.07	80,83,84,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GOL	A	901	6/6	0.82	0.24	6.96	61,63,64,67	0
2	GOL	B	804	6/6	0.89	0.26	4.37	55,56,56,57	0
3	DMS	A	905	4/4	0.82	0.24	2.88	84,86,91,92	0
2	GOL	B	805	6/6	0.88	0.19	2.87	40,44,44,50	0
3	DMS	A	906	4/4	0.80	0.18	2.64	76,79,79,86	0
2	GOL	B	801	6/6	0.87	0.16	1.50	47,55,56,58	0
4	SO4	B	807	5/5	0.95	0.18	1.35	72,74,75,76	0
2	GOL	A	903	6/6	0.89	0.15	1.04	48,53,56,57	0
5	MET	A	908	9/9	0.97	0.20	0.25	27,27,28,29	0
7	ACP	B	809	31/31	0.94	0.12	-0.58	42,49,69,74	0
6	43E	B	808	22/22	0.98	0.11	-0.99	24,31,34,38	0
2	GOL	B	803	6/6	0.95	0.11	-1.09	51,52,53,53	0
2	GOL	A	904	6/6	0.83	0.22	-	67,69,70,70	0
3	DMS	B	806	4/4	0.84	0.30	-	73,81,87,87	0
2	GOL	A	902	6/6	0.90	0.13	-	53,55,56,59	0
2	GOL	B	802	6/6	0.89	0.15	-	46,48,49,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.