



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 01:05 am GMT

PDB ID : 5B2L
Title : A crucial role of Cys218 in the stabilization of an unprecedented auto-inhibition form of MAP2K7
Authors : Sogabe, Y.; Hashimoto, T.; Matsumoto, T.; Kirii, Y.; Sawa, M.; Kinoshita, T.
Deposited on : 2016-01-19
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

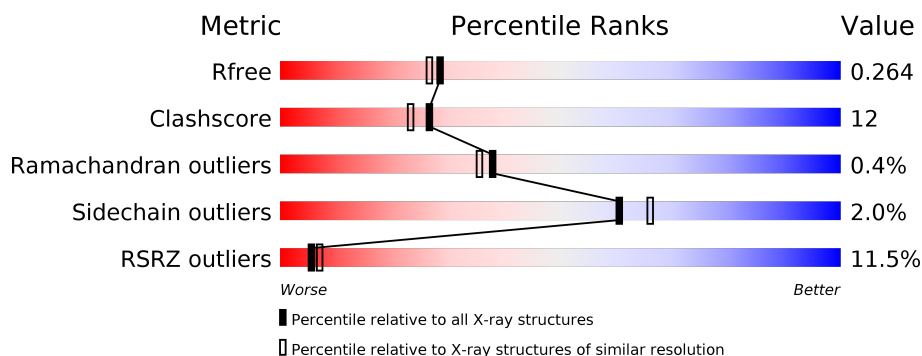
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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 ≥ 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	324	

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
2	EPE	A	501[A]	-	-	-	X
2	EPE	A	501[B]	-	-	X	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EPE	A	502	-	-	-	X
3	GOL	A	503	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2411 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.

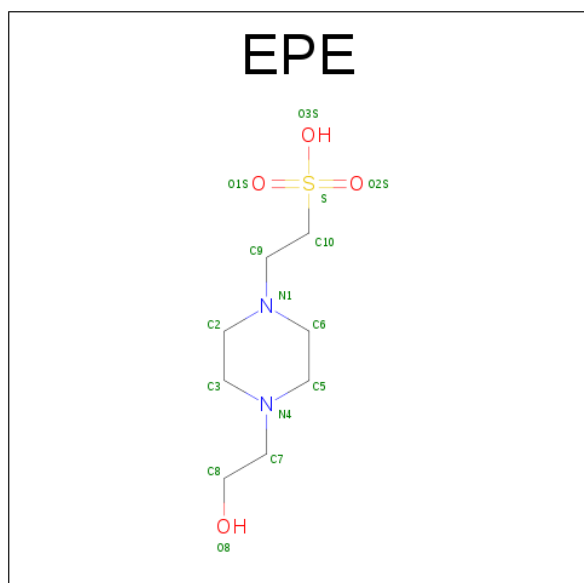
- Molecule 1 is a protein called Dual specificity mitogen-activated protein kinase kinase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2294	1461	395	420	18	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	118	MET	-	initiating methionine	UNP O14733
A	218	SER	CYS	engineered mutation	UNP O14733
A	436	HIS	-	expression tag	UNP O14733
A	437	HIS	-	expression tag	UNP O14733
A	438	HIS	-	expression tag	UNP O14733
A	439	HIS	-	expression tag	UNP O14733
A	440	HIS	-	expression tag	UNP O14733
A	441	HIS	-	expression tag	UNP O14733

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			30	16	4	8	2		
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

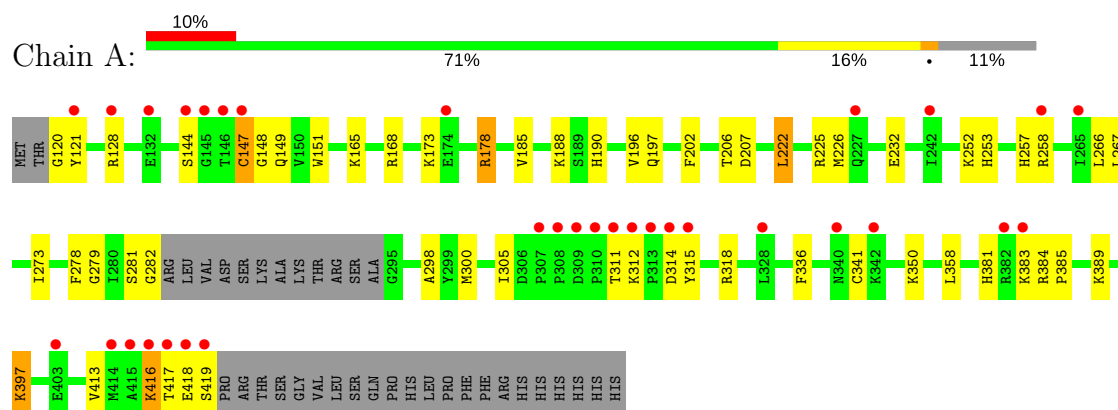
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	66	Total	O	0	0
			66	66		

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: Dual specificity mitogen-activated protein kinase kinase 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.98Å 65.44Å 88.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.94 – 2.10 34.94 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (34.94-2.10) 99.8 (34.94-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.42 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.192 , 0.264 0.191 , 0.264	Depositor DCC
R_{free} test set	989 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2411	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.12% 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, EPE

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	0.99	2/2341 (0.1%)	0.95	2/3149 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	TRP	CD2-CE2	6.50	1.49	1.41
1	A	232	GLU	CD-OE2	-5.73	1.19	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	384	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	222	LEU	CB-CG-CD2	-5.08	102.37	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2294	0	2319	55	0
2	A	45	0	53	14	0
3	A	6	0	8	0	0
4	A	66	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2411	0	2380	55	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 12.

All (55) 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:206:THR:HB	2:A:501[B]:EPE:H82	1.31	1.13
1:A:385:PRO:HB3	1:A:389:LYS:HE2	1.44	0.98
1:A:178:ARG:HG2	1:A:178:ARG:HH21	1.30	0.94
1:A:149:GLN:HE22	2:A:501[A]:EPE:H31	1.48	0.77
1:A:417:THR:HB	1:A:418:GLU:HA	1.65	0.77
1:A:178:ARG:HG2	1:A:178:ARG:NH2	1.97	0.77
1:A:225:ARG:HB3	1:A:417:THR:HG21	1.66	0.76
1:A:385:PRO:CB	1:A:389:LYS:HE2	2.15	0.76
1:A:207:ASP:OD1	2:A:501[B]:EPE:H71	1.84	0.76
1:A:147:CYS:O	1:A:165:LYS:HE2	1.88	0.74
1:A:206:THR:HB	2:A:501[B]:EPE:C8	2.14	0.72
1:A:168:ARG:HB3	2:A:501[B]:EPE:H72	1.71	0.71
1:A:147:CYS:HB2	1:A:278:PHE:HD2	1.55	0.71
1:A:413:VAL:O	1:A:417:THR:OG1	2.07	0.70
1:A:149:GLN:NE2	2:A:501[A]:EPE:H51	2.07	0.69
1:A:385:PRO:HB3	1:A:389:LYS:CE	2.23	0.67
1:A:178:ARG:HH11	1:A:279:GLY:HA2	1.60	0.65
1:A:144:SER:HA	1:A:148:GLY:HA3	1.80	0.63
1:A:178:ARG:HE	1:A:279:GLY:HA2	1.64	0.62
1:A:341:CYS:SG	1:A:350:LYS:HD2	2.39	0.62
1:A:257:HIS:O	1:A:282:GLY:HA2	2.00	0.60
1:A:222:LEU:O	1:A:226:MET:HG3	2.02	0.60
1:A:147:CYS:HB2	1:A:278:PHE:CD2	2.37	0.57
1:A:173:LYS:HE2	4:A:648:HOH:O	2.06	0.56
1:A:300:MET:HE2	1:A:305:ILE:HG12	1.89	0.55
1:A:120:GLY:HA3	1:A:202:PHE:CD1	2.42	0.54
1:A:178:ARG:NH1	1:A:279:GLY:HA2	2.22	0.54
1:A:190:HIS:HA	1:A:197:GLN:OE1	2.09	0.53
1:A:225:ARG:HB3	1:A:417:THR:CG2	2.38	0.52
1:A:252:LYS:HG2	1:A:253:HIS:CE1	2.46	0.51
1:A:168:ARG:CB	2:A:501[B]:EPE:H72	2.42	0.49
1:A:318:ARG:HD2	1:A:381:HIS:O	2.12	0.49
1:A:258:ARG:NE	1:A:315:TYR:OH	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ALA:HB1	1:A:336:PHE:CZ	2.48	0.48
1:A:358:LEU:O	2:A:502:EPE:H101	2.14	0.48
1:A:178:ARG:NE	1:A:279:GLY:HA2	2.28	0.47
1:A:311:THR:HB	1:A:312:LYS:HD3	1.97	0.47
1:A:168:ARG:HD3	2:A:501[B]:EPE:H102	1.97	0.47
1:A:121:TYR:HE2	1:A:128:ARG:HD3	1.80	0.47
1:A:178:ARG:HH21	1:A:178:ARG:CG	2.13	0.46
1:A:416:LYS:HD3	1:A:416:LYS:N	2.31	0.46
1:A:341:CYS:SG	1:A:350:LYS:CD	3.04	0.46
1:A:149:GLN:HE22	2:A:501[A]:EPE:H51	1.79	0.45
1:A:188:LYS:HB3	1:A:253:HIS:CE1	2.52	0.45
1:A:168:ARG:NE	2:A:501[B]:EPE:H51	2.32	0.45
1:A:168:ARG:CD	2:A:501[B]:EPE:H102	2.48	0.44
1:A:206:THR:O	2:A:501[B]:EPE:H82	2.17	0.44
1:A:196:VAL:HG11	1:A:266:LEU:HD12	2.00	0.44
1:A:121:TYR:CE2	1:A:128:ARG:HD3	2.53	0.43
1:A:267:LEU:HG	1:A:273:ILE:HG12	2.00	0.43
1:A:397:LYS:HA	1:A:397:LYS:HD2	1.46	0.42
1:A:311:THR:HB	1:A:312:LYS:CD	2.50	0.41
1:A:185:VAL:HG21	1:A:281:SER:HA	2.03	0.41
1:A:383:LYS:HE3	1:A:383:LYS:HB2	1.91	0.41
1:A:168:ARG:HE	2:A:501[B]:EPE:H51	1.86	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	284/324 (88%)	272 (96%)	11 (4%)	1 (0%)	38 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	314	ASP

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	252/285 (88%)	247 (98%)	5 (2%)	60 66

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	CYS
1	A	178	ARG
1	A	397	LYS
1	A	416	LYS
1	A	419	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

4 ligands are modelled in this entry.

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$
2	EPE	A	501[A]	-	15,15,15	2.15	2 (13%)	18,20,20	2.28	4 (22%)
2	EPE	A	501[B]	-	15,15,15	2.62	2 (13%)	18,20,20	3.14	12 (66%)
2	EPE	A	502	-	15,15,15	2.57	2 (13%)	18,20,20	2.40	4 (22%)
3	GOL	A	503	-	5,5,5	0.88	0	5,5,5	1.37	1 (20%)

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
2	EPE	A	501[A]	-	-	0/9/19/19	0/1/1/1
2	EPE	A	501[B]	-	-	0/9/19/19	0/1/1/1
2	EPE	A	502	-	-	0/9/19/19	0/1/1/1
3	GOL	A	503	-	-	0/4/4/4	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[B]	EPE	C10-S	-7.87	1.65	1.77
2	A	502	EPE	C10-S	-6.55	1.67	1.77
2	A	501[A]	EPE	C10-S	-6.20	1.68	1.77
2	A	501[A]	EPE	O3S-S	5.14	1.64	1.47
2	A	501[B]	EPE	O3S-S	5.54	1.66	1.47
2	A	502	EPE	O2S-S	6.95	1.65	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[B]	EPE	C3-C2-N1	-5.08	100.35	110.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[B]	EPE	C7-N4-C3	-3.96	101.11	111.26
2	A	501[B]	EPE	O3S-S-O2S	-3.68	102.94	111.37
2	A	501[B]	EPE	C6-N1-C2	-3.31	101.36	108.87
2	A	501[B]	EPE	C8-C7-N4	-3.30	101.20	113.33
2	A	501[A]	EPE	C2-C3-N4	-2.85	104.88	110.63
2	A	501[B]	EPE	O2S-S-O1S	-2.21	106.19	113.86
2	A	501[A]	EPE	O3S-S-O2S	-2.17	106.39	111.37
2	A	501[B]	EPE	C2-C3-N4	2.12	114.93	110.63
2	A	502	EPE	C6-N1-C2	2.17	113.78	108.87
2	A	501[B]	EPE	C9-N1-C2	2.30	117.16	111.26
2	A	502	EPE	C5-N4-C3	2.38	114.27	108.87
2	A	502	EPE	O3S-S-C10	2.39	108.99	106.06
3	A	503	GOL	O3-C3-C2	2.67	123.52	110.07
2	A	501[B]	EPE	O1S-S-C10	3.82	110.07	106.79
2	A	501[B]	EPE	C5-N4-C3	3.86	117.62	108.87
2	A	501[B]	EPE	O3S-S-C10	4.53	111.62	106.06
2	A	501[B]	EPE	O2S-S-C10	5.29	111.33	106.79
2	A	501[A]	EPE	O2S-S-C10	5.55	111.56	106.79
2	A	501[A]	EPE	O3S-S-C10	6.38	113.90	106.06
2	A	502	EPE	O2S-S-C10	8.76	114.31	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501[A]	EPE	3	0
2	A	501[B]	EPE	10	0
2	A	502	EPE	1	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, 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	288/324 (88%)	0.60	33 (11%) 5 7	21, 35, 76, 122	4 (1%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	TYR	12.3
1	A	312	LYS	10.5
1	A	314	ASP	9.5
1	A	313	PRO	9.3
1	A	311	THR	8.0
1	A	147	CYS	6.4
1	A	419	SER	5.9
1	A	309	ASP	5.6
1	A	310	PRO	5.0
1	A	417	THR	4.8
1	A	174	GLU	4.0
1	A	308	PRO	4.0
1	A	382	ARG	3.6
1	A	146	THR	3.6
1	A	415	ALA	3.6
1	A	340	ASN	3.1
1	A	418	GLU	3.0
1	A	307	PRO	3.0
1	A	121	TYR	2.9
1	A	342	LYS	2.9
1	A	416	LYS	2.8
1	A	414	MET	2.8
1	A	227	GLN	2.7
1	A	383	LYS	2.6
1	A	132	GLU	2.4
1	A	258	ARG	2.3
1	A	144	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	403	GLU	2.3
1	A	265	ILE	2.2
1	A	328	LEU	2.2
1	A	242	ILE	2.1
1	A	128	ARG	2.1
1	A	145	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	EPE	A	501[A]	15/15	0.68	0.40	9.31	27,35,74,75	15
2	EPE	A	501[B]	15/15	0.68	0.40	8.80	23,31,46,49	15
3	GOL	A	503	6/6	0.68	0.28	6.93	46,57,63,69	0
2	EPE	A	502	15/15	0.65	0.35	5.46	82,100,113,115	0

6.5 Other polymers [i](#)

There are no such residues in this entry.