



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:49 AM UTC

PDB ID : 2PMF / pdb_00002pmf
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : ?? (??), CSD ??CSD?? (????)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

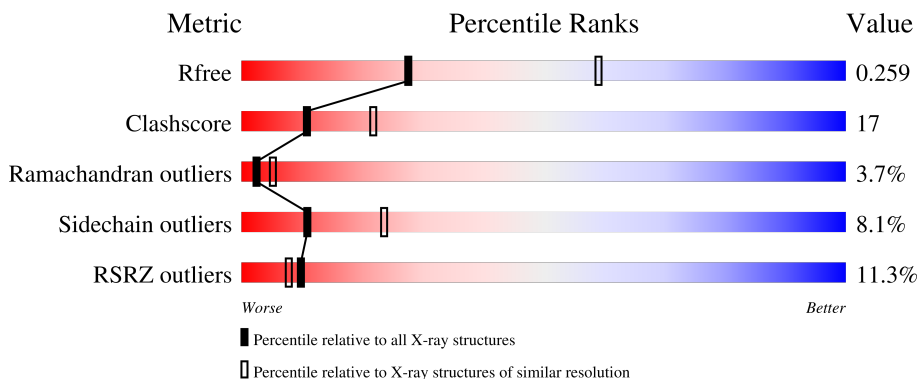
1 Overall quality at a glance

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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 of 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	693	

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
			Total	C	N	O	S			
1	A	522	4144	2631	720	770	23	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	526	ARG	GLY	engineered mutation	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 (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

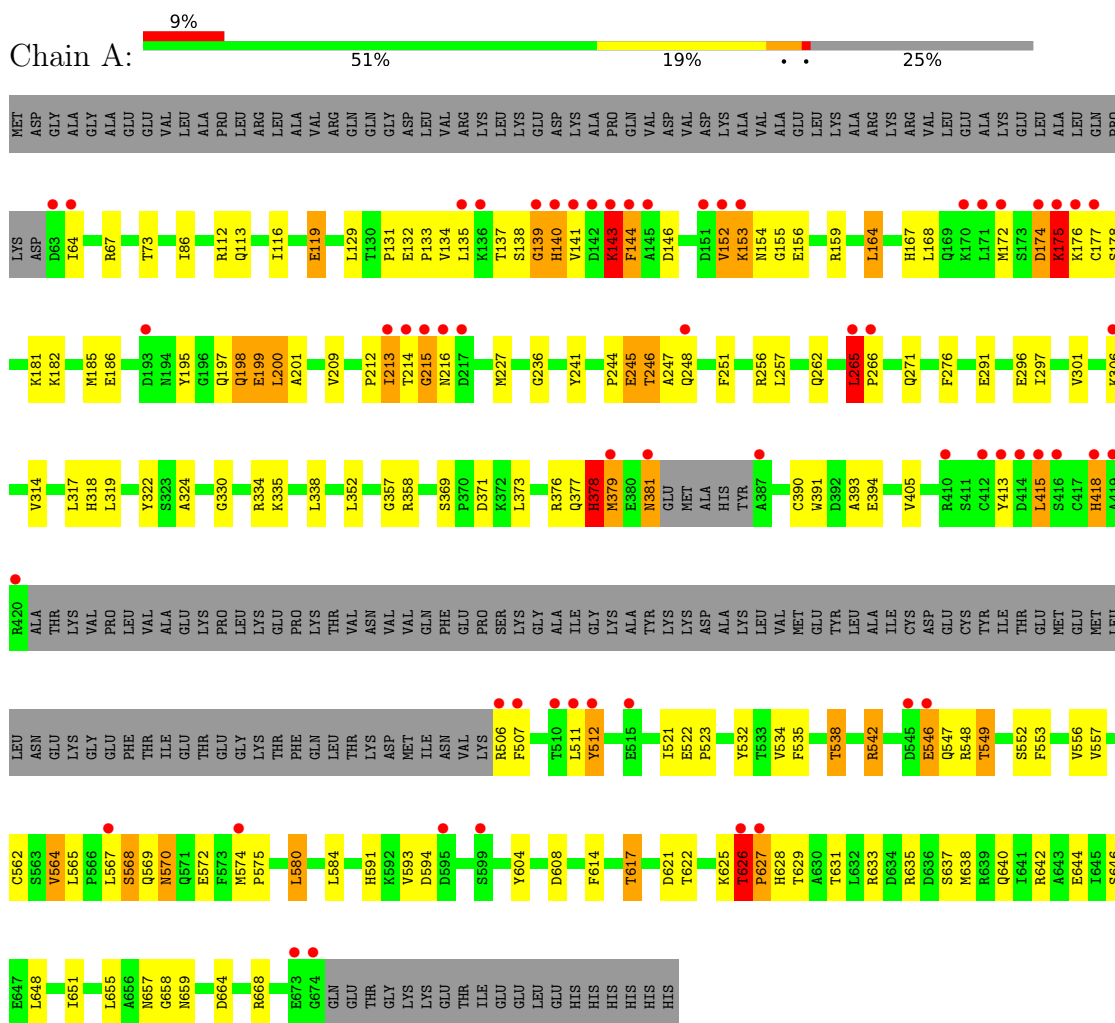
- Molecule 4 is water.

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

3 Residue-property plots

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: Glycyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	91.41Å 91.41Å 246.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.24 – 2.85 29.24 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.24-2.85) 98.7 (29.24-2.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.13 (at 2.85Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.231 , 0.271 0.224 , 0.259	Depositor DCC
R_{free} test set	1272 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtrriage
Anisotropy	0.042	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4353	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtrriage'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.*

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: 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	0.30	0/4237	0.80	10/5722 (0.2%)

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 (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	LEU	N-CA-C	10.10	124.35	109.30
1	A	143	LYS	N-CA-C	-9.55	101.76	113.41
1	A	176	LYS	N-CA-C	-9.06	101.78	112.92
1	A	175	LYS	N-CA-C	8.78	120.92	108.54
1	A	626	THR	N-CA-C	6.54	124.25	109.81
1	A	174	ASP	N-CA-C	-6.23	96.61	107.20
1	A	626	THR	CA-C-N	-5.27	113.26	119.84
1	A	626	THR	C-N-CA	-5.27	113.26	119.84
1	A	140	HIS	N-CA-C	-5.14	107.08	113.19
1	A	153	LYS	N-CA-C	-5.08	101.02	108.79

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 [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	4144	0	4034	136	1
2	A	1	0	0	0	0
3	A	6	0	8	6	0
4	A	202	0	0	2	0
All	All	4353	0	4042	136	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 17.

All (136) 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:O	1:A:379:MET:HG2	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:O	1:A:626:THR:HG22	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:542:ARG:HH11	1:A:542:ARG:CG	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:O	1:A:379:MET:CG	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:VAL:O	1:A:538:THR:HB	1.87	0.74
1:A:626:THR:O	1:A:626:THR:CG2	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
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:172:MET:HE1	1:A:186:GLU:HG3	1.76	0.68
1:A:413:TYR:HE2	1:A:415:LEU:HB2	1.60	0.67
1:A:172:MET:HE3	1:A:186:GLU:HG3	1.75	0.67
1:A:135:LEU:HD12	1:A:241:TYR:HB2	1.79	0.64
1:A:227:MET:HE2	1:A:244:PRO:HG3	1.80	0.63
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:154:ASN:C	1:A:156:GLU:H	2.06	0.59
1:A:570:ASN:C	1:A:572:GLU:H	2.11	0.59
1:A:172:MET:HE1	1:A:186:GLU:CG	2.33	0.58
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:322:TYR:CD2	1:A:376:ARG:HG3	2.41	0.56
1:A:324:ALA:HB1	1:A:379:MET:HB2	1.88	0.56
1:A:648:LEU:HD23	1:A:651:ILE:HD11	1.88	0.55
1:A:381:ASN:ND2	1:A:381:ASN:C	2.64	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: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
1:A:175:LYS:HA	1:A:177:CYS:H	1.73	0.53
1:A:567:LEU:O	1:A:568:SER:C	2.51	0.52
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:CG	1:A:542:ARG:NH1	2.58	0.51
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:569:GLN:H	1:A:569:GLN:CD	2.20	0.50
1:A:542:ARG:HG2	1:A:542:ARG:NH1	2.01	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:570:ASN:C	1:A:572:GLU:N	2.70	0.48
1:A:195:TYR:HD2	1:A:199:GLU:HG2	1.77	0.48
1:A:319:LEU:N	1:A:319:LEU:HD23	2.29	0.48
1:A:319:LEU:HD23	1:A:319:LEU:H	1.79	0.47
1:A:143:LYS:HB2	1:A:227:MET:HE3	1.94	0.47
1:A:181:LYS:HD2	1:A:185:MET:HE3	1.95	0.47
1:A:195:TYR:CD2	1:A:199:GLU:HG2	2.49	0.47
1:A:608:ASP:CG	1:A:633:ARG:HH22	2.18	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:172:MET:CE	1:A:186:GLU:CG	2.82	0.45
1:A:198:GLN:O	1:A:199:GLU:C	2.60	0.45
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:197:GLN:OE1	1:A:198:GLN:N	2.49	0.45
1:A:213:ILE:H	1:A:213:ILE:HG13	1.54	0.45
1:A:139:GLY:C	1:A:141:VAL:H	2.23	0.44
1:A:73:THR:HG21	1:A:549:THR:HG21	1.99	0.44
1:A:143:LYS:O	1:A:144:PHE:HB2	2.16	0.44
1:A:276:PHE:CE2	1:A:291:GLU:HG3	2.53	0.44
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:538:THR:HG21	1:A:553:PHE:CD2	2.53	0.44
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:NH2	2.76	0.42
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: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: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%)	2 5

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%)	410 (92%)	36 (8%)	11 23

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	113	GLN
1	A	119	GLU
1	A	129	LEU
1	A	137	THR
1	A	152	VAL
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	246	THR
1	A	256	ARG
1	A	257	LEU
1	A	262	GLN
1	A	265	LEU
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	418	HIS
1	A	507	PHE
1	A	538	THR
1	A	542	ARG
1	A	546	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	549	THR
1	A	564	VAL
1	A	570	ASN
1	A	580	LEU
1	A	617	THR
1	A	631	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
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	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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.

No monomer is involved in short contacts.

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	522/693 (75%)	0.48	59 (11%) 10 8	26, 53, 117, 133	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	143	LYS	8.0
1	A	415	LEU	6.9
1	A	413	TYR	6.2
1	A	141	VAL	5.9
1	A	152	VAL	5.7
1	A	387	ALA	5.4
1	A	144	PHE	4.8
1	A	171	LEU	4.7
1	A	414	ASP	4.7
1	A	215	GLY	4.6
1	A	381	ASN	4.5
1	A	177	CYS	4.5
1	A	379	MET	4.3
1	A	627	PRO	4.2
1	A	506	ARG	3.9
1	A	512	TYR	3.9
1	A	419	ALA	3.9
1	A	175	LYS	3.9
1	A	63	ASP	3.8
1	A	214	THR	3.8
1	A	216	ASN	3.7
1	A	140	HIS	3.6
1	A	142	ASP	3.5
1	A	306	LYS	3.5
1	A	153	LYS	3.3
1	A	176	LYS	3.3
1	A	213	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	511	LEU	3.2
1	A	248	GLN	3.2
1	A	174	ASP	3.1
1	A	674	GLY	2.9
1	A	416	SER	2.8
1	A	507	PHE	2.8
1	A	136	LYS	2.6
1	A	145	ALA	2.6
1	A	418	HIS	2.6
1	A	64	ILE	2.6
1	A	673	GLU	2.5
1	A	595	ASP	2.4
1	A	574	MET	2.4
1	A	151	ASP	2.4
1	A	135	LEU	2.4
1	A	410	ARG	2.3
1	A	626	THR	2.3
1	A	139	GLY	2.3
1	A	170	LYS	2.3
1	A	599	SER	2.3
1	A	510	THR	2.2
1	A	193	ASP	2.2
1	A	172	MET	2.2
1	A	515	GLU	2.1
1	A	567	LEU	2.1
1	A	546	GLU	2.1
1	A	265	LEU	2.1
1	A	545	ASP	2.1
1	A	412	CYS	2.1
1	A	266	PRO	2.0
1	A	420	ARG	2.0
1	A	217	ASP	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 oligosaccharides 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
3	GOL	A	801	6/6	0.75	0.18	70,74,75,76	0
2	CL	A	901	1/1	0.97	0.08	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.