



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 26, 2018 – 10:17 AM EST

PDB ID : 6B05
Title : The Crystal Structure of the Ferredoxin Protease FusC E83A mutant in complex with Arabidopsis Ferredoxin
Authors : Grinter, R.
Deposited on : 2017-09-13
Resolution : 1.90 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 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 : rb-20031633
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

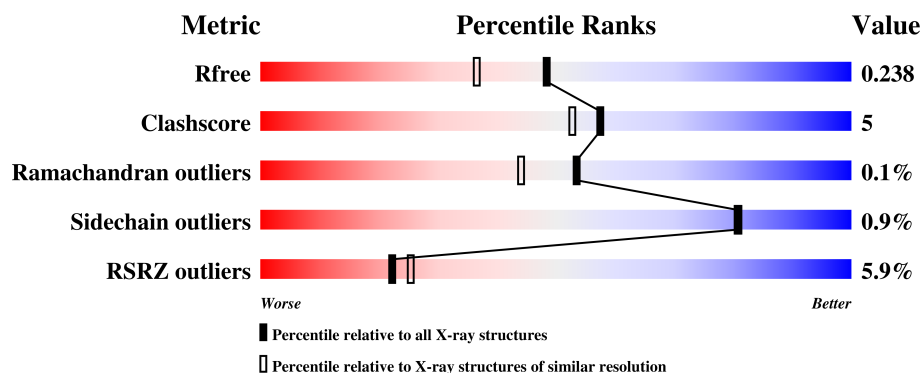
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	111664	5502 (1.90-1.90)
Clashscore	122126	6115 (1.90-1.90)
Ramachandran outliers	120053	6048 (1.90-1.90)
Sidechain outliers	120020	6048 (1.90-1.90)
RSRZ outliers	108989	5379 (1.90-1.90)

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	924	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>.</div> </div>
2	B	104	<div> <div>28%</div> <div>28%</div> <div>11%</div> <div>.</div> <div>61%</div> </div>
2	C	104	<div> <div>5%</div> <div>7%</div> <div>93%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8533 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 Putative zinc protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	896	Total	C	N	O	S	0	12	0
			7203	4522	1291	1367	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	ALA	GLU	conflict	UNP Q6D8U3

- Molecule 2 is a protein called Ferredoxin-2, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	41	Total	C	N	O	S	0	1	0
			324	205	44	74	1			
2	C	7	Total	C	N	O		0	0	0
			48	30	7	11				

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	95	ALA	-	expression tag	UNP P16972
B	96	ILE	-	expression tag	UNP P16972
B	97	MET	-	expression tag	UNP P16972
B	98	LEU	-	expression tag	UNP P16972
B	99	GLU	-	expression tag	UNP P16972
B	100	HIS	-	expression tag	UNP P16972
B	101	HIS	-	expression tag	UNP P16972
B	102	HIS	-	expression tag	UNP P16972
B	103	HIS	-	expression tag	UNP P16972
B	104	HIS	-	expression tag	UNP P16972
B	105	HIS	-	expression tag	UNP P16972
C	95	ALA	-	expression tag	UNP P16972
C	96	ILE	-	expression tag	UNP P16972

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Chain	Residue	Modelled	Actual	Comment	Reference
C	97	MET	-	expression tag	UNP P16972
C	98	LEU	-	expression tag	UNP P16972
C	99	GLU	-	expression tag	UNP P16972
C	100	HIS	-	expression tag	UNP P16972
C	101	HIS	-	expression tag	UNP P16972
C	102	HIS	-	expression tag	UNP P16972
C	103	HIS	-	expression tag	UNP P16972
C	104	HIS	-	expression tag	UNP P16972
C	105	HIS	-	expression tag	UNP P16972

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

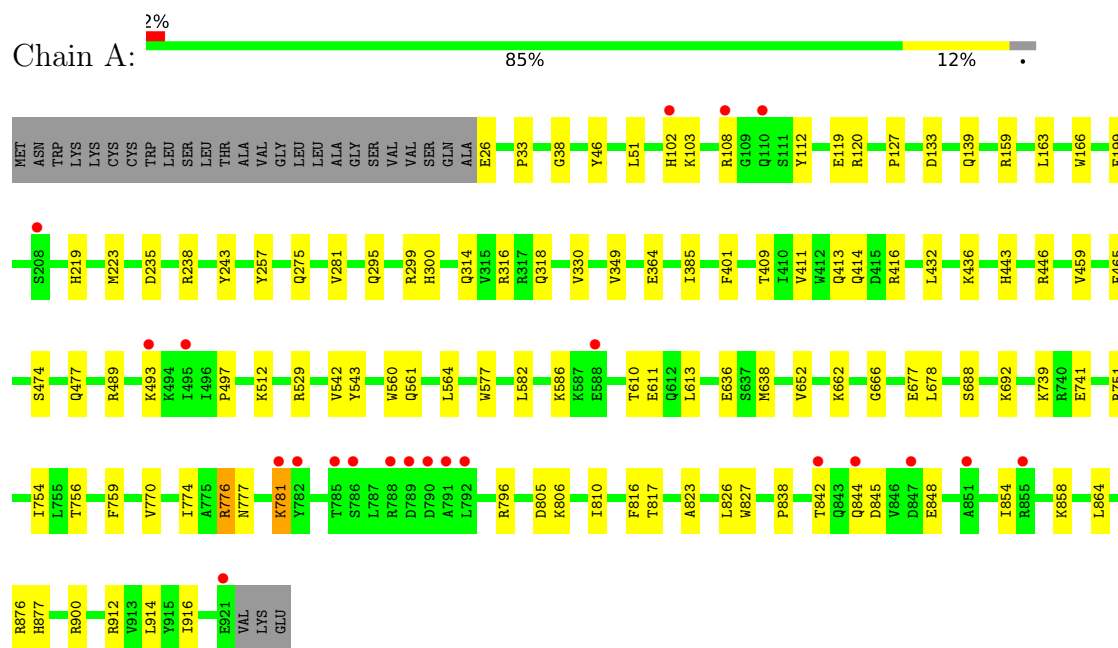
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	938	Total	O	0	0
			938	938		
4	B	16	Total	O	0	0
			16	16		
4	C	3	Total	O	0	0
			3	3		

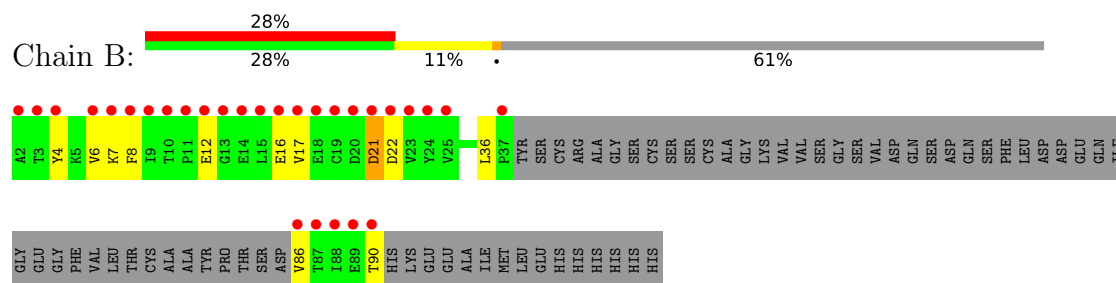
3 Residue-property plots [i](#)

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.

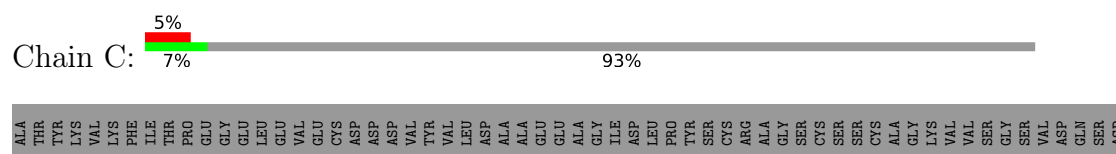
• Molecule 1: Putative zinc protease



• Molecule 2: Ferredoxin-2, chloroplastic



• Molecule 2: Ferredoxin-2, chloroplastic



GLN	SER	PHE	LEU	ASP	GLU	GLN	ILE	GLY	GLY	PHE	VAL	LEU	THR	CYS	ALA	ALA	TYR	PRO	THR	SER	D85	V86	E89	T90	H91	LYS	GLU	GLU	ALA	ILE	MET	LEU	GLU	HIS	HIS	HIS	HIS	HIS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	81.34Å 126.50Å 133.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.99 – 1.90 39.99 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.99-1.90) 99.6 (39.99-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.195 , 0.239 0.194 , 0.238	Depositor DCC
R_{free} test set	5472 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8533	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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: 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	0.40	0/7351	0.58	1/9967 (0.0%)
2	B	0.31	0/327	0.50	0/445
2	C	0.27	0/47	0.44	0/64
All	All	0.39	0/7725	0.58	1/10476 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	529	ARG	NE-CZ-NH2	-6.05	117.27	120.30

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	7203	0	7192	73	0
2	B	324	0	302	10	0
2	C	48	0	43	0	0
3	A	1	0	0	0	0
4	A	938	0	0	9	1
4	B	16	0	0	0	0
4	C	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8533	0	7537	80	1

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.

All (80) 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:512:LYS:NZ	4:A:1101:HOH:O	2.02	0.93
1:A:275:GLN:HE22	1:A:652:VAL:H	1.18	0.89
1:A:318:GLN:HE22	1:A:489:ARG:H	1.19	0.89
1:A:314:GLN:HE21	1:A:318:GLN:HE21	1.28	0.79
1:A:409:THR:HG22	1:A:413:GLN:HE21	1.47	0.78
2:B:6:VAL:HG13	2:B:86:VAL:HG13	1.73	0.71
1:A:677:GLU:OE2	4:A:1102:HOH:O	2.11	0.68
1:A:235:ASP:OD1	1:A:238:ARG:NH2	2.27	0.67
1:A:754:ILE:HB	1:A:816:PHE:HB2	1.77	0.66
1:A:842:THR:HG23	1:A:845:ASP:H	1.61	0.66
2:B:8:PHE:HZ	2:B:90:THR:HB	1.60	0.65
1:A:474:SER:HA	1:A:477:GLN:HE21	1.60	0.64
1:A:805:ASP:HB2	1:A:877:HIS:HE2	1.65	0.62
1:A:159:ARG:NH2	4:A:1114:HOH:O	2.32	0.61
2:B:4:TYR:CE1	2:B:21:ASP:OD1	2.54	0.61
1:A:754:ILE:HD11	1:A:823:ALA:HB1	1.84	0.60
1:A:281:VAL:HG13	1:A:349:VAL:HG21	1.84	0.60
1:A:662:LYS:HD2	1:A:666:GLY:O	2.02	0.59
1:A:119:GLU:OE1	4:A:1103:HOH:O	2.16	0.58
1:A:411:VAL:HG12	1:A:416:ARG:O	2.05	0.57
1:A:776:ARG:NH2	1:A:777:ASN:OD1	2.33	0.57
1:A:275:GLN:NE2	1:A:652:VAL:H	1.98	0.56
2:B:7:LYS:HZ2	2:B:16:GLU:HG2	1.70	0.56
1:A:33:PRO:HB3	1:A:51:LEU:HD23	1.88	0.55
2:B:8:PHE:CZ	2:B:90:THR:HB	2.41	0.54
1:A:26:GLU:CB	1:A:401:PHE:H	2.21	0.54
1:A:805:ASP:HB2	1:A:877:HIS:NE2	2.23	0.53
1:A:838:PRO:O	1:A:900:ARG:HD2	2.09	0.52
1:A:139:GLN:HB2	1:A:243:TYR:CE1	2.45	0.52
1:A:542[B]:VAL:HG23	1:A:610:THR:HG22	1.91	0.52
1:A:166:TRP:CZ2	1:A:199:GLU:HB2	2.45	0.51
1:A:38:GLY:HA3	1:A:46:TYR:CZ	2.46	0.51
1:A:414:GLN:OE1	1:A:416:ARG:NH1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542[B]:VAL:HG21	1:A:613:LEU:HD13	1.95	0.49
1:A:677:GLU:OE1	4:A:1104:HOH:O	2.20	0.49
1:A:446:ARG:NH1	4:A:1112:HOH:O	2.32	0.49
2:B:6:VAL:HB	2:B:17:VAL:HG13	1.94	0.48
1:A:385:ILE:HG22	1:A:432:LEU:HD11	1.95	0.48
1:A:638[B]:MET:HE3	1:A:678:LEU:HD11	1.95	0.48
1:A:842:THR:HG22	1:A:845:ASP:OD2	2.12	0.48
2:B:4:TYR:CZ	2:B:21:ASP:OD1	2.66	0.48
1:A:759:PHE:HA	1:A:810:ILE:O	2.14	0.48
1:A:330:VAL:HG11	2:B:12:GLU:OE1	2.13	0.48
1:A:854:ILE:O	1:A:858:LYS:HG3	2.14	0.48
1:A:127:PRO:HB2	1:A:133:ASP:HB2	1.95	0.47
1:A:805:ASP:O	1:A:877:HIS:HE1	1.98	0.47
1:A:816:PHE:CE2	1:A:826:LEU:HB3	2.51	0.46
1:A:497:PRO:HB2	1:A:577:TRP:CE2	2.51	0.46
1:A:314:GLN:HE21	1:A:318:GLN:NE2	2.04	0.45
1:A:796:ARG:NH1	2:B:22:ASP:HB3	2.31	0.45
1:A:805:ASP:OD2	1:A:876:ARG:HD2	2.17	0.45
1:A:300:HIS:CE1	1:A:443:HIS:HE1	2.36	0.44
1:A:611:GLU:OE1	4:A:1105:HOH:O	2.21	0.44
1:A:459:VAL:HG21	1:A:465:PHE:CD1	2.53	0.44
1:A:582:LEU:HD11	1:A:586:LYS:HE3	2.00	0.44
1:A:739:LYS:HA	1:A:912:ARG:O	2.18	0.44
1:A:806:LYS:HG2	1:A:876:ARG:HD3	2.00	0.43
1:A:754:ILE:HD12	1:A:916:ILE:HG12	2.00	0.43
1:A:796:ARG:NH1	2:B:22:ASP:CG	2.71	0.43
1:A:816:PHE:CD2	1:A:826:LEU:HD13	2.55	0.42
1:A:295:GLN:OE1	1:A:299:ARG:NH1	2.53	0.42
1:A:781:LYS:HD2	1:A:781:LYS:C	2.39	0.42
1:A:108:ARG:HD3	1:A:112:TYR:CE2	2.54	0.42
1:A:102[A]:HIS:NE2	1:A:112:TYR:OH	2.53	0.42
1:A:844:GLN:O	1:A:848:GLU:HG3	2.19	0.42
1:A:636:GLU:HG2	4:A:1592:HOH:O	2.19	0.41
1:A:770:VAL:O	1:A:774:ILE:HG12	2.20	0.41
1:A:741:GLU:HA	1:A:914:LEU:O	2.21	0.41
1:A:543:TYR:CE1	1:A:864:LEU:HD21	2.56	0.41
1:A:219:HIS:O	1:A:223:MET:HG3	2.21	0.41
1:A:688:SER:O	1:A:692:LYS:HG3	2.21	0.41
1:A:805:ASP:CB	1:A:877:HIS:HE2	2.32	0.41
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.95	0.41
1:A:756:THR:HG21	1:A:827:TRP:CH2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:751:ARG:HD2	1:A:817:THR:HG23	2.03	0.40
1:A:316:ARG:NH2	4:A:1161:HOH:O	2.54	0.40
1:A:436:LYS:HB2	1:A:436:LYS:HE2	1.93	0.40
1:A:493:LYS:HD3	1:A:493:LYS:HA	1.87	0.40
1:A:564:LEU:HD21	1:A:638[B]:MET:HE1	2.02	0.40
1:A:560:TRP:CE2	1:A:561:GLN:HG3	2.57	0.40

All (1) 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)
4:A:1126:HOH:O	4:A:1771:HOH:O[2_565]	2.04	0.16

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	906/924 (98%)	896 (99%)	10 (1%)	0	100	100
2	B	38/104 (36%)	35 (92%)	2 (5%)	1 (3%)	6	1
2	C	5/104 (5%)	5 (100%)	0	0	100	100
All	All	949/1132 (84%)	936 (99%)	12 (1%)	1 (0%)	53	44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	36	LEU

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	776/788 (98%)	769 (99%)	7 (1%)	81	81
2	B	36/88 (41%)	35 (97%)	1 (3%)	47	39
2	C	5/88 (6%)	5 (100%)	0	100	100
All	All	817/964 (85%)	809 (99%)	8 (1%)	81	78

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	LYS
1	A	120[A]	ARG
1	A	120[B]	ARG
1	A	257	TYR
1	A	364	GLU
1	A	776	ARG
1	A	781	LYS
2	B	21	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104	GLN
1	A	275	GLN
1	A	318	GLN
1	A	477	GLN
1	A	523	GLN
1	A	601	GLN
1	A	710	GLN

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 [i](#)

Of 1 ligands modelled in this entry, 1 is 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	896/924 (96%)	0.11	22 (2%) 57 61	18, 32, 59, 89	1 (0%)
2	B	41/104 (39%)	3.25	29 (70%) 0 0	29, 92, 136, 140	0
2	C	7/104 (6%)	2.90	5 (71%) 0 0	51, 74, 93, 95	0
All	All	944/1132 (83%)	0.26	56 (5%) 22 25	18, 33, 68, 140	1 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	ILE	8.6
2	B	8	PHE	8.2
2	B	86	VAL	8.0
2	B	87	THR	7.6
2	B	89	GLU	7.1
2	B	9	ILE	6.9
2	B	4	TYR	6.1
2	B	24	TYR	5.8
2	B	37	PRO	4.9
2	C	90	THR	4.7
2	B	2	ALA	4.7
2	B	90	THR	4.5
1	A	855	ARG	4.4
2	B	10	THR	4.4
1	A	788	ARG	4.4
2	B	22	ASP	4.2
2	C	85	ASP	4.1
2	B	3	THR	4.0
1	A	208	SER	4.0
2	B	11	PRO	3.9
2	B	18	GLU	3.9
1	A	791	ALA	3.8
2	C	91	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	13	GLY	3.7
2	B	6	VAL	3.6
2	B	25	VAL	3.6
2	B	17	VAL	3.6
1	A	790	ASP	3.5
2	B	21	ASP	3.4
2	B	14	GLU	3.2
1	A	789	ASP	3.2
2	B	20	ASP	3.2
1	A	782	TYR	3.1
1	A	921	GLU	3.1
2	B	23	VAL	3.1
1	A	495	ILE	3.0
1	A	588	GLU	2.9
1	A	844	GLN	2.9
2	B	12	GLU	2.8
2	B	15	LEU	2.8
2	C	89	GLU	2.8
1	A	108	ARG	2.8
2	B	16	GLU	2.8
1	A	110	GLN	2.7
1	A	493	LYS	2.6
1	A	842	THR	2.5
1	A	786	SER	2.4
2	B	7	LYS	2.4
1	A	781	LYS	2.4
2	B	19	CYS	2.4
1	A	785	THR	2.3
1	A	792	LEU	2.3
1	A	851	ALA	2.2
1	A	102[A]	HIS	2.1
1	A	847	ASP	2.1
2	C	86	VAL	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 carbohydrates 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(\AA^2)	Q<0.9
3	ZN	A	1001	1/1	0.99	0.06	37,37,37,37	0

6.5 Other polymers

There are no such residues in this entry.