



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:32 PM UTC

PDB ID : 4ICS / pdb_00004ics
Title : Crystal structure of PepS from Streptococcus pneumoniae in complex with a substrate
Authors : Lee, S.; Kim, K.K.; Ta, M.H.
Deposited on : 2012-12-11
Resolution : 1.97 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	:	2022.3.0, CSD as543be (2022)
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

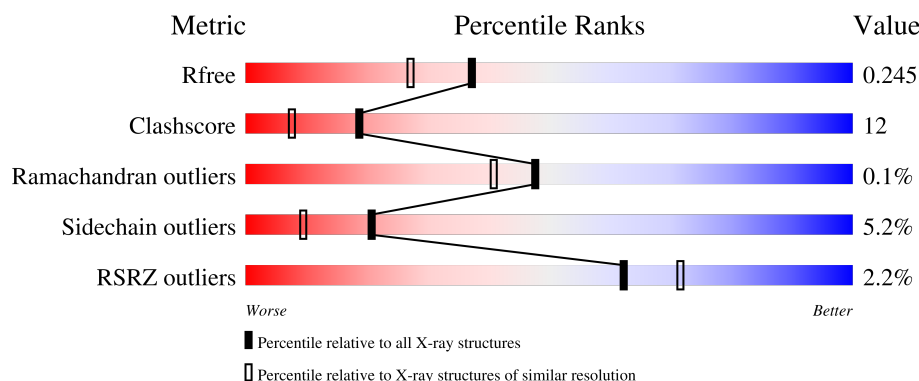
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	413	2% 82% 16% .
1	B	413	2% 80% 17% ..

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
4	GLY	A	504	-	-	X	-
4	GLY	B	504	-	X	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6918 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 Aminopeptidase PepS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	413	Total	C	N	O	S	0	0	0
			3182	2006	541	621	14			
1	B	413	Total	C	N	O	S	0	0	0
			3182	2006	541	621	14			

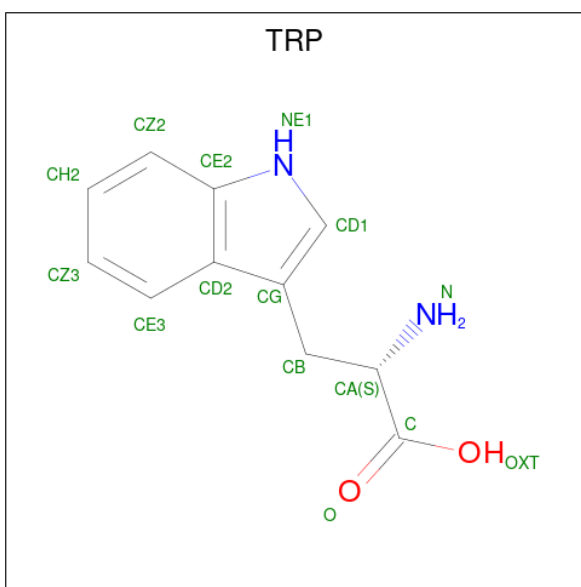
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	343	ASP	GLU	engineered mutation	UNP Q97SP8
B	343	ASP	GLU	engineered mutation	UNP Q97SP8

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

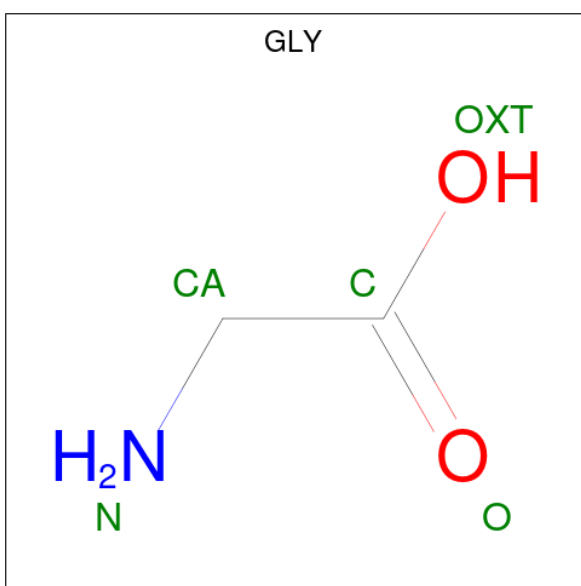
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is TRYPTOPHAN (CCD ID: TRP) (formula: C₁₁H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	11	2	1		
3	B	1	Total	C	N	O	0	0
			14	11	2	1		

- Molecule 4 is GLYCINE (CCD ID: GLY) (formula: $C_2H_5NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			5	2	1	2		
4	B	1	Total	C	N	O	0	0
			5	2	1	2		

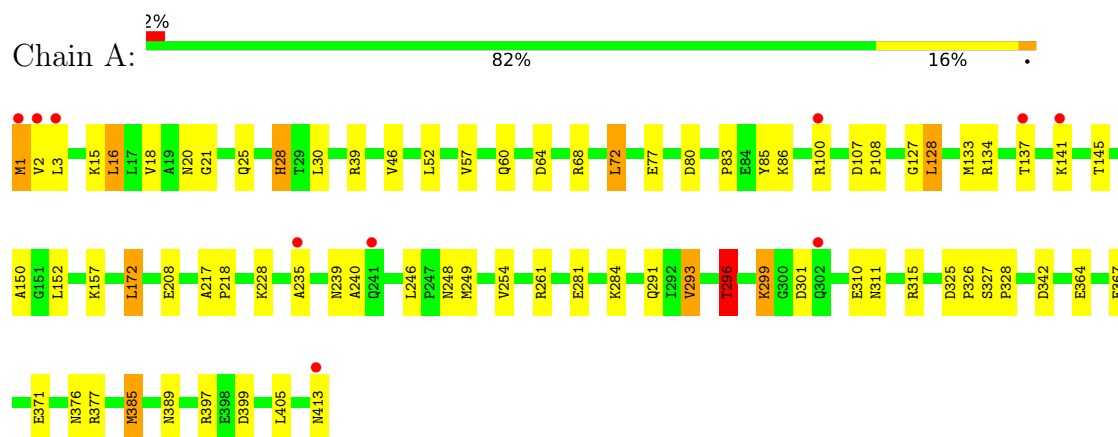
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	238	Total 238	O 238	0	0
5	B	274	Total 274	O 274	0	0

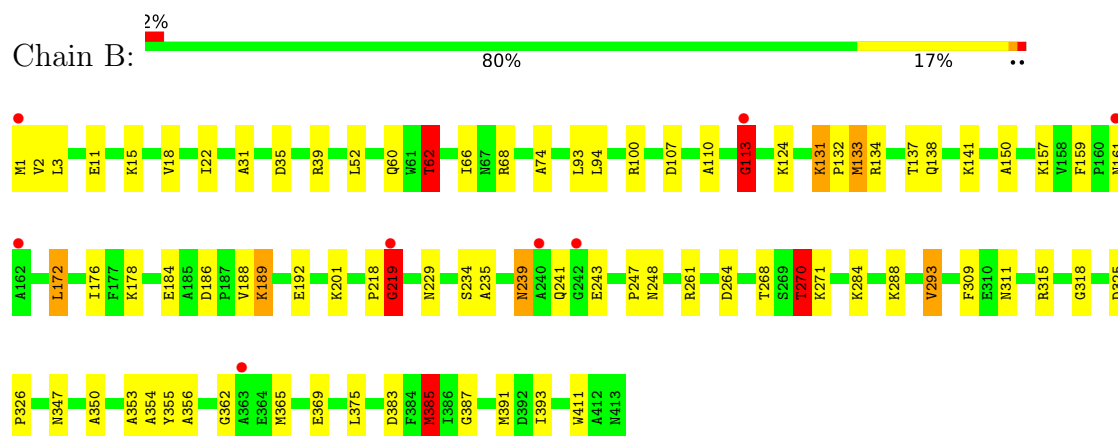
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Aminopeptidase PepS



• Molecule 1: Aminopeptidase PepS



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	126.36Å 126.36Å 139.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.20 – 1.97 41.20 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.6 (41.20-1.97) 99.6 (41.20-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.79 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.225 , 0.257 0.215 , 0.245	Depositor DCC
R_{free} test set	4012 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6918	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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

5.1 Standard geometry

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

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	0.97	1/3247 (0.0%)	1.00	4/4408 (0.1%)
1	B	1.03	2/3247 (0.1%)	1.12	16/4408 (0.4%)
All	All	1.00	3/6494 (0.0%)	1.06	20/8816 (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	B	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	219	GLY	N-CA	9.64	1.59	1.45
1	B	385	MET	SD-CE	-8.62	1.57	1.79
1	A	385	MET	SD-CE	-5.01	1.67	1.79

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	PRO	CA-C-N	-12.91	96.11	121.41
1	B	218	PRO	C-N-CA	-12.91	96.11	121.41
1	B	218	PRO	O-C-N	-11.14	110.15	122.18
1	B	270	THR	N-CA-CB	-8.46	98.76	110.95
1	B	235	ALA	N-CA-C	6.92	119.46	111.02
1	B	176	ILE	N-CA-C	-6.87	104.07	110.53
1	A	293	VAL	N-CA-CB	-6.73	103.06	112.35
1	A	293	VAL	CB-CA-C	6.72	118.21	110.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	VAL	N-CA-C	-6.67	105.62	113.42
1	B	270	THR	OG1-CB-CG2	6.22	121.74	109.30
1	B	293	VAL	N-CA-CB	-5.88	104.23	112.35
1	B	74	ALA	CA-C-N	-5.79	114.30	120.03
1	B	74	ALA	C-N-CA	-5.79	114.30	120.03
1	B	131	LYS	CA-C-N	-5.60	113.12	119.28
1	B	131	LYS	C-N-CA	-5.60	113.12	119.28
1	B	2	VAL	N-CA-C	-5.57	107.32	112.83
1	B	113	GLY	N-CA-C	5.47	121.00	113.99
1	B	353	ALA	N-CA-C	5.24	118.09	109.76
1	B	62	THR	N-CA-CB	-5.07	102.15	111.37
1	A	296	THR	N-CA-CB	-5.06	102.11	111.52

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	113	GLY	Peptide
1	B	219	GLY	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	3182	0	3108	66	2
1	B	3182	0	3107	83	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	14	0	9	0	0
3	B	14	0	9	5	0
4	A	5	0	3	5	0
4	B	5	0	3	4	0
5	A	238	0	0	15	0
5	B	274	0	0	15	0
All	All	6918	0	6239	150	2

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 12.

All (150) 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:21:GLY:CA	1:A:249:MET:HE1	1.30	1.58
1:B:347:ASN:ND2	1:B:391:MET:CE	1.68	1.54
1:A:21:GLY:CA	1:A:249:MET:CE	2.01	1.38
1:A:21:GLY:HA2	1:A:249:MET:CE	1.61	1.25
1:A:291:GLN:HG3	5:A:689:HOH:O	1.06	1.22
1:A:21:GLY:HA3	1:A:249:MET:CE	1.67	1.19
1:B:248:ASN:HD21	4:B:504:GLY:HA3	1.04	1.19
1:B:133:MET:HE3	1:B:133:MET:HA	1.26	1.17
1:B:347:ASN:ND2	1:B:391:MET:HE1	1.39	1.13
1:A:21:GLY:HA2	1:A:249:MET:HE2	1.28	1.09
1:B:271:LYS:HB2	1:B:385:MET:HE3	1.28	1.09
1:B:133:MET:HA	1:B:133:MET:CE	1.83	1.08
1:B:347:ASN:ND2	1:B:391:MET:HE3	1.69	1.06
1:A:15:LYS:HG2	5:A:649:HOH:O	1.53	1.06
1:A:248:ASN:HD21	4:A:504:GLY:HA3	0.89	1.02
1:B:234:SER:O	3:B:503:TRP:CH2	2.12	1.01
1:A:248:ASN:HD21	4:A:504:GLY:CA	1.74	1.01
1:A:248:ASN:ND2	4:A:504:GLY:HA3	1.75	1.00
1:B:68:ARG:HH12	1:B:113:GLY:H	1.08	1.00
1:B:248:ASN:HD21	4:B:504:GLY:CA	1.76	0.99
1:A:100:ARG:HG3	1:A:133:MET:CE	1.95	0.97
1:B:94:LEU:HD21	1:B:133:MET:HE3	1.48	0.94
1:B:271:LYS:HB2	1:B:385:MET:CE	1.97	0.94
1:B:385:MET:HE2	5:B:604:HOH:O	1.66	0.94
1:A:100:ARG:HG3	1:A:133:MET:HE2	1.47	0.94
1:B:347:ASN:ND2	1:B:391:MET:HE2	1.82	0.93
1:B:248:ASN:ND2	4:B:504:GLY:HA3	1.85	0.92
1:B:94:LEU:HD21	1:B:133:MET:CE	2.01	0.89
1:A:246:LEU:HB2	1:A:249:MET:HE2	1.53	0.88
1:B:271:LYS:CB	1:B:385:MET:HE3	2.04	0.87
1:A:1:MET:N	5:A:670:HOH:O	1.93	0.86
1:A:64:ASP:OD1	5:A:830:HOH:O	1.95	0.85
1:B:288:LYS:HE2	5:B:742:HOH:O	1.78	0.84
1:B:288:LYS:CE	5:B:742:HOH:O	2.26	0.84
1:B:60:GLN:CD	5:B:704:HOH:O	2.21	0.84
1:B:234:SER:O	3:B:503:TRP:HH2	1.57	0.83
1:A:291:GLN:NE2	5:A:689:HOH:O	2.09	0.83
1:A:21:GLY:HA3	1:A:249:MET:HE1	0.83	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ASP:OD2	1:B:189:LYS:HE2	1.79	0.82
1:B:347:ASN:HD21	1:B:391:MET:CE	1.93	0.81
1:B:133:MET:CE	1:B:133:MET:CA	2.59	0.80
1:B:270:THR:HG21	1:B:387:GLY:O	1.83	0.78
1:B:35:ASP:HA	1:B:62:THR:HG22	1.66	0.77
1:B:159:PHE:O	5:B:814:HOH:O	2.06	0.72
1:A:367:GLU:OE1	5:A:683:HOH:O	2.07	0.72
1:A:150:ALA:HA	1:A:172:LEU:HD13	1.70	0.72
1:B:264:ASP:OD2	5:B:725:HOH:O	2.07	0.71
1:A:100:ARG:HG3	1:A:133:MET:HE1	1.76	0.68
1:B:134:ARG:HG3	5:B:651:HOH:O	1.94	0.68
1:B:68:ARG:NH1	1:B:113:GLY:H	1.87	0.67
1:A:145:THR:HG21	1:A:249:MET:HE3	1.78	0.66
1:B:239:ASN:C	1:B:239:ASN:HD22	2.03	0.66
1:B:239:ASN:ND2	1:B:241:GLN:H	1.94	0.65
1:B:133:MET:HA	1:B:133:MET:HE2	1.76	0.64
1:B:234:SER:O	3:B:503:TRP:CZ3	2.51	0.63
1:B:189:LYS:N	1:B:189:LYS:HD3	2.13	0.62
1:A:311:ASN:ND2	5:A:665:HOH:O	2.29	0.62
1:B:150:ALA:HA	1:B:172:LEU:HD13	1.82	0.62
1:A:145:THR:CG2	1:A:249:MET:HE3	2.29	0.62
1:B:94:LEU:CD2	1:B:133:MET:CE	2.75	0.62
1:A:107:ASP:OD1	1:A:157:LYS:HE3	2.00	0.61
1:B:94:LEU:CD2	1:B:133:MET:HE1	2.32	0.60
1:A:281:GLU:OE1	1:A:299:LYS:HD3	2.01	0.60
1:A:16:LEU:HD12	1:A:20:ASN:HD22	1.65	0.60
1:A:208:GLU:OE2	1:A:397:ARG:NH1	2.29	0.59
1:A:60:GLN:OE1	1:A:100:ARG:NH1	2.35	0.58
1:B:355:TYR:CZ	3:B:503:TRP:HD1	2.21	0.58
1:A:16:LEU:HD12	1:A:20:ASN:ND2	2.20	0.57
1:B:347:ASN:HD21	1:B:391:MET:HE3	1.63	0.57
1:B:22:ILE:CG2	1:B:22:ILE:O	2.52	0.57
1:B:309:PHE:CE2	1:B:315:ARG:HD3	2.39	0.57
1:B:391:MET:HE3	1:B:393:ILE:HD11	1.86	0.57
1:B:22:ILE:O	1:B:22:ILE:HG22	2.05	0.56
1:B:239:ASN:HD22	1:B:241:GLN:H	1.53	0.56
1:A:141:LYS:HD2	5:A:707:HOH:O	2.05	0.56
4:A:504:GLY:N	5:A:601:HOH:O	2.26	0.55
1:B:133:MET:HE2	1:B:133:MET:O	2.06	0.55
1:A:46:VAL:HG21	1:B:66:ILE:HG12	1.89	0.55
1:B:35:ASP:CA	1:B:62:THR:HG22	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CA	5:A:670:HOH:O	2.45	0.54
1:B:288:LYS:HE3	5:B:742:HOH:O	1.98	0.54
1:B:347:ASN:CG	1:B:391:MET:HE1	2.24	0.54
1:A:21:GLY:N	1:A:249:MET:HE1	2.14	0.53
1:A:291:GLN:CG	5:A:689:HOH:O	1.87	0.53
1:B:219:GLY:HA3	1:B:268:THR:HB	1.91	0.52
1:A:128:LEU:HD13	5:A:702:HOH:O	2.08	0.52
1:A:376:ASN:C	1:A:377:ARG:HD2	2.36	0.51
1:A:83:PRO:HD2	1:A:86:LYS:HD2	1.92	0.50
1:B:239:ASN:ND2	1:B:243:GLU:H	2.08	0.50
1:B:356:ALA:O	1:B:362:GLY:HA3	2.12	0.50
1:B:134:ARG:O	1:B:138:GLN:HG3	2.12	0.49
1:A:399:ASP:OD2	1:A:399:ASP:C	2.52	0.49
1:A:68:ARG:HG2	1:A:72:LEU:HD22	1.92	0.49
1:B:68:ARG:HH12	1:B:113:GLY:N	1.92	0.49
1:B:270:THR:CG2	1:B:387:GLY:O	2.58	0.49
1:A:85:TYR:OH	5:A:700:HOH:O	2.16	0.49
1:A:108:PRO:HD2	1:A:157:LYS:HD2	1.95	0.49
1:B:131:LYS:HB3	1:B:132:PRO:HD3	1.95	0.49
1:B:201:LYS:HE2	1:B:411:TRP:CD2	2.46	0.49
1:B:385:MET:CE	5:B:604:HOH:O	2.42	0.49
1:B:60:GLN:CG	5:B:704:HOH:O	2.56	0.49
4:B:504:GLY:N	5:B:603:HOH:O	2.23	0.49
1:A:325:ASP:N	1:A:326:PRO:CD	2.76	0.48
1:A:342:ASP:HB3	1:A:385:MET:HE3	1.95	0.48
1:B:229:ASN:HA	5:B:682:HOH:O	2.12	0.48
1:B:1:MET:CA	5:B:830:HOH:O	2.46	0.48
1:A:217:ALA:O	1:A:218:PRO:C	2.57	0.47
1:A:39:ARG:HD2	5:A:718:HOH:O	2.15	0.47
1:A:127:GLY:O	1:A:134:ARG:NH1	2.31	0.47
1:A:254:VAL:O	1:A:254:VAL:HG23	2.13	0.47
1:B:325:ASP:N	1:B:326:PRO:CD	2.78	0.47
1:B:18:VAL:HG12	1:B:52:LEU:HD12	1.97	0.47
1:B:133:MET:HE3	1:B:133:MET:CA	2.10	0.46
1:A:377:ARG:HD2	1:A:377:ARG:N	2.30	0.46
1:B:365:MET:HB3	1:B:369:GLU:HB2	1.97	0.46
1:A:239:ASN:OD1	1:A:239:ASN:C	2.59	0.46
1:A:296:THR:HG21	5:A:742:HOH:O	2.16	0.45
1:A:128:LEU:C	1:A:128:LEU:HD22	2.41	0.45
1:B:354:ALA:HB3	1:B:375:LEU:HB3	1.99	0.45
1:B:94:LEU:HD23	1:B:133:MET:HE1	2.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLY:C	1:A:134:ARG:HH12	2.18	0.44
1:B:188:VAL:O	1:B:192:GLU:HG3	2.18	0.43
1:A:284:LYS:HB2	1:A:296:THR:HG22	1.99	0.43
1:B:31:ALA:HB3	1:B:100:ARG:HE	1.82	0.43
1:A:77:GLU:H	1:A:77:GLU:CD	2.26	0.43
1:A:80:ASP:C	1:A:80:ASP:OD1	2.61	0.43
1:B:184:GLU:HA	1:B:184:GLU:OE1	2.18	0.43
1:B:124:LYS:HA	1:B:311:ASN:HD21	1.84	0.43
1:B:350:ALA:HB2	1:B:383:ASP:OD1	2.19	0.43
1:A:46:VAL:HG22	1:A:57:VAL:HG11	1.99	0.42
1:B:141:LYS:HD3	1:B:141:LYS:HA	1.80	0.42
1:A:127:GLY:HA2	1:A:134:ARG:NH1	2.35	0.42
1:A:25:GLN:H	1:A:28:HIS:CD2	2.37	0.42
1:A:296:THR:HA	1:A:301:ASP:OD2	2.19	0.42
1:B:133:MET:CA	1:B:133:MET:HE2	2.39	0.42
1:B:62:THR:HG21	5:B:811:HOH:O	2.20	0.41
1:B:347:ASN:CB	1:B:391:MET:HE1	2.50	0.41
1:A:261:ARG:NH2	1:A:371:GLU:O	2.54	0.41
1:B:247:PRO:HG2	3:B:503:TRP:CZ2	2.56	0.41
1:A:25:GLN:HB2	1:A:28:HIS:CE1	2.56	0.41
1:A:327:SER:HB2	1:A:328:PRO:CD	2.51	0.41
1:B:107:ASP:HB3	1:B:110:ALA:HB2	2.02	0.41
1:A:18:VAL:HG12	1:A:52:LEU:HD12	2.03	0.41
1:A:128:LEU:HD22	1:A:128:LEU:O	2.20	0.41
1:B:261:ARG:HD2	5:B:615:HOH:O	2.20	0.41
1:B:93:LEU:HD23	1:B:93:LEU:HA	1.89	0.40
1:B:318:GLY:O	1:B:354:ALA:HA	2.21	0.40
1:A:248:ASN:ND2	4:A:504:GLY:CA	2.56	0.40
1:A:141:LYS:HA	1:A:240:ALA:HB2	2.04	0.40
1:B:11:GLU:HG2	1:B:15:LYS:HE3	2.04	0.40

All (2) 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:315:ARG:NH2	1:A:413:ASN:OD1[4_455]	1.45	0.75
1:A:315:ARG:NH2	1:A:413:ASN:CG[4_455]	2.18	0.02

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	411/413 (100%)	405 (98%)	5 (1%)	1 (0%)	43	35
1	B	411/413 (100%)	407 (99%)	4 (1%)	0	100	100
All	All	822/826 (100%)	812 (99%)	9 (1%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ALA

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	335/335 (100%)	316 (94%)	19 (6%)	18	8
1	B	335/335 (100%)	320 (96%)	15 (4%)	24	13
All	All	670/670 (100%)	636 (95%)	34 (5%)	21	10

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	VAL
1	A	3	LEU
1	A	16	LEU
1	A	28	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	30	LEU
1	A	72	LEU
1	A	128	LEU
1	A	137	THR
1	A	152	LEU
1	A	172	LEU
1	A	228	LYS
1	A	293	VAL
1	A	296	THR
1	A	299	LYS
1	A	310	GLU
1	A	364	GLU
1	A	389	ASN
1	A	405	LEU
1	B	3	LEU
1	B	39	ARG
1	B	62	THR
1	B	133	MET
1	B	137	THR
1	B	157	LYS
1	B	161	ASN
1	B	172	LEU
1	B	178	LYS
1	B	189	LYS
1	B	239	ASN
1	B	270	THR
1	B	284	LYS
1	B	293	VAL
1	B	385	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	28	HIS
1	A	81	ASN
1	A	209	GLN
1	A	248	ASN
1	A	311	ASN
1	A	389	ASN
1	B	20	ASN
1	B	25	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	81	ASN
1	B	138	GLN
1	B	209	GLN
1	B	239	ASN
1	B	248	ASN
1	B	311	ASN
1	B	410	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	TRP	B	503	2,4	14,15,16	2.28	5 (35%)	15,20,22	0.97	0
4	GLY	A	504	3	4,4,4	1.14	0	3,4,4	0.89	0
3	TRP	A	503	2,4	14,15,16	1.23	1 (7%)	15,20,22	0.69	0
4	GLY	B	504	3	4,4,4	1.27	1 (25%)	3,4,4	1.52	1 (33%)

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	TRP	B	503	2,4	-	2/5/6/8	0/2/2/2
4	GLY	A	504	3	-	2/2/2/2	-
3	TRP	A	503	2,4	-	2/5/6/8	0/2/2/2
4	GLY	B	504	3	-	2/2/2/2	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	503	TRP	CB-CG	-5.77	1.39	1.50
3	B	503	TRP	CZ3-CE3	-3.90	1.32	1.38
3	A	503	TRP	CB-CG	-2.98	1.44	1.50
3	B	503	TRP	CH2-CZ2	-2.63	1.34	1.38
3	B	503	TRP	CD2-CG	-2.52	1.39	1.44
4	B	504	GLY	O-C	2.33	1.29	1.22
3	B	503	TRP	CD1-CG	2.21	1.40	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	504	GLY	OXT-C-O	2.06	128.63	123.33

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	TRP	N-CA-CB-CG
3	B	503	TRP	C-CA-CB-CG
4	A	504	GLY	OXT-C-CA-N
4	B	504	GLY	OXT-C-CA-N
3	A	503	TRP	CA-CB-CG-CD2
4	A	504	GLY	O-C-CA-N
4	B	504	GLY	O-C-CA-N
3	A	503	TRP	CA-CB-CG-CD1

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	TRP	5	0
4	A	504	GLY	5	0
4	B	504	GLY	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	413/413 (100%)	0.29	10 (2%) 59 69	20, 28, 40, 59	0
1	B	413/413 (100%)	0.18	8 (1%) 66 75	18, 27, 38, 46	0
All	All	826/826 (100%)	0.23	18 (2%) 62 71	18, 27, 39, 59	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	161	ASN	5.0
1	A	1	MET	4.0
1	A	302	GLN	3.9
1	B	113	GLY	3.8
1	B	240	ALA	3.8
1	A	2	VAL	3.7
1	A	413	ASN	3.6
1	B	219	GLY	2.7
1	A	241	GLN	2.6
1	A	235	ALA	2.6
1	A	3	LEU	2.4
1	A	141	LYS	2.4
1	B	363	ALA	2.4
1	B	1	MET	2.2
1	A	100	ARG	2.2
1	A	137	THR	2.1
1	B	162	ALA	2.1
1	B	242	GLY	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($\text{\AA}^2$)	Q<0.9
4	GLY	B	504	5/5	0.62	0.37	35,36,36,37	0
4	GLY	A	504	5/5	0.76	0.25	38,38,40,40	0
3	TRP	B	503	14/15	0.79	0.18	29,32,36,38	0
3	TRP	A	503	14/15	0.82	0.15	33,35,37,39	0
2	ZN	B	501	1/1	0.99	0.11	37,37,37,37	0
2	ZN	B	502	1/1	0.99	0.02	25,25,25,25	0
2	ZN	A	502	1/1	0.99	0.03	27,27,27,27	0
2	ZN	A	501	1/1	1.00	0.13	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.