



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:07 PM UTC

PDB ID : 5A40 / pdb_00005a40
Title : Crystal structure of a dual topology fluoride ion channel.
Authors : Stockbridge, R.B.; Kolmakova-Partensky, L.; Shane, T.; Koide, A.; Koide, S.;
Miller, C.; Newstead, S.
Deposited on : 2015-06-04
Resolution : 3.60 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

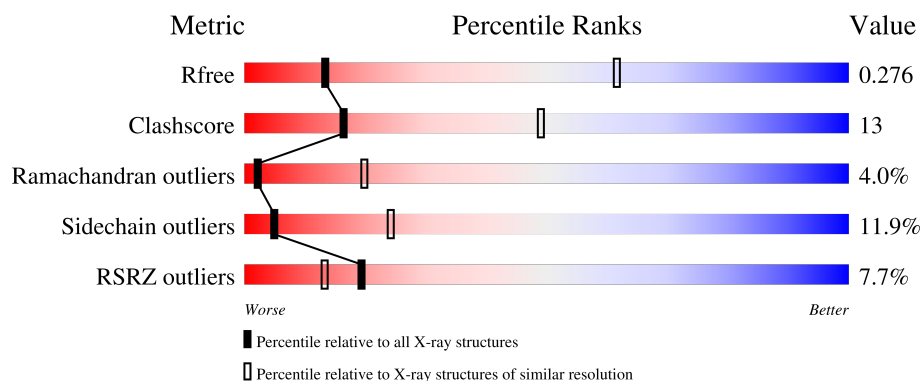
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	128	6% 80% 17% ...
1	B	128	11% 78% 17% ..
1	C	128	4% 81% 16% ...
1	D	128	5% 78% 19% .
2	E	90	8% 59% 26% 10% 6%

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Mol	Chain	Length	Quality of chain
2	F	90	12% 52% 31% 12%
2	G	90	14% 52% 34% 9%
2	H	90	2% 59% 26% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6488 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 FLUORIDE ION TRANSPORTER CRCB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			929	614	154	157	4			
1	B	124	Total	C	N	O	S	0	0	0
			902	595	151	152	4			
1	C	127	Total	C	N	O	S	0	0	0
			929	614	154	157	4			
1	D	124	Total	C	N	O	S	0	0	0
			902	595	151	152	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	LYS	ARG	conflict	UNP Q7VYU0
A	94	CYS	GLU	engineered mutation	UNP Q7VYU0
B	29	LYS	ARG	conflict	UNP Q7VYU0
B	94	CYS	GLU	engineered mutation	UNP Q7VYU0
C	29	LYS	ARG	conflict	UNP Q7VYU0
C	94	CYS	GLU	engineered mutation	UNP Q7VYU0
D	29	LYS	ARG	conflict	UNP Q7VYU0
D	94	CYS	GLU	engineered mutation	UNP Q7VYU0

- Molecule 2 is a protein called MONOBODIES.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	90	Total	C	N	O	S	0	0	0
			712	466	107	138	1			
2	F	88	Total	C	N	O	S	0	0	0
			699	458	105	135	1			
2	G	88	Total	C	N	O	S	0	0	0
			699	458	105	135	1			
2	H	90	Total	C	N	O	S	0	0	0
			712	466	107	138	1			

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

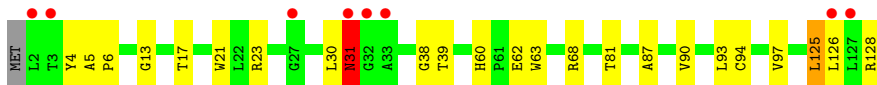
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Hg	0	0
			1	1		
3	F	1	Total	Hg	0	0
			1	1		
3	G	1	Total	Hg	0	0
			1	1		
3	H	1	Total	Hg	0	0
			1	1		

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.

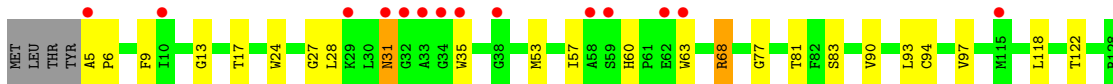
• Molecule 1: PUTATIVE FLUORIDE ION TRANSPORTER CRCB

Chain A: 



• Molecule 1: PUTATIVE FLUORIDE ION TRANSPORTER CRCB

Chain B: 



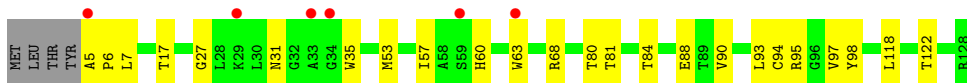
• Molecule 1: PUTATIVE FLUORIDE ION TRANSPORTER CRCB

Chain C: 



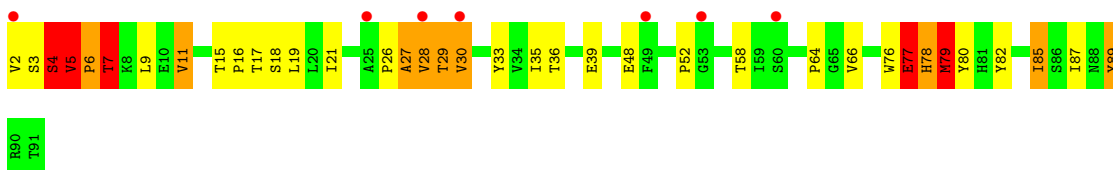
• Molecule 1: PUTATIVE FLUORIDE ION TRANSPORTER CRCB

Chain D: 



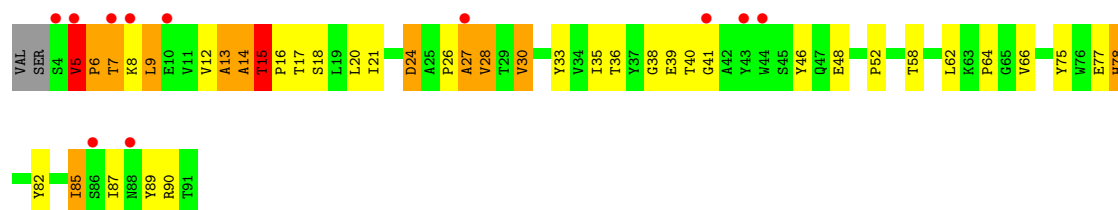
• Molecule 2: MONOBODIES

Chain E: 



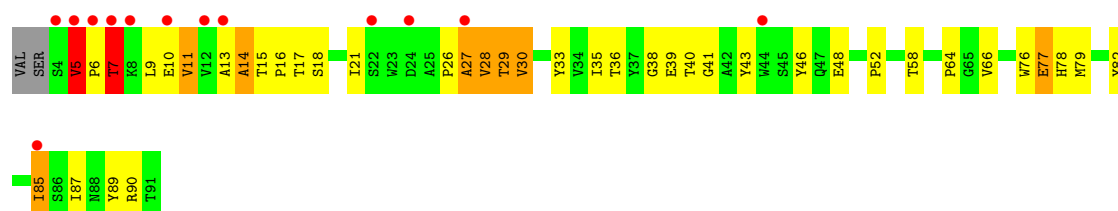
● Molecule 2: MONOBODIES

Chain F: 



● Molecule 2: MONOBODIES

Chain G: 



● Molecule 2: MONOBODIES

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	146.79Å 183.70Å 72.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.71 – 3.60 114.67 – 3.60	Depositor EDS
% Data completeness (in resolution range)	94.2 (114.71-3.60) 94.2 (114.67-3.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.18 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.235 , 0.270 0.239 , 0.276	Depositor DCC
R_{free} test set	1134 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	84.0	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	6488	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.43% 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: HG

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	0.70	0/953	1.08	4/1306 (0.3%)
1	B	0.69	0/925	0.96	1/1267 (0.1%)
1	C	0.73	0/953	1.02	1/1306 (0.1%)
1	D	0.73	0/925	1.00	0/1267
2	E	0.88	0/737	1.05	2/1016 (0.2%)
2	F	0.88	0/724	1.08	1/998 (0.1%)
2	G	0.79	1/724 (0.1%)	1.15	3/998 (0.3%)
2	H	0.92	3/737 (0.4%)	1.00	2/1016 (0.2%)
All	All	0.78	4/6678 (0.1%)	1.04	14/9174 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1
2	F	0	2
2	H	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	5	VAL	N-CA	6.12	1.54	1.46
2	H	3	SER	CA-C	6.07	1.59	1.52
2	H	4	SER	N-CA	5.87	1.53	1.46
2	H	3	SER	N-CA	5.24	1.52	1.46

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	5	VAL	CA-C-N	-11.91	104.96	119.84
2	G	5	VAL	C-N-CA	-11.91	104.96	119.84
2	G	5	VAL	N-CA-C	9.86	130.17	108.88
2	H	3	SER	N-CA-C	8.01	121.48	108.34
1	A	31	ASN	N-CA-C	7.79	121.12	108.34
2	F	13	ALA	N-CA-C	7.37	121.49	109.85
1	A	30	LEU	CA-C-N	-7.01	112.89	122.77
1	A	30	LEU	C-N-CA	-7.01	112.89	122.77
1	A	31	ASN	CB-CA-C	6.58	120.68	110.14
2	E	77	GLU	N-CA-C	5.20	121.87	110.80
2	E	79	MET	N-CA-C	5.14	121.76	110.80
2	H	5	VAL	C-N-CD	-5.11	109.35	120.60
1	C	81	THR	CB-CA-C	-5.09	101.15	109.80
1	B	31	ASN	N-CA-C	5.02	116.80	108.02

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	5	VAL	Peptide
2	F	14	ALA	Peptide
2	F	5	VAL	Peptide
2	H	3	SER	Peptide

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	929	0	957	17	0
1	B	902	0	930	15	0
1	C	929	0	957	13	0
1	D	902	0	931	19	0
2	E	712	0	681	33	0
2	F	699	0	667	38	0
2	G	699	0	667	36	0
2	H	712	0	681	22	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
3	H	1	0	0	0	0
All	All	6488	0	6471	169	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 13.

All (169) 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)
2:F:5:VAL:O	2:F:7:THR:N	2.12	0.82
2:E:78:HIS:O	2:E:80:TYR:N	2.15	0.79
1:A:87:ALA:HB3	2:E:79:MET:HE1	1.67	0.75
2:F:5:VAL:HG12	2:F:6:PRO:N	2.03	0.74
2:E:5:VAL:HG12	2:E:6:PRO:N	2.06	0.71
2:F:5:VAL:C	2:F:7:THR:H	1.98	0.71
2:G:5:VAL:C	2:G:7:THR:H	1.99	0.71
2:F:26:PRO:O	2:F:27:ALA:C	2.35	0.69
1:D:7:LEU:HB2	2:F:15:THR:HG23	1.75	0.68
2:G:13:ALA:CB	2:G:89:TYR:OH	2.41	0.68
2:F:6:PRO:O	2:F:7:THR:O	2.11	0.68
2:F:24:ASP:N	2:F:24:ASP:OD1	2.28	0.66
2:G:11:VAL:HG11	2:G:89:TYR:CD2	2.30	0.66
2:F:30:VAL:HG11	2:F:33:TYR:CZ	2.32	0.64
2:G:30:VAL:HG11	2:G:33:TYR:CZ	2.32	0.64
2:H:30:VAL:HG11	2:H:33:TYR:CZ	2.31	0.64
1:D:27:GLY:O	1:D:31:ASN:HB2	1.97	0.64
2:E:30:VAL:HG11	2:E:33:TYR:CZ	2.33	0.64
1:D:88:GLU:HG3	2:H:79:MET:CE	2.27	0.64
1:B:27:GLY:O	1:B:31:ASN:HB2	1.99	0.62
2:G:5:VAL:HG21	2:G:82:TYR:CB	2.28	0.62
1:A:87:ALA:HB3	2:E:79:MET:CE	2.28	0.62
2:G:5:VAL:HG12	2:G:6:PRO:HD3	1.82	0.62
1:C:27:GLY:O	1:C:31:ASN:HB2	2.00	0.61
2:G:6:PRO:O	2:G:7:THR:O	2.19	0.60
2:E:5:VAL:HG12	2:E:6:PRO:CD	2.32	0.59
2:E:11:VAL:HG12	2:E:11:VAL:O	2.02	0.59
2:F:5:VAL:HG21	2:F:82:TYR:CB	2.33	0.59
2:F:12:VAL:HB	2:F:20:LEU:HD23	1.85	0.58
2:F:5:VAL:HG12	2:F:6:PRO:CD	2.33	0.58
2:E:5:VAL:HG21	2:E:82:TYR:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:5:VAL:HG21	2:G:82:TYR:CG	2.40	0.57
2:E:6:PRO:O	2:E:7:THR:O	2.23	0.57
2:F:5:VAL:HG21	2:F:82:TYR:CG	2.40	0.57
1:A:87:ALA:CB	2:E:79:MET:CE	2.83	0.56
2:E:26:PRO:O	2:E:27:ALA:C	2.48	0.56
2:G:11:VAL:HG12	2:G:11:VAL:O	2.05	0.56
2:H:9:LEU:HD21	2:H:21:ILE:CG2	2.35	0.56
1:D:6:PRO:HD2	2:F:15:THR:HG21	1.87	0.56
2:G:5:VAL:C	2:G:7:THR:N	2.61	0.56
2:H:11:VAL:O	2:H:11:VAL:HG12	2.04	0.56
2:F:14:ALA:C	2:F:15:THR:O	2.48	0.56
2:G:13:ALA:HB2	2:G:89:TYR:OH	2.05	0.56
1:A:31:ASN:HB3	1:A:38:GLY:H	1.71	0.56
1:D:7:LEU:CB	2:F:15:THR:HG23	2.36	0.56
2:E:5:VAL:HG21	2:E:82:TYR:CG	2.41	0.56
2:F:5:VAL:C	2:F:7:THR:N	2.62	0.55
2:G:5:VAL:HG12	2:G:6:PRO:CD	2.37	0.55
1:D:88:GLU:HG3	2:H:79:MET:HE3	1.87	0.55
2:E:5:VAL:HG12	2:E:6:PRO:HD3	1.87	0.55
1:A:87:ALA:CB	2:E:79:MET:HE1	2.34	0.54
2:G:26:PRO:O	2:G:27:ALA:C	2.49	0.54
2:F:5:VAL:CG1	2:F:6:PRO:N	2.70	0.54
1:D:98:TYR:CE2	2:H:43:TYR:HB3	2.42	0.53
2:F:5:VAL:HG12	2:F:6:PRO:HD3	1.89	0.53
2:G:5:VAL:O	2:G:7:THR:N	2.41	0.53
2:H:19:LEU:HD13	2:H:89:TYR:CZ	2.43	0.53
1:A:17:THR:HG23	1:B:13:GLY:HA2	1.91	0.53
2:G:5:VAL:HG12	2:G:6:PRO:N	2.23	0.53
1:A:13:GLY:HA2	1:B:17:THR:HG23	1.91	0.52
2:H:26:PRO:O	2:H:27:ALA:C	2.53	0.52
2:E:19:LEU:HD13	2:E:89:TYR:CZ	2.46	0.51
2:E:5:VAL:CG1	2:E:6:PRO:N	2.72	0.50
1:C:13:GLY:HA2	1:D:17:THR:HG23	1.94	0.50
2:G:6:PRO:O	2:G:7:THR:C	2.55	0.50
2:E:5:VAL:O	2:E:7:THR:N	2.45	0.49
2:E:4:SER:O	2:E:5:VAL:HG23	2.13	0.49
2:E:77:GLU:O	2:E:78:HIS:O	2.30	0.49
1:B:118:LEU:O	1:B:122:THR:HG23	2.13	0.48
2:F:17:THR:HG22	2:F:62:LEU:O	2.13	0.48
1:A:17:THR:HG23	1:B:13:GLY:CA	2.44	0.48
2:E:39:GLU:HG2	2:E:66:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:ALA:HB1	1:C:6:PRO:HD2	1.96	0.48
1:A:5:ALA:HB1	1:A:6:PRO:HD2	1.96	0.47
1:B:90:VAL:HA	1:B:93:LEU:HD12	1.95	0.47
2:F:77:GLU:O	2:F:78:HIS:C	2.55	0.47
1:B:68:ARG:NE	2:E:77:GLU:OE1	2.47	0.47
2:E:5:VAL:C	2:E:7:THR:H	2.22	0.47
2:G:9:LEU:HD23	2:G:87:ILE:HG13	1.96	0.47
2:E:39:GLU:HG2	2:E:66:VAL:CG1	2.45	0.47
1:C:81:THR:HG21	1:C:84:THR:OG1	2.14	0.47
1:D:118:LEU:O	1:D:122:THR:HG23	2.14	0.46
2:E:9:LEU:HD22	2:E:85:ILE:HG22	1.97	0.46
2:E:78:HIS:CG	2:E:79:MET:H	2.32	0.46
1:A:60:HIS:HB3	1:A:63:TRP:NE1	2.30	0.46
2:G:9:LEU:HD22	2:G:85:ILE:HG22	1.97	0.46
1:B:5:ALA:HB1	1:B:6:PRO:HD2	1.98	0.46
2:E:28:VAL:HG12	2:E:29:THR:H	1.80	0.46
2:E:76:TRP:CD2	2:E:76:TRP:O	2.69	0.46
2:H:28:VAL:HB	2:H:82:TYR:OH	2.16	0.46
1:A:90:VAL:HA	1:A:93:LEU:HD12	1.97	0.46
2:H:39:GLU:HG2	2:H:66:VAL:HG11	1.97	0.46
2:G:28:VAL:HB	2:G:82:TYR:OH	2.16	0.46
1:C:90:VAL:HA	1:C:93:LEU:HD12	1.98	0.46
2:H:28:VAL:HG12	2:H:29:THR:H	1.80	0.46
1:D:90:VAL:HA	1:D:93:LEU:HD12	1.98	0.45
1:B:97:VAL:O	1:B:97:VAL:HG23	2.16	0.45
2:F:16:PRO:HB2	2:F:64:PRO:HB3	1.97	0.45
2:E:6:PRO:O	2:E:7:THR:C	2.58	0.45
1:B:60:HIS:HB3	1:B:63:TRP:NE1	2.31	0.45
1:C:125:LEU:HD13	1:C:126:LEU:CD2	2.46	0.45
2:G:9:LEU:HD23	2:G:87:ILE:HD11	1.99	0.45
2:G:39:GLU:HG2	2:G:66:VAL:HG11	1.99	0.45
1:A:97:VAL:O	1:A:97:VAL:HG23	2.16	0.45
2:H:39:GLU:HG2	2:H:66:VAL:CG1	2.47	0.45
2:H:39:GLU:O	2:H:40:THR:C	2.60	0.45
2:E:9:LEU:HD23	2:E:87:ILE:HD11	1.99	0.45
2:G:9:LEU:HD23	2:G:87:ILE:CD1	2.47	0.45
1:C:97:VAL:HG23	1:C:97:VAL:O	2.16	0.45
1:A:125:LEU:HD13	1:A:126:LEU:CD2	2.47	0.44
1:D:53:MET:HE3	1:D:57:ILE:HD11	1.99	0.44
2:E:28:VAL:HB	2:E:82:TYR:OH	2.17	0.44
1:D:97:VAL:HG23	1:D:97:VAL:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:75:TYR:CD2	2:F:78:HIS:O	2.71	0.44
2:H:76:TRP:O	2:H:76:TRP:CG	2.69	0.44
2:G:10:GLU:HG2	2:G:11:VAL:N	2.32	0.44
1:C:13:GLY:CA	1:D:17:THR:HG23	2.48	0.44
1:C:68:ARG:NE	2:H:77:GLU:OE1	2.51	0.44
2:F:39:GLU:HG2	2:F:66:VAL:HG11	1.98	0.44
2:G:13:ALA:O	2:G:14:ALA:O	2.35	0.44
2:G:14:ALA:HA	2:G:15:THR:C	2.42	0.44
2:G:28:VAL:HG12	2:G:29:THR:H	1.83	0.44
2:H:9:LEU:HD21	2:H:21:ILE:HG23	1.99	0.43
2:H:78:HIS:O	2:H:79:MET:CB	2.66	0.43
1:C:60:HIS:HB3	1:C:63:TRP:NE1	2.33	0.43
1:D:5:ALA:HB1	1:D:6:PRO:HD2	1.99	0.43
1:A:21:TRP:NE1	1:B:9:PHE:O	2.43	0.43
2:F:13:ALA:HB2	2:F:20:LEU:HB3	1.99	0.43
1:B:53:MET:HE3	1:B:57:ILE:HD11	2.00	0.43
2:F:39:GLU:HG2	2:F:66:VAL:CG1	2.48	0.43
2:F:9:LEU:HD23	2:F:87:ILE:HG13	2.01	0.43
2:G:39:GLU:HG2	2:G:66:VAL:CG1	2.49	0.43
1:A:23:ARG:NH2	1:B:77:GLY:HA3	2.34	0.43
2:E:35:ILE:O	2:E:48:GLU:HA	2.19	0.43
1:A:13:GLY:CA	1:B:17:THR:HG23	2.48	0.42
1:A:31:ASN:HD22	1:A:39:THR:H	1.67	0.42
2:F:89:TYR:CE1	2:F:90:ARG:O	2.72	0.42
2:E:76:TRP:O	2:E:76:TRP:CG	2.71	0.42
2:F:12:VAL:HG12	2:F:12:VAL:O	2.19	0.42
2:H:76:TRP:O	2:H:76:TRP:CD2	2.72	0.42
2:E:16:PRO:HB2	2:E:64:PRO:HB3	2.00	0.42
2:F:9:LEU:HD23	2:F:87:ILE:HD11	2.02	0.42
2:F:35:ILE:O	2:F:48:GLU:HA	2.20	0.42
2:G:89:TYR:CE1	2:G:90:ARG:O	2.73	0.42
2:G:5:VAL:HG21	2:G:82:TYR:HB2	2.00	0.42
1:C:98:TYR:CE2	2:G:43:TYR:HB3	2.54	0.42
2:G:78:HIS:O	2:G:79:MET:CB	2.68	0.42
2:F:39:GLU:O	2:F:40:THR:C	2.62	0.42
1:D:84:THR:HG23	2:H:79:MET:HE1	2.02	0.42
2:F:9:LEU:HD23	2:F:87:ILE:CD1	2.50	0.42
2:F:38:GLY:HA3	2:F:46:TYR:CD1	2.55	0.42
2:G:16:PRO:HB2	2:G:64:PRO:HB3	2.01	0.42
1:C:83:SER:HB3	1:D:80:THR:HG21	2.02	0.41
2:G:39:GLU:O	2:G:40:THR:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:13:ALA:HB3	2:F:20:LEU:N	2.34	0.41
2:H:6:PRO:HB3	2:H:25:ALA:HB2	2.03	0.41
2:G:38:GLY:HA3	2:G:46:TYR:CD1	2.55	0.41
1:D:27:GLY:O	1:D:31:ASN:CB	2.68	0.41
2:F:30:VAL:HG11	2:F:33:TYR:CE2	2.56	0.41
2:G:35:ILE:O	2:G:48:GLU:HA	2.21	0.41
1:D:60:HIS:HB3	1:D:63:TRP:NE1	2.35	0.41
2:G:76:TRP:O	2:G:76:TRP:CG	2.74	0.40
1:B:24:TRP:O	1:B:28:LEU:HG	2.22	0.40
2:F:9:LEU:HD22	2:F:85:ILE:HG22	2.02	0.40
1:C:35:TRP:HA	1:C:36:PRO:HD3	1.85	0.40
2:F:5:VAL:HG21	2:F:82:TYR:HB2	2.04	0.40
1:D:95:ARG:HH21	2:H:48:GLU:CD	2.29	0.40
2:F:75:TYR:HD2	2:F:78:HIS:O	2.04	0.40
2:H:5:VAL:HG13	2:H:6:PRO:HA	2.03	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	125/128 (98%)	114 (91%)	11 (9%)	0	100	100
1	B	122/128 (95%)	110 (90%)	11 (9%)	1 (1%)	16	49
1	C	125/128 (98%)	111 (89%)	14 (11%)	0	100	100
1	D	122/128 (95%)	108 (88%)	14 (12%)	0	100	100
2	E	88/90 (98%)	69 (78%)	11 (12%)	8 (9%)	0	6
2	F	86/90 (96%)	68 (79%)	7 (8%)	11 (13%)	0	3
2	G	86/90 (96%)	68 (79%)	11 (13%)	7 (8%)	1	8
2	H	88/90 (98%)	71 (81%)	10 (11%)	7 (8%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	842/872 (97%)	719 (85%)	89 (11%)	34 (4%)	2	20

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	4	SER
2	E	5	VAL
2	E	6	PRO
2	E	7	THR
2	E	78	HIS
2	E	79	MET
2	F	5	VAL
2	F	6	PRO
2	F	7	THR
2	G	7	THR
2	G	14	ALA
2	H	4	SER
2	E	27	ALA
2	F	41	GLY
2	G	27	ALA
2	G	41	GLY
2	G	77	GLU
2	H	7	THR
2	H	41	GLY
2	H	77	GLU
2	F	9	LEU
2	F	27	ALA
2	G	5	VAL
2	H	27	ALA
2	F	28	VAL
2	F	8	LYS
2	F	15	THR
1	B	83	SER
2	E	52	PRO
2	F	52	PRO
2	F	78	HIS
2	G	52	PRO
2	H	6	PRO
2	H	52	PRO

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	88/89 (99%)	80 (91%)	8 (9%)	9	33
1	B	85/89 (96%)	81 (95%)	4 (5%)	23	50
1	C	88/89 (99%)	81 (92%)	7 (8%)	11	37
1	D	85/89 (96%)	81 (95%)	4 (5%)	23	50
2	E	78/78 (100%)	61 (78%)	17 (22%)	1	7
2	F	76/78 (97%)	67 (88%)	9 (12%)	5	24
2	G	76/78 (97%)	64 (84%)	12 (16%)	2	15
2	H	78/78 (100%)	61 (78%)	17 (22%)	1	7
All	All	654/668 (98%)	576 (88%)	78 (12%)	5	24

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	TYR
1	A	31	ASN
1	A	62	GLU
1	A	68	ARG
1	A	81	THR
1	A	94	CYS
1	A	125	LEU
1	A	128	ARG
1	B	35	TRP
1	B	68	ARG
1	B	81	THR
1	B	94	CYS
1	C	4	TYR
1	C	62	GLU
1	C	68	ARG
1	C	81	THR
1	C	94	CYS
1	C	125	LEU
1	C	128	ARG

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Mol	Chain	Res	Type
1	D	35	TRP
1	D	68	ARG
1	D	81	THR
1	D	94	CYS
2	E	2	VAL
2	E	3	SER
2	E	4	SER
2	E	7	THR
2	E	11	VAL
2	E	15	THR
2	E	17	THR
2	E	18	SER
2	E	21	ILE
2	E	28	VAL
2	E	29	THR
2	E	30	VAL
2	E	36	THR
2	E	58	THR
2	E	77	GLU
2	E	85	ILE
2	E	89	TYR
2	F	15	THR
2	F	18	SER
2	F	21	ILE
2	F	24	ASP
2	F	28	VAL
2	F	30	VAL
2	F	36	THR
2	F	58	THR
2	F	85	ILE
2	G	7	THR
2	G	11	VAL
2	G	17	THR
2	G	18	SER
2	G	21	ILE
2	G	28	VAL
2	G	29	THR
2	G	30	VAL
2	G	36	THR
2	G	58	THR
2	G	77	GLU
2	G	85	ILE

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Mol	Chain	Res	Type
2	H	2	VAL
2	H	3	SER
2	H	7	THR
2	H	9	LEU
2	H	11	VAL
2	H	15	THR
2	H	17	THR
2	H	18	SER
2	H	21	ILE
2	H	28	VAL
2	H	29	THR
2	H	30	VAL
2	H	36	THR
2	H	58	THR
2	H	83	SER
2	H	85	ILE
2	H	89	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	60	HIS
1	B	60	HIS
1	C	60	HIS
1	D	60	HIS
2	G	78	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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	127/128 (99%)	0.19	8 (6%) 26 16	44, 71, 126, 153	0
1	B	124/128 (96%)	0.53	14 (11%) 10 8	47, 74, 116, 129	0
1	C	127/128 (99%)	0.10	5 (3%) 43 24	40, 60, 98, 147	0
1	D	124/128 (96%)	0.13	6 (4%) 35 20	44, 63, 102, 134	0
2	E	90/90 (100%)	0.80	7 (7%) 19 13	54, 77, 113, 129	0
2	F	88/90 (97%)	0.75	11 (12%) 8 7	59, 84, 116, 137	0
2	G	88/90 (97%)	0.75	13 (14%) 5 5	59, 94, 136, 151	0
2	H	90/90 (100%)	0.37	2 (2%) 62 36	58, 82, 110, 142	0
All	All	858/872 (98%)	0.41	66 (7%) 19 13	40, 75, 121, 153	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	10	GLU	6.0
2	F	88	ASN	5.7
2	E	2	VAL	5.1
2	F	8	LYS	4.9
1	B	62	GLU	4.5
1	B	33	ALA	4.2
1	C	33	ALA	4.0
1	B	38	GLY	3.9
1	A	31	ASN	3.8
1	D	33	ALA	3.7
2	G	6	PRO	3.6
1	A	2	LEU	3.6
1	D	29	LYS	3.5
1	C	29	LYS	3.4
2	G	5	VAL	3.3
2	G	7	THR	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	27	ALA	3.2
2	E	60	SER	3.2
2	F	44	TRP	3.1
1	A	127	LEU	3.1
2	F	43	TYR	3.1
1	B	34	GLY	2.9
1	B	59	SER	2.9
1	B	5	ALA	2.9
2	E	25	ALA	2.9
2	F	86	SER	2.8
1	D	34	GLY	2.7
1	B	35	TRP	2.7
2	G	12	VAL	2.6
1	C	2	LEU	2.6
2	G	22	SER	2.6
2	G	44	TRP	2.6
2	F	10	GLU	2.5
2	E	30	VAL	2.5
1	A	126	LEU	2.5
1	B	10	ILE	2.4
2	G	13	ALA	2.4
1	B	29	LYS	2.4
1	B	31	ASN	2.4
2	G	27	ALA	2.3
1	C	124	ARG	2.3
2	F	41	GLY	2.3
2	G	4	SER	2.3
2	E	53	GLY	2.3
2	G	24	ASP	2.3
1	B	63	TRP	2.3
1	D	59	SER	2.3
2	G	8	LYS	2.3
2	H	8	LYS	2.3
1	B	58	ALA	2.2
1	A	33	ALA	2.2
1	D	63	TRP	2.2
2	F	4	SER	2.2
2	G	85	ILE	2.2
2	H	2	VAL	2.2
1	A	3	THR	2.2
1	C	3	THR	2.2
1	D	5	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	49	PHE	2.2
2	F	5	VAL	2.1
2	E	28	VAL	2.1
2	F	7	THR	2.1
1	B	32	GLY	2.0
1	A	32	GLY	2.0
1	B	115	MET	2.0
1	A	27	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	HG	E	1092	1/1	0.97	0.06	184,184,184,184	0
3	HG	G	1092	1/1	0.98	0.06	187,187,187,187	0
3	HG	F	1092	1/1	0.99	0.08	183,183,183,183	0
3	HG	H	1092	1/1	0.99	0.10	182,182,182,182	0

6.5 Other polymers [i](#)

There are no such residues in this entry.