



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:34 AM UTC

PDB ID : 2ZVD / pdb_00002zvd
Title : Crystal structure of Pseudomonas sp. MIS38 lipase in an open conformation
Authors : Angkawidjaja, C.; Matsumura, H.; Koga, Y.; Takano, K.; Kanaya, S.
Deposited on : 2008-11-05
Resolution : 2.15 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
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

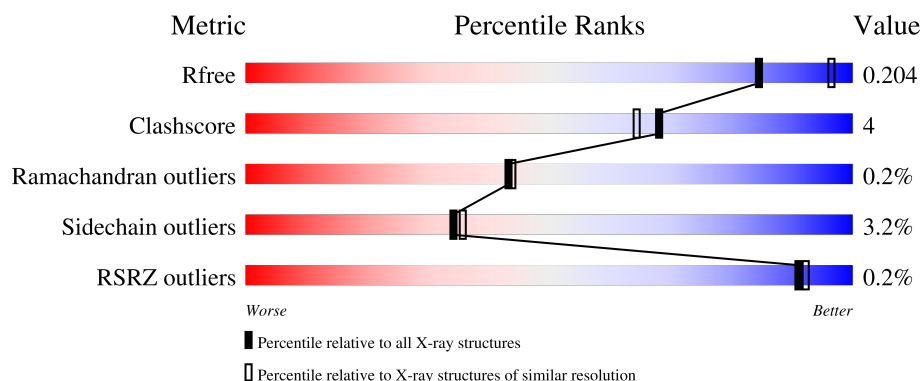
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	617	 87% 10% ..
1	C	617	 89% 10% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10287 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 Lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	608	Total	C	N	O	S	0	0	0
			4484	2812	759	908	5			
1	C	616	Total	C	N	O	S	0	0	0
			4553	2863	769	916	5			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	11	Total	Ca	0	0
			11	11		
2	C	11	Total	Ca	0	0
			11	11		

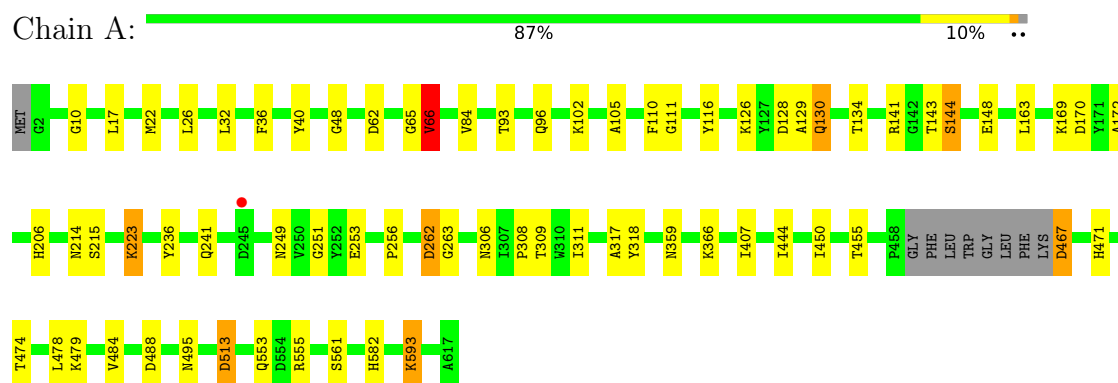
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	623	Total	O	0	0
			623	623		
3	C	605	Total	O	0	0
			605	605		

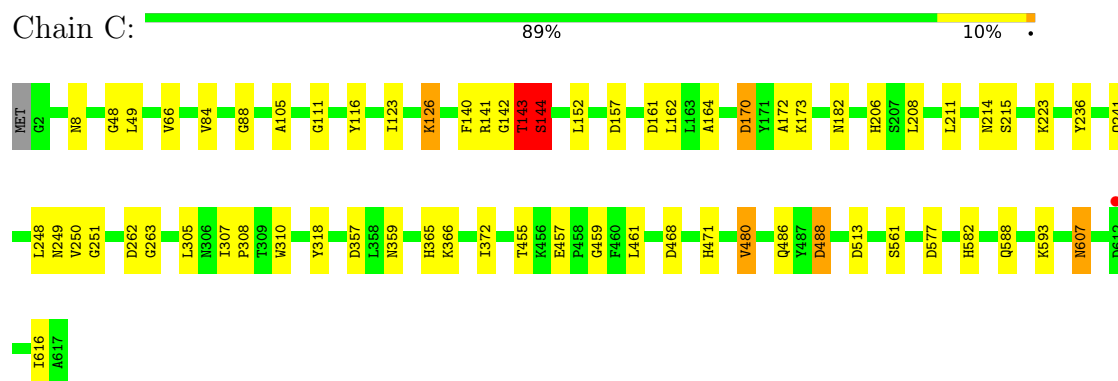
3 Residue-property plots

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: Lipase



• Molecule 1: Lipase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	104.78Å 104.78Å 497.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.15 40.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (40.00-2.15) 100.0 (40.00-2.15)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.210 (Not available) , 0.204	Depositor DCC
R_{free} test set	4473 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10287	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: CA

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	1.09	9/4574 (0.2%)	1.01	6/6214 (0.1%)
1	C	1.10	14/4648 (0.3%)	1.04	6/6315 (0.1%)
All	All	1.09	23/9222 (0.2%)	1.02	12/12529 (0.1%)

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	2
1	C	0	1
All	All	0	3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	164	ALA	C-O	-7.95	1.14	1.24
1	A	170	ASP	C-O	-7.55	1.14	1.24
1	C	144	SER	C-O	-7.47	1.14	1.24
1	C	488	ASP	C-O	-7.18	1.15	1.23
1	C	142	GLY	C-O	-6.53	1.16	1.23
1	A	144	SER	C-O	-6.24	1.16	1.24
1	C	48	GLY	C-O	-6.21	1.16	1.23
1	A	141	ARG	C-O	-6.16	1.16	1.23
1	A	66	VAL	C-O	-5.95	1.16	1.24
1	A	65	GLY	C-O	-5.95	1.16	1.24
1	A	444	ILE	CA-CB	5.90	1.61	1.54
1	C	49	LEU	C-O	-5.87	1.18	1.24
1	C	459	GLY	C-O	-5.81	1.16	1.23
1	C	162	LEU	C-O	-5.74	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	THR	C-O	-5.57	1.17	1.24
1	C	372	ILE	CA-CB	5.41	1.60	1.54
1	C	123	ILE	CA-CB	5.29	1.60	1.54
1	A	62	ASP	C-O	-5.27	1.16	1.24
1	C	105	ALA	C-O	-5.21	1.17	1.24
1	C	141	ARG	C-O	-5.16	1.17	1.23
1	A	48	GLY	C-O	-5.11	1.18	1.24
1	C	140	PHE	C-O	-5.05	1.17	1.24
1	C	461	LEU	C-O	-5.04	1.16	1.23

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	513	ASP	N-CA-C	-10.12	95.53	110.52
1	C	480	VAL	CB-CA-C	-8.70	100.80	111.32
1	A	513	ASP	N-CA-C	-7.48	99.45	110.52
1	C	305	LEU	CA-C-N	-6.48	114.15	122.77
1	C	305	LEU	C-N-CA	-6.48	114.15	122.77
1	C	170	ASP	N-CA-C	5.95	119.85	112.24
1	C	143	THR	CB-CA-C	5.81	118.97	109.90
1	A	143	THR	CB-CA-C	5.59	116.68	109.80
1	A	262	ASP	O-C-N	-5.48	116.22	123.13
1	A	148	GLU	CB-CA-C	-5.47	101.38	110.68
1	A	488	ASP	CB-CA-C	5.46	117.30	109.71
1	A	262	ASP	N-CA-C	5.08	116.98	107.99

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	130	GLN	Peptide
1	A	262	ASP	Peptide
1	C	262	ASP	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	4484	0	4269	34	0
1	C	4553	0	4339	29	0
2	A	11	0	0	0	0
2	C	11	0	0	0	0
3	A	623	0	0	8	0
3	C	605	0	0	8	0
All	All	10287	0	8608	63	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 4.

All (63) 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:593:LYS:HG2	3:A:923:HOH:O	1.52	1.10
1:C:182:ASN:HB2	3:C:1204:HOH:O	1.66	0.95
1:A:214:ASN:HD21	1:A:249:ASN:HD21	1.20	0.85
1:C:170:ASP:HA	3:C:636:HOH:O	1.79	0.83
1:C:214:ASN:HD21	1:C:249:ASN:HD21	1.31	0.76
1:C:471:HIS:HD2	3:C:781:HOH:O	1.69	0.75
1:C:170:ASP:HB2	1:C:173:LYS:HB3	1.67	0.75
1:C:468:ASP:HB2	3:C:1051:HOH:O	1.87	0.75
1:A:10:GLY:HA3	3:A:1178:HOH:O	1.85	0.74
1:A:241:GLN:OE1	1:A:263:GLY:HA2	1.91	0.70
1:A:129:ALA:HB2	3:A:1420:HOH:O	1.94	0.66
1:A:471:HIS:HD2	3:A:825:HOH:O	1.79	0.64
1:A:129:ALA:CB	3:A:1420:HOH:O	2.46	0.63
1:C:241:GLN:OE1	1:C:263:GLY:HA2	2.01	0.60
1:A:32:LEU:HD11	1:A:66:VAL:HG22	1.87	0.56
1:C:593:LYS:HG2	3:C:1181:HOH:O	2.06	0.56
1:C:223:LYS:HD3	3:C:1157:HOH:O	2.04	0.56
1:C:143:THR:HG22	1:C:208:LEU:HB2	1.88	0.56
1:A:455:THR:OG1	1:A:471:HIS:HE1	1.89	0.55
1:C:170:ASP:HB3	3:C:1045:HOH:O	2.06	0.54
1:A:111:GLY:HA3	1:A:116:TYR:O	2.08	0.53
1:A:93:THR:OG1	1:A:96:GLN:HG3	2.09	0.52
1:C:251:GLY:HA2	1:C:318:TYR:HE1	1.75	0.52
1:C:588:GLN:NE2	3:C:1161:HOH:O	2.43	0.51
1:A:317:ALA:HB3	3:A:1059:HOH:O	2.10	0.51
1:C:111:GLY:HA3	1:C:116:TYR:O	2.11	0.51
1:A:306:ASN:ND2	1:A:308:PRO:HD2	2.27	0.49
1:C:206:HIS:HA	1:C:236:TYR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:THR:HB	1:C:157:ASP:HB3	1.95	0.47
1:A:582:HIS:HD2	1:A:593:LYS:O	1.96	0.47
1:A:407:ILE:HG22	1:A:450:ILE:HD11	1.97	0.47
1:C:143:THR:HG21	1:C:161:ASP:OD2	2.15	0.47
1:A:102:LYS:HD2	1:A:110:PHE:HB2	1.96	0.46
1:A:40:TYR:CE1	1:A:311:ILE:HD11	2.51	0.46
1:A:172:ALA:O	1:A:215:SER:HB2	2.16	0.46
1:A:251:GLY:HA2	1:A:318:TYR:HE1	1.81	0.45
1:A:479:LYS:HG2	1:A:484:VAL:HG22	1.97	0.45
1:A:555:ARG:NH2	3:A:959:HOH:O	2.30	0.45
1:C:607:ASN:ND2	1:C:607:ASN:H	2.16	0.44
1:A:223:LYS:HB3	1:A:223:LYS:HE3	1.67	0.44
1:A:306:ASN:HD22	1:A:308:PRO:HD2	1.83	0.44
1:C:307:ILE:O	1:C:310:TRP:HB2	2.18	0.44
1:A:105:ALA:HB2	3:A:1135:HOH:O	2.17	0.43
1:C:88:GLY:O	1:C:126:LYS:HG3	2.18	0.43
1:A:471:HIS:HB3	1:A:478:LEU:HB3	2.00	0.43
1:C:455:THR:OG1	1:C:457:GLU:OE2	2.33	0.42
1:A:128:ASP:HB3	1:A:134:THR:HG21	2.00	0.42
1:C:172:ALA:O	1:C:215:SER:HB2	2.19	0.42
1:C:248:LEU:HG	1:C:250:VAL:HG23	2.01	0.42
1:A:256:PRO:HG3	1:A:309:THR:OG1	2.19	0.42
1:C:455:THR:OG1	1:C:471:HIS:HE1	2.03	0.42
1:A:474:THR:HG21	1:A:479:LYS:HD3	2.00	0.42
1:C:582:HIS:HD2	1:C:593:LYS:O	2.03	0.42
1:C:357:ASP:CG	1:C:365:HIS:HD1	2.27	0.41
1:C:307:ILE:N	1:C:308:PRO:CD	2.83	0.41
1:A:22:MET:O	1:A:26:LEU:HG	2.21	0.41
1:A:36:PHE:CD2	1:A:36:PHE:C	2.99	0.41
1:A:495:ASN:HD22	1:A:513:ASP:H	1.69	0.41
1:A:206:HIS:HA	1:A:236:TYR:O	2.21	0.40
1:C:143:THR:O	1:C:144:SER:CB	2.69	0.40
1:A:102:LYS:HD2	1:A:110:PHE:CB	2.51	0.40
1:A:467:ASP:OD2	1:A:467:ASP:N	2.54	0.40
1:C:577:ASP:OD2	1:C:582:HIS:HE1	2.04	0.40

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	604/617 (98%)	588 (97%)	15 (2%)	1 (0%)	43	44
1	C	614/617 (100%)	599 (98%)	14 (2%)	1 (0%)	43	44
All	All	1218/1234 (99%)	1187 (98%)	29 (2%)	2 (0%)	43	44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	C	144	SER

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	464/471 (98%)	449 (97%)	15 (3%)	34	36
1	C	470/471 (100%)	455 (97%)	15 (3%)	34	36
All	All	934/942 (99%)	904 (97%)	30 (3%)	34	36

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	66	VAL
1	A	84	VAL
1	A	126	LYS

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Mol	Chain	Res	Type
1	A	130	GLN
1	A	163	LEU
1	A	169	LYS
1	A	223	LYS
1	A	253	GLU
1	A	359	ASN
1	A	366	LYS
1	A	467	ASP
1	A	553	GLN
1	A	561	SER
1	A	593	LYS
1	C	8	ASN
1	C	66	VAL
1	C	84	VAL
1	C	126	LYS
1	C	143	THR
1	C	152	LEU
1	C	211	LEU
1	C	359	ASN
1	C	366	LYS
1	C	480	VAL
1	C	486	GLN
1	C	488	ASP
1	C	561	SER
1	C	607	ASN
1	C	616	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	42	HIS
1	A	43	ASN
1	A	64	GLN
1	A	160	ASN
1	A	249	ASN
1	A	306	ASN
1	A	423	ASN
1	A	471	HIS
1	A	495	ASN
1	A	553	GLN
1	A	571	GLN

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Mol	Chain	Res	Type
1	A	582	HIS
1	C	8	ASN
1	C	130	GLN
1	C	149	ASN
1	C	160	ASN
1	C	182	ASN
1	C	249	ASN
1	C	298	ASN
1	C	381	GLN
1	C	423	ASN
1	C	471	HIS
1	C	495	ASN
1	C	553	GLN
1	C	571	GLN
1	C	582	HIS
1	C	607	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 22 ligands modelled in this entry, 22 are monoatomic - leaving 0 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 [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	608/617 (98%)	-0.47	1 (0%) 91 92	10, 18, 32, 54	0
1	C	616/617 (99%)	-0.39	1 (0%) 91 92	10, 20, 34, 49	0
All	All	1224/1234 (99%)	-0.43	2 (0%) 91 92	10, 19, 33, 54	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	612	ASP	3.3
1	A	245	ASP	2.7

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
2	CA	C	625	1/1	0.97	0.04	27,27,27,27	0
2	CA	C	627	1/1	0.97	0.04	36,36,36,36	0
2	CA	A	620	1/1	0.98	0.02	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	C	623	1/1	0.98	0.03	27,27,27,27	0
2	CA	A	622	1/1	0.99	0.05	17,17,17,17	0
2	CA	A	623	1/1	0.99	0.02	17,17,17,17	0
2	CA	A	625	1/1	0.99	0.03	18,18,18,18	0
2	CA	A	626	1/1	0.99	0.02	16,16,16,16	0
2	CA	A	628	1/1	0.99	0.03	21,21,21,21	0
2	CA	C	618	1/1	0.99	0.01	15,15,15,15	0
2	CA	C	621	1/1	0.99	0.01	15,15,15,15	0
2	CA	C	622	1/1	0.99	0.03	17,17,17,17	0
2	CA	A	619	1/1	0.99	0.02	16,16,16,16	0
2	CA	A	618	1/1	0.99	0.01	12,12,12,12	0
2	CA	C	626	1/1	0.99	0.02	20,20,20,20	0
2	CA	A	621	1/1	0.99	0.01	12,12,12,12	0
2	CA	C	628	1/1	0.99	0.01	20,20,20,20	0
2	CA	C	624	1/1	1.00	0.03	20,20,20,20	0
2	CA	C	620	1/1	1.00	0.01	13,13,13,13	0
2	CA	A	624	1/1	1.00	0.01	15,15,15,15	0
2	CA	A	627	1/1	1.00	0.03	23,23,23,23	0
2	CA	C	619	1/1	1.00	0.01	17,17,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.