



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:30 PM UTC

PDB ID : 2FZV / pdb_00002fzv
Title : Crystal Structure of an apo form of a Flavin-binding Protein from *Shigella flexneri*
Authors : Vorontsov, I.I.; Minasov, G.; Brunzelle, J.S.; Shuvalova, L.; Collart, F.R.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-02-10
Resolution : 1.70 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

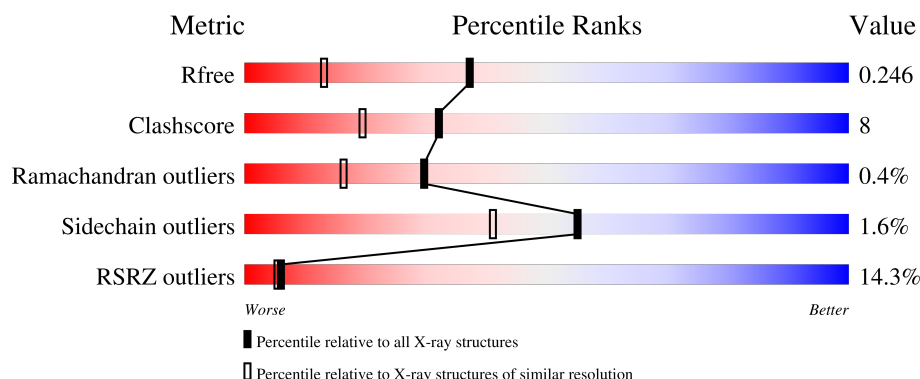
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	279	5% 73% 10% • 16%
1	B	279	14% 75% 14% 11%
1	C	279	10% 74% 10% • 15%
1	D	279	20% 70% 14% • 15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9117 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 arsenical resistance protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	19	0
			2009	1255	375	370	9			
1	B	247	Total	C	N	O	S	0	19	0
			2090	1307	383	391	9			
1	C	236	Total	C	N	O	S	0	12	0
			1977	1242	368	359	8			
1	D	236	Total	C	N	O	S	0	6	0
			1909	1197	351	353	8			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	GB 30042143
A	-22	HIS	-	expression tag	GB 30042143
A	-21	HIS	-	expression tag	GB 30042143
A	-20	HIS	-	expression tag	GB 30042143
A	-19	HIS	-	expression tag	GB 30042143
A	-18	HIS	-	expression tag	GB 30042143
A	-17	HIS	-	expression tag	GB 30042143
A	-16	SER	-	cloning artifact	GB 30042143
A	-15	SER	-	cloning artifact	GB 30042143
A	-14	GLY	-	cloning artifact	GB 30042143
A	-13	VAL	-	cloning artifact	GB 30042143
A	-12	ASP	-	cloning artifact	GB 30042143
A	-11	LEU	-	cloning artifact	GB 30042143
A	-10	GLY	-	cloning artifact	GB 30042143
A	-9	THR	-	cloning artifact	GB 30042143
A	-8	GLU	-	cloning artifact	GB 30042143
A	-7	ASN	-	cloning artifact	GB 30042143
A	-6	LEU	-	cloning artifact	GB 30042143
A	-5	TYR	-	cloning artifact	GB 30042143
A	-4	PHE	-	cloning artifact	GB 30042143
A	-3	GLN	-	cloning artifact	GB 30042143

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	cloning artifact	GB 30042143
A	-1	ASN	-	cloning artifact	GB 30042143
A	0	ALA	-	cloning artifact	GB 30042143
B	-23	MET	-	initiating methionine	GB 30042143
B	-22	HIS	-	expression tag	GB 30042143
B	-21	HIS	-	expression tag	GB 30042143
B	-20	HIS	-	expression tag	GB 30042143
B	-19	HIS	-	expression tag	GB 30042143
B	-18	HIS	-	expression tag	GB 30042143
B	-17	HIS	-	expression tag	GB 30042143
B	-16	SER	-	cloning artifact	GB 30042143
B	-15	SER	-	cloning artifact	GB 30042143
B	-14	GLY	-	cloning artifact	GB 30042143
B	-13	VAL	-	cloning artifact	GB 30042143
B	-12	ASP	-	cloning artifact	GB 30042143
B	-11	LEU	-	cloning artifact	GB 30042143
B	-10	GLY	-	cloning artifact	GB 30042143
B	-9	THR	-	cloning artifact	GB 30042143
B	-8	GLU	-	cloning artifact	GB 30042143
B	-7	ASN	-	cloning artifact	GB 30042143
B	-6	LEU	-	cloning artifact	GB 30042143
B	-5	TYR	-	cloning artifact	GB 30042143
B	-4	PHE	-	cloning artifact	GB 30042143
B	-3	GLN	-	cloning artifact	GB 30042143
B	-2	SER	-	cloning artifact	GB 30042143
B	-1	ASN	-	cloning artifact	GB 30042143
B	0	ALA	-	cloning artifact	GB 30042143
C	-23	MET	-	initiating methionine	GB 30042143
C	-22	HIS	-	expression tag	GB 30042143
C	-21	HIS	-	expression tag	GB 30042143
C	-20	HIS	-	expression tag	GB 30042143
C	-19	HIS	-	expression tag	GB 30042143
C	-18	HIS	-	expression tag	GB 30042143
C	-17	HIS	-	expression tag	GB 30042143
C	-16	SER	-	cloning artifact	GB 30042143
C	-15	SER	-	cloning artifact	GB 30042143
C	-14	GLY	-	cloning artifact	GB 30042143
C	-13	VAL	-	cloning artifact	GB 30042143
C	-12	ASP	-	cloning artifact	GB 30042143
C	-11	LEU	-	cloning artifact	GB 30042143
C	-10	GLY	-	cloning artifact	GB 30042143
C	-9	THR	-	cloning artifact	GB 30042143

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLU	-	cloning artifact	GB 30042143
C	-7	ASN	-	cloning artifact	GB 30042143
C	-6	LEU	-	cloning artifact	GB 30042143
C	-5	TYR	-	cloning artifact	GB 30042143
C	-4	PHE	-	cloning artifact	GB 30042143
C	-3	GLN	-	cloning artifact	GB 30042143
C	-2	SER	-	cloning artifact	GB 30042143
C	-1	ASN	-	cloning artifact	GB 30042143
C	0	ALA	-	cloning artifact	GB 30042143
D	-23	MET	-	initiating methionine	GB 30042143
D	-22	HIS	-	expression tag	GB 30042143
D	-21	HIS	-	expression tag	GB 30042143
D	-20	HIS	-	expression tag	GB 30042143
D	-19	HIS	-	expression tag	GB 30042143
D	-18	HIS	-	expression tag	GB 30042143
D	-17	HIS	-	expression tag	GB 30042143
D	-16	SER	-	cloning artifact	GB 30042143
D	-15	SER	-	cloning artifact	GB 30042143
D	-14	GLY	-	cloning artifact	GB 30042143
D	-13	VAL	-	cloning artifact	GB 30042143
D	-12	ASP	-	cloning artifact	GB 30042143
D	-11	LEU	-	cloning artifact	GB 30042143
D	-10	GLY	-	cloning artifact	GB 30042143
D	-9	THR	-	cloning artifact	GB 30042143
D	-8	GLU	-	cloning artifact	GB 30042143
D	-7	ASN	-	cloning artifact	GB 30042143
D	-6	LEU	-	cloning artifact	GB 30042143
D	-5	TYR	-	cloning artifact	GB 30042143
D	-4	PHE	-	cloning artifact	GB 30042143
D	-3	GLN	-	cloning artifact	GB 30042143
D	-2	SER	-	cloning artifact	GB 30042143
D	-1	ASN	-	cloning artifact	GB 30042143
D	0	ALA	-	cloning artifact	GB 30042143

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	1

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

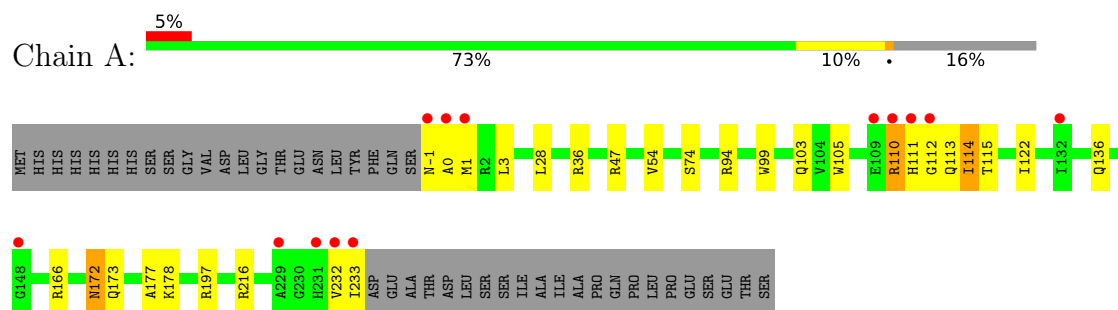
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	357	Total	O	0	16
			366	366		
4	B	285	Total	O	0	6
			288	288		
4	C	285	Total	O	0	5
			286	286		
4	D	184	Total	O	0	6
			189	189		

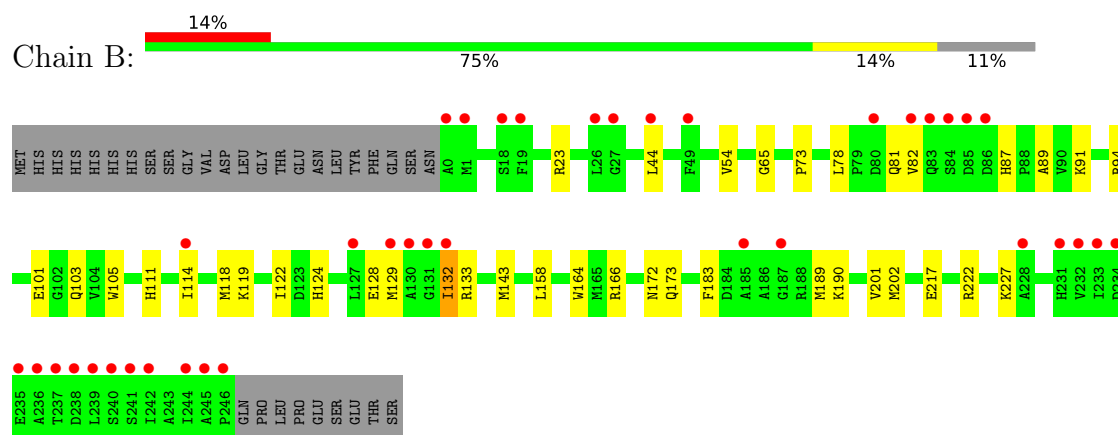
3 Residue-property plots [i](#)

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.

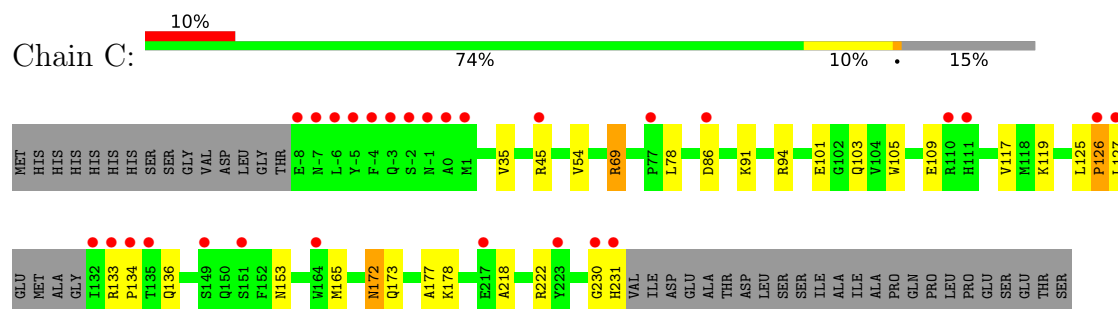
- Molecule 1: putative arsenical resistance protein



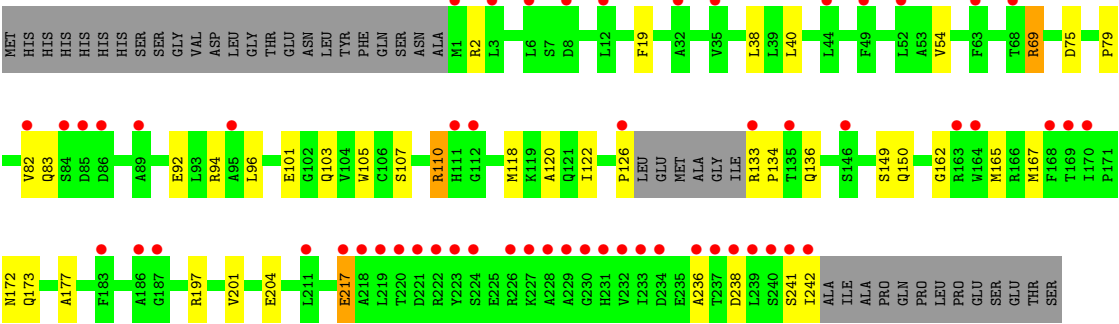
- Molecule 1: putative arsenical resistance protein



- Molecule 1: putative arsenical resistance protein



- Molecule 1: putative arsenical resistance protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	117.82Å 117.82Å 154.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 1.70 29.81 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.81-1.70) 98.3 (29.81-1.70)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.199 , 0.246 0.200 , 0.246	Depositor DCC
R_{free} test set	5843 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9117	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CL

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	0.58	0/2052	0.81	0/2774
1	B	0.52	0/2133	0.84	1/2888 (0.0%)
1	C	0.52	0/2023	0.85	1/2738 (0.0%)
1	D	0.70	2/1950 (0.1%)	0.88	1/2640 (0.0%)
All	All	0.58	2/8158 (0.0%)	0.85	3/11040 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	238	ASP	CG-OD1	18.84	1.61	1.25
1	D	238	ASP	CG-OD2	13.35	1.50	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	101	GLU	N-CA-C	-6.21	106.02	113.97
1	B	101	GLU	N-CA-C	-5.91	106.41	113.97
1	C	101	GLU	N-CA-C	-5.71	106.86	113.88

There are no chirality outliers.

There are no planarity outliers.

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	2009	0	1993	40	0
1	B	2090	0	2077	36	0
1	C	1977	0	1959	26	0
1	D	1909	0	1898	34	0
2	A	1	0	0	0	0
3	A	2	0	0	0	0
4	A	366	0	0	7	0
4	B	288	0	0	7	0
4	C	286	0	0	2	0
4	D	189	0	0	3	0
All	All	9117	0	7927	128	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 (128) 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:B:129:MET:O	1:B:132[A]:ILE:HG22	1.65	0.96
1:B:23[B]:ARG:HH21	1:B:65:GLY:HA3	1.31	0.94
1:D:133:ARG:O	1:D:136:GLN:HG3	1.74	0.88
1:C:69:ARG:HH21	1:C:69:ARG:CG	1.88	0.86
1:B:23[B]:ARG:NH2	1:B:65:GLY:HA3	1.88	0.85
1:D:2:ARG:HD2	4:D:370:HOH:O	1.76	0.83
1:D:110[B]:ARG:HG3	1:D:110[B]:ARG:HH21	1.40	0.83
1:A:110[A]:ARG:O	1:A:111[A]:HIS:CG	2.32	0.83
1:A:110[B]:ARG:HH11	1:A:110[B]:ARG:HG3	1.44	0.80
1:C:105:TRP:CH2	1:C:165:MET:HE1	2.18	0.79
1:C:69:ARG:HH21	1:C:69:ARG:HG3	1.47	0.77
1:C:105:TRP:HH2	1:C:165:MET:HE1	1.49	0.77
1:C:105:TRP:HH2	1:C:165:MET:CE	1.97	0.76
1:A:0:ALA:H	1:A:1:MET:HA	1.52	0.74
1:A:110[A]:ARG:C	1:A:111[A]:HIS:CG	2.68	0.72
1:D:92:GLU:HB2	4:D:370:HOH:O	1.89	0.71
1:D:110[A]:ARG:HH11	1:D:110[A]:ARG:HG2	1.56	0.71
1:A:0:ALA:N	1:A:1:MET:HA	2.06	0.70
1:A:114[A]:ILE:O	1:B:119[A]:LYS:NZ	2.23	0.70
1:B:94:ARG:HD2	1:B:124:HIS:O	1.92	0.70
1:A:103:GLN:HE21	1:A:105:TRP:HE1	1.39	0.69
1:D:110[A]:ARG:HH11	1:D:110[A]:ARG:CG	2.05	0.69
1:D:69:ARG:HG2	1:D:96:LEU:HD22	1.77	0.67
1:A:110[B]:ARG:HH11	1:A:110[B]:ARG:CG	2.07	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLN:HE21	1:B:105:TRP:HE1	1.43	0.67
1:D:217[A]:GLU:H	1:D:217[A]:GLU:CD	2.04	0.65
1:B:94:ARG:NH2	1:B:129:MET:SD	2.70	0.65
1:D:241:SER:HB3	1:D:242:ILE:HG13	1.77	0.65
1:C:103:GLN:HE21	1:C:105:TRP:HE1	1.43	0.64
1:B:114[B]:ILE:HD11	1:B:158:LEU:HG	1.79	0.64
1:B:82:VAL:HG22	4:B:368:HOH:O	1.98	0.63
1:C:136:GLN:HE22	1:C:222:ARG:HH22	1.47	0.62
1:D:241:SER:HB3	1:D:242:ILE:CG1	2.30	0.62
1:B:87:HIS:HD2	1:B:89:ALA:H	1.47	0.61
1:B:82:VAL:HG21	1:B:87:HIS:HB2	1.81	0.61
1:A:110[A]:ARG:C	1:A:111[A]:HIS:CD2	2.79	0.61
1:A:110[B]:ARG:HD2	4:B:533:HOH:O	2.02	0.60
1:C:69:ARG:HH21	1:C:69:ARG:HG2	1.67	0.60
1:D:110[B]:ARG:HH21	1:D:110[B]:ARG:CG	2.10	0.59
1:B:87:HIS:CD2	1:B:89:ALA:H	2.20	0.59
1:B:172:ASN:HD22	1:B:173:GLN:H	1.49	0.58
1:A:110[A]:ARG:HG3	4:A:598:HOH:O	2.03	0.58
1:A:0:ALA:H	1:A:1:MET:CA	2.17	0.58
1:D:172:ASN:HD22	1:D:173:GLN:H	1.52	0.58
1:D:105:TRP:CZ2	1:D:167:MET:HE1	2.39	0.57
1:A:103:GLN:NE2	1:A:105:TRP:HE1	2.03	0.57
1:B:103:GLN:NE2	1:B:105:TRP:HE1	2.01	0.57
1:A:1:MET:HG3	1:A:3:LEU:H	1.71	0.55
1:A:197[A]:ARG:NH2	4:A:353:HOH:O	2.40	0.55
1:D:103:GLN:HE21	1:D:105:TRP:HE1	1.55	0.55
1:A:94:ARG:NH1	4:A:550:HOH:O	2.39	0.54
1:B:166[A]:ARG:NH1	1:D:204:GLU:OE1	2.41	0.54
1:B:166[A]:ARG:HH12	1:D:172:ASN:HB2	1.72	0.54
1:B:217[B]:GLU:H	1:B:217[B]:GLU:CD	2.17	0.53
1:B:44:LEU:HD21	1:B:73:PRO:HG2	1.90	0.53
1:A:110[A]:ARG:O	1:A:111[A]:HIS:ND1	2.42	0.53
1:C:78:LEU:HD21	1:C:117[A]:VAL:HG12	1.90	0.53
1:A:36[B]:ARG:HD2	1:A:99:TRP:CE2	2.44	0.53
1:C:103:GLN:NE2	1:C:105:TRP:HE1	2.07	0.52
1:C:86:ASP:HA	1:C:91:LYS:HE3	1.92	0.52
1:A:113[B]:GLN:O	1:A:114[B]:ILE:O	2.28	0.51
1:C:136:GLN:NE2	1:C:222:ARG:HH12	2.08	0.51
1:C:230:GLY:O	1:C:231:HIS:HB2	2.10	0.51
1:C:119[B]:LYS:HE2	1:C:119[B]:LYS:HA	1.93	0.51
1:D:38:LEU:HB3	1:D:103:GLN:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ARG:CG	1:C:69:ARG:NH2	2.58	0.51
1:C:45[B]:ARG:NH2	4:C:446:HOH:O	2.44	0.51
1:A:74[B]:SER:O	1:B:81:GLN:HG3	2.11	0.51
1:D:110[A]:ARG:CG	1:D:110[A]:ARG:NH1	2.71	0.49
1:C:133:ARG:HD3	1:C:165:MET:HA	1.94	0.49
1:B:183:PHE:CE2	1:B:189:MET:HG3	2.48	0.49
1:C:172:ASN:HD22	1:C:173:GLN:H	1.61	0.49
1:A:113[B]:GLN:O	1:A:114[B]:ILE:C	2.56	0.48
1:B:166[A]:ARG:HE	1:B:222:ARG:NH1	2.11	0.48
1:B:227:LYS:HG3	1:D:19:PHE:CD2	2.48	0.48
1:D:236:ALA:HA	4:D:306:HOH:O	2.12	0.48
1:A:28:LEU:HD21	1:C:218:ALA:HB3	1.96	0.48
1:C:133:ARG:O	1:C:136:GLN:HG2	2.13	0.48
1:A:172:ASN:HD22	1:A:173:GLN:H	1.61	0.48
1:D:40:LEU:HD12	1:D:105:TRP:CD1	2.48	0.48
1:A:136:GLN:HG2	1:A:166:ARG:HB2	1.97	0.46
1:D:83:GLN:HE21	1:D:83:GLN:HA	1.80	0.46
4:A:325:HOH:O	1:B:111:HIS:HD2	1.98	0.46
1:C:69:ARG:HG3	1:C:69:ARG:NH2	2.18	0.46
1:D:105:TRP:CH2	1:D:167:MET:HE1	2.51	0.46
1:A:0:ALA:N	1:A:1:MET:CA	2.75	0.46
1:D:162:GLY:HA2	1:D:167:MET:HE3	1.98	0.46
1:A:110[B]:ARG:CG	1:A:110[B]:ARG:NH1	2.74	0.46
1:A:112[A]:GLY:O	1:A:113[A]:GLN:CD	2.58	0.46
1:B:23[B]:ARG:NH2	4:B:362:HOH:O	2.48	0.46
1:B:78:LEU:H	1:B:81:GLN:NE2	2.15	0.45
1:C:125:LEU:N	1:C:126:PRO:CD	2.78	0.45
1:B:91[B]:LYS:HD2	4:B:453:HOH:O	2.17	0.45
1:A:-1:ASN:HB3	1:A:1:MET:HA	1.97	0.45
1:D:126:PRO:HB2	1:D:134:PRO:HB2	1.98	0.45
1:B:132[A]:ILE:HG12	1:B:133:ARG:N	2.32	0.45
1:A:115:THR:HA	4:B:533:HOH:O	2.16	0.45
4:A:503:HOH:O	1:D:149:SER:HB3	2.17	0.45
1:B:201:VAL:HG12	1:B:202:MET:HE2	1.99	0.45
1:A:113[B]:GLN:C	1:A:114[B]:ILE:O	2.60	0.44
1:B:128[A]:GLU:HG2	1:B:133:ARG:HG2	1.98	0.44
1:A:110[A]:ARG:HB3	1:A:111[A]:HIS:CD2	2.52	0.44
1:C:109:GLU:CD	1:C:153:ASN:HB2	2.42	0.44
1:D:122:ILE:O	1:D:165:MET:HE1	2.18	0.44
1:D:79:PRO:HD3	1:D:120:ALA:HB2	1.99	0.44
1:D:103:GLN:NE2	1:D:105:TRP:HE1	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:150:GLN:HB2	1:D:177:ALA:HB2	2.00	0.43
1:D:241:SER:HA	1:D:242:ILE:HA	1.66	0.43
1:A:110[A]:ARG:O	1:A:111[A]:HIS:CD2	2.69	0.43
1:A:47[B]:ARG:NH2	4:A:379:HOH:O	2.51	0.43
1:B:172:ASN:HD22	1:B:173:GLN:N	2.17	0.43
1:D:197:ARG:O	1:D:201:VAL:HG23	2.20	0.42
1:A:111[A]:HIS:HA	1:B:164:TRP:CE2	2.55	0.42
1:C:94:ARG:HD3	1:C:127:LEU:HD11	2.02	0.42
1:A:232:VAL:CG1	1:A:233:ILE:HB	2.49	0.42
1:A:232:VAL:HA	1:A:233:ILE:HA	1.77	0.42
1:D:107:SER:HB2	1:D:118:MET:HG2	2.02	0.42
1:D:2:ARG:HE	1:D:75:ASP:CG	2.28	0.41
1:A:177:ALA:O	1:A:178:LYS:C	2.62	0.41
1:B:103:GLN:HE21	1:B:105:TRP:NE1	2.14	0.41
1:C:177:ALA:O	1:C:178:LYS:C	2.62	0.41
1:A:36[B]:ARG:HD2	1:A:99:TRP:NE1	2.36	0.41
1:A:216:ARG:NH1	4:A:417:HOH:O	2.54	0.41
1:B:143:MET:HE2	4:B:299:HOH:O	2.21	0.41
1:B:190:LYS:HE2	4:B:523:HOH:O	2.20	0.40
1:B:118:MET:HE2	1:B:122:ILE:HD11	2.03	0.40
1:C:134:PRO:HD2	4:C:534:HOH:O	2.21	0.40
1:A:122:ILE:O	1:B:111:HIS:HE1	2.05	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	252/279 (90%)	244 (97%)	4 (2%)	4 (2%)	7	1
1	B	264/279 (95%)	254 (96%)	10 (4%)	0	100	100
1	C	244/279 (88%)	237 (97%)	6 (2%)	1 (0%)	30	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	237/279 (85%)	229 (97%)	7 (3%)	1 (0%)	30	16
All	All	997/1116 (89%)	964 (97%)	27 (3%)	6 (1%)	30	9

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114[A]	ILE
1	A	114[B]	ILE
1	C	126	PRO
1	A	110[A]	ARG
1	A	110[B]	ARG
1	D	82	VAL

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	215/236 (91%)	213 (99%)	2 (1%)	70	62
1	B	225/236 (95%)	222 (99%)	3 (1%)	61	48
1	C	212/236 (90%)	208 (98%)	4 (2%)	50	34
1	D	205/236 (87%)	198 (97%)	7 (3%)	32	16
All	All	857/944 (91%)	841 (98%)	16 (2%)	55	34

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	172	ASN
1	B	54	VAL
1	B	132[A]	ILE
1	B	132[B]	ILE
1	C	35	VAL
1	C	54	VAL
1	C	69	ARG

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Mol	Chain	Res	Type
1	C	172	ASN
1	D	54	VAL
1	D	69	ARG
1	D	94	ARG
1	D	110[A]	ARG
1	D	110[B]	ARG
1	D	217[A]	GLU
1	D	217[B]	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	172	ASN
1	A	181	GLN
1	B	81	GLN
1	B	87	HIS
1	B	103	GLN
1	B	111	HIS
1	B	172	ASN
1	B	181	GLN
1	C	-3	GLN
1	C	83	GLN
1	C	103	GLN
1	C	136	GLN
1	C	150	GLN
1	C	172	ASN
1	C	181	GLN
1	D	62	GLN
1	D	83	GLN
1	D	103	GLN
1	D	111	HIS
1	D	113	GLN
1	D	172	ASN
1	D	181	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 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	235/279 (84%)	0.49	13 (5%) 30 34	8, 19, 33, 49	19 (8%)
1	B	247/279 (88%)	1.07	38 (15%) 5 4	8, 20, 41, 49	19 (7%)
1	C	236/279 (84%)	0.99	28 (11%) 9 8	8, 20, 36, 55	12 (5%)
1	D	236/279 (84%)	1.55	57 (24%) 2 2	9, 21, 35, 57	5 (2%)
All	All	954/1116 (85%)	1.03	136 (14%) 6 5	8, 20, 36, 57	55 (5%)

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	238	ASP	7.8
1	D	239	LEU	6.4
1	C	-1	ASN	6.2
1	D	232	VAL	6.1
1	A	0	ALA	6.1
1	A	111[A]	HIS	5.9
1	D	237	THR	5.6
1	B	239	LEU	5.5
1	B	246	PRO	5.5
1	C	164[A]	TRP	5.5
1	C	126	PRO	5.4
1	D	223	TYR	5.4
1	C	127	LEU	5.3
1	C	132	ILE	5.3
1	B	132[A]	ILE	5.2
1	C	-6	LEU	5.2
1	B	82	VAL	5.2
1	D	236	ALA	5.2
1	C	0	ALA	5.0
1	C	-3	GLN	5.0
1	C	-4	PHE	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	242	ILE	4.9
1	B	231	HIS	4.9
1	A	233	ILE	4.8
1	B	235	GLU	4.4
1	D	224	SER	4.4
1	D	228	ALA	4.4
1	D	230	GLY	4.4
1	B	241	SER	4.3
1	D	233	ILE	4.3
1	B	233	ILE	4.2
1	D	240	SER	4.2
1	C	-2	SER	4.1
1	B	236	ALA	4.1
1	B	245	ALA	4.1
1	D	111	HIS	4.0
1	C	-5	TYR	4.0
1	B	131	GLY	4.0
1	B	232	VAL	4.0
1	B	244	ILE	3.9
1	A	110[A]	ARG	3.9
1	A	112[A]	GLY	3.7
1	A	1	MET	3.7
1	C	231	HIS	3.7
1	B	242	ILE	3.6
1	D	231	HIS	3.6
1	D	135	THR	3.5
1	A	232	VAL	3.5
1	D	234	ASP	3.5
1	B	237	THR	3.5
1	B	127[A]	LEU	3.5
1	D	164	TRP	3.2
1	D	85	ASP	3.2
1	D	63	PHE	3.2
1	D	187	GLY	3.2
1	B	187	GLY	3.2
1	B	129	MET	3.2
1	B	238	ASP	3.2
1	B	240	SER	3.1
1	B	86[A]	ASP	3.1
1	D	133	ARG	3.0
1	C	230	GLY	3.0
1	D	222	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	223	TYR	2.9
1	C	217	GLU	2.9
1	A	132	ILE	2.9
1	C	133	ARG	2.9
1	D	226	ARG	2.9
1	B	0	ALA	2.9
1	D	6	LEU	2.9
1	D	221	ASP	2.9
1	D	168	PHE	2.9
1	B	228	ALA	2.9
1	D	219	LEU	2.9
1	B	85[A]	ASP	2.8
1	D	126	PRO	2.8
1	B	234	ASP	2.8
1	D	183	PHE	2.8
1	D	112	GLY	2.7
1	D	1	MET	2.7
1	D	82	VAL	2.7
1	D	3	LEU	2.7
1	D	49	PHE	2.7
1	D	84	SER	2.7
1	D	12	LEU	2.7
1	C	1	MET	2.7
1	C	134	PRO	2.6
1	B	83	GLN	2.6
1	A	148	GLY	2.6
1	D	170	ILE	2.6
1	D	32	ALA	2.6
1	D	52	LEU	2.6
1	B	114[A]	ILE	2.6
1	B	84[A]	SER	2.6
1	D	218	ALA	2.6
1	B	130	ALA	2.5
1	C	149	SER	2.5
1	C	-7	ASN	2.5
1	D	220	THR	2.5
1	D	227	LYS	2.5
1	C	-8	GLU	2.5
1	C	45[A]	ARG	2.5
1	C	151	SER	2.5
1	A	-1	ASN	2.5
1	D	8	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	86	ASP	2.4
1	D	89	ALA	2.4
1	C	110[A]	ARG	2.4
1	B	1	MET	2.4
1	D	95	ALA	2.3
1	D	229	ALA	2.3
1	D	241	SER	2.3
1	D	186	ALA	2.3
1	C	111[A]	HIS	2.2
1	C	135	THR	2.2
1	B	185	ALA	2.2
1	D	163	ARG	2.2
1	B	44	LEU	2.2
1	D	86	ASP	2.2
1	B	19	PHE	2.2
1	D	35[A]	VAL	2.2
1	B	26	LEU	2.2
1	B	27	GLY	2.2
1	A	229	ALA	2.1
1	D	44	LEU	2.1
1	D	169	THR	2.1
1	D	146	SER	2.1
1	D	68	THR	2.1
1	A	109	GLU	2.1
1	B	18[A]	SER	2.1
1	B	80	ASP	2.0
1	D	211	LEU	2.0
1	A	231	HIS	2.0
1	C	77	PRO	2.0
1	D	217[A]	GLU	2.0
1	B	49	PHE	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 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	256[B]	1/1	0.98	0.14	8,8,8,8	1
3	CL	A	257	1/1	0.99	0.18	13,13,13,13	0
3	CL	A	258	1/1	0.99	0.22	11,11,11,11	0

6.5 Other polymers

There are no such residues in this entry.