



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 11:53 am GMT

PDB ID : 2PMF  
Title : The crystal structure of a human glycyl-tRNA synthetase mutant  
Authors : Xie, W.  
Deposited on : 2007-04-21  
Resolution : 2.85 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

<https://www.wwpdb.org/validation/2017/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  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

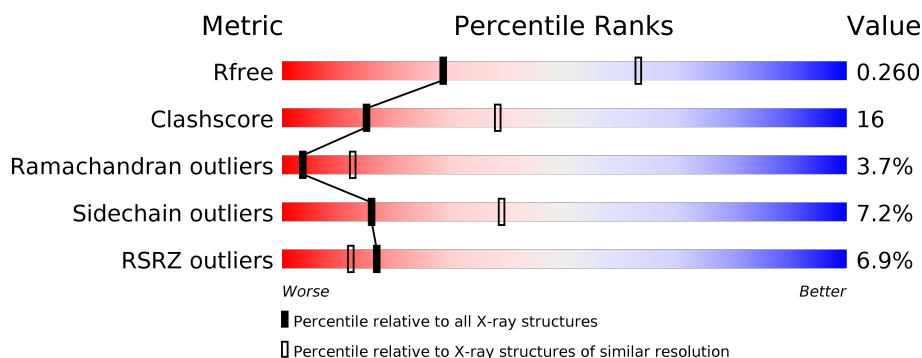
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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))
$R_{free}$	111664	2715 (2.90-2.82)
Clashscore	122126	2976 (2.90-2.82)
Ramachandran outliers	120053	2913 (2.90-2.82)
Sidechain outliers	120020	2916 (2.90-2.82)
RSRZ outliers	108989	2654 (2.90-2.82)

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	693	<div> <div>5%</div> <div>52%</div> <div>19%</div> <div>•</div> <div>25%</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
3	GOL	A	801	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4353 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 Glycyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4144	2631	720	770	23			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	526	ARG	GLY	ENGINEERED	UNP P41250
A	686	LEU	-	CLONING ARTIFACT	UNP P41250
A	687	GLU	-	CLONING ARTIFACT	UNP P41250
A	688	HIS	-	CLONING ARTIFACT	UNP P41250
A	689	HIS	-	CLONING ARTIFACT	UNP P41250
A	690	HIS	-	CLONING ARTIFACT	UNP P41250
A	691	HIS	-	CLONING ARTIFACT	UNP P41250
A	692	HIS	-	CLONING ARTIFACT	UNP P41250
A	693	HIS	-	CLONING ARTIFACT	UNP P41250

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 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
3	A	1	Total	C	O	0	0
			6	3	3		

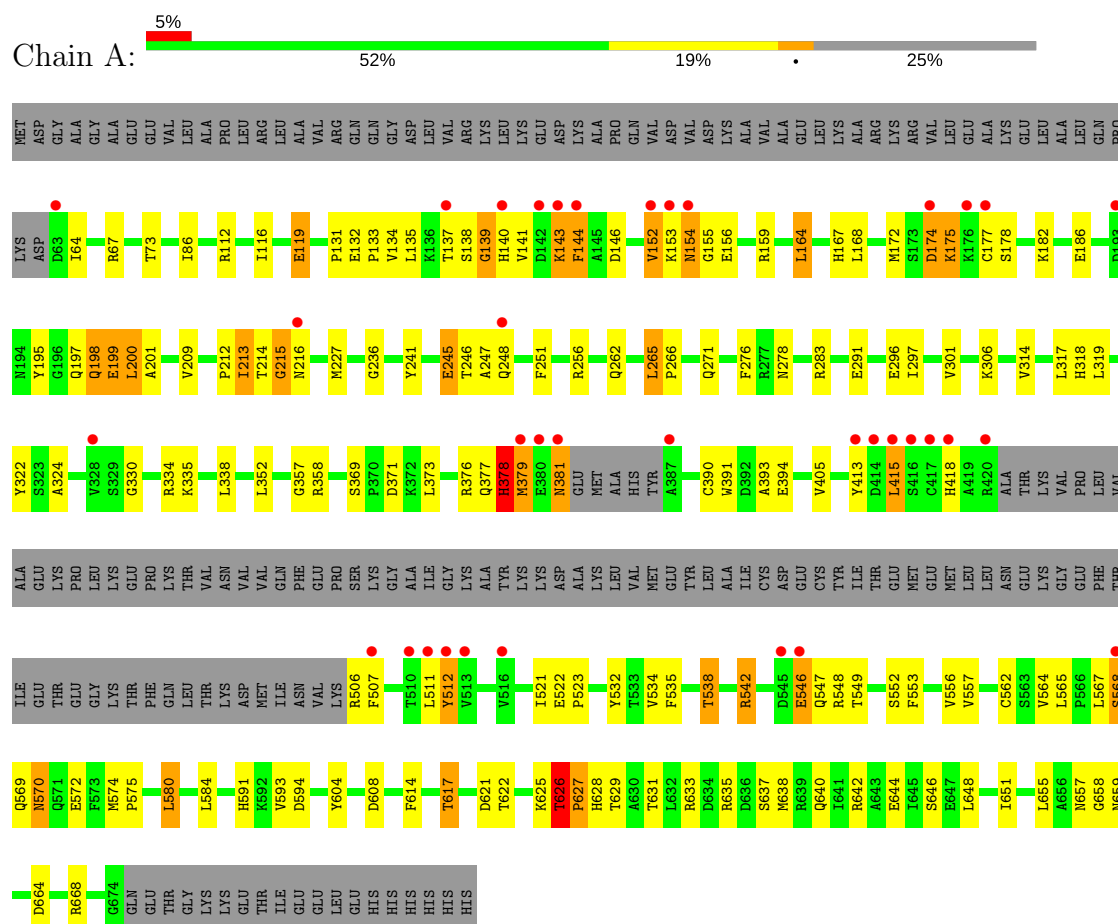
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	202	Total	O	0	0
			202	202		

### 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 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: Glycyl-tRNA synthetase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.41Å 91.41Å 246.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.24 – 2.85 29.23 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.24-2.85) 98.8 (29.23-2.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.13 (at 2.85Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.231 , 0.271 0.224 , 0.260	Depositor DCC
$R_{free}$ test set	1272 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4353	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL

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	0.24	0/4237	0.44	1/5722 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

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	A	174	ASP	N-CA-C	-5.33	96.61	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	LYS	Peptide
1	A	175	LYS	Peptide
1	A	265	LEU	Peptide
1	A	378	HIS	Peptide
1	A	626	THR	Peptide

## 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	4144	0	4034	133	1
2	A	1	0	0	0	0
3	A	6	0	8	7	0
4	A	202	0	0	2	0
All	All	4353	0	4042	133	1

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 16.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ARG:HG2	1:A:542:ARG:HH11	1.19	1.03
1:A:379:MET:HG2	1:A:379:MET:O	1.64	0.98
1:A:621:ASP:HB3	3:A:801:GOL:H11	1.43	0.98
1:A:314:VAL:HG11	1:A:357:GLY:HA3	1.50	0.94
1:A:626:THR:HG22	1:A:626:THR:O	1.68	0.92
1:A:154:ASN:O	1:A:156:GLU:N	2.00	0.92
1:A:172:MET:CE	1:A:186:GLU:HG3	2.00	0.91
1:A:664:ASP:O	1:A:668:ARG:HD2	1.69	0.91
1:A:172:MET:HE3	1:A:186:GLU:HG3	1.56	0.85
1:A:542:ARG:CG	1:A:542:ARG:HH11	1.90	0.84
1:A:633:ARG:HG3	1:A:640:GLN:HG2	1.61	0.82
1:A:413:TYR:CE2	1:A:415:LEU:HB2	2.15	0.81
1:A:379:MET:CG	1:A:379:MET:O	2.28	0.81
1:A:629:THR:OG1	3:A:801:GOL:H2	1.81	0.79
1:A:657:ASN:O	1:A:659:ASN:N	2.15	0.79
1:A:622:THR:O	1:A:628:HIS:HD2	1.68	0.75
1:A:534:VAL:O	1:A:538:THR:HB	1.87	0.74
1:A:626:THR:CG2	1:A:626:THR:O	2.34	0.73
1:A:140:HIS:HE1	1:A:241:TYR:OH	1.70	0.73
1:A:198:GLN:O	1:A:201:ALA:N	2.22	0.72
1:A:168:LEU:O	1:A:172:MET:HB2	1.89	0.72
1:A:135:LEU:HD23	1:A:248:GLN:HE22	1.56	0.71
1:A:664:ASP:O	1:A:668:ARG:CD	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:VAL:CG1	1:A:357:GLY:HA3	2.21	0.69
1:A:248:GLN:HG3	1:A:418:HIS:CE1	2.28	0.69
1:A:604:TYR:OH	1:A:617:THR:HG22	1.93	0.69
1:A:413:TYR:HE2	1:A:415:LEU:HB2	1.60	0.67
1:A:135:LEU:HD12	1:A:241:TYR:HB2	1.79	0.64
1:A:138:SER:HB3	1:A:143:LYS:HE2	1.79	0.63
1:A:369:SER:HB3	1:A:371:ASP:OD1	1.99	0.63
1:A:297:ILE:HB	1:A:523:PRO:HG2	1.80	0.62
1:A:621:ASP:HB3	3:A:801:GOL:C1	2.26	0.62
1:A:553:PHE:O	1:A:635:ARG:NH2	2.32	0.62
1:A:538:THR:HG23	1:A:552:SER:N	2.14	0.62
1:A:644:GLU:HG3	1:A:646:SER:H	1.65	0.62
1:A:140:HIS:CE1	1:A:241:TYR:OH	2.52	0.61
1:A:134:VAL:HG12	1:A:248:GLN:HE21	1.65	0.61
1:A:246:THR:HB	1:A:296:GLU:HG3	1.82	0.61
1:A:175:LYS:HD3	1:A:182:LYS:HE3	1.80	0.61
1:A:248:GLN:HG3	1:A:418:HIS:HE1	1.66	0.60
1:A:522:GLU:O	1:A:522:GLU:HG3	2.00	0.60
1:A:177:CYS:SG	1:A:178:SER:N	2.75	0.60
1:A:627:PRO:O	1:A:629:THR:HG23	2.02	0.59
1:A:622:THR:O	1:A:628:HIS:CD2	2.55	0.58
1:A:132:GLU:HG3	1:A:241:TYR:HE1	1.68	0.58
1:A:314:VAL:HG13	1:A:317:LEU:HD12	1.84	0.58
1:A:538:THR:HG23	1:A:552:SER:H	1.68	0.58
1:A:134:VAL:HG12	1:A:248:GLN:NE2	2.19	0.57
1:A:637:SER:O	1:A:638:MET:HB2	2.05	0.57
1:A:625:LYS:HB2	3:A:801:GOL:H32	1.85	0.57
1:A:322:TYR:HD2	1:A:376:ARG:HG3	1.69	0.56
1:A:135:LEU:HD23	1:A:248:GLN:NE2	2.20	0.56
1:A:251:PHE:HB3	1:A:415:LEU:HG	1.88	0.56
1:A:324:ALA:HB1	1:A:379:MET:HB2	1.88	0.56
1:A:322:TYR:CD2	1:A:376:ARG:HG3	2.41	0.56
1:A:648:LEU:HD23	1:A:651:ILE:HD11	1.88	0.55
1:A:378:HIS:CE1	1:A:390:CYS:HB2	2.42	0.55
1:A:608:ASP:OD2	1:A:633:ARG:NH2	2.32	0.55
1:A:154:ASN:C	1:A:156:GLU:H	2.06	0.54
1:A:172:MET:CE	1:A:186:GLU:CG	2.82	0.54
1:A:570:ASN:C	1:A:572:GLU:H	2.11	0.54
1:A:358:ARG:HD3	4:A:1093:HOH:O	2.07	0.53
1:A:393:ALA:HB3	1:A:405:VAL:HB	1.90	0.53
1:A:314:VAL:HG12	1:A:338:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:HA	1:A:177:CYS:H	1.73	0.53
1:A:413:TYR:CD2	1:A:415:LEU:HB2	2.43	0.52
1:A:565:LEU:HD22	1:A:594:ASP:HB3	1.93	0.51
1:A:198:GLN:O	1:A:200:LEU:N	2.43	0.51
1:A:251:PHE:O	1:A:415:LEU:HD21	2.11	0.51
1:A:580:LEU:O	1:A:584:LEU:HB2	2.10	0.51
1:A:642:ARG:NH2	3:A:801:GOL:H12	2.25	0.51
1:A:542:ARG:NH1	1:A:542:ARG:CG	2.58	0.51
1:A:381:ASN:C	1:A:381:ASN:ND2	2.64	0.50
1:A:245:GLU:HG2	1:A:246:THR:N	2.25	0.50
1:A:642:ARG:HH21	3:A:801:GOL:H12	1.77	0.50
1:A:167:HIS:HD2	1:A:209:VAL:HG22	1.77	0.50
1:A:245:GLU:HG2	1:A:247:ALA:H	1.76	0.50
1:A:542:ARG:NH1	1:A:542:ARG:HG2	2.01	0.49
1:A:172:MET:HE3	1:A:186:GLU:CG	2.34	0.49
1:A:119:GLU:HG3	4:A:946:HOH:O	2.13	0.49
1:A:556:VAL:HG13	1:A:557:VAL:HG23	1.95	0.49
1:A:195:TYR:HD2	1:A:199:GLU:HG2	1.77	0.48
1:A:567:LEU:O	1:A:568:SER:C	2.51	0.48
1:A:319:LEU:N	1:A:319:LEU:HD23	2.29	0.48
1:A:319:LEU:H	1:A:319:LEU:HD23	1.79	0.47
1:A:195:TYR:CD2	1:A:199:GLU:HG2	2.49	0.47
1:A:112:ARG:HG2	1:A:116:ILE:HD12	1.95	0.47
1:A:306:LYS:NZ	1:A:521:ILE:HD11	2.29	0.47
1:A:132:GLU:HB3	1:A:133:PRO:HD3	1.97	0.47
1:A:546:GLU:O	1:A:548:ARG:N	2.48	0.47
1:A:511:LEU:O	1:A:512:TYR:CB	2.63	0.47
1:A:376:ARG:NH1	1:A:394:GLU:OE2	2.48	0.46
1:A:415:LEU:HD22	1:A:506:ARG:N	2.31	0.46
1:A:564:VAL:HG22	1:A:593:VAL:HA	1.98	0.46
1:A:153:LYS:O	1:A:154:ASN:HB3	2.16	0.46
1:A:614:PHE:CZ	1:A:655:LEU:HB3	2.51	0.46
1:A:246:THR:CG2	1:A:271:GLN:HB3	2.46	0.45
1:A:146:ASP:OD1	1:A:159:ARG:NH1	2.49	0.45
1:A:569:GLN:H	1:A:569:GLN:CD	2.20	0.45
1:A:197:GLN:OE1	1:A:198:GLN:N	2.49	0.45
1:A:143:LYS:O	1:A:144:PHE:HB2	2.16	0.45
1:A:213:ILE:H	1:A:213:ILE:HG13	1.54	0.45
1:A:73:THR:HG21	1:A:549:THR:HG21	1.99	0.44
1:A:276:PHE:CE2	1:A:291:GLU:HG3	2.53	0.44
1:A:570:ASN:C	1:A:572:GLU:N	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ALA:HB1	1:A:379:MET:CB	2.47	0.44
1:A:153:LYS:O	1:A:154:ASN:CB	2.65	0.44
1:A:143:LYS:O	1:A:144:PHE:CB	2.66	0.44
1:A:143:LYS:HB2	1:A:227:MET:HE3	1.99	0.44
1:A:538:THR:HG21	1:A:553:PHE:CD2	2.53	0.44
1:A:629:THR:HG1	3:A:801:GOL:H2	1.77	0.43
1:A:135:LEU:CD1	1:A:241:TYR:HB2	2.46	0.43
1:A:565:LEU:HD22	1:A:594:ASP:CB	2.48	0.43
1:A:574:MET:N	1:A:575:PRO:HD2	2.34	0.43
1:A:377:GLN:HB2	1:A:391:TRP:CE2	2.54	0.43
1:A:546:GLU:HA	1:A:546:GLU:OE1	2.19	0.43
1:A:608:ASP:CG	1:A:633:ARG:HH22	2.18	0.43
1:A:306:LYS:HZ2	1:A:521:ILE:HD11	1.84	0.42
1:A:251:PHE:CB	1:A:415:LEU:HG	2.50	0.42
1:A:532:TYR:HA	1:A:535:PHE:CD1	2.54	0.42
1:A:164:LEU:HD12	1:A:200:LEU:HD21	2.02	0.42
1:A:135:LEU:HD12	1:A:241:TYR:CB	2.48	0.42
1:A:413:TYR:HE2	1:A:415:LEU:CB	2.31	0.42
1:A:139:GLY:C	1:A:141:VAL:H	2.23	0.41
1:A:318:HIS:HB3	1:A:335:LYS:HE2	2.01	0.41
1:A:143:LYS:HD3	1:A:143:LYS:HA	1.70	0.41
1:A:154:ASN:O	1:A:154:ASN:ND2	2.50	0.41
1:A:167:HIS:CD2	1:A:209:VAL:HG22	2.54	0.41
1:A:214:THR:HA	1:A:215:GLY:HA2	1.99	0.41
1:A:131:PRO:HG2	1:A:134:VAL:HG23	2.03	0.40
1:A:132:GLU:N	1:A:133:PRO:CD	2.84	0.40
1:A:198:GLN:O	1:A:199:GLU:C	2.60	0.40
1:A:562:CYS:O	1:A:591:HIS:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:SER:OG	1:A:668:ARG:O[7_455]	2.14	0.06

## 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	516/693 (74%)	468 (91%)	29 (6%)	19 (4%)	4	12

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	PHE
1	A	155	GLY
1	A	198	GLN
1	A	199	GLU
1	A	547	GLN
1	A	266	PRO
1	A	330	GLY
1	A	658	GLY
1	A	212	PRO
1	A	215	GLY
1	A	512	TYR
1	A	64	ILE
1	A	627	PRO
1	A	568	SER
1	A	626	THR
1	A	152	VAL
1	A	139	GLY
1	A	236	GLY
1	A	86	ILE

### 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	446/601 (74%)	414 (93%)	32 (7%)	16	39

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	119	GLU
1	A	137	THR
1	A	152	VAL
1	A	154	ASN
1	A	164	LEU
1	A	174	ASP
1	A	200	LEU
1	A	213	ILE
1	A	216	ASN
1	A	245	GLU
1	A	256	ARG
1	A	262	GLN
1	A	265	LEU
1	A	278	ASN
1	A	283	ARG
1	A	301	VAL
1	A	334	ARG
1	A	352	LEU
1	A	373	LEU
1	A	378	HIS
1	A	379	MET
1	A	381	ASN
1	A	415	LEU
1	A	507	PHE
1	A	538	THR
1	A	542	ARG
1	A	546	GLU
1	A	570	ASN
1	A	580	LEU
1	A	617	THR
1	A	631	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN

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Mol	Chain	Res	Type
1	A	113	GLN
1	A	140	HIS
1	A	167	HIS
1	A	206	ASN
1	A	248	GLN
1	A	278	ASN
1	A	378	HIS
1	A	381	ASN
1	A	418	HIS
1	A	570	ASN
1	A	628	HIS
1	A	640	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	GOL	A	801	-	5,5,5	0.37	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
3	GOL	A	801	-	-	0/4/4/4	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.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	GOL	7	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	522/693 (75%)	-0.01	36 (6%) <b>17</b> <b>12</b>	26, 53, 117, 133	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	415	LEU	6.4
1	A	413	TYR	6.4
1	A	143	LYS	5.8
1	A	545	ASP	5.0
1	A	142	ASP	4.6
1	A	414	ASP	4.3
1	A	63	ASP	4.3
1	A	140	HIS	4.2
1	A	512	TYR	4.0
1	A	176	LYS	3.9
1	A	387	ALA	3.5
1	A	418	HIS	3.4
1	A	420	ARG	3.4
1	A	416	SER	3.2
1	A	546	GLU	3.1
1	A	381	ASN	3.0
1	A	177	CYS	2.9
1	A	154	ASN	2.8
1	A	507	PHE	2.8
1	A	328	VAL	2.8
1	A	144	PHE	2.7
1	A	153	LYS	2.7
1	A	380	GLU	2.7
1	A	152	VAL	2.6
1	A	137	THR	2.5
1	A	417	CYS	2.4
1	A	568	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	379	MET	2.4
1	A	511	LEU	2.4
1	A	174	ASP	2.3
1	A	510	THR	2.3
1	A	516	VAL	2.3
1	A	193	ASP	2.2
1	A	248	GLN	2.1
1	A	513	VAL	2.0
1	A	216	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	GOL	A	801	6/6	0.81	0.28	70,74,75,76	0
2	CL	A	901	1/1	0.97	0.19	51,51,51,51	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.