



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:19 PM GMT

PDB ID : 4EG3  
Title : Trypanosoma brucei methionyl-tRNA synthetase in complex with product methionyl-adenylate  
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 : 2.94 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](mailto: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.

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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

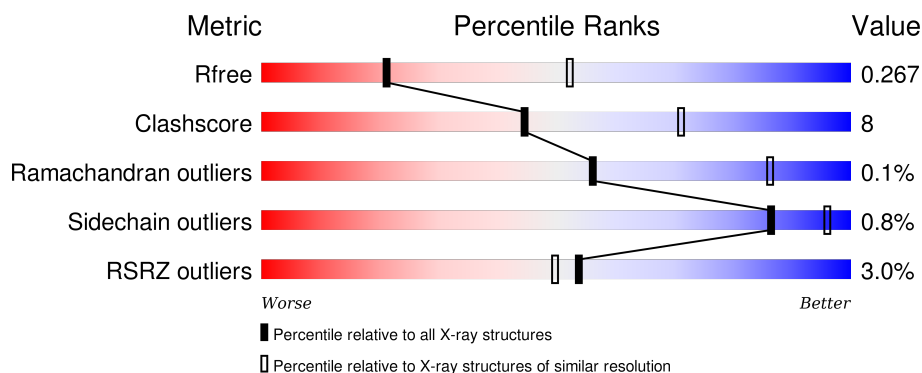
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 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	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (2.98-2.90)

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  $\geq 3$ , 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>4%</div> <div>81%</div> <div>16%</div> <div>.</div> </div>
1	B	542	<div> <div>2%</div> <div>77%</div> <div>20%</div> <div>..</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	805	-	-	-	X
2	GOL	B	802	-	-	-	X
2	GOL	B	803	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8666 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	527	Total	As	C	N	O	S	0	0	0
			4210	1	2712	713	773	11			
1	B	529	Total	As	C	N	O	S	0	0	0
			4225	1	2720	712	780	12			

There are 22 discrepancies between the modelled and reference sequences:

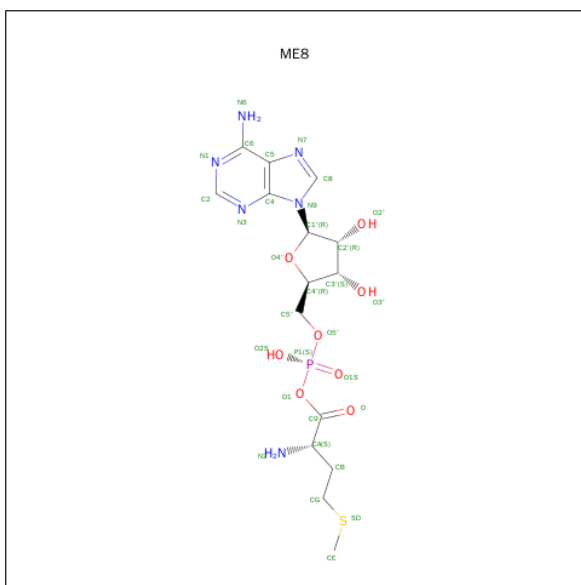
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q38C91
A	-3	PRO	-	EXPRESSION TAG	UNP Q38C91
A	-2	GLY	-	EXPRESSION TAG	UNP Q38C91
A	-1	SER	-	EXPRESSION TAG	UNP Q38C91
A	0	MET	-	EXPRESSION TAG	UNP Q38C91
A	309	THR	ALA	CONFLICT	UNP Q38C91
A	452	ALA	LYS	ENGINEERED MUTATION	UNP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

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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	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 [[(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHOXY-HYDROXY-PHOSPHORYL] (2S)-2-AZANYL-4-METHYLSULFANYL-BUTANOATE (three-letter code: ME8) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>6</sub>O<sub>8</sub>PS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 31	C 15	N 6	O 8	P 1	S 1	0	0
3	B	1	Total 31	C 15	N 6	O 8	P 1	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	40	Total O 40 40	0	0
4	B	63	Total O 63 63	0	0



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.48Å 105.91Å 208.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.94 44.00 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.94) 99.1 (44.00-2.94)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.212 , 0.266 0.214 , 0.267	Depositor DCC
$R_{free}$ test set	2056 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.891	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 40851 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8666	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CAS, GOL, ME8

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	0.51	3/4309 (0.1%)	0.59	0/5856
1	B	0.51	0/4323	0.58	0/5874
All	All	0.51	3/8632 (0.0%)	0.58	0/11730

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	547	TRP	CD2-CE2	5.33	1.47	1.41
1	A	345	TRP	CD2-CE2	5.16	1.47	1.41
1	A	685	TRP	CD2-CE2	5.15	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4210	0	4155	55	0
1	B	4225	0	4162	79	0
2	A	42	0	56	0	0
2	B	24	0	32	0	0
3	A	31	0	22	0	0
3	B	31	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	40	0	0	0	0
4	B	63	0	0	0	0
All	All	8666	0	8449	134	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 8.

All (134) 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:244:VAL:HG22	1:B:266:THR:HG23	1.53	0.90
1:B:271:ARG:O	1:B:275:VAL:HG23	1.77	0.84
1:B:284:THR:HG22	1:B:326:ILE:HG21	1.64	0.79
1:B:719:ARG:O	1:B:722:VAL:HG12	1.88	0.74
1:B:582:LEU:HD12	1:B:716:ILE:HG23	1.71	0.73
1:B:251:VAL:HG21	1:B:288:GLU:HG2	1.72	0.72
1:A:648:LEU:HD11	1:A:668:VAL:HA	1.73	0.71
1:A:670:ASP:OD1	1:A:673:ARG:NH2	2.25	0.69
1:B:238:VAL:HG22	1:B:278:GLU:OE2	1.93	0.69
1:A:641:LEU:HD23	1:A:701:ILE:HG21	1.75	0.68
1:A:505:LEU:HD13	1:A:507:ARG:NH2	2.09	0.68
1:B:460:ALA:HB3	1:B:470:CAS:SG	2.34	0.67
1:B:389:VAL:HG12	1:B:396:VAL:HA	1.77	0.66
1:B:707:ARG:NH1	1:B:745:ALA:HB3	2.12	0.65
1:B:405:TYR:HB2	1:B:450:SER:HB3	1.79	0.64
1:A:641:LEU:HD23	1:A:701:ILE:CG2	2.27	0.64
1:B:707:ARG:HH12	1:B:745:ALA:HB3	1.63	0.64
1:A:244:VAL:HG22	1:A:266:THR:HG23	1.81	0.63
1:A:324:TYR:HB3	1:A:326:ILE:HD12	1.81	0.63
1:B:499:VAL:HG11	1:B:504:GLU:HB3	1.80	0.62
1:B:377:THR:HG22	1:B:378:ASP:H	1.64	0.62
1:A:641:LEU:HD11	1:A:675:ILE:HA	1.82	0.61
1:B:760:VAL:HG21	1:B:763:SER:OG	2.00	0.61
1:B:286:THR:HG23	1:B:329:PHE:CZ	2.36	0.60
1:B:273:HIS:ND1	1:B:278:GLU:OE1	2.26	0.60
1:B:456:LEU:HD23	1:B:460:ALA:HB2	1.83	0.60
1:B:260:VAL:HG11	1:B:322:MET:HE2	1.82	0.60
1:B:455:THR:HB	1:B:456:LEU:HD12	1.86	0.58
1:B:562:VAL:HG22	1:B:563:PHE:H	1.68	0.58
1:A:471:VAL:HG11	1:A:475:LEU:HD22	1.85	0.57
1:A:291:GLN:HB2	1:A:456:LEU:HD23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:LEU:C	1:B:711:LEU:HD23	2.25	0.57
1:B:635:THR:HG22	1:B:637:GLU:H	1.69	0.57
1:B:499:VAL:HG11	1:B:504:GLU:CB	2.34	0.57
1:B:260:VAL:HG11	1:B:322:MET:CE	2.35	0.56
1:B:672:LEU:HA	1:B:675:ILE:HD12	1.86	0.56
1:B:378:ASP:N	1:B:378:ASP:OD1	2.39	0.55
1:A:487:LEU:O	1:A:507:ARG:NH2	2.38	0.55
1:A:292:LYS:HE2	1:A:366:SER:O	2.06	0.55
1:A:326:ILE:HG22	1:A:328:TYR:H	1.72	0.55
1:A:632:ALA:HB3	1:A:697:THR:OG1	2.07	0.55
1:A:635:THR:HG22	1:A:637:GLU:H	1.71	0.55
1:B:473:VAL:O	1:B:477:ALA:N	2.38	0.55
1:A:640:SER:O	1:A:644:LEU:HD12	2.07	0.54
1:A:382:LYS:O	1:A:383:ASP:CB	2.56	0.54
1:A:641:LEU:HD22	1:A:678:TYR:CD2	2.42	0.54
1:B:656:TYR:O	1:B:659:PRO:HB3	2.07	0.54
1:B:251:VAL:HG13	1:B:286:THR:HB	1.90	0.54
1:B:286:THR:HG23	1:B:329:PHE:CE1	2.42	0.54
1:B:641:LEU:HD22	1:B:678:TYR:CG	2.43	0.54
1:A:527:TRP:CE2	1:A:531:LEU:HD11	2.44	0.53
1:B:284:THR:O	1:B:329:PHE:HA	2.07	0.53
1:B:668:VAL:HG11	1:B:713:LEU:HG	1.90	0.53
1:B:685:TRP:O	1:B:688:VAL:HG22	2.08	0.53
1:A:648:LEU:HB2	1:A:671:VAL:HG21	1.90	0.52
1:A:268:VAL:HG13	1:A:715:PRO:HB2	1.91	0.52
1:A:641:LEU:HD22	1:A:678:TYR:CG	2.46	0.51
1:A:430:GLU:OE2	1:A:433:ARG:NH1	2.43	0.51
1:A:288:GLU:HB2	1:A:333:THR:HG23	1.91	0.51
1:B:724:ILE:HD11	1:B:761:LEU:HD21	1.93	0.51
1:A:727:MET:HE3	1:A:761:LEU:HD13	1.91	0.51
1:A:460:ALA:O	1:A:470:CAS:CE1	2.58	0.51
1:A:471:VAL:CG1	1:A:475:LEU:HD22	2.42	0.50
1:B:635:THR:HG22	1:B:636:GLU:N	2.24	0.50
1:B:432:ARG:NH1	1:B:544:ALA:O	2.44	0.50
1:A:617:CYS:SG	1:A:703:LEU:HD23	2.51	0.50
1:B:582:LEU:CD1	1:B:716:ILE:HG23	2.40	0.50
1:B:260:VAL:HG21	1:B:565:PRO:HG3	1.92	0.50
1:B:582:LEU:HD13	1:B:716:ILE:HD12	1.93	0.50
1:B:688:VAL:HG12	1:B:695:LEU:HD22	1.93	0.50
1:A:336:GLN:HB3	1:A:498:LEU:HD22	1.93	0.50
1:B:261:TYR:O	1:B:265:ILE:HD12	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:707:ARG:NH2	1:B:740:ASN:O	2.45	0.49
1:A:685:TRP:O	1:A:688:VAL:HG12	2.12	0.49
1:B:652:ALA:CB	1:B:712:LEU:HD22	2.42	0.49
1:B:521:LYS:HA	1:B:525:ILE:HD13	1.95	0.49
1:A:260:VAL:HG21	1:A:565:PRO:HG3	1.95	0.48
1:B:669:PHE:HA	1:B:672:LEU:HD12	1.95	0.48
1:B:268:VAL:HG11	1:B:661:ILE:HD13	1.96	0.48
1:B:652:ALA:HB3	1:B:712:LEU:HD22	1.96	0.47
1:A:668:VAL:HG11	1:A:713:LEU:HG	1.97	0.47
1:A:261:TYR:CZ	1:A:265:ILE:HD11	2.50	0.47
1:A:322:MET:HE2	1:A:566:VAL:HA	1.96	0.47
1:A:242:PHE:CE1	1:A:273:HIS:CD2	3.03	0.47
1:A:251:VAL:O	1:A:311:VAL:HG11	2.14	0.47
1:A:648:LEU:HD13	1:A:671:VAL:HG21	1.97	0.47
1:B:337:HIS:O	1:B:341:VAL:HG23	2.15	0.46
1:B:756:VAL:HG23	1:B:756:VAL:O	2.14	0.46
1:B:377:THR:HG22	1:B:378:ASP:N	2.29	0.46
1:A:648:LEU:HD13	1:A:671:VAL:CG2	2.45	0.46
1:A:649:PRO:HA	1:A:712:LEU:HD11	1.97	0.46
1:B:478:LEU:HD22	1:B:527:TRP:HB2	1.98	0.46
1:A:613:LEU:HD21	1:A:675:ILE:HG21	1.98	0.46
1:B:528:PRO:HB3	1:B:538:LEU:HD23	1.98	0.46
1:A:251:VAL:HG23	1:A:293:VAL:HG11	1.97	0.45
1:A:543:VAL:HG21	1:A:659:PRO:CG	2.46	0.45
1:B:520:LEU:HD13	1:B:544:ALA:HB2	1.97	0.45
1:B:261:TYR:CE1	1:B:265:ILE:HD11	2.52	0.45
1:B:251:VAL:CG2	1:B:288:GLU:HG2	2.43	0.45
1:B:365:ILE:H	1:B:365:ILE:HD12	1.81	0.45
1:A:569:ALA:HB1	1:A:574:TYR:CD2	2.52	0.45
1:B:487:LEU:HD13	1:B:495:GLU:HG3	1.99	0.45
1:A:430:GLU:O	1:A:433:ARG:HB3	2.17	0.44
1:B:690:THR:HG22	1:B:691:ASP:HB2	2.00	0.44
1:A:549:THR:HG22	1:A:554:LYS:HD2	1.99	0.44
1:B:688:VAL:HG12	1:B:695:LEU:CD2	2.48	0.44
1:B:532:LEU:HG	1:B:538:LEU:HD21	1.99	0.44
1:A:543:VAL:HG21	1:A:659:PRO:HG3	2.00	0.44
1:B:612:ASN:O	1:B:616:ARG:N	2.50	0.43
1:A:648:LEU:CD1	1:A:668:VAL:HA	2.46	0.43
1:B:630:SER:O	1:B:696:ARG:NH1	2.50	0.43
1:B:671:VAL:O	1:B:674:ALA:HB3	2.18	0.43
1:A:655:TYR:CE1	1:A:663:LYS:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:TYR:CD2	1:A:593:TYR:C	2.92	0.42
1:B:594:SER:HB3	1:B:597:ASN:ND2	2.33	0.42
1:A:486:ARG:O	1:A:499:VAL:HG22	2.20	0.42
1:B:252:ASN:HD22	1:B:252:ASN:H	1.66	0.42
1:B:488:ARG:O	1:B:496:VAL:HG22	2.20	0.42
1:B:330:ILE:HD13	1:B:480:ASN:HB2	2.02	0.42
1:B:653:ASP:O	1:B:657:LEU:HD13	2.19	0.42
1:A:251:VAL:HG13	1:A:286:THR:HB	2.02	0.42
1:A:676:ASN:O	1:A:679:VAL:HG22	2.20	0.42
1:B:610:LEU:O	1:B:614:VAL:HG23	2.20	0.41
1:B:728:LEU:O	1:B:752:LEU:HD23	2.21	0.41
1:B:378:ASP:HA	1:B:388:LYS:HA	2.03	0.41
1:B:426:CYS:SG	1:B:427:ILE:HD12	2.61	0.41
1:B:304:PRO:O	1:B:308:THR:HG23	2.20	0.41
1:A:723:VAL:HG12	1:A:727:MET:HE3	2.02	0.41
1:B:258:GLY:HA3	3:B:805:ME8:C5	2.51	0.41
1:B:405:TYR:HB2	1:B:450:SER:CB	2.49	0.41
1:B:290:GLY:HA3	1:B:473:VAL:HG11	2.03	0.41
1:A:527:TRP:HB3	1:A:528:PRO:HD3	2.02	0.41
1:B:593:TYR:CD2	1:B:594:SER:N	2.89	0.41
1:A:413:ARG:NH2	1:A:441:GLU:O	2.54	0.41

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	522/542 (96%)	497 (95%)	24 (5%)	1 (0%)	52	83
1	B	522/542 (96%)	502 (96%)	20 (4%)	0	100	100
All	All	1044/1084 (96%)	999 (96%)	44 (4%)	1 (0%)	56	86

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	759	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	451/468 (96%)	448 (99%)	3 (1%)	88	96
1	B	453/468 (97%)	449 (99%)	4 (1%)	84	95
All	All	904/936 (97%)	897 (99%)	7 (1%)	86	96

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

Mol	Chain	Res	Type
1	A	284	THR
1	A	563	PHE
1	A	766	SER
1	B	252	ASN
1	B	378	ASP
1	B	473	VAL
1	B	651	THR

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

Mol	Chain	Res	Type
1	B	404	ASN

### 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	0.86	0	2,9,11	1.39	0
1	CAS	B	470	1	5,8,9	0.96	0	2,9,11	1.60	1 (50%)

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	0/0/0/0
1	CAS	B	470	1	-	0/0/7/9	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	470	CAS	O-C-CA	-2.16	119.87	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

13 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	0.60	0	5,5,5	0.83	0
2	GOL	A	802	-	5,5,5	0.36	0	5,5,5	0.32	0
2	GOL	A	803	-	5,5,5	0.24	0	5,5,5	0.37	0
2	GOL	A	804	-	5,5,5	0.34	0	5,5,5	0.26	0
2	GOL	A	805	-	5,5,5	0.31	0	5,5,5	0.30	0
2	GOL	A	806	-	5,5,5	0.24	0	5,5,5	0.26	0
2	GOL	A	807	-	5,5,5	0.27	0	5,5,5	0.26	0
3	ME8	A	808	-	26,33,33	0.71	0	26,48,48	2.48	4 (15%)
2	GOL	B	801	-	5,5,5	0.16	0	5,5,5	0.38	0
2	GOL	B	802	-	5,5,5	0.41	0	5,5,5	0.36	0
2	GOL	B	803	-	5,5,5	0.26	0	5,5,5	0.59	0
2	GOL	B	804	-	5,5,5	0.32	0	5,5,5	0.21	0
3	ME8	B	805	-	26,33,33	0.80	1 (3%)	26,48,48	2.38	3 (11%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	807	-	-	0/4/4/4	0/0/0/0
3	ME8	A	808	-	-	0/17/39/39	0/3/3/3
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	ME8	B	805	-	-	0/17/39/39	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	805	ME8	P1-O2S	2.03	1.63	1.54

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	808	ME8	N3-C2-N1	-10.84	120.59	128.89
3	B	805	ME8	N3-C2-N1	-10.57	120.80	128.89
3	A	808	ME8	C4-C5-N7	-2.17	107.48	109.48
3	A	808	ME8	CE-SD-CG	2.14	107.69	100.37
3	B	805	ME8	O2S-P1-O1	3.21	114.09	104.16
3	B	805	ME8	CE-SD-CG	3.22	111.36	100.37
3	A	808	ME8	O2S-P1-O1	3.87	116.12	104.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	805	ME8	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	526/542 (97%)	-0.02	21 (3%)	42 38	33, 54, 89, 123	0
1	B	528/542 (97%)	-0.12	11 (2%)	67 65	36, 56, 100, 135	0
All	All	1054/1084 (97%)	-0.07	32 (3%)	54 50	33, 55, 96, 135	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	562	VAL	5.4
1	B	561	ASN	3.7
1	A	767	THR	3.5
1	A	561	ASN	3.1
1	A	766	SER	3.0
1	B	551	ASP	3.0
1	B	563	PHE	3.0
1	A	551	ASP	2.9
1	A	622	ILE	2.8
1	A	382	LYS	2.8
1	A	552	ARG	2.7
1	A	558	SER	2.7
1	A	625	ASN	2.6
1	A	381	ASP	2.6
1	A	301	GLN	2.6
1	B	767	THR	2.6
1	B	380	VAL	2.5
1	B	562	VAL	2.5
1	A	302	VAL	2.4
1	A	757	GLU	2.4
1	A	756	VAL	2.3
1	A	299	GLN	2.3
1	B	758	GLY	2.2
1	A	624	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	552	ARG	2.1
1	A	685	TRP	2.1
1	A	620	ALA	2.1
1	B	391	LEU	2.1
1	B	387	CYS	2.0
1	A	755	ALA	2.0
1	A	385	ASN	2.0
1	B	744	GLY	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CAS	A	470	9/10	0.96	0.17	-	53,54,58,58	3
1	CAS	B	470	9/10	0.96	0.20	-	57,62,68,68	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	GOL	A	805	6/6	0.88	0.26	4.42	48,51,53,58	0
2	GOL	B	803	6/6	0.89	0.26	3.14	53,56,56,58	0
2	GOL	B	802	6/6	0.88	0.31	2.39	68,72,72,73	0
2	GOL	A	803	6/6	0.89	0.23	1.98	71,76,78,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	804	6/6	0.88	0.23	1.89	67,72,72,73	0
2	GOL	A	802	6/6	0.95	0.19	1.33	64,66,69,71	0
3	ME8	A	808	31/31	0.97	0.17	-0.60	34,43,48,51	0
3	ME8	B	805	31/31	0.95	0.15	-0.74	36,47,58,60	0
2	GOL	B	804	6/6	0.70	0.40	-	75,82,87,89	0
2	GOL	A	807	6/6	0.87	0.20	-	74,75,76,76	0
2	GOL	A	806	6/6	0.85	0.27	-	68,73,74,74	0
2	GOL	A	801	6/6	0.97	0.11	-	22,23,24,24	0
2	GOL	B	801	6/6	0.90	0.17	-	41,46,47,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.