



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:12 pm BST

PDB ID : 3M6M  
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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

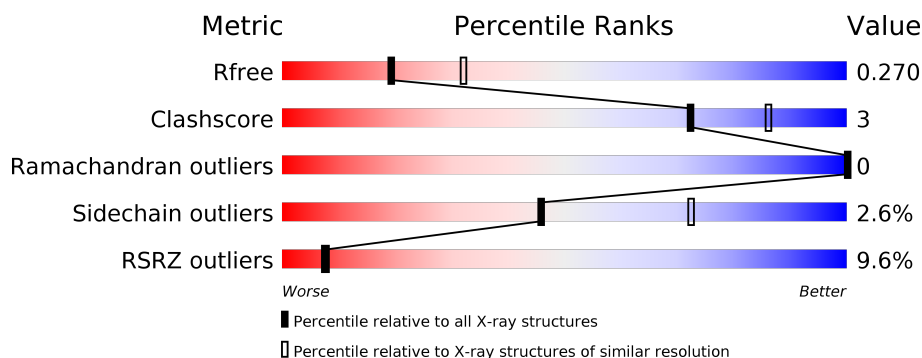
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>0%</div> <div> <div></div> <div>78%</div> <div>7%</div> <div>14%</div> </div> </div>
1	B	305	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>5%</div> <div>14%</div> </div> </div>
1	C	305	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>7%</div> <div>14%</div> </div> </div>
2	D	143	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>13%</div> <div>17%</div> </div> </div>
2	E	143	<div> <div>34%</div> <div> <div></div> <div>70%</div> <div>8%</div> <div>21%</div> </div> </div>
2	F	143	<div> <div>17%</div> <div> <div></div> <div>69%</div> <div>10%</div> <div>20%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit 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			

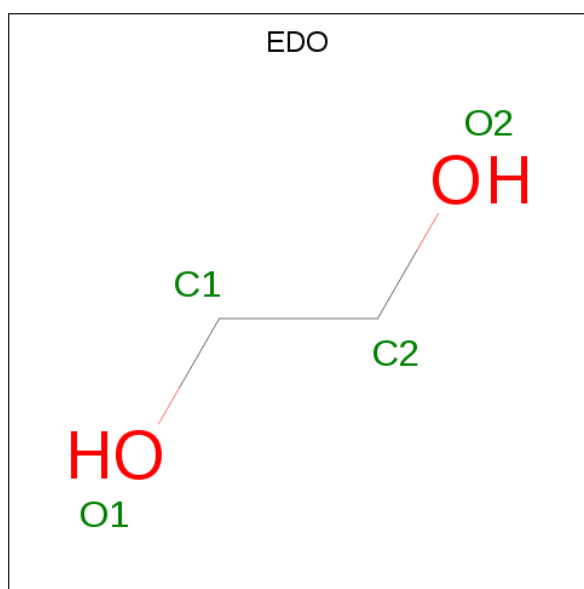
There are 3 discrepancies between the modelled and reference sequences:

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 (three-letter code: IOD) (formula: I).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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 (three-letter code: MG) (formula: Mg).

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

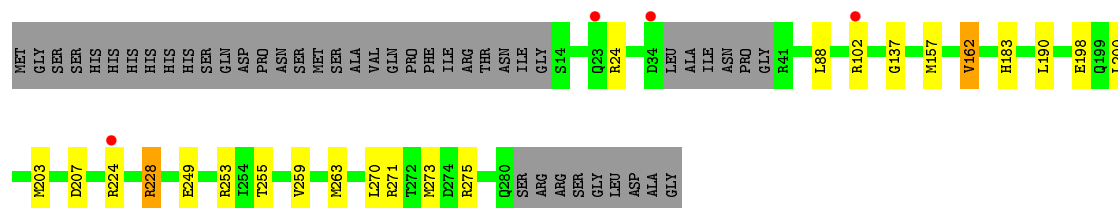
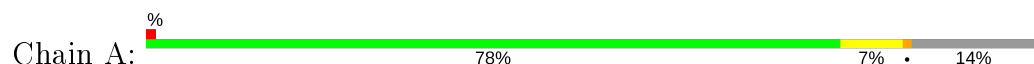
- Molecule 6 is water.

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

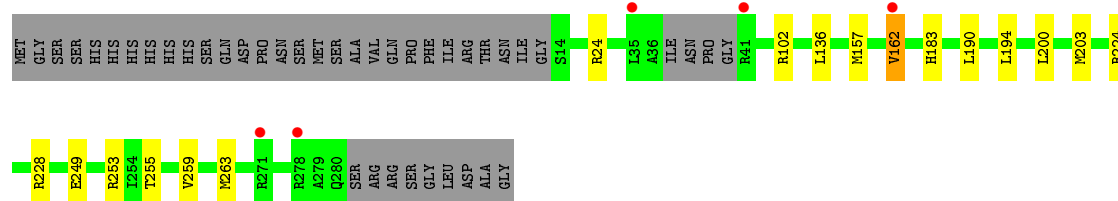
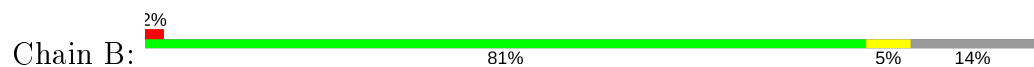
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

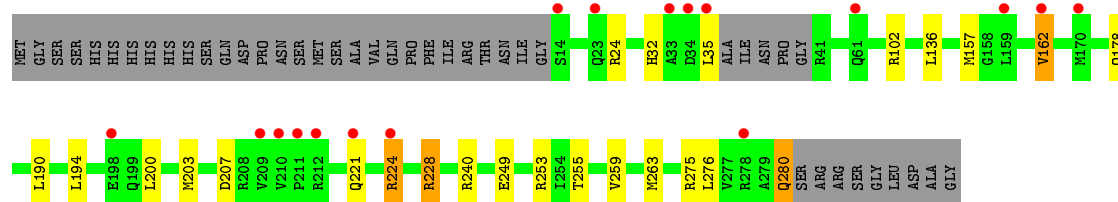
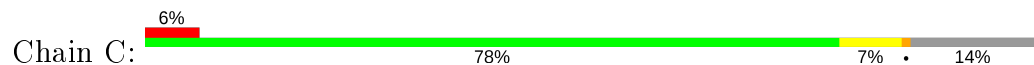
#### • Molecule 1: Rpff protein



#### • Molecule 1: Rpff protein



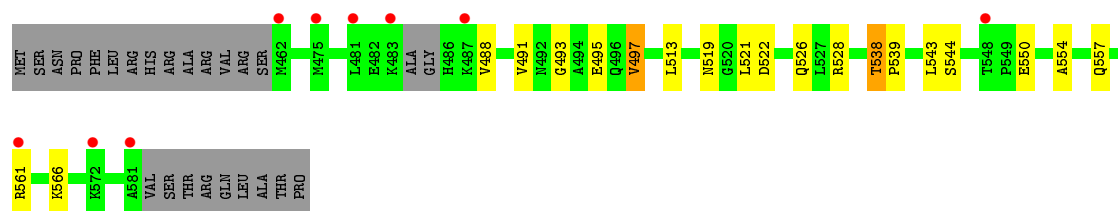
#### • Molecule 1: Rpff protein



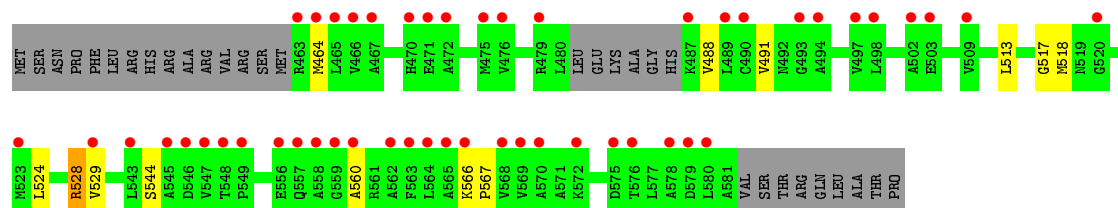
#### • Molecule 2: Sensory/regulatory protein rpfc



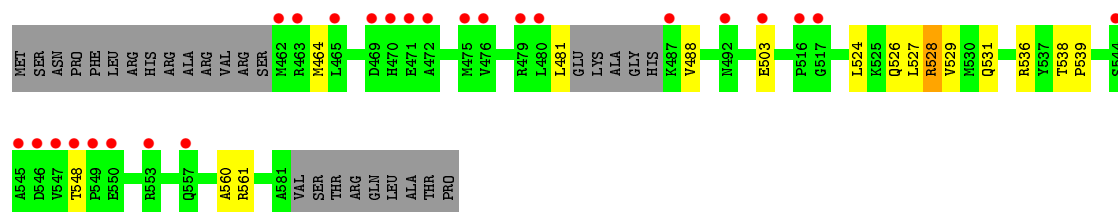




• Molecule 2: Sensory/regulatory protein rpfc



• Molecule 2: Sensory/regulatory protein rpfc



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.91Å 130.91Å 156.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 29.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.50) 100.0 (29.18-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	8.32 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, $R_{free}$	0.250 , 0.271 0.250 , 0.270	Depositor DCC
$R_{free}$ test set	2667 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 27.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, IOD, EDO

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	0.33	0/2049	0.64	8/2768 (0.3%)
1	B	0.32	0/2062	0.68	9/2786 (0.3%)
1	C	0.32	0/2057	0.72	10/2779 (0.4%)
2	D	0.31	0/904	0.50	0/1220
2	E	0.30	0/859	0.46	0/1161
2	F	0.30	0/875	0.48	0/1182
All	All	0.32	0/8806	0.63	27/11896 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	ARG	NE-CZ-NH2	-13.84	113.38	120.30
1	C	24	ARG	NE-CZ-NH1	-13.53	113.54	120.30
1	B	224	ARG	NE-CZ-NH1	13.40	127.00	120.30
1	C	24	ARG	NE-CZ-NH2	12.80	126.70	120.30
1	C	102	ARG	NE-CZ-NH1	-11.57	114.52	120.30
1	A	253	ARG	NE-CZ-NH1	-11.43	114.59	120.30
1	C	102	ARG	NE-CZ-NH2	11.41	126.00	120.30
1	A	253	ARG	NE-CZ-NH2	11.03	125.81	120.30
1	A	224	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	C	224	ARG	NE-CZ-NH1	-7.05	116.78	120.30
1	A	224	ARG	NE-CZ-NH2	6.83	123.72	120.30
1	B	24	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	24	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	224	ARG	CD-NE-CZ	6.67	132.94	123.60
1	C	224	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	B	253	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	24	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	B	24	ARG	NE-CZ-NH2	-6.31	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	253	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	102	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	102	ARG	NE-CZ-NH2	-6.09	117.26	120.30
1	B	253	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	102	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	24	ARG	CD-NE-CZ	5.90	131.86	123.60
1	C	253	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	102	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	102	ARG	CD-NE-CZ	5.40	131.16	123.60

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	17	0
1	B	2029	0	2033	8	0
1	C	2024	0	2028	21	0
2	D	896	0	921	19	0
2	E	852	0	875	8	0
2	F	868	0	895	9	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	59	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 3.

All (59) 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:OD2	2.23	0.72
1:C:228:ARG:NH2	2:D:522:ASP:CG	2.45	0.70
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
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:C:228:ARG:NH2	2:D:522:ASP:OD1	2.35	0.59
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
2:F:524:LEU:HD21	2:F:560:ALA:HB2	1.88	0.55
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: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:271:ARG:HH12	2:D:495:GLU:CD	2.15	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
1:C:200:LEU:HA	1:C:203:MET:HE3	1.97	0.47
2:F:531:GLN:NE2	2:F:538:THR:H	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:194:LEU:HD12	2:F:528:ARG:HG3	1.98	0.46
1:B:200:LEU:HA	1:B:203: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:221:GLN:CG	2:D:550:GLU:HG3	2.46	0.45
2:D:543:LEU:HB3	2:D:566:LYS:HD2	1.97	0.45
1:A:271:ARG:NH1	2:D:495:GLU:CD	2.69	0.45
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:E:566:LYS:HA	2:E:567:PRO:C	2.41	0.41
1:A:200:LEU:HA	1:A:203:MET:HE3	2.03	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:E:524:LEU:HD21	2:E:560:ALA:HB2	2.02	0.40
1:A:270:LEU:HA	1:A:273:MET:HE3	2.04	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	206 (98%)	4 (2%)	57	80
1	B	211/246 (86%)	207 (98%)	4 (2%)	57	80
1	C	211/246 (86%)	206 (98%)	5 (2%)	49	74
2	D	95/116 (82%)	91 (96%)	4 (4%)	30	54
2	E	90/116 (78%)	88 (98%)	2 (2%)	52	77
2	F	92/116 (79%)	87 (95%)	5 (5%)	22	42
All	All	909/1086 (84%)	885 (97%)	24 (3%)	46	72

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	VAL
1	A	228	ARG
1	A	249	GLU
1	A	255	THR
1	B	162	VAL
1	B	228	ARG
1	B	249	GLU
1	B	255	THR
1	C	162	VAL
1	C	228	ARG

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Mol	Chain	Res	Type
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	538	THR
2	E	491	VAL
2	E	528	ARG
2	F	503	GLU
2	F	527	LEU
2	F	528	ARG
2	F	536	ARG
2	F	548	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
1	B	183	HIS
1	B	280	GLN
1	C	183	HIS
1	C	221	GLN
1	C	231	HIS
2	D	486	HIS
2	D	492	ASN
2	E	514	HIS
2	F	526	GLN
2	F	531	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 carbohydrates 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	C	904	-	3,3,3	0.32	0	2,2,2	0.55	0
4	EDO	B	903	-	3,3,3	0.35	0	2,2,2	0.50	0
4	EDO	A	902	-	3,3,3	0.39	0	2,2,2	0.32	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	C	904	-	-	1/1/1/1	-
4	EDO	B	903	-	-	1/1/1/1	-
4	EDO	A	902	-	-	0/1/1/1	-

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	B	903	EDO	O1-C1-C2-O2
4	C	904	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	261/305 (85%)	0.01	4 (1%) 73 75	25, 39, 51, 61	0
1	B	263/305 (86%)	0.18	5 (1%) 66 69	26, 41, 56, 69	0
1	C	262/305 (85%)	0.33	17 (6%) 18 19	27, 45, 61, 74	0
2	D	118/143 (82%)	0.43	9 (7%) 13 14	42, 62, 88, 97	0
2	E	113/143 (79%)	1.90	49 (43%) 0 0	60, 110, 148, 154	0
2	F	115/143 (80%)	1.45	25 (21%) 0 0	58, 88, 121, 136	0
All	All	1132/1344 (84%)	0.50	109 (9%) 8 7	25, 45, 119, 154	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	553	ARG	8.4
2	F	547	VAL	7.1
2	E	471	GLU	6.0
2	F	516	PRO	5.5
2	E	564	LEU	5.5
2	F	549	PRO	5.3
2	F	462	MET	5.2
2	F	548	THR	5.1
2	E	503	GLU	5.0
2	E	578	ALA	4.8
1	C	33	ALA	4.7
2	E	487	LYS	4.5
2	F	470	HIS	4.4
2	F	517	GLY	4.3
2	E	465	LEU	4.3
1	B	278	ARG	4.2
2	F	475	MET	4.2
1	C	34	ASP	4.2
2	F	550	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
2	E	472	ALA	4.0
1	C	210	VAL	4.0
2	E	489	LEU	3.9
2	E	557	GLN	3.9
2	E	575	ASP	3.6
2	F	479	ARG	3.6
2	E	467	ALA	3.6
2	E	543	LEU	3.5
2	E	547	VAL	3.5
2	E	470	HIS	3.4
1	C	23	GLN	3.4
2	E	549	PRO	3.4
1	B	271	ARG	3.4
1	C	14	SER	3.3
2	E	569	VAL	3.3
2	E	479	ARG	3.3
2	F	503	GLU	3.3
2	E	502	ALA	3.2
2	D	572	LYS	3.2
2	E	475	MET	3.1
2	E	558	ALA	3.1
2	E	493	GLY	3.1
2	E	565	ALA	3.1
2	F	492	ASN	3.0
2	E	572	LYS	3.0
1	C	198	GLU	3.0
1	C	170	MET	3.0
2	E	579	ASP	3.0
2	E	576	THR	2.9
2	F	476	VAL	2.9
2	E	580	LEU	2.9
1	C	212	ARG	2.8
2	E	563	PHE	2.8
2	E	568	VAL	2.7
2	E	494	ALA	2.7
2	E	560	ALA	2.7
2	E	566	LYS	2.7
2	E	545	ALA	2.7
2	E	570	ALA	2.7
2	F	557	GLN	2.7
2	E	498	LEU	2.6
2	E	466	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	481	LEU	2.6
1	B	162	VAL	2.6
2	F	472	ALA	2.6
1	A	102	ARG	2.6
1	C	224	ARG	2.6
1	C	278	ARG	2.5
2	E	476	VAL	2.5
2	F	471	GLU	2.5
2	D	483	LYS	2.5
2	F	480	LEU	2.5
2	E	548	THR	2.5
2	E	562	ALA	2.5
1	C	61	GLN	2.4
1	A	23	GLN	2.4
2	D	581	ALA	2.4
1	C	209	VAL	2.4
2	E	556	GLU	2.4
1	A	224	ARG	2.4
2	F	469	ASP	2.4
1	C	35	LEU	2.4
2	D	561	ARG	2.4
1	C	159	LEU	2.4
2	D	475	MET	2.3
2	F	544	SER	2.3
1	B	35	LEU	2.3
2	F	546	ASP	2.3
1	B	41	ARG	2.3
1	A	34	ASP	2.3
2	E	559	GLY	2.2
1	C	162	VAL	2.2
2	E	520	GLY	2.2
2	E	463	ARG	2.2
2	E	529	VAL	2.2
2	F	465	LEU	2.2
2	E	464	MET	2.2
2	D	487	LYS	2.2
1	C	211	PRO	2.2
2	F	545	ALA	2.1
2	D	548	THR	2.1
2	F	487	LYS	2.1
2	F	463	ARG	2.1
2	E	490	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	523	MET	2.1
1	C	221	GLN	2.1
2	E	546	ASP	2.0
2	E	497	VAL	2.0
2	E	509	VAL	2.0
2	D	462	MET	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	IOD	E	3	1/1	0.64	0.10	121,121,121,121	0
5	MG	D	591	1/1	0.78	0.31	53,53,53,53	0
5	MG	E	591	1/1	0.83	0.09	63,63,63,63	0
5	MG	F	3	1/1	0.84	0.14	76,76,76,76	0
3	IOD	F	7	1/1	0.88	0.06	119,119,119,119	0
4	EDO	C	904	4/4	0.92	0.44	28,28,29,30	0
4	EDO	A	902	4/4	0.92	0.32	26,26,27,29	0
3	IOD	B	291	1/1	0.94	0.13	116,116,116,116	0
3	IOD	A	291	1/1	0.94	0.13	120,120,120,120	0
4	EDO	B	903	4/4	0.95	0.50	35,35,36,36	0
3	IOD	F	4	1/1	0.95	0.11	126,126,126,126	0
3	IOD	C	291	1/1	0.95	0.15	117,117,117,117	0
3	IOD	C	293	1/1	0.96	0.11	105,105,105,105	0
3	IOD	C	292	1/1	0.96	0.13	103,103,103,103	0
3	IOD	D	6	1/1	0.97	0.07	131,131,131,131	0
3	IOD	D	1	1/1	0.97	0.05	64,64,64,64	0
3	IOD	C	290	1/1	0.97	0.17	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	IOD	B	290	1/1	0.98	0.14	102,102,102,102	0
3	IOD	E	2	1/1	0.98	0.05	86,86,86,86	0
3	IOD	A	290	1/1	0.99	0.15	123,123,123,123	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.