



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:31 am GMT

PDB ID : 1XFO
Title : Crystal Structure of an archaeal aminopeptidase
Authors : Russo, S.; Baumann, U.
Deposited on : 2004-09-15
Resolution : 1.96 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
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

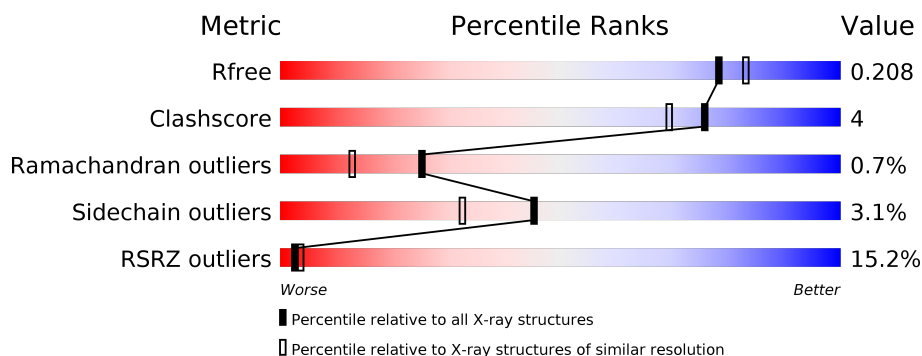
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2004 (1.96-1.96)
Clashscore	112137	2136 (1.96-1.96)
Ramachandran outliers	110173	2117 (1.96-1.96)
Sidechain outliers	110143	2117 (1.96-1.96)
RSRZ outliers	101464	2018 (1.96-1.96)

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	357	<div> <div>13%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	357	<div> <div>14%</div> <div> <div></div> <div>85%</div> <div>9%</div> <div>6%</div> </div> </div>
1	C	357	<div> <div>18%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	D	357	<div> <div>12%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ZN	A	382	-	-	-	X
2	ZN	B	354	-	-	-	X
2	ZN	C	354	-	-	-	X
2	ZN	C	355	-	-	-	X
2	ZN	D	355	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11167 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 Frv operon protein FrvX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	346	Total	C	N	O	S	0	0	0
			2684	1716	458	501	9			
1	B	337	Total	C	N	O	S	0	0	0
			2610	1674	440	488	8			
1	C	337	Total	C	N	O	S	0	0	0
			2610	1674	440	488	8			
1	D	337	Total	C	N	O	S	0	0	0
			2610	1674	440	488	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ARG	-	EXPRESSION TAG	UNP O59196
A	-2	GLY	-	EXPRESSION TAG	UNP O59196
A	-1	SER	-	EXPRESSION TAG	UNP O59196
A	0	HIS	-	EXPRESSION TAG	UNP O59196
B	-3	ARG	-	EXPRESSION TAG	UNP O59196
B	-2	GLY	-	EXPRESSION TAG	UNP O59196
B	-1	SER	-	EXPRESSION TAG	UNP O59196
B	0	HIS	-	EXPRESSION TAG	UNP O59196
C	-3	ARG	-	EXPRESSION TAG	UNP O59196
C	-2	GLY	-	EXPRESSION TAG	UNP O59196
C	-1	SER	-	EXPRESSION TAG	UNP O59196
C	0	HIS	-	EXPRESSION TAG	UNP O59196
D	-3	ARG	-	EXPRESSION TAG	UNP O59196
D	-2	GLY	-	EXPRESSION TAG	UNP O59196
D	-1	SER	-	EXPRESSION TAG	UNP O59196
D	0	HIS	-	EXPRESSION TAG	UNP O59196

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

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

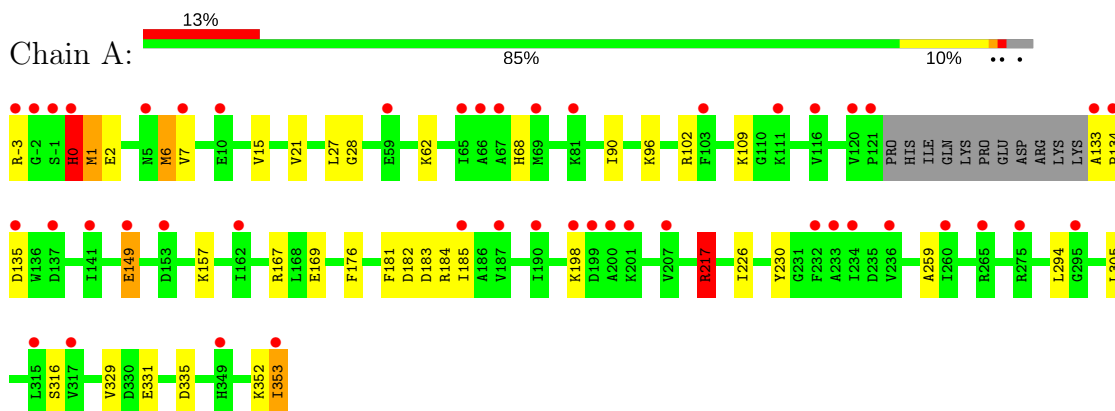
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	179	Total 179	O 179	0	0
3	B	140	Total 140	O 140	0	0
3	C	133	Total 133	O 133	0	0
3	D	193	Total 193	O 193	0	0

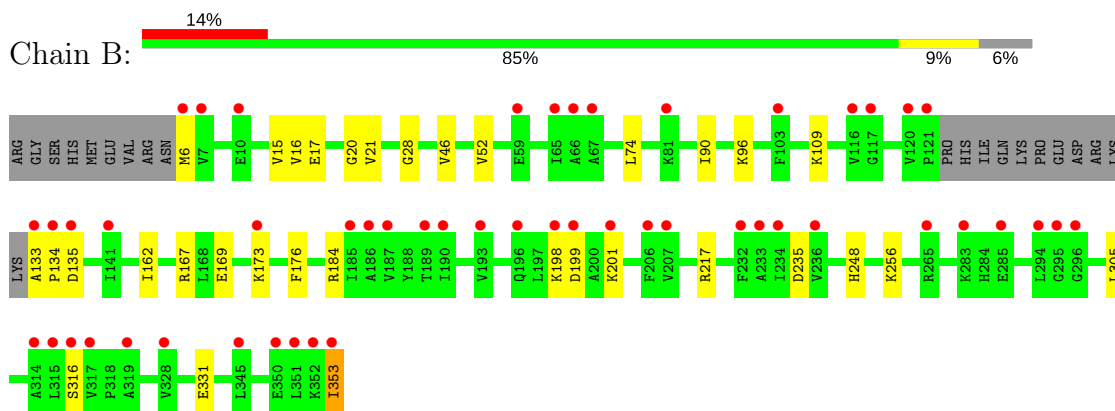
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

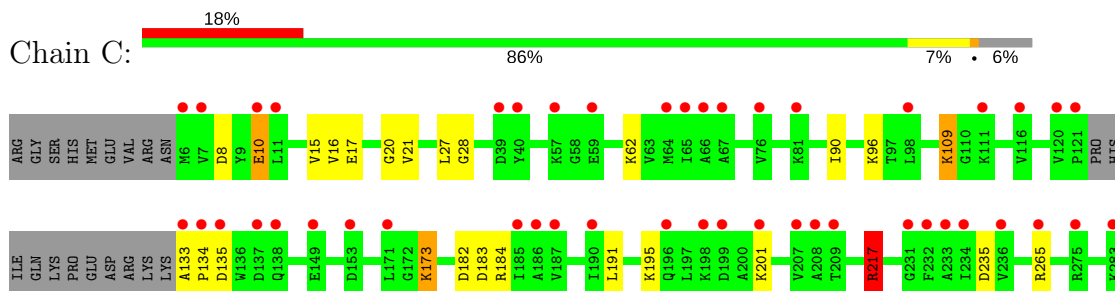
- Molecule 1: Frv operon protein FrvX

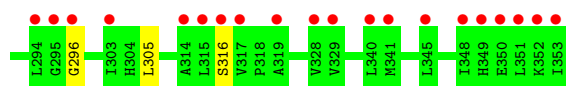


- Molecule 1: Frv operon protein FrvX

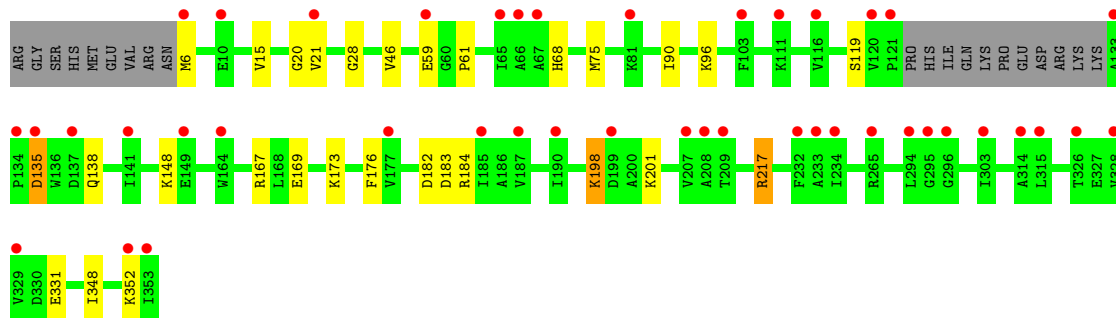
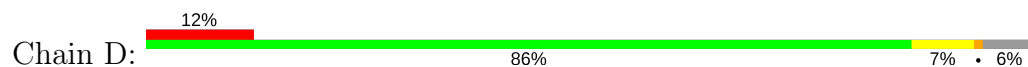


- Molecule 1: Frv operon protein FrvX





● Molecule 1: Frv operon protein FrvX



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	158.34Å 158.34Å 114.46Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.92 – 1.96 29.92 – 1.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.92-1.96) 94.3 (29.92-1.96)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.96Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.183 , 0.209 0.183 , 0.208	Depositor DCC
R_{free} test set	2423 reflections (2.25%)	DCC
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.028 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11167	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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	0.45	0/2734	0.68	2/3697 (0.1%)
1	B	0.41	0/2659	0.56	0/3598
1	C	0.42	0/2659	0.57	2/3598 (0.1%)
1	D	0.47	0/2659	0.61	1/3598 (0.0%)
All	All	0.44	0/10711	0.61	5/14491 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	ILE	CA-C-O	19.59	161.24	120.10
1	C	217	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	A	217	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	217	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	C	217	ARG	NE-CZ-NH2	-5.19	117.71	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	2684	0	2730	29	0
1	B	2610	0	2656	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2610	0	2656	16	0
1	D	2610	0	2656	16	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	179	0	0	5	0
3	B	140	0	0	1	0
3	C	133	0	0	2	0
3	D	193	0	0	4	0
All	All	11167	0	10698	76	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 (76) 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:D:46:VAL:HB	3:D:532:HOH:O	1.50	1.08
1:A:21:VAL:HG11	1:A:90:ILE:CD1	2.15	0.77
1:A:167:ARG:NE	1:A:169:GLU:OE2	2.24	0.67
1:A:21:VAL:HG11	1:A:90:ILE:HD13	1.75	0.67
1:B:21:VAL:HG11	1:B:90:ILE:CD1	2.25	0.65
1:C:173:LYS:HE3	1:C:173:LYS:HA	1.80	0.64
1:A:21:VAL:CG1	1:A:90:ILE:HD13	2.29	0.63
1:D:15:VAL:HG12	1:D:184:ARG:HB3	1.81	0.62
1:A:21:VAL:HG11	1:A:90:ILE:HD12	1.80	0.62
1:C:21:VAL:HG11	1:C:90:ILE:HD12	1.82	0.62
1:C:21:VAL:HG12	1:C:90:ILE:HG21	1.81	0.61
1:D:135:ASP:HB2	3:D:546:HOH:O	2.00	0.61
1:A:217:ARG:HB3	1:B:305:LEU:HD21	1.82	0.60
1:A:176:PHE:HE2	1:A:331:GLU:HB3	1.66	0.60
1:D:6:MET:N	3:D:417:HOH:O	2.35	0.59
1:D:21:VAL:HG11	1:D:90:ILE:CD1	2.34	0.58
1:D:148:LYS:HE3	3:D:485:HOH:O	2.04	0.58
1:C:27:LEU:HA	1:C:109:LYS:HD2	1.85	0.57
1:B:21:VAL:HG11	1:B:90:ILE:HD12	1.86	0.57
1:C:133:ALA:N	1:C:134:PRO:CD	2.68	0.56
1:A:157:LYS:HD3	3:A:549:HOH:O	2.05	0.56
1:B:21:VAL:HG11	1:B:90:ILE:HD13	1.88	0.55
1:D:21:VAL:HG11	1:D:90:ILE:HD12	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-3:ARG:HB3	1:A:2:GLU:O	2.07	0.55
1:B:176:PHE:HE2	1:B:331:GLU:HB3	1.72	0.54
1:C:15:VAL:HG12	1:C:184:ARG:HB3	1.90	0.53
1:B:15:VAL:HG12	1:B:184:ARG:HB3	1.90	0.52
1:C:191:LEU:O	1:C:195:LYS:HG3	2.10	0.51
1:B:167:ARG:NE	1:B:169:GLU:OE2	2.40	0.51
1:B:217:ARG:HB3	1:C:305:LEU:HD21	1.93	0.50
1:A:305:LEU:HD21	1:C:217:ARG:HB3	1.94	0.50
1:A:133:ALA:N	1:A:134:PRO:HD2	2.27	0.50
1:D:176:PHE:HE2	1:D:331:GLU:HB3	1.77	0.50
1:A:15:VAL:HG12	1:A:184:ARG:HB3	1.95	0.49
1:A:68:HIS:NE2	1:A:183:ASP:HB2	2.28	0.48
1:A:7:VAL:HG21	1:A:176:PHE:CZ	2.49	0.47
1:A:6:MET:HG3	1:A:335:ASP:HB2	1.94	0.47
1:B:217:ARG:HD3	3:B:438:HOH:O	2.14	0.47
1:A:217:ARG:HD3	3:A:449:HOH:O	2.14	0.47
1:A:21:VAL:CG1	1:A:90:ILE:CD1	2.89	0.47
1:B:21:VAL:CG1	1:B:90:ILE:HD13	2.43	0.47
1:B:133:ALA:N	1:B:134:PRO:CD	2.78	0.46
1:A:259:ALA:HB3	1:A:316:SER:HB2	1.97	0.46
1:C:8:ASP:OD1	1:C:10:GLU:HG3	2.16	0.46
1:A:0:HIS:CD2	1:A:0:HIS:O	2.70	0.45
1:A:230:TYR:HE1	1:A:353:ILE:HD12	1.81	0.45
1:D:198:LYS:HD3	1:D:198:LYS:N	2.32	0.45
1:C:182:ASP:HA	1:C:183:ASP:HA	1.81	0.44
1:D:75:MET:HB2	1:D:90:ILE:HD11	1.99	0.44
1:B:16:VAL:HG23	1:B:17:GLU:HG3	1.99	0.44
3:A:532:HOH:O	1:B:248:HIS:HE1	2.00	0.44
1:A:133:ALA:N	1:A:134:PRO:CD	2.82	0.43
1:C:265:ARG:HD2	1:C:265:ARG:HA	1.87	0.43
1:D:182:ASP:HA	1:D:183:ASP:HA	1.82	0.43
1:A:0:HIS:O	1:A:1:MET:O	2.36	0.42
1:C:217:ARG:HD3	3:C:428:HOH:O	2.18	0.42
1:D:68:HIS:NE2	1:D:183:ASP:HB2	2.33	0.42
1:A:102:ARG:HD3	3:A:435:HOH:O	2.19	0.42
1:A:182:ASP:HA	1:A:183:ASP:HA	1.79	0.42
1:C:133:ALA:N	1:C:134:PRO:HD2	2.34	0.42
1:D:167:ARG:NE	1:D:169:GLU:OE2	2.36	0.42
1:A:294:LEU:HD21	3:C:482:HOH:O	2.18	0.41
1:C:235:ASP:O	1:C:316:SER:HA	2.20	0.41
1:B:235:ASP:O	1:B:316:SER:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:LEU:HA	1:A:109:LYS:HD3	2.02	0.41
1:A:181:PHE:O	1:A:185:ILE:HG22	2.21	0.41
1:B:46:VAL:HG12	1:B:52:VAL:HG22	2.01	0.41
1:B:353:ILE:H	1:B:353:ILE:HD12	1.86	0.41
1:C:16:VAL:HG23	1:C:17:GLU:HG3	2.03	0.41
1:D:61:PRO:HG2	1:D:348:ILE:HG23	2.03	0.41
1:A:149:GLU:HB3	3:A:482:HOH:O	2.19	0.40
1:B:256:LYS:HD3	1:B:256:LYS:HA	1.90	0.40
1:D:119:SER:HA	1:D:138:GLN:O	2.21	0.40
1:A:62:LYS:HE3	1:A:226:ILE:O	2.21	0.40
1:B:74:LEU:HB2	1:B:162:ILE:HB	2.04	0.40
1:D:21:VAL:HG11	1:D:90:ILE:HD13	2.02	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	342/357 (96%)	329 (96%)	10 (3%)	3 (1%)	20	9
1	B	333/357 (93%)	326 (98%)	5 (2%)	2 (1%)	28	15
1	C	333/357 (93%)	322 (97%)	8 (2%)	3 (1%)	20	9
1	D	333/357 (93%)	325 (98%)	6 (2%)	2 (1%)	28	15
All	All	1341/1428 (94%)	1302 (97%)	29 (2%)	10 (1%)	25	13

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	B	28	GLY
1	A	28	GLY

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Mol	Chain	Res	Type
1	D	28	GLY
1	A	0	HIS
1	C	28	GLY
1	C	296	GLY
1	C	20	GLY
1	D	20	GLY
1	B	20	GLY

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	284/295 (96%)	275 (97%)	9 (3%)	44	31
1	B	276/295 (94%)	267 (97%)	9 (3%)	43	30
1	C	276/295 (94%)	268 (97%)	8 (3%)	48	35
1	D	276/295 (94%)	268 (97%)	8 (3%)	48	35
All	All	1112/1180 (94%)	1078 (97%)	34 (3%)	45	32

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	6	MET
1	A	96	LYS
1	A	135	ASP
1	A	149	GLU
1	A	198	LYS
1	A	217	ARG
1	A	329	VAL
1	A	352	LYS
1	B	6	MET
1	B	96	LYS
1	B	109	LYS
1	B	135	ASP
1	B	173	LYS

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Mol	Chain	Res	Type
1	B	198	LYS
1	B	199	ASP
1	B	201	LYS
1	B	353	ILE
1	C	10	GLU
1	C	62	LYS
1	C	96	LYS
1	C	109	LYS
1	C	135	ASP
1	C	173	LYS
1	C	201	LYS
1	C	217	ARG
1	D	59	GLU
1	D	96	LYS
1	D	135	ASP
1	D	173	LYS
1	D	198	LYS
1	D	201	LYS
1	D	217	ARG
1	D	352	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	82	ASN
1	B	349	HIS
1	D	349	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	346/357 (96%)	0.88	46 (13%) 4 6	32, 37, 45, 61	0
1	B	337/357 (94%)	0.93	51 (15%) 3 4	32, 37, 43, 51	0
1	C	337/357 (94%)	1.07	66 (19%) 1 1	32, 37, 44, 52	0
1	D	337/357 (94%)	0.83	43 (12%) 4 7	32, 37, 44, 52	0
All	All	1357/1428 (95%)	0.93	206 (15%) 2 4	32, 37, 44, 61	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	353	ILE	9.2
1	C	121	PRO	8.6
1	C	353	ILE	8.2
1	A	121	PRO	7.8
1	D	353	ILE	7.2
1	C	133	ALA	6.9
1	B	121	PRO	6.7
1	C	120	VAL	6.6
1	D	121	PRO	6.5
1	C	6	MET	6.2
1	B	6	MET	6.2
1	C	66	ALA	5.6
1	A	353	ILE	5.6
1	B	352	LYS	5.6
1	A	198	LYS	5.6
1	C	352	LYS	5.5
1	C	234	ILE	5.3
1	C	233	ALA	5.3
1	A	120	VAL	5.1
1	B	65	ILE	5.0
1	A	0	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	232	PHE	4.9
1	A	59	GLU	4.8
1	A	5	ASN	4.8
1	A	133	ALA	4.7
1	C	65	ILE	4.6
1	B	234	ILE	4.5
1	C	294	LEU	4.4
1	A	199	ASP	4.4
1	C	67	ALA	4.3
1	D	133	ALA	4.3
1	A	-1	SER	4.1
1	D	352	LYS	4.0
1	B	207	VAL	4.0
1	A	65	ILE	3.9
1	A	234	ILE	3.9
1	B	59	GLU	3.9
1	A	134	PRO	3.8
1	B	66	ALA	3.8
1	A	-2	GLY	3.8
1	C	199	ASP	3.8
1	B	187	VAL	3.8
1	D	234	ILE	3.8
1	B	315	LEU	3.8
1	A	162	ILE	3.7
1	B	198	LYS	3.7
1	C	190	ILE	3.7
1	B	120	VAL	3.7
1	B	196	GLN	3.7
1	D	120	VAL	3.6
1	C	134	PRO	3.6
1	C	59	GLU	3.6
1	A	67	ALA	3.6
1	D	296	GLY	3.5
1	C	341	MET	3.5
1	C	207	VAL	3.5
1	B	190	ILE	3.5
1	C	198	LYS	3.5
1	C	315	LEU	3.5
1	D	67	ALA	3.4
1	B	67	ALA	3.3
1	C	7	VAL	3.3
1	A	10	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	201	LYS	3.3
1	D	295	GLY	3.3
1	B	199	ASP	3.2
1	D	328	VAL	3.2
1	D	6	MET	3.2
1	A	200	ALA	3.2
1	B	233	ALA	3.2
1	C	111	LYS	3.2
1	C	265	ARG	3.1
1	B	232	PHE	3.1
1	B	201	LYS	3.1
1	D	199	ASP	3.1
1	D	10	GLU	3.1
1	A	7	VAL	3.1
1	D	294	LEU	3.1
1	C	350	GLU	3.0
1	C	349	HIS	3.0
1	B	116	VAL	3.0
1	D	233	ALA	3.0
1	A	149	GLU	3.0
1	C	149	GLU	3.0
1	B	186	ALA	3.0
1	C	116	VAL	3.0
1	A	66	ALA	2.9
1	D	59	GLU	2.9
1	A	233	ALA	2.9
1	A	153	ASP	2.9
1	C	351	LEU	2.9
1	D	190	ILE	2.9
1	D	208	ALA	2.9
1	C	328	VAL	2.9
1	A	349	HIS	2.9
1	B	185	ILE	2.9
1	B	133	ALA	2.9
1	B	351	LEU	2.8
1	A	190	ILE	2.8
1	D	232	PHE	2.8
1	A	116	VAL	2.8
1	C	11	LEU	2.8
1	B	317	VAL	2.8
1	D	66	ALA	2.8
1	C	10	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	328	VAL	2.8
1	A	265	ARG	2.8
1	A	187	VAL	2.8
1	C	196	GLN	2.7
1	C	348	ILE	2.7
1	B	236	VAL	2.7
1	B	7	VAL	2.7
1	B	350	GLU	2.7
1	C	209	THR	2.7
1	D	81	LYS	2.6
1	D	141	ILE	2.6
1	D	185	ILE	2.6
1	D	329	VAL	2.6
1	B	314	ALA	2.6
1	D	135	ASP	2.6
1	C	138	GLN	2.6
1	B	193	VAL	2.6
1	B	283	LYS	2.6
1	B	117	GLY	2.6
1	B	134	PRO	2.6
1	B	294	LEU	2.6
1	C	319	ALA	2.6
1	A	185	ILE	2.6
1	B	295	GLY	2.6
1	B	135	ASP	2.5
1	A	236	VAL	2.5
1	D	207	VAL	2.5
1	B	10	GLU	2.5
1	A	111	LYS	2.5
1	A	135	ASP	2.5
1	C	329	VAL	2.5
1	D	116	VAL	2.5
1	A	141	ILE	2.4
1	B	345	LEU	2.4
1	C	340	LEU	2.4
1	B	141	ILE	2.4
1	D	265	ARG	2.4
1	C	345	LEU	2.4
1	C	296	GLY	2.4
1	C	186	ALA	2.4
1	C	135	ASP	2.4
1	B	296	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	64	MET	2.4
1	C	185	ILE	2.4
1	A	207	VAL	2.4
1	A	137	ASP	2.3
1	A	-3	ARG	2.3
1	D	314	ALA	2.3
1	B	189	THR	2.3
1	A	260	ILE	2.3
1	C	98	LEU	2.3
1	C	81	LYS	2.3
1	D	149	GLU	2.3
1	A	315	LEU	2.3
1	C	39	ASP	2.3
1	C	40	TYR	2.3
1	C	231	GLY	2.3
1	C	317	VAL	2.3
1	D	177	VAL	2.3
1	B	206	PHE	2.3
1	C	57	LYS	2.3
1	C	137	ASP	2.3
1	C	187	VAL	2.3
1	C	236	VAL	2.3
1	C	314	ALA	2.3
1	A	317	VAL	2.2
1	B	173	LYS	2.2
1	D	21	VAL	2.2
1	B	316	SER	2.2
1	D	303	ILE	2.2
1	C	295	GLY	2.2
1	D	111	LYS	2.2
1	B	285	GLU	2.2
1	B	319	ALA	2.2
1	C	275	ARG	2.2
1	D	103	PHE	2.2
1	C	153	ASP	2.2
1	A	103	PHE	2.2
1	D	134	PRO	2.1
1	D	209	THR	2.1
1	C	208	ALA	2.1
1	C	283	LYS	2.1
1	A	232	PHE	2.1
1	B	81	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	171	LEU	2.1
1	B	265	ARG	2.1
1	C	316	SER	2.1
1	C	76	VAL	2.1
1	D	187	VAL	2.1
1	D	326	THR	2.1
1	A	275	ARG	2.1
1	D	315	LEU	2.1
1	A	69	MET	2.1
1	B	103	PHE	2.1
1	D	65	ILE	2.1
1	C	201	LYS	2.1
1	D	164	TRP	2.0
1	D	137	ASP	2.0
1	A	295	GLY	2.0
1	C	303	ILE	2.0
1	A	81	LYS	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(Å ²)	Q<0.9
2	ZN	C	355	1/1	0.99	0.40	20.18	69,69,69,69	0
2	ZN	A	382	1/1	0.97	0.39	9.95	61,61,61,61	0
2	ZN	B	354	1/1	0.97	0.39	9.78	66,66,66,66	0
2	ZN	D	355	1/1	0.98	0.31	5.13	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	ZN	C	354	1/1	0.99	0.22	2.23	41,41,41,41	0
2	ZN	D	354	1/1	0.99	0.18	1.10	34,34,34,34	0
2	ZN	A	354	1/1	0.99	0.18	1.09	39,39,39,39	0
2	ZN	B	371	1/1	0.99	0.19	0.87	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.