



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:16 PM GMT

PDB ID : 4OCM
Title : Crystal Structure of the Rpn8-Rpn11 MPN domain heterodimer, crystal form Ib
Authors : Pathare, G.R.; Bracher, A.
Deposited on : 2014-01-09
Resolution : 1.99 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

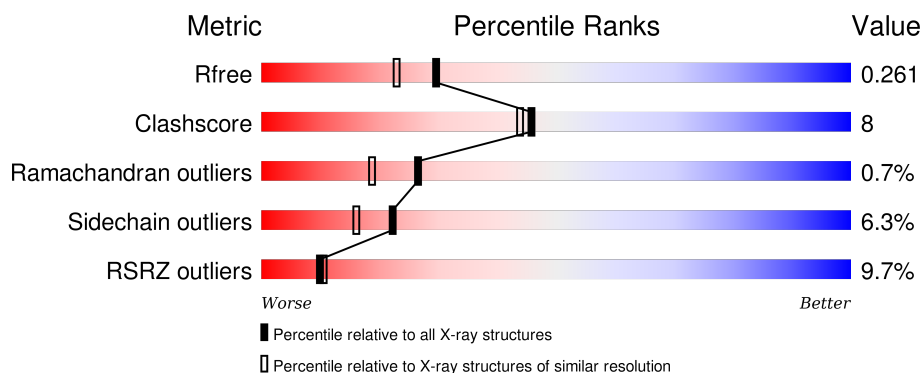
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	187	<div> <div>8%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	187	<div> <div>7%</div> <div> <div></div> <div>65%</div> <div>20%</div> <div>• •</div> <div>11%</div> </div> </div>
2	B	220	<div> <div>7%</div> <div> <div></div> <div>64%</div> <div>14%</div> <div>•</div> <div>20%</div> </div> </div>
2	E	220	<div> <div>12%</div> <div> <div></div> <div>71%</div> <div>10%</div> <div>•</div> <div>16%</div> </div> </div>
3	C	133	<div> <div>9%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>•</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	F	133	<div><div></div><div>6%</div><div>77%</div><div>14%</div><div>•• 6%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7521 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 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1277	814	215	243	5			
1	D	166	Total	C	N	O	S	0	1	0
			1299	828	218	248	5			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q08723
A	0	HIS	-	CLONING ARTIFACT	UNP Q08723
A	177	GLY	-	SEE REMARK 999	UNP Q08723
A	178	SER	-	SEE REMARK 999	UNP Q08723
A	179	GLY	-	SEE REMARK 999	UNP Q08723
A	180	GLY	-	SEE REMARK 999	UNP Q08723
A	181	SER	-	SEE REMARK 999	UNP Q08723
A	182	GLY	-	SEE REMARK 999	UNP Q08723
A	183	GLY	-	SEE REMARK 999	UNP Q08723
A	184	SER	-	SEE REMARK 999	UNP Q08723
A	185	GLY	-	SEE REMARK 999	UNP Q08723
D	-1	GLY	-	CLONING ARTIFACT	UNP Q08723
D	0	HIS	-	CLONING ARTIFACT	UNP Q08723
D	177	GLY	-	SEE REMARK 999	UNP Q08723
D	178	SER	-	SEE REMARK 999	UNP Q08723
D	179	GLY	-	SEE REMARK 999	UNP Q08723
D	180	GLY	-	SEE REMARK 999	UNP Q08723
D	181	SER	-	SEE REMARK 999	UNP Q08723
D	182	GLY	-	SEE REMARK 999	UNP Q08723
D	183	GLY	-	SEE REMARK 999	UNP Q08723
D	184	SER	-	SEE REMARK 999	UNP Q08723
D	185	GLY	-	SEE REMARK 999	UNP Q08723

- Molecule 2 is a protein called 26S proteasome regulatory subunit RPN11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	0	0	0
			1376	879	236	249	12			
2	E	184	Total	C	N	O	S	0	1	0
			1420	903	242	263	12			

- Molecule 3 is a protein called Nb1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	125	Total	C	N	O	S	0	1	0
			981	615	175	187	4			
3	F	125	Total	C	N	O	S	0	0	0
			969	609	173	183	4			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	K	0	0
			1	1		

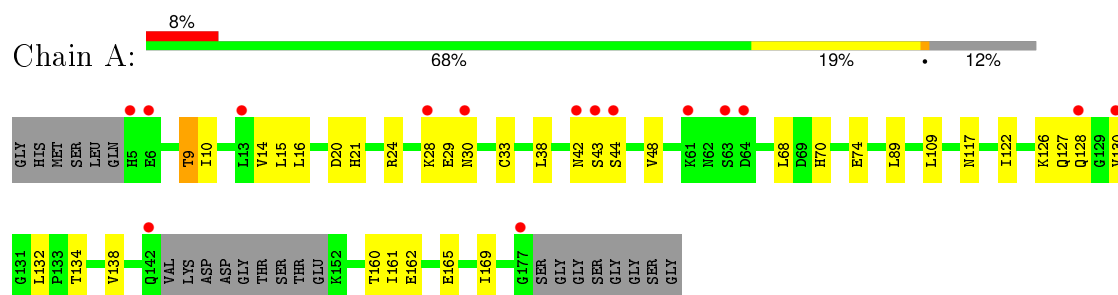
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total	O	0	0
			23	23		
6	B	31	Total	O	0	0
			31	31		
6	C	23	Total	O	0	0
			23	23		
6	D	33	Total	O	0	0
			33	33		
6	E	43	Total	O	0	0
			43	43		
6	F	43	Total	O	0	0
			43	43		

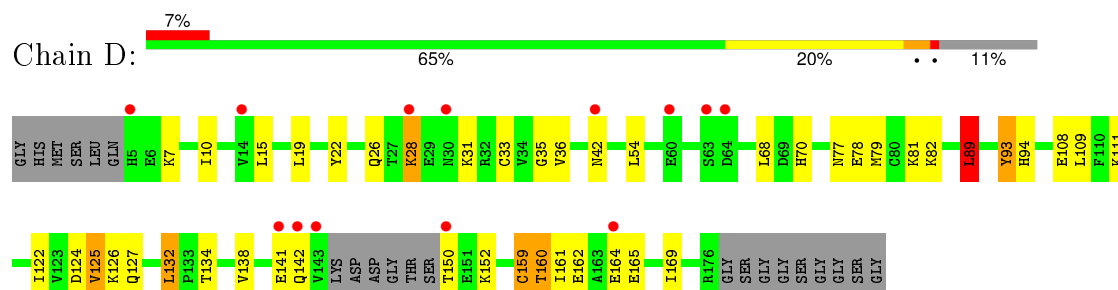
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

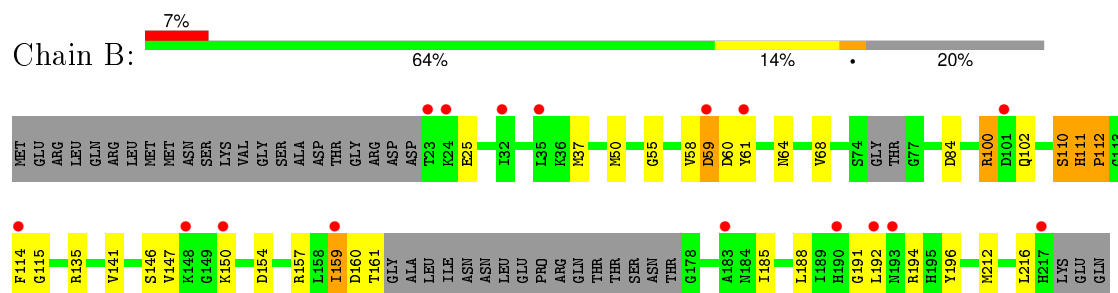
- Molecule 1: 26S proteasome regulatory subunit RPN8



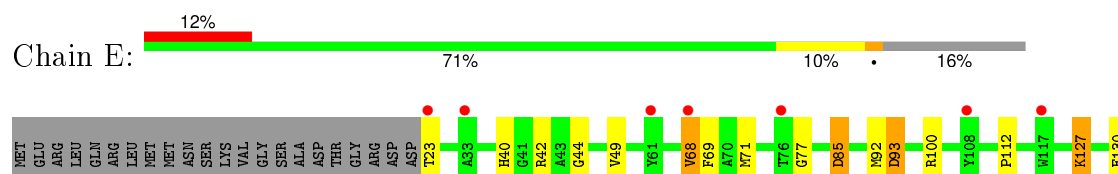
- Molecule 1: 26S proteasome regulatory subunit RPN8

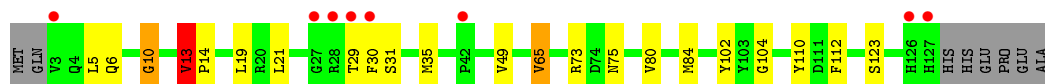


- Molecule 2: 26S proteasome regulatory subunit RPN11



- Molecule 2: 26S proteasome regulatory subunit RPN11





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	63.40 Å 44.97 Å 200.04 Å 90.00° 98.40° 90.00°	Depositor
Resolution (Å)	30.00 – 1.99 29.71 – 1.99	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-1.99) 96.5 (29.71-1.99)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.00 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.216 , 0.262 0.214 , 0.261	Depositor DCC
R_{free} test set	3757 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	33.1	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.8	EDS
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	2 of 74685 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7521	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.20 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.5806e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, K

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	0.86	0/1301	0.91	5/1766 (0.3%)
1	D	1.16	6/1322 (0.5%)	1.00	2/1793 (0.1%)
2	B	0.93	0/1400	0.90	2/1889 (0.1%)
2	E	1.10	2/1445 (0.1%)	1.02	5/1957 (0.3%)
3	C	0.88	0/1007	0.91	0/1365
3	F	1.26	2/995 (0.2%)	1.01	2/1349 (0.1%)
All	All	1.04	10/7470 (0.1%)	0.96	16/10119 (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
1	A	0	1
2	B	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	159	CYS	CB-SG	-7.79	1.69	1.82
2	E	130	GLU	CG-CD	6.66	1.61	1.51
1	D	93	TYR	CD2-CE2	6.44	1.49	1.39
1	D	125	VAL	CB-CG1	-5.88	1.40	1.52
3	F	49	VAL	CB-CG1	5.87	1.65	1.52
1	D	138	VAL	CB-CG1	-5.71	1.40	1.52
1	D	93	TYR	CD1-CE1	5.57	1.47	1.39
2	E	130	GLU	CD-OE2	5.32	1.31	1.25
3	F	110	TYR	CD2-CE2	5.29	1.47	1.39
1	D	78	GLU	CG-CD	5.09	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	92	MET	CG-SD-CE	-8.27	86.97	100.20
3	F	65	VAL	CG1-CB-CG2	7.26	122.51	110.90
1	A	24	ARG	NE-CZ-NH1	-7.19	116.71	120.30
2	E	68	VAL	CA-CB-CG1	6.65	120.88	110.90
2	E	68	VAL	CG1-CB-CG2	6.43	121.18	110.90
1	A	68	LEU	CA-CB-CG	6.32	129.83	115.30
3	F	13	VAL	CB-CA-C	-5.96	100.08	111.40
2	E	85	ASP	CB-CG-OD1	5.94	123.65	118.30
1	D	132	LEU	CB-CG-CD2	-5.84	101.07	111.00
2	B	84	ASP	CB-CG-OD2	5.80	123.52	118.30
2	B	100	ARG	NE-CZ-NH2	-5.70	117.45	120.30
2	E	157	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	109	LEU	CB-CG-CD2	5.54	120.41	111.00
1	D	89	LEU	CB-CG-CD1	5.25	119.92	111.00
1	A	10	ILE	CG1-CB-CG2	-5.04	100.31	111.40
1	A	126	LYS	CD-CE-NZ	-5.02	100.15	111.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	GLN	Peptide
2	B	110	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	1277	0	1247	17	0
1	D	1299	0	1270	34	0
2	B	1376	0	1385	29	0
2	E	1420	0	1403	13	0
3	C	981	0	917	12	0
3	F	969	0	908	15	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
6	A	23	0	0	0	0
6	B	31	0	0	1	0
6	C	23	0	0	0	0
6	D	33	0	0	4	0
6	E	43	0	0	1	0
6	F	43	0	0	0	0
All	All	7521	0	7130	111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (111) 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:70:HIS:HE1	1:D:109:LEU:HD21	1.11	1.14
1:D:70:HIS:CE1	1:D:109:LEU:HD21	1.95	1.01
3:C:75[B]:ASN:HD22	3:C:75[B]:ASN:H	1.23	0.84
3:C:75[B]:ASN:ND2	3:C:75[B]:ASN:H	1.81	0.79
1:A:9:THR:HG23	1:A:162:GLU:HB3	1.65	0.79
2:B:37:MET:CE	2:B:68:VAL:HG11	2.16	0.76
1:D:15:LEU:HD21	1:D:134:THR:HG21	1.67	0.75
1:D:142:GLN:O	1:D:150:THR:HA	1.87	0.74
1:D:15:LEU:HD21	1:D:134:THR:CG2	2.21	0.71
3:F:35:MET:HG3	3:F:80:VAL:HG21	1.74	0.69
3:C:7:GLU:HG3	3:C:97:CYS:SG	2.34	0.67
2:B:59:ASP:O	2:B:135:ARG:NH1	2.26	0.67
2:B:37:MET:HE2	2:B:68:VAL:HG11	1.76	0.67
2:B:100:ARG:HD3	2:B:102:GLN:OE1	1.95	0.67
3:C:15:ALA:HB3	3:C:126:HIS:HD2	1.60	0.66
2:B:25:GLU:OE2	2:B:157:ARG:NH1	2.28	0.65
2:B:111:HIS:HB2	2:B:114:PHE:HD1	1.62	0.65
2:B:59:ASP:HB3	2:B:61:TYR:H	1.61	0.65
3:F:5:LEU:HD21	3:F:112:PHE:HE1	1.64	0.62
1:D:15:LEU:CD2	1:D:134:THR:CG2	2.78	0.62
2:E:93:ASP:OD1	6:E:535:HOH:O	2.16	0.62
2:E:211:LYS:HB2	2:E:211:LYS:NZ	2.15	0.61
2:B:37:MET:HE3	2:B:68:VAL:HG11	1.84	0.60
2:E:146:SER:HA	2:E:150:LYS:O	2.02	0.59
2:B:25:GLU:OE2	2:B:157:ARG:CZ	2.52	0.58
1:D:7:LYS:HG2	6:D:528:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:25:ASP:OD1	3:C:27:GLY:N	2.32	0.57
3:C:75[B]:ASN:N	3:C:75[B]:ASN:HD22	1.98	0.57
1:D:10:ILE:HD11	1:D:159:CYS:HB2	1.87	0.57
1:D:70:HIS:HE1	1:D:109:LEU:CD2	2.02	0.56
1:A:16:LEU:HG	2:B:212:MET:CE	2.36	0.56
3:F:19:LEU:HB2	3:F:84:MET:HE3	1.86	0.55
1:D:22:TYR:CD2	1:D:125:VAL:HG11	2.40	0.55
2:B:111:HIS:HB2	2:B:114:PHE:CD1	2.43	0.54
3:C:15:ALA:HB3	3:C:126:HIS:CD2	2.41	0.54
1:A:21:HIS:CE1	1:A:33:CYS:HB2	2.43	0.54
2:B:188:LEU:O	2:B:192:LEU:HG	2.08	0.53
1:A:9:THR:CG2	1:A:162:GLU:HB3	2.37	0.53
3:F:10:GLY:HA2	3:F:19:LEU:HD22	1.91	0.53
3:C:30:PHE:HB3	3:C:112:PHE:CE2	2.44	0.52
1:D:68:LEU:HD12	1:D:109:LEU:HD23	1.92	0.52
1:D:81:LYS:HG2	6:D:505:HOH:O	2.10	0.51
2:B:157:ARG:NH1	6:B:520:HOH:O	2.43	0.51
1:D:124:ASP:OD1	6:D:532:HOH:O	2.19	0.51
1:D:164:GLU:OE1	2:E:42:ARG:HG2	2.11	0.51
1:D:19:LEU:CD1	1:D:125:VAL:HG13	2.42	0.50
1:D:124:ASP:OD2	1:D:127:GLN:HA	2.12	0.50
3:C:75[B]:ASN:N	3:C:75[B]:ASN:ND2	2.55	0.50
1:D:132:LEU:HD23	1:D:161:ILE:HD11	1.94	0.49
1:D:160:THR:HB	6:D:528:HOH:O	2.13	0.49
1:D:79:MET:HA	1:D:82:LYS:HE3	1.95	0.49
2:B:111:HIS:CD2	2:B:115:GLY:O	2.66	0.48
3:F:13:VAL:HG12	3:F:14:PRO:HD2	1.95	0.48
1:D:28:LYS:HG3	1:D:31:LYS:HG3	1.95	0.48
1:D:164:GLU:CD	2:E:42:ARG:HG2	2.34	0.48
2:B:146:SER:HA	2:B:150:LYS:O	2.14	0.47
2:B:37:MET:HE2	2:B:68:VAL:CG1	2.44	0.47
2:E:69:PHE:HE1	2:E:71:MET:CE	2.27	0.47
1:D:141:GLU:HG2	1:D:152:LYS:HG2	1.96	0.47
1:D:10:ILE:CD1	1:D:159:CYS:HB2	2.45	0.47
3:F:21:LEU:HG	3:F:84:MET:CE	2.45	0.46
1:A:169:ILE:HD13	2:B:147:VAL:HA	1.98	0.46
1:A:16:LEU:HA	2:B:212:MET:HE1	1.97	0.46
3:F:30:PHE:CB	3:F:112:PHE:CD2	2.99	0.46
1:A:117:ASN:ND2	1:A:138:VAL:HG22	2.30	0.45
2:B:37:MET:CE	2:B:68:VAL:CG1	2.91	0.45
1:D:35:GLY:HA3	1:D:93:TYR:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:TYR:CG	1:D:125:VAL:HG11	2.51	0.45
3:F:75:ASN:ND2	3:F:75:ASN:H	2.14	0.45
1:A:165:GLU:O	1:A:169:ILE:HD12	2.16	0.45
2:E:40:HIS:CE1	2:E:49:VAL:HB	2.52	0.44
1:A:38:LEU:HD23	1:A:89:LEU:HA	1.99	0.44
3:C:26:SER:HB2	3:C:28:ARG:HD2	1.99	0.44
2:B:159:ILE:HD11	2:B:191:GLY:C	2.37	0.44
1:A:70:HIS:O	1:A:74:GLU:HG3	2.17	0.44
1:A:20:ASP:OD2	2:B:100:ARG:NH2	2.50	0.44
2:E:204:HIS:CE1	3:F:102:TYR:HB2	2.53	0.43
1:D:54:LEU:HD13	1:D:68:LEU:HD22	1.99	0.43
1:A:15:LEU:HD12	2:B:216:LEU:HD21	2.00	0.43
2:E:212:MET:O	2:E:216:LEU:HG	2.19	0.43
1:A:14:VAL:HG21	1:A:48:VAL:HG12	2.00	0.43
1:A:169:ILE:CD1	2:B:147:VAL:HA	2.48	0.43
1:A:29:GLU:O	1:A:30:ASN:CB	2.66	0.43
2:B:110:SER:HA	2:B:141:VAL:O	2.19	0.43
2:B:111:HIS:HA	2:B:112:PRO:HD3	1.45	0.43
2:B:55:GLY:HA3	2:B:64:ASN:O	2.19	0.43
1:D:33:CYS:O	1:D:94:HIS:HA	2.19	0.42
3:F:13:VAL:HG12	3:F:14:PRO:CD	2.49	0.42
3:F:10:GLY:HA2	3:F:19:LEU:HD13	2.02	0.41
2:E:127:LYS:HE3	2:E:158:LEU:HD13	2.02	0.41
1:D:165:GLU:O	1:D:169:ILE:HG13	2.20	0.41
1:A:9:THR:O	1:A:9:THR:HG22	2.20	0.41
1:A:122:ILE:O	1:A:134:THR:HA	2.20	0.41
1:D:122:ILE:O	1:D:134:THR:HA	2.20	0.41
3:C:30:PHE:CB	3:C:112:PHE:CE2	3.03	0.41
2:B:160:ASP:O	2:B:161:THR:C	2.59	0.41
2:B:194:ARG:HD2	2:B:196:TYR:CZ	2.55	0.41
3:F:30:PHE:CB	3:F:112:PHE:CE2	3.03	0.41
1:D:132:LEU:HD23	1:D:161:ILE:CD1	2.50	0.41
2:E:44:GLY:HA3	2:E:49:VAL:HG11	2.02	0.41
3:F:102:TYR:CE2	3:F:104:GLY:HA3	2.56	0.41
1:D:108:GLU:OE2	1:D:111:LYS:HE3	2.21	0.41
2:B:50:MET:HB2	2:B:50:MET:HE3	1.91	0.41
3:C:13:VAL:HG21	3:C:19:LEU:HG	2.04	0.40
2:E:148:LYS:H	2:E:148:LYS:HG2	1.70	0.40
3:F:30:PHE:HB2	3:F:112:PHE:CE2	2.56	0.40
1:D:15:LEU:HD22	1:D:134:THR:CG2	2.51	0.40
3:F:21:LEU:HD21	3:F:84:MET:HE1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ASN:ND2	1:D:81:LYS:HE3	2.36	0.40
2:E:44:GLY:HA3	2:E:49:VAL:CG1	2.51	0.40
1:D:36:VAL:HG13	1:D:89:LEU:HD13	2.02	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	160/187 (86%)	153 (96%)	7 (4%)	0	100	100
1	D	163/187 (87%)	157 (96%)	6 (4%)	0	100	100
2	B	171/220 (78%)	164 (96%)	4 (2%)	3 (2%)	11	4
2	E	181/220 (82%)	171 (94%)	8 (4%)	2 (1%)	17	9
3	C	124/133 (93%)	121 (98%)	3 (2%)	0	100	100
3	F	123/133 (92%)	118 (96%)	4 (3%)	1 (1%)	24	15
All	All	922/1080 (85%)	884 (96%)	32 (4%)	6 (1%)	26	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	59	ASP
3	F	10	GLY
2	E	112	PRO
2	B	58	VAL
2	E	77	GLY
2	B	112	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	137/162 (85%)	127 (93%)	10 (7%)	17	11
1	D	139/162 (86%)	132 (95%)	7 (5%)	30	24
2	B	151/191 (79%)	146 (97%)	5 (3%)	45	43
2	E	154/191 (81%)	144 (94%)	10 (6%)	21	15
3	C	102/109 (94%)	92 (90%)	10 (10%)	10	5
3	F	100/109 (92%)	93 (93%)	7 (7%)	19	12
All	All	783/924 (85%)	734 (94%)	49 (6%)	22	16

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	28	LYS
1	A	42	ASN
1	A	43	SER
1	A	44	SER
1	A	127	GLN
1	A	130	VAL
1	A	132	LEU
1	A	160	THR
1	A	161	ILE
2	B	60	ASP
2	B	111	HIS
2	B	154	ASP
2	B	159	ILE
2	B	185	ILE
3	C	6	GLN
3	C	8	SER
3	C	13	VAL
3	C	18	SER
3	C	28	ARG
3	C	29	THR
3	C	31	SER

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Mol	Chain	Res	Type
3	C	46	ARG
3	C	65	VAL
3	C	73	ARG
1	D	26	GLN
1	D	28	LYS
1	D	42	ASN
1	D	89	LEU
1	D	126	LYS
1	D	160	THR
1	D	162	GLU
2	E	23	THR
2	E	68	VAL
2	E	85	ASP
2	E	93	ASP
2	E	100	ARG
2	E	127	LYS
2	E	168	LEU
2	E	185	ILE
2	E	193	ASN
2	E	211	LYS
3	F	6	GLN
3	F	13	VAL
3	F	29	THR
3	F	31	SER
3	F	65	VAL
3	F	73	ARG
3	F	123	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	115	GLN
2	B	73	GLN
2	B	111	HIS
3	C	78	ASN
3	C	126	HIS
1	D	26	GLN
1	D	42	ASN
1	D	70	HIS
1	D	77	ASN
1	D	115	GLN

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Mol	Chain	Res	Type
2	E	186	GLN
2	E	204	HIS
3	F	75	ASN

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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

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	164/187 (87%)	0.66	15 (9%)	11 12	27, 45, 71, 87	0
1	D	166/187 (88%)	0.52	13 (7%)	16 17	14, 36, 62, 83	0
2	B	177/220 (80%)	0.53	16 (9%)	12 12	24, 40, 68, 73	0
2	E	184/220 (83%)	0.90	27 (14%)	3 4	15, 33, 87, 134	0
3	C	125/133 (93%)	0.65	12 (9%)	10 11	24, 40, 64, 91	0
3	F	125/133 (93%)	0.34	8 (6%)	23 24	16, 30, 56, 76	0
All	All	941/1080 (87%)	0.61	91 (9%)	10 10	14, 38, 69, 134	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	185	ILE	15.7
1	D	143	VAL	9.6
2	E	183	ALA	8.7
2	E	181	ASN	7.2
3	C	28	ARG	6.8
2	E	184	ASN	6.8
2	E	23	THR	6.5
2	E	186	GLN	6.3
2	E	187	ALA	6.2
3	C	30	PHE	5.9
2	E	188	LEU	5.5
3	F	3	VAL	5.4
1	A	5	HIS	5.3
2	B	23	THR	5.2
3	F	29	THR	5.2
3	C	29	THR	5.0
2	E	148	LYS	5.0
1	A	128	GLN	4.8
3	F	30	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
3	C	42	PRO	4.5
2	E	190	HIS	4.5
2	E	166	ASN	4.4
2	E	182	LYS	4.4
3	F	28	ARG	4.3
1	D	150	THR	4.2
2	E	218	LYS	4.2
2	E	149	GLY	4.2
2	E	76	THR	3.9
2	B	193	ASN	3.8
3	C	27	GLY	3.7
2	B	148	LYS	3.5
2	B	217	HIS	3.5
3	F	27	GLY	3.5
1	A	43	SER	3.4
2	B	114	PHE	3.4
1	A	28	LYS	3.4
2	E	147	VAL	3.4
1	A	63	SER	3.3
2	B	61	TYR	3.3
3	C	3	VAL	3.2
3	C	31	SER	3.2
1	A	13	LEU	3.2
3	C	21	LEU	3.2
2	E	217	HIS	3.2
2	B	190	HIS	3.1
1	A	130	VAL	3.0
3	C	97	CYS	3.0
1	A	6	GLU	2.9
2	B	192	LEU	2.9
2	E	168	LEU	2.9
2	E	193	ASN	2.9
1	D	30	ASN	2.8
2	E	191	GLY	2.8
2	E	189	ILE	2.8
2	E	108	TYR	2.8
3	F	42	PRO	2.7
1	A	142	GLN	2.7
1	D	63	SER	2.7
1	A	64	ASP	2.7
1	A	44	SER	2.6
2	B	35	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	82	LEU	2.5
2	E	117	TRP	2.5
2	E	61	TYR	2.5
2	B	101	ASP	2.4
3	C	43	GLY	2.4
2	E	33	ALA	2.4
1	A	61	LYS	2.4
2	E	68	VAL	2.4
2	B	59	ASP	2.4
3	F	127	HIS	2.4
2	B	183	ALA	2.3
2	B	150	LYS	2.3
1	D	60	GLU	2.3
2	B	32	ILE	2.2
3	C	127	HIS	2.2
2	B	159	ILE	2.2
1	D	164	GLU	2.2
1	D	14	VAL	2.2
1	D	64	ASP	2.1
2	B	24	LYS	2.1
1	A	42	ASN	2.1
1	D	42	ASN	2.1
1	D	28	LYS	2.1
1	D	5	HIS	2.1
1	D	142	GLN	2.1
1	D	141	GLU	2.1
1	A	30	ASN	2.0
1	A	177	GLY	2.0
3	F	126	HIS	2.0
2	E	139	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
4	ZN	E	401	1/1	0.99	0.04	-2.64	59,59,59,59	0
4	ZN	B	401	1/1	0.97	0.07	-2.87	77,77,77,77	0
5	K	D	301	1/1	0.94	0.15	-	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.