Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 03:23 am GMT

PDB ID	:	6HFB
Title	:	Outward-facing conformation of a multidrug resistance MATE family transporter of the MOP superfamily.
Authors	:	Nonaka, T.; Zakrzewska, S.; Safarian, S.; Michel, H.
Deposited on	:	2018-08-21
Resolution	:	3.50 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:

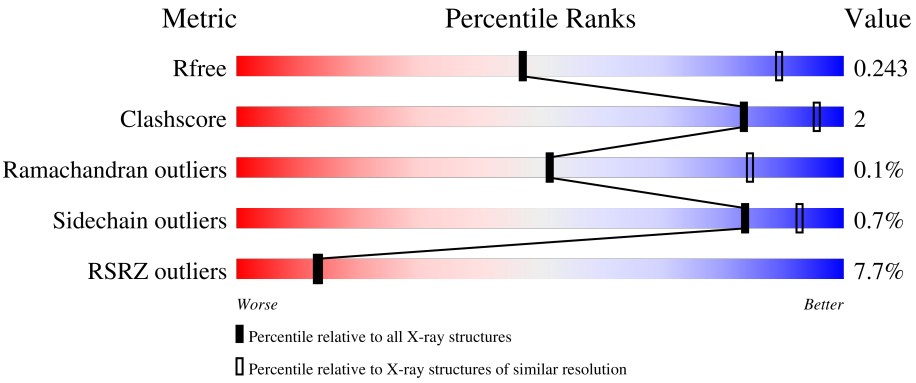
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	485	8% 85% 9% 7%
1	B	485	4% 87% 6% 7%
1	C	485	8% 86% 7% 7%
1	D	485	8% 86% 7% 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13638 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	1	0
			3412	2237	557	597	21			
1	B	453	Total	C	N	O	S	0	0	0
			3404	2232	554	597	21			
1	C	451	Total	C	N	O	S	0	2	0
			3409	2236	558	594	21			
1	D	451	Total	C	N	O	S	0	1	0
			3401	2231	554	595	21			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	THR	ALA	engineered mutation	UNP Q8U2X0
A	462	ARG	-	expression tag	UNP Q8U2X0
A	463	ASN	-	expression tag	UNP Q8U2X0
A	464	SER	-	expression tag	UNP Q8U2X0
A	465	GLU	-	expression tag	UNP Q8U2X0
A	466	ASN	-	expression tag	UNP Q8U2X0
A	467	LEU	-	expression tag	UNP Q8U2X0
A	468	TYR	-	expression tag	UNP Q8U2X0
A	469	PHE	-	expression tag	UNP Q8U2X0
A	470	GLN	-	expression tag	UNP Q8U2X0
A	471	GLY	-	expression tag	UNP Q8U2X0
A	472	GLY	-	expression tag	UNP Q8U2X0
A	473	ARG	-	expression tag	UNP Q8U2X0
A	474	GLY	-	expression tag	UNP Q8U2X0
A	475	SER	-	expression tag	UNP Q8U2X0
A	476	HIS	-	expression tag	UNP Q8U2X0
A	477	HIS	-	expression tag	UNP Q8U2X0
A	478	HIS	-	expression tag	UNP Q8U2X0
A	479	HIS	-	expression tag	UNP Q8U2X0
A	480	HIS	-	expression tag	UNP Q8U2X0
A	481	HIS	-	expression tag	UNP Q8U2X0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	482	HIS	-	expression tag	UNP Q8U2X0
A	483	HIS	-	expression tag	UNP Q8U2X0
A	484	HIS	-	expression tag	UNP Q8U2X0
A	485	HIS	-	expression tag	UNP Q8U2X0
B	298	THR	ALA	engineered mutation	UNP Q8U2X0
B	462	ARG	-	expression tag	UNP Q8U2X0
B	463	ASN	-	expression tag	UNP Q8U2X0
B	464	SER	-	expression tag	UNP Q8U2X0
B	465	GLU	-	expression tag	UNP Q8U2X0
B	466	ASN	-	expression tag	UNP Q8U2X0
B	467	LEU	-	expression tag	UNP Q8U2X0
B	468	TYR	-	expression tag	UNP Q8U2X0
B	469	PHE	-	expression tag	UNP Q8U2X0
B	470	GLN	-	expression tag	UNP Q8U2X0
B	471	GLY	-	expression tag	UNP Q8U2X0
B	472	GLY	-	expression tag	UNP Q8U2X0
B	473	ARG	-	expression tag	UNP Q8U2X0
B	474	GLY	-	expression tag	UNP Q8U2X0
B	475	SER	-	expression tag	UNP Q8U2X0
B	476	HIS	-	expression tag	UNP Q8U2X0
B	477	HIS	-	expression tag	UNP Q8U2X0
B	478	HIS	-	expression tag	UNP Q8U2X0
B	479	HIS	-	expression tag	UNP Q8U2X0
B	480	HIS	-	expression tag	UNP Q8U2X0
B	481	HIS	-	expression tag	UNP Q8U2X0
B	482	HIS	-	expression tag	UNP Q8U2X0
B	483	HIS	-	expression tag	UNP Q8U2X0
B	484	HIS	-	expression tag	UNP Q8U2X0
B	485	HIS	-	expression tag	UNP Q8U2X0
C	298	THR	ALA	engineered mutation	UNP Q8U2X0
C	462	ARG	-	expression tag	UNP Q8U2X0
C	463	ASN	-	expression tag	UNP Q8U2X0
C	464	SER	-	expression tag	UNP Q8U2X0
C	465	GLU	-	expression tag	UNP Q8U2X0
C	466	ASN	-	expression tag	UNP Q8U2X0
C	467	LEU	-	expression tag	UNP Q8U2X0
C	468	TYR	-	expression tag	UNP Q8U2X0
C	469	PHE	-	expression tag	UNP Q8U2X0
C	470	GLN	-	expression tag	UNP Q8U2X0
C	471	GLY	-	expression tag	UNP Q8U2X0
C	472	GLY	-	expression tag	UNP Q8U2X0
C	473	ARG	-	expression tag	UNP Q8U2X0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	474	GLY	-	expression tag	UNP Q8U2X0
C	475	SER	-	expression tag	UNP Q8U2X0
C	476	HIS	-	expression tag	UNP Q8U2X0
C	477	HIS	-	expression tag	UNP Q8U2X0
C	478	HIS	-	expression tag	UNP Q8U2X0
C	479	HIS	-	expression tag	UNP Q8U2X0
C	480	HIS	-	expression tag	UNP Q8U2X0
C	481	HIS	-	expression tag	UNP Q8U2X0
C	482	HIS	-	expression tag	UNP Q8U2X0
C	483	HIS	-	expression tag	UNP Q8U2X0
C	484	HIS	-	expression tag	UNP Q8U2X0
C	485	HIS	-	expression tag	UNP Q8U2X0
D	298	THR	ALA	engineered mutation	UNP Q8U2X0
D	462	ARG	-	expression tag	UNP Q8U2X0
D	463	ASN	-	expression tag	UNP Q8U2X0
D	464	SER	-	expression tag	UNP Q8U2X0
D	465	GLU	-	expression tag	UNP Q8U2X0
D	466	ASN	-	expression tag	UNP Q8U2X0
D	467	LEU	-	expression tag	UNP Q8U2X0
D	468	TYR	-	expression tag	UNP Q8U2X0
D	469	PHE	-	expression tag	UNP Q8U2X0
D	470	GLN	-	expression tag	UNP Q8U2X0
D	471	GLY	-	expression tag	UNP Q8U2X0
D	472	GLY	-	expression tag	UNP Q8U2X0
D	473	ARG	-	expression tag	UNP Q8U2X0
D	474	GLY	-	expression tag	UNP Q8U2X0
D	475	SER	-	expression tag	UNP Q8U2X0
D	476	HIS	-	expression tag	UNP Q8U2X0
D	477	HIS	-	expression tag	UNP Q8U2X0
D	478	HIS	-	expression tag	UNP Q8U2X0
D	479	HIS	-	expression tag	UNP Q8U2X0
D	480	HIS	-	expression tag	UNP Q8U2X0
D	481	HIS	-	expression tag	UNP Q8U2X0
D	482	HIS	-	expression tag	UNP Q8U2X0
D	483	HIS	-	expression tag	UNP Q8U2X0
D	484	HIS	-	expression tag	UNP Q8U2X0
D	485	HIS	-	expression tag	UNP Q8U2X0

- Molecule 2 is CESIUM ION (three-letter code: CS) (formula: Cs).

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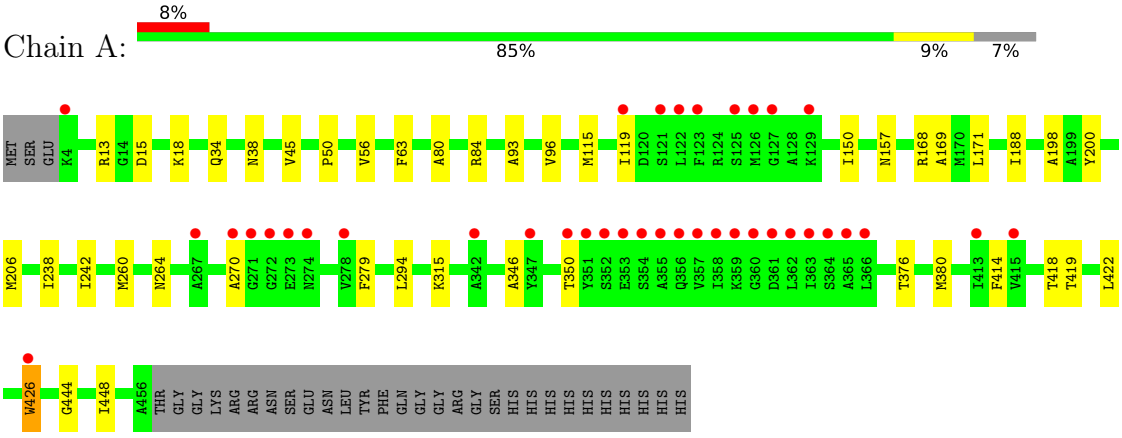
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Cs 4 4	0	0
2	B	2	Total Cs 2 2	0	0
2	C	3	Total Cs 3 3	0	0
2	D	3	Total Cs 3 3	0	0

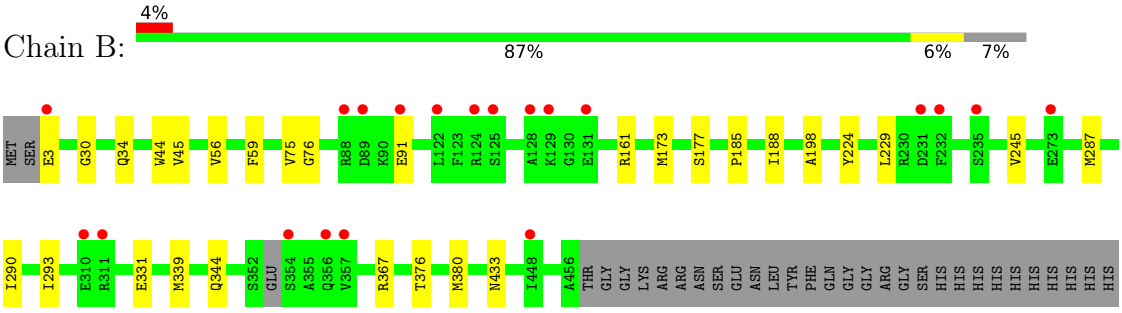
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

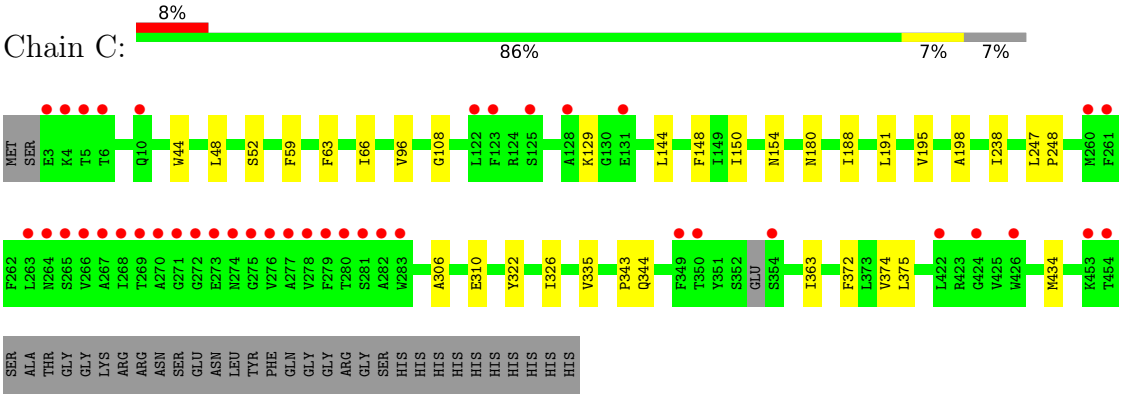
• Molecule 1: Uncharacterized protein



• Molecule 1: Uncharacterized protein

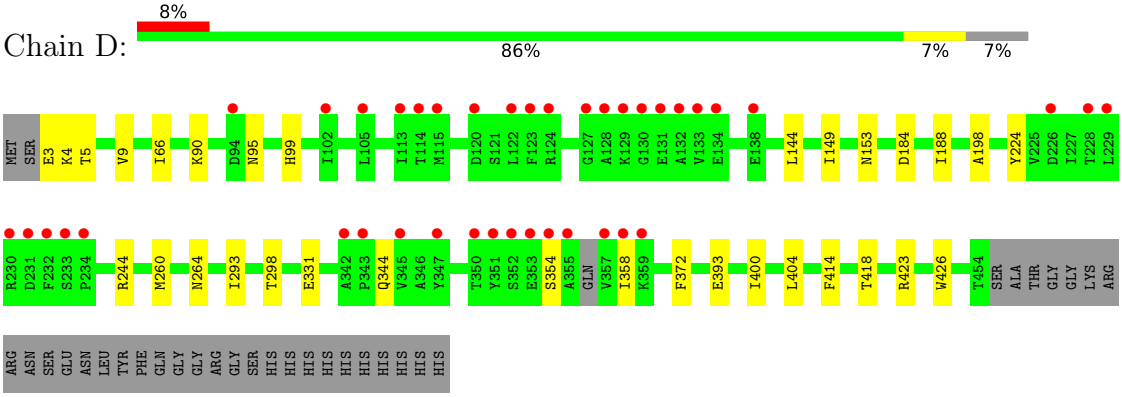


• Molecule 1: Uncharacterized protein



• Molecule 1: Uncharacterized protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	219.75Å 94.25Å 138.78Å 90.00° 126.48° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 47.12 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.2 (20.00-3.50) 93.1 (47.12-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.48Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.189 , 0.239 0.196 , 0.243	Depositor DCC
R_{free} test set	1396 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	70.0	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 63.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.021 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	13638	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CS

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	0.24	0/3476	0.38	0/4714
1	B	0.24	0/3464	0.38	0/4697
1	C	0.24	0/3475	0.38	0/4710
1	D	0.24	0/3464	0.38	0/4696
All	All	0.24	0/13879	0.38	0/18817

There are no bond length outliers.

There are no bond angle outliers.

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	3412	0	3601	22	0
1	B	3404	0	3587	16	0
1	C	3409	0	3603	16	0
1	D	3401	0	3588	15	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
All	All	13638	0	14379	67	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 2.

All (67) 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:149:ILE:O	1:D:153:ASN:ND2	2.26	0.68
1:A:15:ASP:HB3	1:A:18:LYS:HB3	1.80	0.64
1:D:260:MET:O	1:D:264:ASN:ND2	2.32	0.61
1:A:188:ILE:HD11	1:A:198:ALA:HB2	1.81	0.61
1:D:400:ILE:HG23	1:D:404:LEU:HD12	1.84	0.59
1:D:95:ASN:O	1:D:99:HIS:ND1	2.37	0.58
1:A:260:MET:O	1:A:264:ASN:ND2	2.38	0.57
1:A:34:GLN:O	1:A:38:ASN:ND2	2.36	0.57
1:B:45:VAL:HG11	1:B:56:VAL:HG21	1.86	0.57
1:A:13:ARG:O	1:A:315:LYS:NZ	2.38	0.55
1:A:279:PHE:HD1	1:A:426:TRP:HZ3	1.56	0.53
1:D:423:ARG:HA	1:D:426:TRP:CD1	2.44	0.52
1:B:3:GLU:OE2	1:B:224:TYR:OH	2.23	0.52
1:A:84:ARG:HH22	1:A:238:ILE:HG12	1.75	0.52
1:A:45:VAL:HG11	1:A:56:VAL:HG21	1.91	0.52
1:D:414:PHE:O	1:D:418:THR:OG1	2.28	0.51
1:A:84:ARG:HB2	1:A:93:ALA:HB2	1.92	0.51
1:C:150:ILE:O	1:C:154:ASN:ND2	2.39	0.51
1:C:375:LEU:HD12	1:C:434:MET:HG2	1.92	0.51
1:C:52:SER:HB3	1:C:195:VAL:HB	1.92	0.51
1:A:294:LEU:HD23	1:A:380:MET:HE1	1.93	0.50
1:A:200:TYR:CE1	1:C:344:GLN:HG2	2.47	0.49
1:D:4:LYS:HD3	1:D:5:THR:H	1.78	0.49
1:D:354:SER:HA	1:D:358:ILE:HD12	1.95	0.48
1:A:115:MET:O	1:A:119:ILE:HG13	2.15	0.47
1:B:56:VAL:HA	1:B:59:PHE:CE2	2.50	0.47
1:A:157:ASN:ND2	1:A:169:ALA:O	2.46	0.47
1:D:244[A]:ARG:NE	1:D:393:GLU:OE1	2.31	0.47
1:A:346:ALA:O	1:A:350:THR:HG22	2.15	0.46
1:C:66:ILE:HD11	1:C:144:LEU:HD23	1.97	0.46
1:D:188:ILE:HD11	1:D:198:ALA:HB2	1.98	0.46
1:A:376:THR:HG22	1:A:380:MET:HG3	1.97	0.46
1:A:414:PHE:O	1:A:418:THR:OG1	2.34	0.45
1:D:3:GLU:HA	1:D:90:LYS:HE3	1.98	0.45
1:B:344:GLN:OE1	1:B:344:GLN:N	2.48	0.45
1:C:59:PHE:CE2	1:C:63:PHE:HB2	2.52	0.45
1:A:96:VAL:HG13	1:A:242:ILE:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:VAL:HA	1:B:59:PHE:CZ	2.52	0.44
1:C:322:TYR:CE2	1:C:326:ILE:HD11	2.52	0.44
1:A:80:ALA:O	1:A:84:ARG:HG2	2.17	0.44
1:B:293:ILE:HD11	1:B:331:GLU:HG3	1.99	0.44
1:D:344:GLN:OE1	1:D:344:GLN:N	2.48	0.44
1:D:9:VAL:HG21	1:D:224:TYR:CG	2.53	0.43
1:C:343:PRO:HG3	1:C:363:ILE:HG23	2.00	0.43
1:B:339:MET:O	1:B:367:ARG:NE	2.51	0.43
1:C:108:GLY:HA3	1:C:148:PHE:HA	2.00	0.43
1:C:188:ILE:HD11	1:C:198:ALA:HB2	2.00	0.43
1:B:34:GLN:HG2	1:B:177:SER:OG	2.18	0.43
1:D:66:ILE:HD11	1:D:144:LEU:HD23	2.00	0.43
1:C:247:LEU:HB3	1:C:248:PRO:HD3	2.01	0.42
1:A:150:ILE:HG12	1:A:206:MET:SD	2.60	0.42
1:A:270:ALA:HB1	1:A:422:LEU:HA	2.01	0.42
1:A:444:GLY:O	1:A:448:ILE:HG12	2.19	0.42
1:A:168:ARG:HA	1:A:171:LEU:HD12	2.01	0.42
1:C:335:VAL:HG21	1:C:374:VAL:HG22	2.00	0.42
1:B:188:ILE:HD11	1:B:198:ALA:HB2	2.02	0.41
1:C:96:VAL:HG22	1:C:238:ILE:HG23	2.02	0.41
1:D:293:ILE:HD11	1:D:331:GLU:HG3	2.01	0.41
1:B:30:GLY:HA3	1:B:173:MET:HE3	2.02	0.41
1:B:75:VAL:HG22	1:B:161:ARG:HH22	1.86	0.41
1:B:287:MET:O	1:B:290:ILE:HG12	2.20	0.41
1:B:376:THR:HG22	1:B:380:MET:HG3	2.01	0.41
1:B:76:GLY:HA2	1:B:245:VAL:HB	2.03	0.40
1:C:44:TRP:O	1:C:48:LEU:HD13	2.21	0.40
1:B:44:TRP:CE2	1:B:185:PRO:HB3	2.56	0.40
1:B:229:LEU:HD11	1:C:191:LEU:HD23	2.03	0.40
1:C:306:ALA:O	1:C:310:GLU:HG3	2.21	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	452/485 (93%)	434 (96%)	17 (4%)	1 (0%)	47 81
1	B	449/485 (93%)	443 (99%)	6 (1%)	0	100 100
1	C	449/485 (93%)	437 (97%)	11 (2%)	1 (0%)	47 81
1	D	448/485 (92%)	440 (98%)	8 (2%)	0	100 100
All	All	1798/1940 (93%)	1754 (98%)	42 (2%)	2 (0%)	51 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	129	LYS
1	A	50	PRO

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	358/384 (93%)	355 (99%)	3 (1%)	81 91
1	B	357/384 (93%)	355 (99%)	2 (1%)	86 94
1	C	358/384 (93%)	356 (99%)	2 (1%)	86 94
1	D	357/384 (93%)	354 (99%)	3 (1%)	81 91
All	All	1430/1536 (93%)	1420 (99%)	10 (1%)	84 93

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	PHE
1	A	419	THR
1	A	426	TRP
1	B	91	GLU
1	B	433	ASN
1	C	180	ASN

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Mol	Chain	Res	Type
1	C	372	PHE
1	D	184	ASP
1	D	298	THR
1	D	372	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 12 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 (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, 95^{th} 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	453/485 (93%)	0.41	38 (8%)	11 11	23, 49, 107, 178	0
1	B	453/485 (93%)	0.07	20 (4%)	34 30	21, 50, 95, 143	0
1	C	451/485 (92%)	0.21	41 (9%)	9 9	22, 49, 139, 174	0
1	D	451/485 (92%)	0.22	40 (8%)	9 10	32, 62, 114, 151	0
All	All	1808/1940 (93%)	0.23	139 (7%)	13 13	21, 54, 119, 178	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	THR	7.5
1	A	358	ILE	7.1
1	C	266	VAL	6.5
1	C	276	VAL	6.4
1	A	361	ASP	6.4
1	C	268	ILE	6.1
1	C	454	THR	6.1
1	C	274	ASN	6.0
1	A	356	GLN	5.8
1	C	267	ALA	5.7
1	C	272	GLY	5.7
1	A	359	LYS	5.5
1	C	264	ASN	5.4
1	D	232	PHE	5.2
1	C	263	LEU	5.1
1	A	360	GLY	5.1
1	A	357	VAL	5.0
1	C	273	GLU	5.0
1	D	129	LYS	4.9
1	D	128	ALA	4.9
1	A	121	SER	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	357	VAL	4.7
1	B	356	GLN	4.6
1	C	3	GLU	4.6
1	C	279	PHE	4.5
1	D	229	LEU	4.5
1	C	281	SER	4.4
1	D	127	GLY	4.4
1	A	362	LEU	4.3
1	A	351	TYR	4.3
1	A	347	TYR	4.3
1	D	234	PRO	4.2
1	C	271	GLY	4.2
1	A	274	ASN	4.0
1	C	5	THR	4.0
1	C	265	SER	4.0
1	A	278	VAL	3.9
1	B	3	GLU	3.9
1	A	352	SER	3.7
1	B	89	ASP	3.7
1	D	130	GLY	3.7
1	D	233	SER	3.6
1	C	270	ALA	3.6
1	D	231	ASP	3.6
1	A	127	GLY	3.6
1	A	271	GLY	3.6
1	C	260	MET	3.5
1	B	88	ARG	3.4
1	A	122	LEU	3.4
1	D	357	VAL	3.4
1	D	94	ASP	3.4
1	A	125	SER	3.4
1	D	355	ALA	3.3
1	D	353	GLU	3.3
1	C	350	THR	3.3
1	B	124	ARG	3.3
1	C	275	GLY	3.2
1	C	349	PHE	3.2
1	D	347	TYR	3.1
1	A	272	GLY	3.1
1	D	230	ARG	3.1
1	C	128	ALA	3.1
1	A	273	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	114	THR	3.1
1	D	350	THR	3.0
1	B	273	GLU	3.0
1	A	126	MET	3.0
1	C	278	VAL	3.0
1	B	129	LYS	3.0
1	D	102	ILE	2.9
1	D	123	PHE	2.9
1	A	119	ILE	2.9
1	D	133	VAL	2.9
1	A	426	TRP	2.9
1	C	282	ALA	2.9
1	D	115	MET	2.9
1	D	354	SER	2.9
1	A	355	ALA	2.9
1	D	120	ASP	2.9
1	A	123	PHE	2.8
1	D	359	LYS	2.8
1	A	363	ILE	2.8
1	A	270	ALA	2.8
1	A	342	ALA	2.8
1	D	124	ARG	2.8
1	C	6	THR	2.7
1	D	228	THR	2.7
1	B	354	SER	2.7
1	B	310	GLU	2.7
1	C	354	SER	2.7
1	B	232	PHE	2.7
1	D	134	GLU	2.7
1	D	113	ILE	2.6
1	C	4	LYS	2.6
1	C	280	THR	2.6
1	D	345	VAL	2.5
1	A	366	LEU	2.5
1	C	269	THR	2.5
1	B	125	SER	2.5
1	A	415	VAL	2.5
1	D	132	ALA	2.5
1	C	123	PHE	2.5
1	D	105	LEU	2.5
1	B	231	ASP	2.5
1	D	131	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	342	ALA	2.4
1	B	311	ARG	2.4
1	C	422	LEU	2.4
1	D	358	ILE	2.4
1	A	413	ILE	2.4
1	B	91	GLU	2.4
1	B	128	ALA	2.4
1	C	283	TRP	2.4
1	D	352	SER	2.3
1	C	131	GLU	2.3
1	C	125	SER	2.3
1	C	277	ALA	2.3
1	C	122	LEU	2.3
1	A	353	GLU	2.2
1	A	364	SER	2.2
1	B	448	ILE	2.2
1	B	122	LEU	2.2
1	A	354	SER	2.1
1	C	453	LYS	2.1
1	D	138	GLU	2.1
1	C	426	TRP	2.1
1	A	267	ALA	2.1
1	C	10	GLN	2.1
1	D	343	PRO	2.1
1	B	235	SER	2.1
1	D	351	TYR	2.1
1	C	424	GLY	2.1
1	A	4	LYS	2.1
1	A	365	ALA	2.1
1	D	122	LEU	2.1
1	A	129	LYS	2.0
1	C	261	PHE	2.0
1	D	226	ASP	2.0
1	B	131	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CS	C	503	1/1	0.54	0.11	211,211,211,211	0
2	CS	A	502	1/1	0.63	0.19	213,213,213,213	0
2	CS	A	504	1/1	0.67	0.10	204,204,204,204	0
2	CS	A	503	1/1	0.76	0.09	201,201,201,201	0
2	CS	D	502	1/1	0.81	0.20	197,197,197,197	0
2	CS	D	501	1/1	0.89	0.09	123,123,123,123	0
2	CS	C	502	1/1	0.96	0.09	138,138,138,138	0
2	CS	A	501	1/1	0.97	0.09	74,74,74,74	0
2	CS	B	502	1/1	0.97	0.13	120,120,120,120	1
2	CS	C	501	1/1	0.98	0.04	75,75,75,75	0
2	CS	B	501	1/1	0.99	0.08	80,80,80,80	0
2	CS	D	503	1/1	0.99	0.07	82,82,82,82	0

6.5 Other polymers (i)

There are no such residues in this entry.