



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:26 PM UTC

PDB ID : 4Y8E / pdb_00004y8e
Title : PA3825-EAL Ca-Apo Structure
Authors : Horrell, S.; Bellini, D.; Strange, R.; Wagner, A.; Walsh, M.
Deposited on : 2015-02-16
Resolution : 1.61 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

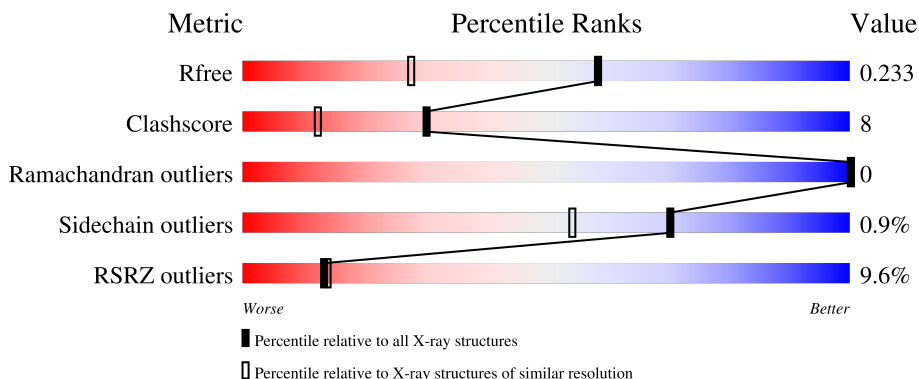
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.61 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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	263	12% 79% 16% ..
1	B	263	7% 81% 15% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4354 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 PA3825 EAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	6	0
			2029	1290	351	381	7			
1	B	254	Total	C	N	O	S	0	2	0
			2000	1271	347	375	7			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Ca	0	0
			3	3		
2	B	3	Total	Ca	0	0
			3	3		

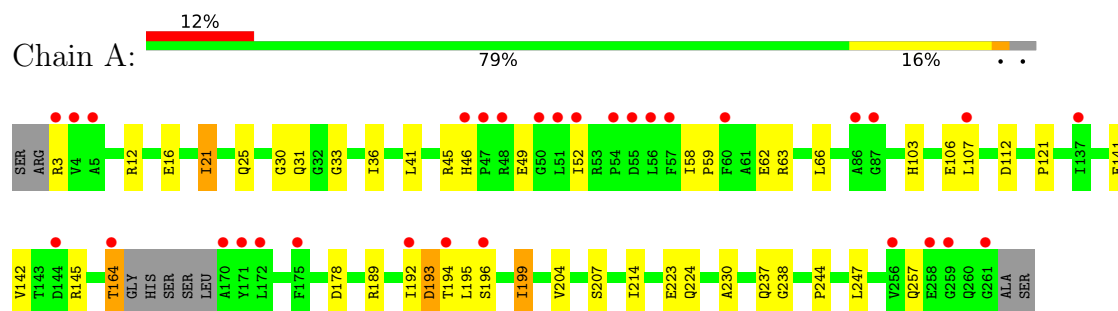
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	166	Total	O	0	0
			166	166		
3	B	153	Total	O	0	0
			153	153		

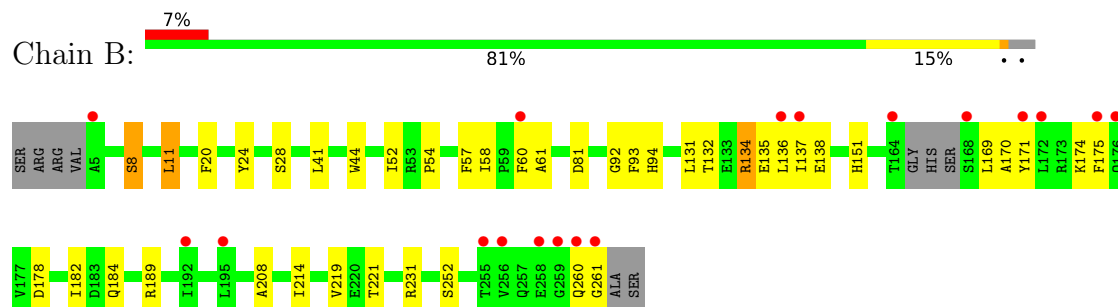
3 Residue-property plots [i](#)

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: PA3825 EAL



• Molecule 1: PA3825 EAL



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.44Å 59.82Å 96.69Å 90.00° 116.94° 90.00°	Depositor
Resolution (Å)	40.21 – 1.61 40.21 – 1.61	Depositor EDS
% Data completeness (in resolution range)	97.0 (40.21-1.61) 97.0 (40.21-1.61)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.61Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.185 , 0.223 0.195 , 0.233	Depositor DCC
R_{free} test set	3641 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 27.5	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	0.96	EDS
Total number of atoms	4354	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 20.74 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.1376e-03.*

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	1.51	15/2069 (0.7%)	1.32	10/2804 (0.4%)
1	B	1.47	10/2040 (0.5%)	1.29	6/2764 (0.2%)
All	All	1.49	25/4109 (0.6%)	1.31	16/5568 (0.3%)

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

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	GLY	C-O	-7.08	1.16	1.23
1	B	221	THR	N-CA	-6.75	1.40	1.45
1	A	224	GLN	N-CA	6.75	1.54	1.46
1	A	230	ALA	N-CA	6.52	1.54	1.46
1	A	199	ILE	N-CA	-6.40	1.39	1.46
1	B	219	VAL	N-CA	-6.26	1.39	1.46
1	B	20	PHE	N-CA	5.95	1.53	1.46
1	B	11	LEU	N-CA	5.82	1.53	1.46
1	A	237	GLN	CD-NE2	-5.82	1.21	1.33
1	B	219	VAL	C-O	5.81	1.29	1.24
1	A	25	GLN	CD-NE2	-5.68	1.21	1.33
1	A	107	LEU	N-CA	5.64	1.53	1.46
1	A	58	ILE	CA-CB	5.52	1.56	1.54
1	A	207	SER	CA-C	-5.51	1.45	1.52
1	B	41	LEU	C-O	-5.42	1.17	1.24
1	B	131	LEU	N-CA	5.34	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	ASP	CA-CB	-5.28	1.46	1.54
1	B	208	ALA	N-CA	-5.26	1.39	1.46
1	A	214	ILE	N-CA	-5.20	1.40	1.46
1	A	223	GLU	CA-CB	-5.20	1.45	1.53
1	A	121	PRO	CA-C	5.14	1.54	1.51
1	A	204	VAL	N-CA	-5.12	1.40	1.46
1	A	247	LEU	N-CA	-5.12	1.40	1.46
1	B	8	SER	CA-CB	5.08	1.61	1.53
1	B	24	TYR	CA-CB	-5.05	1.46	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	GLU	CA-C-N	-7.38	109.07	122.50
1	A	106	GLU	C-N-CA	-7.38	109.07	122.50
1	A	257	GLN	N-CA-C	7.03	119.02	111.36
1	A	52	ILE	N-CA-C	6.20	117.86	108.80
1	A	145	ARG	N-CA-C	6.12	118.03	111.36
1	A	142	VAL	N-CA-C	6.04	120.02	113.43
1	B	61	ALA	N-CA-C	-5.67	105.18	111.36
1	B	28	SER	CA-C-N	-5.62	114.00	119.78
1	B	28	SER	C-N-CA	-5.62	114.00	119.78
1	A	238	GLY	CA-C-O	-5.43	116.21	121.86
1	B	189	ARG	N-CA-C	5.35	119.80	113.16
1	A	214	ILE	CB-CA-C	5.27	118.60	110.28
1	B	81	ASP	N-CA-C	5.22	116.78	111.14
1	A	30	GLY	N-CA-C	5.13	118.89	112.73
1	B	231	ARG	N-CA-C	5.11	119.15	113.02
1	A	21	ILE	O-C-N	5.02	124.85	121.69

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	193	ASP	Mainchain

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	2029	0	2025	41	0
1	B	2000	0	1995	28	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	166	0	0	14	0
3	B	153	0	0	8	0
All	All	4354	0	4020	68	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 (68) 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:194[A]:THR:HB	3:A:530:HOH:O	1.31	1.24
1:A:195[B]:LEU:O	1:A:195[B]:LEU:HD13	1.39	1.23
1:A:194[A]:THR:O	3:A:401:HOH:O	1.60	1.18
1:A:195[B]:LEU:HD13	1:A:195[B]:LEU:C	1.76	1.07
1:B:171:TYR:HA	1:B:174:LYS:HE3	1.38	1.04
1:A:195[B]:LEU:C	1:A:195[B]:LEU:CD1	2.32	1.00
1:B:135:GLU:OE1	3:B:401:HOH:O	1.81	0.97
1:B:132:THR:HG23	3:B:401:HOH:O	1.68	0.93
1:B:171:TYR:CA	1:B:174:LYS:HE3	2.01	0.90
1:A:164:THR:HG22	3:A:536:HOH:O	1.75	0.85
1:A:62:GLU:OE2	3:A:402:HOH:O	1.99	0.80
1:B:136:LEU:HD21	1:B:175:PHE:CD2	2.20	0.77
1:A:195[B]:LEU:O	1:A:195[B]:LEU:CD1	2.26	0.74
1:A:12:ARG:NH1	1:A:16:GLU:OE2	2.20	0.74
1:A:195[B]:LEU:O	1:A:199:ILE:HG12	1.89	0.72
1:A:196[A]:SER:OG	3:A:404:HOH:O	2.06	0.72
1:A:196[A]:SER:HB2	3:A:424:HOH:O	1.90	0.71
1:B:184:GLN:OE1	3:B:402:HOH:O	2.09	0.69
1:A:62:GLU:CD	3:A:402:HOH:O	2.36	0.67
1:A:193:ASP:OD1	1:A:194[B]:THR:N	2.28	0.66
1:A:164:THR:CG2	3:A:536:HOH:O	2.37	0.65
1:B:11:LEU:HD12	1:B:60:PHE:CD2	2.33	0.63
1:B:54:PRO:HA	1:B:57:PHE:CE1	2.33	0.63
1:B:151:HIS:HE1	1:B:178:ASP:OD2	1.80	0.62
1:A:195[B]:LEU:C	1:A:195[B]:LEU:HD12	2.25	0.61
1:A:196[B]:SER:CB	3:A:403:HOH:O	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLU:HG2	3:A:486:HOH:O	2.02	0.60
1:B:170:ALA:O	1:B:174:LYS:HG3	2.03	0.59
1:A:103:HIS:HE1	1:A:112:ASP:OD2	1.87	0.58
1:A:196[A]:SER:CB	3:A:424:HOH:O	2.49	0.57
1:B:8:SER:HG	1:B:60:PHE:HZ	1.50	0.57
1:B:134:ARG:NE	3:B:406:HOH:O	2.39	0.55
1:B:138:GLU:OE1	3:B:403:HOH:O	2.18	0.55
1:B:11:LEU:HD12	1:B:60:PHE:HD2	1.72	0.54
1:A:36:ILE:C	1:A:36:ILE:HD12	2.32	0.54
1:B:151:HIS:HD2	3:B:432:HOH:O	1.89	0.54
1:B:171:TYR:N	1:B:174:LYS:HE3	2.23	0.54
1:A:195[B]:LEU:CD1	1:A:199:ILE:HG13	2.38	0.53
1:B:54:PRO:HB3	1:B:58:ILE:HD12	1.92	0.52
1:A:196[B]:SER:HB3	3:A:419:HOH:O	2.10	0.52
1:B:136:LEU:HD21	1:B:175:PHE:CE2	2.44	0.52
1:A:195[B]:LEU:CD1	1:A:199:ILE:CG1	2.87	0.52
1:A:193:ASP:OD1	1:A:193:ASP:C	2.54	0.51
1:B:260:GLN:O	1:B:261:GLY:C	2.54	0.50
1:A:195[B]:LEU:HD11	1:A:199:ILE:HG13	1.95	0.49
1:A:193:ASP:OD2	1:A:196[A]:SER:OG	2.31	0.48
1:A:189:ARG:HA	1:A:192:ILE:HD12	1.96	0.48
1:B:94:HIS:HD2	3:B:542:HOH:O	1.95	0.48
1:A:45:ARG:CG	1:A:45:ARG:O	2.62	0.48
1:B:44:TRP:CD2	1:B:52:ILE:HD12	2.48	0.47
1:B:8:SER:OG	1:B:60:PHE:HZ	1.97	0.47
1:A:195[B]:LEU:HD13	1:A:199:ILE:HG12	1.96	0.46
1:A:195[A]:LEU:O	1:A:196[A]:SER:C	2.58	0.44
1:A:195[B]:LEU:HD11	1:A:199:ILE:CG1	2.47	0.44
1:A:31:GLN:HB2	3:A:412:HOH:O	2.17	0.44
1:A:41[A]:LEU:HD22	1:A:244:PRO:CG	2.48	0.44
1:B:134:ARG:CZ	3:B:406:HOH:O	2.66	0.43
1:A:192:ILE:O	1:B:252:SER:HB3	2.19	0.43
1:B:182:ILE:HD11	1:B:214:ILE:HD11	2.00	0.42
1:A:12:ARG:HD3	1:A:66:LEU:HD21	2.00	0.42
1:A:195[B]:LEU:CD1	1:A:199:ILE:HG12	2.50	0.42
1:A:21:ILE:HG21	1:A:45:ARG:HH11	1.85	0.41
1:B:134:ARG:O	1:B:137:ILE:HG12	2.19	0.41
1:B:92:GLY:O	1:B:93:PHE:C	2.64	0.41
1:A:103:HIS:HD2	3:A:475:HOH:O	2.02	0.41
1:A:59:PRO:O	1:A:63:ARG:HG3	2.20	0.41
1:A:46:HIS:CD2	1:A:49:GLU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:TYR:N	1:B:174:LYS:CE	2.84	0.40

There are no symmetry-related clashes.

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	256/263 (97%)	253 (99%)	3 (1%)	0	100	100
1	B	252/263 (96%)	246 (98%)	6 (2%)	0	100	100
All	All	508/526 (97%)	499 (98%)	9 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	218/220 (99%)	216 (99%)	2 (1%)	70	54
1	B	215/220 (98%)	213 (99%)	2 (1%)	70	54
All	All	433/440 (98%)	429 (99%)	4 (1%)	70	54

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	164	THR
1	B	134	ARG
1	B	169	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	103	HIS
1	A	237	GLN
1	B	94	HIS
1	B	151	HIS

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 6 ligands modelled in this entry, 6 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 ⓘ

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	254/263 (96%)	0.57	31 (12%) 8 9	12, 28, 65, 98	6 (2%)
1	B	254/263 (96%)	0.43	18 (7%) 22 23	15, 27, 50, 99	2 (0%)
All	All	508/526 (96%)	0.50	49 (9%) 13 14	12, 27, 56, 99	8 (1%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	LEU	5.6
1	A	170	ALA	5.6
1	A	171	TYR	5.0
1	A	4	VAL	4.9
1	B	261	GLY	4.5
1	A	175	PHE	4.4
1	A	51	LEU	4.2
1	A	56	LEU	4.2
1	A	54	PRO	4.1
1	A	164	THR	4.0
1	B	164	THR	3.9
1	B	5	ALA	3.8
1	B	137	ILE	3.6
1	A	5	ALA	3.4
1	A	192	ILE	3.1
1	A	60	PHE	2.9
1	B	255	THR	2.9
1	B	260	GLN	2.8
1	B	175	PHE	2.7
1	A	46	HIS	2.7
1	B	176	GLN	2.7
1	A	55	ASP	2.7
1	A	107	LEU	2.7
1	A	258	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	60	PHE	2.6
1	A	47	PRO	2.6
1	A	48	ARG	2.6
1	B	168	SER	2.6
1	A	194[A]	THR	2.5
1	B	171	TYR	2.5
1	A	256	VAL	2.5
1	A	87	GLY	2.4
1	B	256	VAL	2.4
1	A	261	GLY	2.3
1	B	259	GLY	2.3
1	B	136	LEU	2.3
1	A	259	GLY	2.3
1	B	172	LEU	2.2
1	B	192	ILE	2.2
1	A	86	ALA	2.2
1	A	57	PHE	2.2
1	A	52	ILE	2.1
1	B	258	GLU	2.1
1	A	196[A]	SER	2.1
1	A	137	ILE	2.1
1	A	144	ASP	2.0
1	A	3	ARG	2.0
1	B	195	LEU	2.0
1	A	50	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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
2	CA	A	303	1/1	0.98	0.05	23,23,23,23	0
2	CA	A	302	1/1	0.99	0.06	29,29,29,29	0
2	CA	A	301	1/1	0.99	0.02	21,21,21,21	0
2	CA	B	301	1/1	0.99	0.05	25,25,25,25	0
2	CA	B	302	1/1	0.99	0.05	28,28,28,28	0
2	CA	B	303	1/1	0.99	0.06	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.