



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 27, 2023 – 04:17 am BST

PDB ID : 8ACG
Title : Structure of Pseudomonas aeruginosa aminopeptidase, PaAP_T E340A mutant
Authors : Harding, C.J.; Czekster, C.M.
Deposited on : 2022-07-05
Resolution : 2.84 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

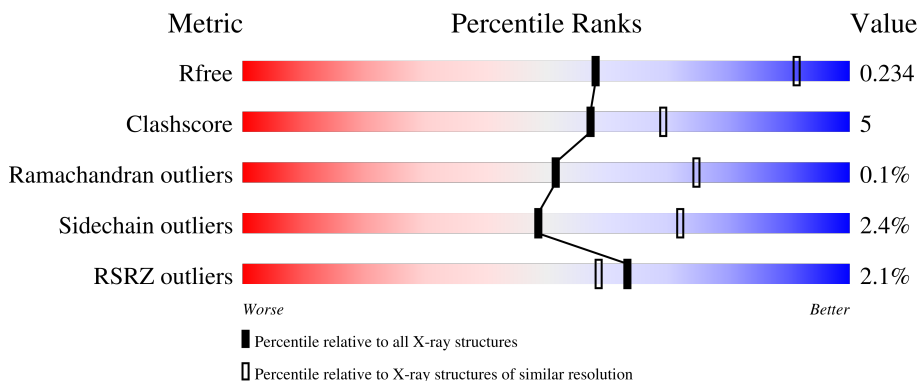
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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	490	 4% 81% 14% .
1	B	490	 82% 13% . 5%
1	C	490	 4% 84% 11% . .
1	D	490	 2% 84% 12% .
1	E	490	 4% 84% 12% .

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Mol	Chain	Length	Quality of chain
1	F	490	 84% 12% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21300 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 Keratinase KP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	F	471	3554	2241	600	703	10	0	0	0
1	D	474	3575	2255	603	707	10	0	0	0
1	A	468	3525	2222	593	700	10	0	0	0
1	E	470	3548	2238	599	702	9	0	0	0
1	B	465	3506	2212	589	695	10	0	0	0
1	C	472	3562	2247	601	704	10	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	340	ALA	GLU	engineered mutation	UNP E3ULB5
F	513	LEU	ALA	conflict	UNP E3ULB5
F	514	VAL	GLN	conflict	UNP E3ULB5
F	515	PRO	SER	conflict	UNP E3ULB5
D	340	ALA	GLU	engineered mutation	UNP E3ULB5
D	513	LEU	ALA	conflict	UNP E3ULB5
D	514	VAL	GLN	conflict	UNP E3ULB5
D	515	PRO	SER	conflict	UNP E3ULB5
A	340	ALA	GLU	engineered mutation	UNP E3ULB5
A	513	LEU	ALA	conflict	UNP E3ULB5
A	514	VAL	GLN	conflict	UNP E3ULB5
A	515	PRO	SER	conflict	UNP E3ULB5
E	340	ALA	GLU	engineered mutation	UNP E3ULB5
E	513	LEU	ALA	conflict	UNP E3ULB5
E	514	VAL	GLN	conflict	UNP E3ULB5
E	515	PRO	SER	conflict	UNP E3ULB5
B	340	ALA	GLU	engineered mutation	UNP E3ULB5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	513	LEU	ALA	conflict	UNP E3ULB5
B	514	VAL	GLN	conflict	UNP E3ULB5
B	515	PRO	SER	conflict	UNP E3ULB5
C	340	ALA	GLU	engineered mutation	UNP E3ULB5
C	513	LEU	ALA	conflict	UNP E3ULB5
C	514	VAL	GLN	conflict	UNP E3ULB5
C	515	PRO	SER	conflict	UNP E3ULB5

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	3	Total Zn 3 3	0	0
2	D	3	Total Zn 3 3	0	0
2	A	3	Total Zn 3 3	0	0
2	E	3	Total Zn 3 3	0	0
2	B	3	Total Zn 3 3	0	0
2	C	3	Total Zn 3 3	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	3	Total O 3 3	0	0
4	D	1	Total O 1 1	0	0

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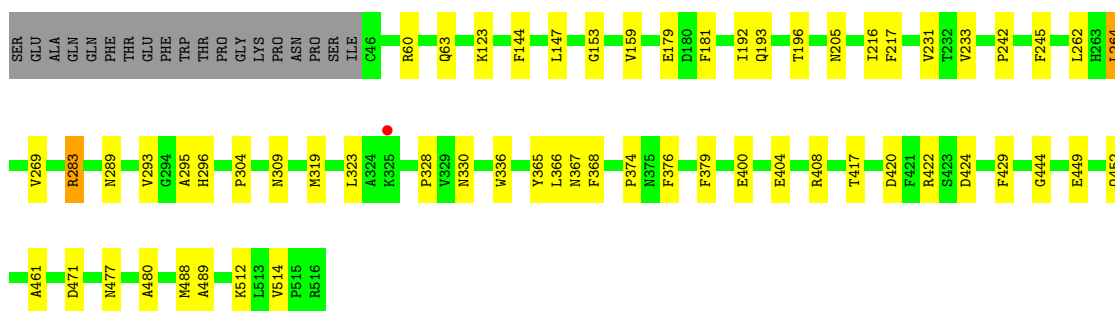
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0
4	B	1	Total O 1 1	0	0
4	C	2	Total O 2 2	0	0

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.

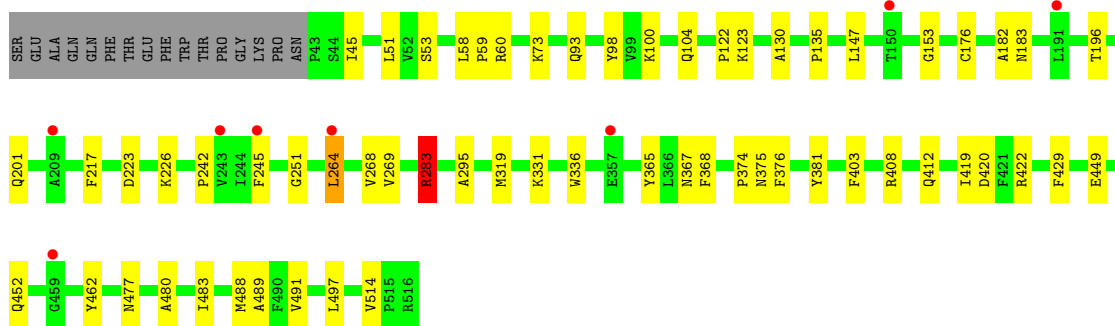
- Molecule 1: Keratinase KP1

Chain F: 




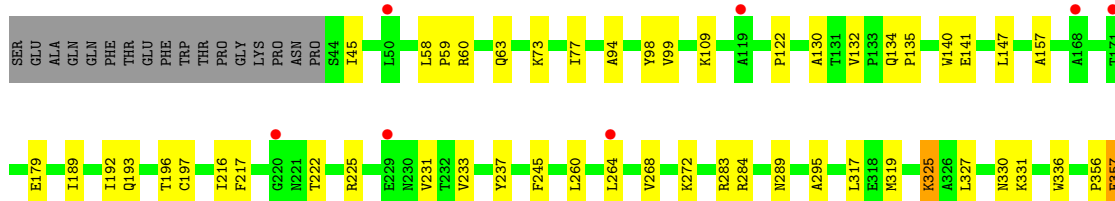
- Molecule 1: Keratinase KP1

Chain D: 



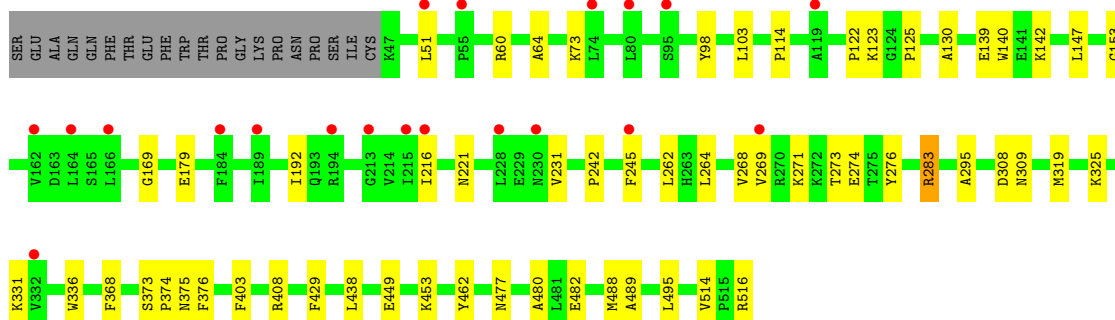
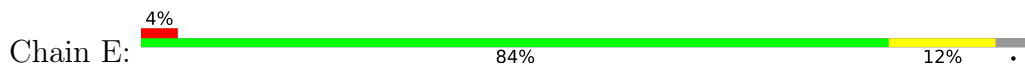
- Molecule 1: Keratinase KP1

Chain A: 

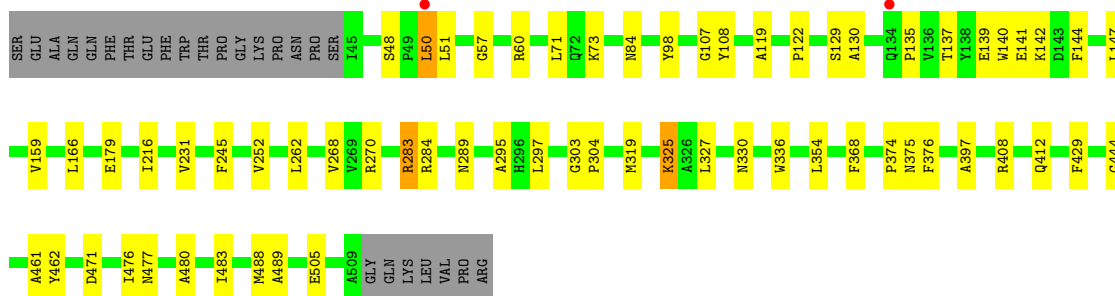
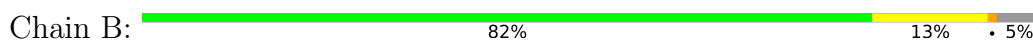




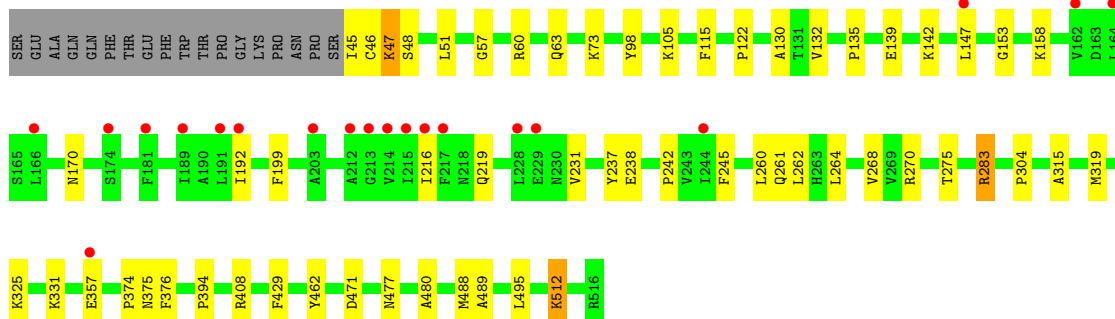
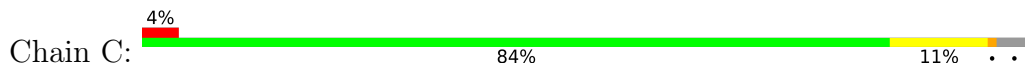
• Molecule 1: Keratinase KP1



• Molecule 1: Keratinase KP1



• Molecule 1: Keratinase KP1



4 Data and refinement statistics i

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	186.74Å 186.74Å 84.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.57 – 2.84 61.13 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.57-2.84) 99.8 (61.13-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.86Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.191 , 0.239 0.191 , 0.234	Depositor DCC
R_{free} test set	3812 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	101.8	Xtrriage
Anisotropy	0.016	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l 0.007 for h,-h-k,-l 0.004 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	21300	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.64 % 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 6.7167e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN, MG

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	0.48	0/3600	0.62	0/4891
1	B	0.49	0/3581	0.63	1/4866 (0.0%)
1	C	0.54	0/3638	0.66	1/4941 (0.0%)
1	D	0.53	1/3652 (0.0%)	0.68	2/4960 (0.0%)
1	E	0.46	0/3624	0.63	1/4922 (0.0%)
1	F	0.52	0/3630	0.67	1/4930 (0.0%)
All	All	0.51	1/21725 (0.0%)	0.65	6/29510 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	283	ARG	CG-CD	5.01	1.64	1.51

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	264	LEU	CA-CB-CG	7.86	133.38	115.30
1	D	51	LEU	CA-CB-CG	-6.51	100.33	115.30
1	F	264	LEU	CA-CB-CG	6.21	129.57	115.30
1	E	264	LEU	CA-CB-CG	6.14	129.43	115.30
1	C	325	LYS	CD-CE-NZ	5.65	124.69	111.70

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	3525	0	3396	42	0
1	B	3506	0	3378	36	0
1	C	3562	0	3442	31	0
1	D	3575	0	3455	33	0
1	E	3548	0	3428	36	0
1	F	3554	0	3433	31	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	3	0	0	0	0
All	All	21300	0	20532	204	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 5.

The worst 5 of 204 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:C:374:PRO:HA	1:C:477:ASN:HB2	1.72	0.71
1:A:196:THR:O	1:E:516:ARG:NH1	2.24	0.69
1:C:130:ALA:O	1:C:135:PRO:HA	1.93	0.69
1:B:130:ALA:O	1:B:135:PRO:HA	1.93	0.69
1:E:374:PRO:HA	1:E:477:ASN:HB2	1.76	0.68

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	466/490 (95%)	449 (96%)	17 (4%)	0	100	100
1	B	463/490 (94%)	447 (96%)	16 (4%)	0	100	100
1	C	470/490 (96%)	453 (96%)	17 (4%)	0	100	100
1	D	472/490 (96%)	456 (97%)	15 (3%)	1 (0%)	47	69
1	E	468/490 (96%)	453 (97%)	15 (3%)	0	100	100
1	F	469/490 (96%)	450 (96%)	18 (4%)	1 (0%)	47	69
All	All	2808/2940 (96%)	2708 (96%)	98 (4%)	2 (0%)	51	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	196	THR
1	D	196	THR

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	366/386 (95%)	354 (97%)	12 (3%)	38	63
1	B	364/386 (94%)	358 (98%)	6 (2%)	62	81
1	C	370/386 (96%)	358 (97%)	12 (3%)	39	63
1	D	372/386 (96%)	364 (98%)	8 (2%)	52	75
1	E	368/386 (95%)	363 (99%)	5 (1%)	67	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	369/386 (96%)	359 (97%)	10 (3%)	44 69
All	All	2209/2316 (95%)	2156 (98%)	53 (2%)	49 72

5 of 53 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	408	ARG
1	B	50	LEU
1	C	357	GLU
1	A	429	PHE
1	E	283	ARG

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

Mol	Chain	Res	Type
1	D	93	GLN
1	D	104	GLN
1	A	289	ASN
1	A	330	ASN
1	B	430	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 21 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	468/490 (95%)	0.02	7 (1%) 73 70	84, 106, 140, 166	0
1	B	465/490 (94%)	-0.07	2 (0%) 92 91	75, 101, 123, 140	0
1	C	472/490 (96%)	0.20	20 (4%) 36 28	71, 97, 187, 208	0
1	D	474/490 (96%)	0.05	8 (1%) 70 66	68, 96, 136, 161	0
1	E	470/490 (95%)	0.16	20 (4%) 35 27	79, 113, 145, 169	0
1	F	471/490 (96%)	0.04	1 (0%) 95 94	76, 94, 113, 137	0
All	All	2820/2940 (95%)	0.07	58 (2%) 63 58	68, 101, 146, 208	0

The worst 5 of 58 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	212	ALA	4.8
1	E	51	LEU	4.5
1	C	215	ILE	4.4
1	E	119	ALA	4.3
1	C	181	PHE	3.5

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 monosaccharides 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	MG	D	604	1/1	0.73	0.23	82,82,82,82	0
3	MG	A	604	1/1	0.82	0.29	105,105,105,105	0
3	MG	F	604	1/1	0.86	0.27	88,88,88,88	0
2	ZN	D	601	1/1	0.94	0.20	88,88,88,88	0
2	ZN	E	601	1/1	0.95	0.22	104,104,104,104	0
2	ZN	F	601	1/1	0.95	0.22	97,97,97,97	0
2	ZN	A	602	1/1	0.96	0.20	96,96,96,96	0
2	ZN	F	603	1/1	0.96	0.20	114,114,114,114	0
2	ZN	F	602	1/1	0.96	0.23	86,86,86,86	0
2	ZN	D	602	1/1	0.96	0.19	98,98,98,98	0
2	ZN	A	601	1/1	0.96	0.20	107,107,107,107	0
2	ZN	C	601	1/1	0.97	0.23	97,97,97,97	0
2	ZN	E	602	1/1	0.97	0.24	99,99,99,99	0
2	ZN	B	601	1/1	0.97	0.21	99,99,99,99	0
2	ZN	B	603	1/1	0.97	0.13	111,111,111,111	0
2	ZN	C	603	1/1	0.98	0.17	110,110,110,110	0
2	ZN	C	602	1/1	0.98	0.23	98,98,98,98	0
2	ZN	B	602	1/1	0.99	0.22	93,93,93,93	0
2	ZN	A	603	1/1	0.99	0.17	113,113,113,113	0
2	ZN	E	603	1/1	0.99	0.24	113,113,113,113	0
2	ZN	D	603	1/1	0.99	0.19	116,116,116,116	0

6.5 Other polymers [i](#)

There are no such residues in this entry.