



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:37 PM UTC

PDB ID : 3M6M / pdb_00003m6m
Title : Crystal structure of RpffF complexed with REC domain of RpfC
Authors : Cheng, Z.; Lim, S.C.; Qamra, R.; Song, H.
Deposited on : 2010-03-16
Resolution : 2.50 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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

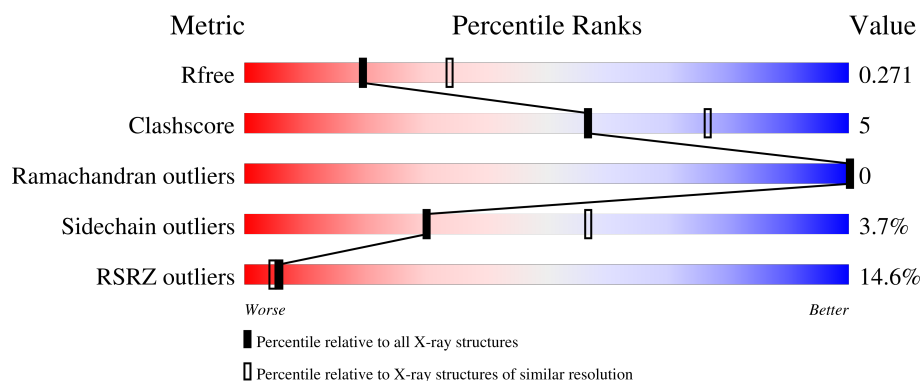
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	305	2% 76% 9% 14%
1	B	305	3% 78% 7% 14%
1	C	305	5% 74% 10% 14%
2	D	143	9% 66% 15% 17%
2	E	143	52% 69% 9% 21%

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Mol	Chain	Length	Quality of chain
2	F	143	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	IOD	C	292	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8717 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 RpPf protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			2016	1263	368	367	18			
1	B	263	Total	C	N	O	S	0	0	0
			2029	1272	370	369	18			
1	C	262	Total	C	N	O	S	0	0	0
			2024	1269	369	368	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP Q7CLS3
A	-14	GLY	-	expression tag	UNP Q7CLS3
A	-13	SER	-	expression tag	UNP Q7CLS3
A	-12	SER	-	expression tag	UNP Q7CLS3
A	-11	HIS	-	expression tag	UNP Q7CLS3
A	-10	HIS	-	expression tag	UNP Q7CLS3
A	-9	HIS	-	expression tag	UNP Q7CLS3
A	-8	HIS	-	expression tag	UNP Q7CLS3
A	-7	HIS	-	expression tag	UNP Q7CLS3
A	-6	HIS	-	expression tag	UNP Q7CLS3
A	-5	SER	-	expression tag	UNP Q7CLS3
A	-4	GLN	-	expression tag	UNP Q7CLS3
A	-3	ASP	-	expression tag	UNP Q7CLS3
A	-2	PRO	-	expression tag	UNP Q7CLS3
A	-1	ASN	-	expression tag	UNP Q7CLS3
A	0	SER	-	expression tag	UNP Q7CLS3
B	-15	MET	-	expression tag	UNP Q7CLS3
B	-14	GLY	-	expression tag	UNP Q7CLS3
B	-13	SER	-	expression tag	UNP Q7CLS3
B	-12	SER	-	expression tag	UNP Q7CLS3
B	-11	HIS	-	expression tag	UNP Q7CLS3
B	-10	HIS	-	expression tag	UNP Q7CLS3
B	-9	HIS	-	expression tag	UNP Q7CLS3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP Q7CLS3
B	-7	HIS	-	expression tag	UNP Q7CLS3
B	-6	HIS	-	expression tag	UNP Q7CLS3
B	-5	SER	-	expression tag	UNP Q7CLS3
B	-4	GLN	-	expression tag	UNP Q7CLS3
B	-3	ASP	-	expression tag	UNP Q7CLS3
B	-2	PRO	-	expression tag	UNP Q7CLS3
B	-1	ASN	-	expression tag	UNP Q7CLS3
B	0	SER	-	expression tag	UNP Q7CLS3
C	-15	MET	-	expression tag	UNP Q7CLS3
C	-14	GLY	-	expression tag	UNP Q7CLS3
C	-13	SER	-	expression tag	UNP Q7CLS3
C	-12	SER	-	expression tag	UNP Q7CLS3
C	-11	HIS	-	expression tag	UNP Q7CLS3
C	-10	HIS	-	expression tag	UNP Q7CLS3
C	-9	HIS	-	expression tag	UNP Q7CLS3
C	-8	HIS	-	expression tag	UNP Q7CLS3
C	-7	HIS	-	expression tag	UNP Q7CLS3
C	-6	HIS	-	expression tag	UNP Q7CLS3
C	-5	SER	-	expression tag	UNP Q7CLS3
C	-4	GLN	-	expression tag	UNP Q7CLS3
C	-3	ASP	-	expression tag	UNP Q7CLS3
C	-2	PRO	-	expression tag	UNP Q7CLS3
C	-1	ASN	-	expression tag	UNP Q7CLS3
C	0	SER	-	expression tag	UNP Q7CLS3

- Molecule 2 is a protein called Sensory/regulatory protein rpfC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	118	Total	C	N	O	S	0	0	0
			896	560	158	167	11			
2	E	113	Total	C	N	O	S	0	0	0
			852	532	150	160	10			
2	F	115	Total	C	N	O	S	0	0	0
			868	543	152	162	11			

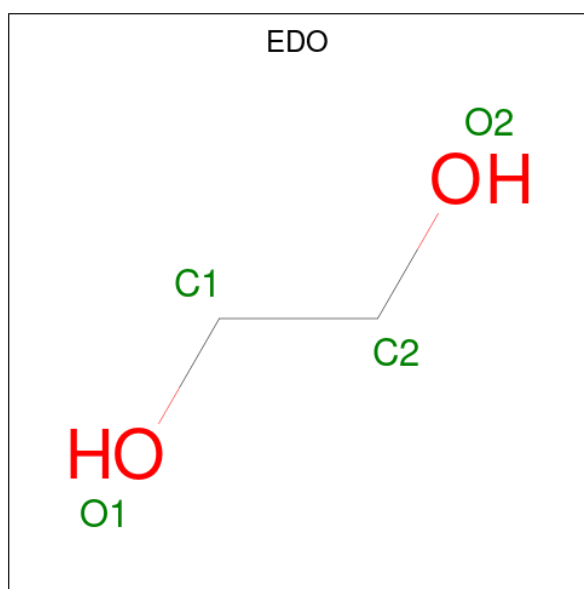
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	448	MET	-	expression tag	UNP P0C0F6
E	448	MET	-	expression tag	UNP P0C0F6
F	448	MET	-	expression tag	UNP P0C0F6

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total I 2 2	0	0
3	B	2	Total I 2 2	0	0
3	C	4	Total I 4 4	0	0
3	D	2	Total I 2 2	0	0
3	E	2	Total I 2 2	0	0
3	F	2	Total I 2 2	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total 1	Mg 1	0	0
5	E	1	Total 1	Mg 1	0	0
5	F	1	Total 1	Mg 1	0	0

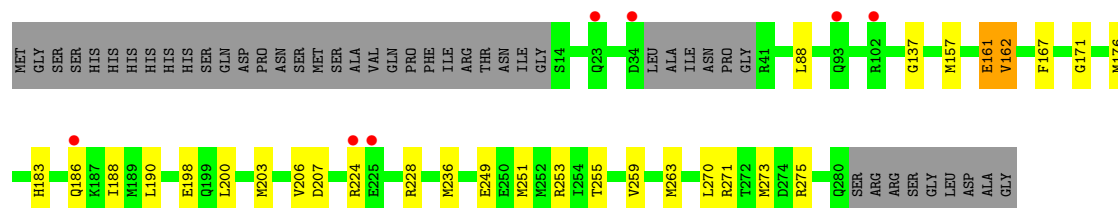
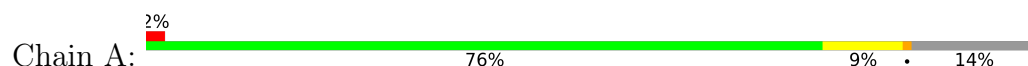
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total 3	O 3	0	0

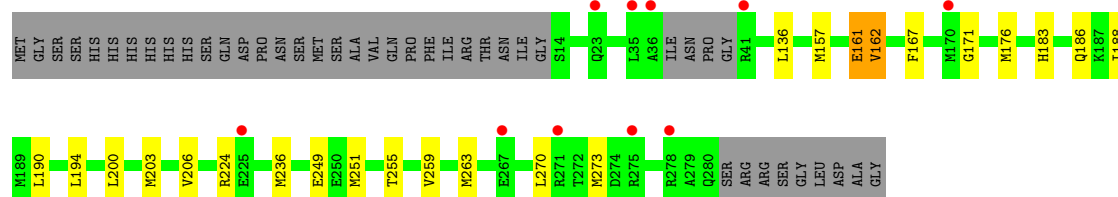
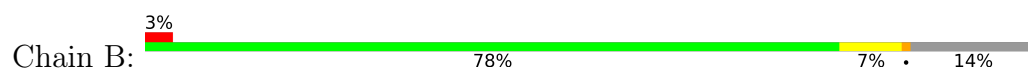
3 Residue-property plots [i](#)

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.

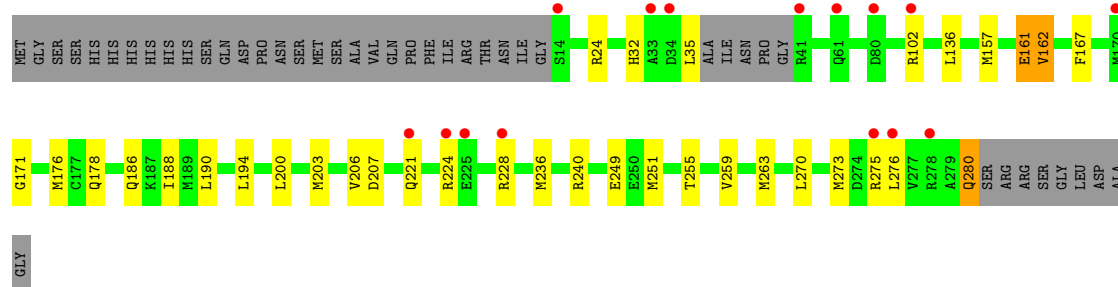
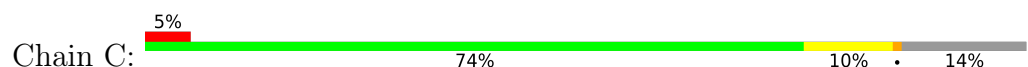
- Molecule 1: RpPf protein



- Molecule 1: RpPf protein

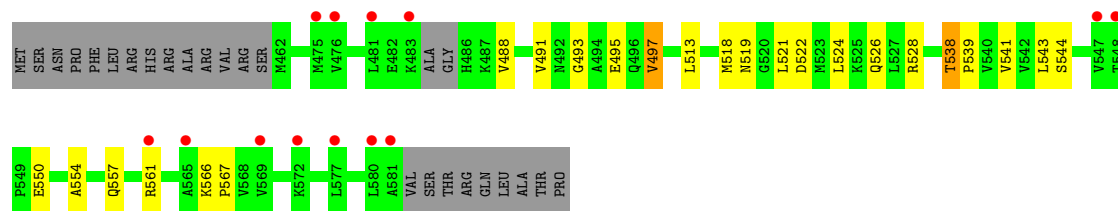


- Molecule 1: RpPf protein

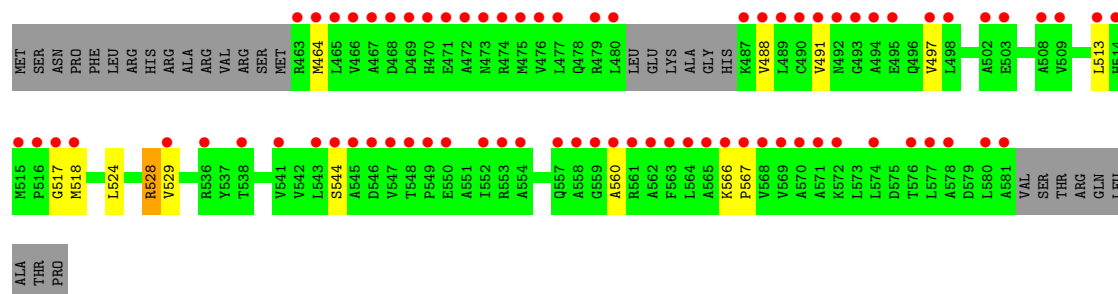


- Molecule 2: Sensory/regulatory protein rpfC

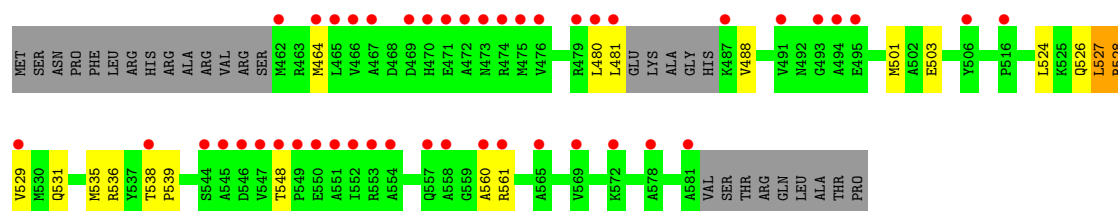




● Molecule 2: Sensory/regulatory protein rpfc



● Molecule 2: Sensory/regulatory protein rpfc



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	130.91Å 130.91Å 156.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.50) 99.8 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.32 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.250 , 0.271 0.250 , 0.271	Depositor DCC
R_{free} test set	2667 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 18.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8717	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: EDO, IOD, MG

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	0.44	0/2049	0.81	3/2768 (0.1%)
1	B	0.42	0/2062	0.80	3/2786 (0.1%)
1	C	0.43	0/2057	0.85	5/2779 (0.2%)
2	D	0.44	0/904	0.81	0/1220
2	E	0.44	0/859	0.75	0/1161
2	F	0.43	0/875	0.77	0/1182
All	All	0.43	0/8806	0.81	11/11896 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	24	ARG	NE-CZ-NH2	8.34	126.70	119.20
1	C	24	ARG	NE-CZ-NH1	-7.96	113.54	121.50
1	C	102	ARG	NE-CZ-NH2	7.56	126.00	119.20
1	A	253	ARG	NE-CZ-NH2	7.35	125.81	119.20
1	C	102	ARG	NE-CZ-NH1	-6.99	114.52	121.50
1	A	253	ARG	NE-CZ-NH1	-6.91	114.59	121.50
1	B	224	ARG	NE-CZ-NH2	-6.47	113.38	119.20
1	B	224	ARG	CD-NE-CZ	6.10	132.94	124.40
1	B	224	ARG	NE-CZ-NH1	5.50	127.00	121.50
1	C	24	ARG	CD-NE-CZ	5.33	131.86	124.40
1	A	224	ARG	NE-CZ-NH2	5.02	123.72	119.20

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	2016	0	2017	25	0
1	B	2029	0	2033	14	0
1	C	2024	0	2028	28	0
2	D	896	0	921	23	0
2	E	852	0	875	8	0
2	F	868	0	895	11	0
3	A	2	0	0	1	0
3	B	2	0	0	0	0
3	C	4	0	0	2	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	4	0	6	2	0
4	B	4	0	6	0	0
4	C	4	0	6	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	B	3	0	0	0	0
All	All	8717	0	8787	81	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 5.

All (81) 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:C:178:GLN:OE1	3:C:292:IOD:I	2.51	0.98
1:C:275:ARG:HH21	2:F:526:GLN:HE22	1.28	0.81
1:C:228:ARG:NH2	2:D:522:ASP:CG	2.45	0.74
1:A:275:ARG:NH2	2:D:518:MET:HE1	2.03	0.74
1:C:228:ARG:NH2	2:D:522:ASP:OD2	2.23	0.72
1:A:88:LEU:HD21	4:A:902:EDO:H22	1.76	0.67
1:C:228:ARG:CZ	2:D:522:ASP:OD1	2.43	0.66
1:A:207:ASP:OD1	1:B:183:HIS:HE1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:GLN:HE22	2:D:554:ALA:HB2	1.63	0.64
1:A:137:GLY:HA3	4:A:902:EDO:H12	1.79	0.64
1:B:162:VAL:HG11	1:B:190:LEU:HA	1.80	0.63
1:C:162:VAL:HG11	1:C:190:LEU:HA	1.82	0.62
1:C:221:GLN:HG3	2:D:550:GLU:HG3	1.80	0.62
1:A:162:VAL:HG11	1:A:190:LEU:HA	1.83	0.61
1:B:236:MET:HA	1:B:236:MET:HE2	1.83	0.61
1:C:236:MET:HA	1:C:236:MET:HE2	1.83	0.60
1:A:236:MET:HA	1:A:236:MET:HE2	1.83	0.59
1:C:228:ARG:NH2	2:D:522:ASP:OD1	2.35	0.59
1:A:200:LEU:HA	1:A:203:MET:HE3	1.86	0.58
1:A:275:ARG:HH22	2:D:518:MET:HE1	1.69	0.58
1:A:228:ARG:NH2	2:E:518:MET:HA	2.19	0.58
2:D:513:LEU:HB3	2:D:544:SER:HB3	1.86	0.58
1:C:200:LEU:HA	1:C:203:MET:HE3	1.87	0.57
1:B:200:LEU:HA	1:B:203:MET:HE3	1.86	0.57
1:A:176:MET:HE1	1:A:188:ILE:HG21	1.87	0.56
1:B:176:MET:HE1	1:B:188:ILE:HG21	1.87	0.55
1:C:176:MET:HE1	1:C:188:ILE:HG21	1.88	0.55
2:F:524:LEU:HD21	2:F:560:ALA:HB2	1.88	0.55
1:A:271:ARG:HH12	2:D:495:GLU:CD	2.15	0.54
1:C:157:MET:HB2	1:C:200:LEU:HD11	1.90	0.54
1:A:183:HIS:HE1	1:C:207:ASP:OD1	1.90	0.54
1:C:32:HIS:HB3	1:C:35:LEU:HD12	1.90	0.54
1:B:157:MET:HB2	1:B:200:LEU:HD11	1.90	0.53
1:A:167:PHE:CD1	1:C:236:MET:HE3	2.44	0.53
1:A:157:MET:HB2	1:A:200:LEU:HD11	1.90	0.53
1:C:275:ARG:HH21	2:F:526:GLN:NE2	2.03	0.53
1:A:228:ARG:NH2	2:E:517:GLY:O	2.42	0.52
1:C:276:LEU:O	1:C:280:GLN:HB3	2.10	0.52
1:A:207:ASP:OD1	1:B:183:HIS:CE1	2.61	0.52
1:C:259:VAL:O	1:C:263:MET:HG2	2.10	0.51
1:A:236:MET:HE3	1:B:167:PHE:CD1	2.45	0.50
1:A:271:ARG:NH1	2:D:495:GLU:CD	2.69	0.50
2:E:513:LEU:HB3	2:E:544:SER:HB3	1.93	0.49
1:C:136:LEU:HD13	2:F:529:VAL:HG23	1.94	0.49
1:B:259:VAL:O	1:B:263:MET:HG2	2.13	0.48
1:B:194:LEU:HD12	2:E:528:ARG:HG3	1.95	0.48
1:B:136:LEU:HD13	2:E:529:VAL:HG23	1.95	0.48
1:A:259:VAL:O	1:A:263:MET:HG2	2.14	0.47
1:A:275:ARG:HH21	2:D:526:GLN:HE22	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:531:GLN:NE2	2:F:538:THR:H	2.13	0.46
1:C:194:LEU:HD12	2:F:528:ARG:HG3	1.98	0.46
1:C:240:ARG:NE	3:C:292:IOD:I	3.18	0.46
2:D:513:LEU:O	2:D:519:ASN:HB2	2.16	0.46
1:A:171:GLY:HA3	1:A:251:MET:HE3	1.98	0.46
2:D:493:GLY:O	2:D:497:VAL:HG12	2.16	0.46
1:A:275:ARG:HH21	2:D:526:GLN:NE2	2.14	0.46
1:C:224:ARG:HH22	2:D:521:LEU:HD23	1.81	0.46
2:D:539:PRO:HB3	2:D:561:ARG:HD3	1.98	0.46
1:C:171:GLY:HA3	1:C:251:MET:HE3	1.98	0.45
1:C:221:GLN:CG	2:D:550:GLU:HG3	2.46	0.45
1:A:270:LEU:HA	1:A:273:MET:HE3	1.98	0.45
2:D:543:LEU:HB3	2:D:566:LYS:HD2	1.97	0.45
2:E:566:LYS:HA	2:E:567:PRO:C	2.41	0.45
1:B:171:GLY:HA3	1:B:251:MET:HE3	1.99	0.45
1:C:270:LEU:HA	1:C:273:MET:HE3	1.99	0.45
1:B:270:LEU:HA	1:B:273:MET:HE3	1.99	0.45
1:C:228:ARG:CZ	2:D:522:ASP:CG	2.89	0.44
1:B:161:GLU:HG3	1:B:167:PHE:C	2.43	0.44
1:A:161:GLU:HG3	1:A:167:PHE:C	2.43	0.43
1:C:161:GLU:HG3	1:C:167:PHE:C	2.43	0.43
2:F:539:PRO:HB3	2:F:561:ARG:HD3	2.01	0.42
2:E:464:MET:HB2	2:E:488:VAL:HG22	2.01	0.42
2:D:538:THR:HA	2:D:539:PRO:HD3	1.85	0.42
2:D:528:ARG:NH2	2:D:557:GLN:O	2.53	0.41
2:F:464:MET:HB2	2:F:488:VAL:HG22	2.02	0.41
2:F:501:MET:HB3	2:F:535:MET:HE1	2.03	0.41
2:F:501:MET:HE1	2:F:527:LEU:HD21	2.02	0.41
2:F:464:MET:HG3	2:F:481:LEU:HD23	2.03	0.41
1:A:198:GLU:HB2	3:A:290:IOD:I	2.91	0.41
2:D:566:LYS:HA	2:D:567:PRO:C	2.46	0.40
2:E:524:LEU:HD21	2:E:560:ALA:HB2	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	257/305 (84%)	254 (99%)	3 (1%)	0	100	100
1	B	259/305 (85%)	255 (98%)	4 (2%)	0	100	100
1	C	258/305 (85%)	254 (98%)	4 (2%)	0	100	100
2	D	114/143 (80%)	113 (99%)	1 (1%)	0	100	100
2	E	109/143 (76%)	107 (98%)	2 (2%)	0	100	100
2	F	111/143 (78%)	109 (98%)	2 (2%)	0	100	100
All	All	1108/1344 (82%)	1092 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	210/246 (85%)	204 (97%)	6 (3%)	37	65
1	B	211/246 (86%)	205 (97%)	6 (3%)	38	66
1	C	211/246 (86%)	204 (97%)	7 (3%)	33	61
2	D	95/116 (82%)	89 (94%)	6 (6%)	16	34
2	E	90/116 (78%)	87 (97%)	3 (3%)	33	61
2	F	92/116 (79%)	86 (94%)	6 (6%)	15	32
All	All	909/1086 (84%)	875 (96%)	34 (4%)	30	57

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

Mol	Chain	Res	Type
1	A	161	GLU
1	A	162	VAL
1	A	186	GLN

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Mol	Chain	Res	Type
1	A	206	VAL
1	A	249	GLU
1	A	255	THR
1	B	161	GLU
1	B	162	VAL
1	B	186	GLN
1	B	206	VAL
1	B	249	GLU
1	B	255	THR
1	C	161	GLU
1	C	162	VAL
1	C	186	GLN
1	C	206	VAL
1	C	249	GLU
1	C	255	THR
1	C	280	GLN
2	D	488	VAL
2	D	491	VAL
2	D	497	VAL
2	D	524	LEU
2	D	538	THR
2	D	541	VAL
2	E	491	VAL
2	E	497	VAL
2	E	528	ARG
2	F	480	LEU
2	F	503	GLU
2	F	527	LEU
2	F	528	ARG
2	F	536	ARG
2	F	548	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	HIS
1	A	231	HIS
1	B	32	HIS
1	B	183	HIS
1	B	193	ASN
1	C	32	HIS
1	C	183	HIS

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Mol	Chain	Res	Type
1	C	193	ASN
1	C	221	GLN
1	C	231	HIS
2	D	478	GLN
2	D	486	HIS
2	D	492	ASN
2	D	526	GLN
2	D	557	GLN
2	F	526	GLN
2	F	557	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 17 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	A	902	-	3,3,3	0.37	0	2,2,2	0.36	0
4	EDO	B	903	-	3,3,3	0.33	0	2,2,2	0.54	0
4	EDO	C	904	-	3,3,3	0.29	0	2,2,2	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	902	-	-	0/1/1/1	-
4	EDO	B	903	-	-	1/1/1/1	-
4	EDO	C	904	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	904	EDO	O1-C1-C2-O2
4	B	903	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	902	EDO	2	0

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	261/305 (85%)	0.15	7 (2%) 56 51	25, 39, 51, 61	0
1	B	263/305 (86%)	0.20	10 (3%) 44 39	26, 41, 56, 69	0
1	C	262/305 (85%)	0.33	15 (5%) 29 26	27, 45, 61, 74	0
2	D	118/143 (82%)	0.83	13 (11%) 10 8	42, 62, 88, 97	0
2	E	113/143 (79%)	2.48	75 (66%) 0 0	60, 110, 148, 154	0
2	F	115/143 (80%)	1.84	45 (39%) 1 0	58, 88, 121, 136	0
All	All	1132/1344 (84%)	0.68	165 (14%) 6 4	25, 45, 119, 154	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	581	ALA	7.6
2	F	462	MET	6.3
2	F	547	VAL	6.1
2	F	581	ALA	5.4
2	E	465	LEU	4.9
2	E	558	ALA	4.6
2	E	547	VAL	4.4
2	E	557	GLN	4.3
2	E	494	ALA	4.3
2	F	481	LEU	4.3
1	C	224	ARG	4.0
2	E	567	PRO	4.0
2	F	475	MET	4.0
2	E	470	HIS	3.9
2	E	564	LEU	3.9
2	F	476	VAL	3.9
2	F	548	THR	3.8
1	C	170	MET	3.8
2	E	503	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	581	ALA	3.7
2	E	548	THR	3.7
2	F	465	LEU	3.7
2	E	549	PRO	3.7
2	E	473	ASN	3.6
2	F	491	VAL	3.6
2	E	472	ALA	3.6
1	B	278	ARG	3.5
1	C	225	GLU	3.5
2	E	569	VAL	3.5
1	A	102	ARG	3.5
2	E	574	LEU	3.5
1	A	23	GLN	3.4
2	F	565	ALA	3.4
2	E	577	LEU	3.4
2	E	468	ASP	3.4
2	E	509	VAL	3.4
2	E	580	LEU	3.4
2	E	552	ILE	3.4
2	E	563	PHE	3.3
2	E	571	ALA	3.3
2	F	472	ALA	3.3
1	A	93	GLN	3.3
1	C	221	GLN	3.3
2	F	551	ALA	3.3
2	E	476	VAL	3.3
2	E	469	ASP	3.3
2	E	565	ALA	3.3
2	E	488	VAL	3.2
2	E	554	ALA	3.2
2	E	475	MET	3.2
2	E	480	LEU	3.2
2	E	487	LYS	3.2
2	E	493	GLY	3.2
2	E	560	ALA	3.2
2	E	570	ALA	3.2
2	E	489	LEU	3.2
2	E	492	ASN	3.2
2	E	529	VAL	3.2
2	E	576	THR	3.1
1	B	275	ARG	3.1
2	E	550	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	464	MET	3.1
1	B	23	GLN	3.1
2	D	548	THR	3.0
1	B	225	GLU	3.0
2	E	502	ALA	3.0
2	F	464	MET	3.0
2	D	481	LEU	3.0
1	C	14	SER	3.0
2	F	516	PRO	3.0
2	E	498	LEU	3.0
1	C	34	ASP	3.0
2	E	559	GLY	3.0
2	E	491	VAL	3.0
2	E	518	MET	3.0
2	F	560	ALA	3.0
2	F	544	SER	3.0
2	E	471	GLU	2.9
2	F	553	ARG	2.9
1	B	36	ALA	2.9
2	F	550	GLU	2.9
2	E	477	LEU	2.9
2	E	566	LYS	2.8
1	B	41	ARG	2.8
2	E	568	VAL	2.8
2	D	483	LYS	2.8
2	E	546	ASP	2.8
2	F	493	GLY	2.8
2	F	552	ILE	2.8
2	E	543	LEU	2.8
2	E	561	ARG	2.8
2	F	549	PRO	2.7
2	E	508	ALA	2.7
2	E	466	VAL	2.7
2	E	544	SER	2.7
1	B	35	LEU	2.7
2	F	578	ALA	2.7
2	E	490	CYS	2.7
1	B	271	ARG	2.7
2	E	463	ARG	2.7
2	E	497	VAL	2.7
2	F	554	ALA	2.7
2	E	467	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	F	494	ALA	2.6
2	F	473	ASN	2.6
2	E	495	GLU	2.6
2	F	545	ALA	2.6
1	A	224	ARG	2.6
1	A	34	ASP	2.6
2	D	547	VAL	2.6
2	E	541	VAL	2.5
2	F	467	ALA	2.5
2	D	561	ARG	2.5
2	F	487	LYS	2.5
1	C	33	ALA	2.5
2	F	495	GLU	2.5
2	F	557	GLN	2.5
2	E	562	ALA	2.5
2	D	475	MET	2.5
2	F	469	ASP	2.4
1	C	278	ARG	2.4
2	E	536	ARG	2.4
2	E	553	ARG	2.4
1	C	275	ARG	2.4
2	E	514	HIS	2.4
2	D	572	LYS	2.4
2	F	538	THR	2.3
2	F	474	ARG	2.3
1	C	276	LEU	2.3
2	F	558	ALA	2.3
1	C	61	GLN	2.3
1	B	267	GLU	2.3
2	D	476	VAL	2.3
2	F	506	TYR	2.3
2	F	470	HIS	2.3
2	E	513	LEU	2.3
2	F	529	VAL	2.3
1	A	186	GLN	2.2
2	D	577	LEU	2.2
2	D	580	LEU	2.2
1	C	102	ARG	2.2
1	C	228	ARG	2.2
2	D	569	VAL	2.2
2	E	517	GLY	2.2
1	C	80	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	479	ARG	2.2
2	E	516	PRO	2.2
2	E	572	LYS	2.2
2	E	515	MET	2.2
1	A	225	GLU	2.2
2	F	561	ARG	2.2
2	D	565	ALA	2.1
2	E	545	ALA	2.1
2	F	480	LEU	2.1
2	F	479	ARG	2.1
1	B	170	MET	2.1
2	F	569	VAL	2.1
2	E	578	ALA	2.1
2	E	474	ARG	2.1
2	F	546	ASP	2.1
2	E	538	THR	2.1
2	F	471	GLU	2.1
2	F	572	LYS	2.0
1	C	41	ARG	2.0
2	F	466	VAL	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(Å ²)	Q<0.9
5	MG	E	591	1/1	0.77	0.17	63,63,63,63	0
5	MG	F	3	1/1	0.77	0.23	76,76,76,76	0
3	IOD	E	3	1/1	0.78	0.13	121,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	D	591	1/1	0.84	0.27	53,53,53,53	0
4	EDO	C	904	4/4	0.86	0.18	28,28,29,30	0
3	IOD	F	7	1/1	0.90	0.10	119,119,119,119	0
4	EDO	B	903	4/4	0.91	0.18	35,35,36,36	0
4	EDO	A	902	4/4	0.93	0.13	26,26,27,29	0
3	IOD	A	291	1/1	0.93	0.20	120,120,120,120	0
3	IOD	A	290	1/1	0.94	0.17	123,123,123,123	0
3	IOD	C	293	1/1	0.94	0.13	105,105,105,105	0
3	IOD	C	290	1/1	0.95	0.19	130,130,130,130	0
3	IOD	B	291	1/1	0.95	0.14	116,116,116,116	0
3	IOD	B	290	1/1	0.96	0.16	102,102,102,102	0
3	IOD	D	6	1/1	0.97	0.16	131,131,131,131	0
3	IOD	C	292	1/1	0.97	0.26	103,103,103,103	0
3	IOD	F	4	1/1	0.97	0.12	126,126,126,126	0
3	IOD	C	291	1/1	0.97	0.19	117,117,117,117	0
3	IOD	D	1	1/1	0.97	0.06	64,64,64,64	0
3	IOD	E	2	1/1	0.98	0.08	86,86,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.