



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:16 PM GMT

PDB ID : 4OCL  
Title : Crystal Structure of the Rpn8-Rpn11 MPN domain heterodimer, crystal form Ia  
Authors : Pathare, G.R.; Bracher, A.  
Deposited on : 2014-01-09  
Resolution : 2.40 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (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

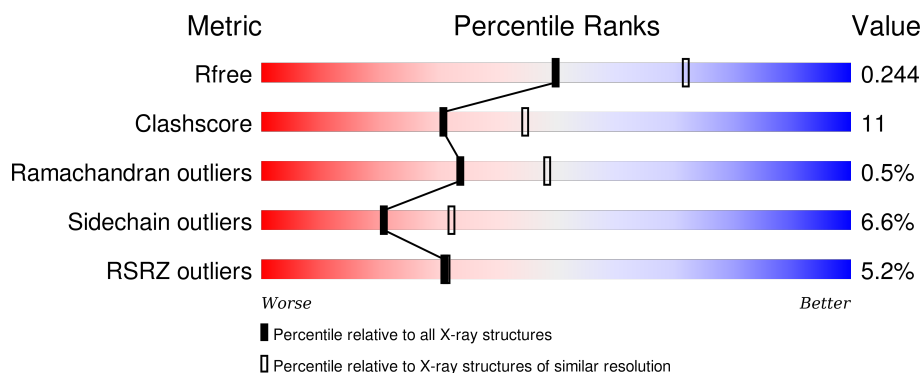
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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>4%</div> <div>69% 16% • 13%</div> </div>
1	D	187	<div> <div>2%</div> <div>63% 21% • • 12%</div> </div>
2	B	220	<div> <div>3%</div> <div>59% 20% • 18%</div> </div>
2	E	220	<div> <div>8%</div> <div>63% 20% • 16%</div> </div>
3	C	133	<div> <div>6%</div> <div>73% 20% • 6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	133	<div><div></div><div>5%</div><div>69%</div><div>23%</div><div>• 6%</div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7359 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	163	Total	C	N	O	S	0	0	0
			1252	800	211	236	5			
1	D	164	Total	C	N	O	S	0	0	0
			1265	808	213	239	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	181	Total	C	N	O	S	0	0	0
			1396	890	240	254	12			
2	E	184	Total	C	N	O	S	0	0	0
			1402	893	240	257	12			

- Molecule 3 is a protein called Nb1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	125	Total	C	N	O	S	0	0	0
			973	611	173	185	4			
3	F	125	Total	C	N	O	S	0	0	0
			975	612	176	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		

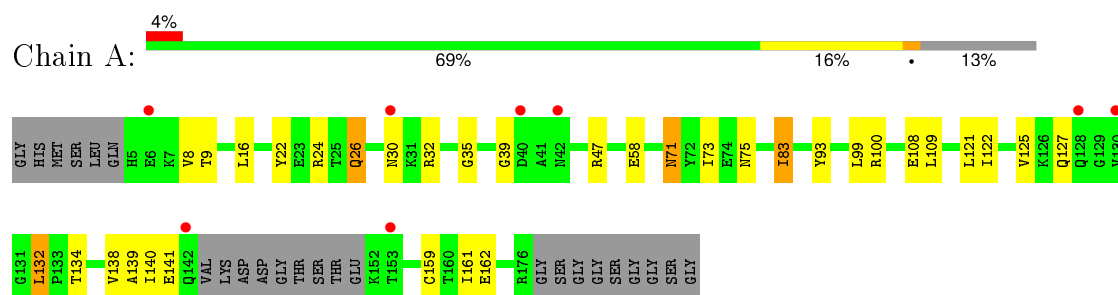
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total	O	0	0
			11	11		
5	B	21	Total	O	0	0
			21	21		
5	C	14	Total	O	0	0
			14	14		
5	D	17	Total	O	0	0
			17	17		
5	E	11	Total	O	0	0
			11	11		
5	F	20	Total	O	0	0
			20	20		

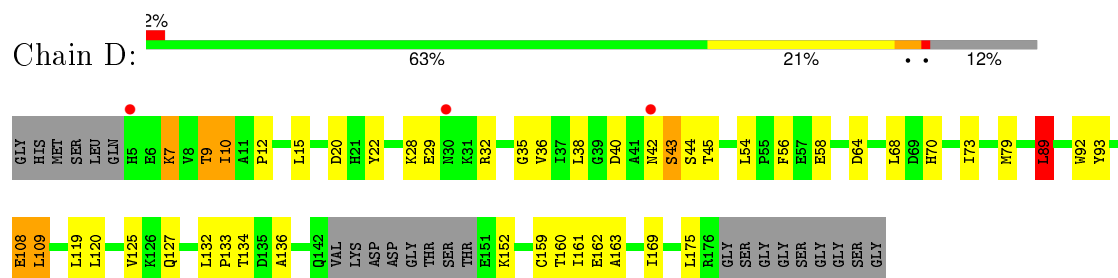
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

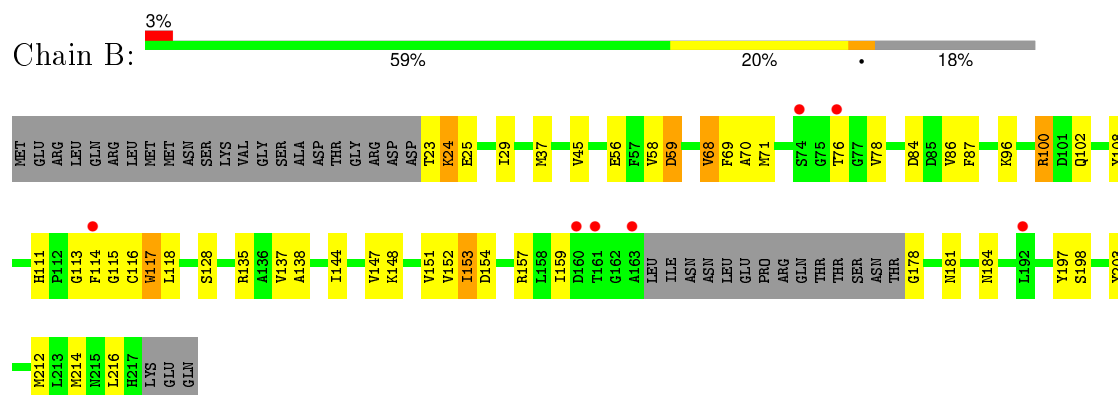
- Molecule 1: 26S proteasome regulatory subunit RPN8



- Molecule 1: 26S proteasome regulatory subunit RPN8

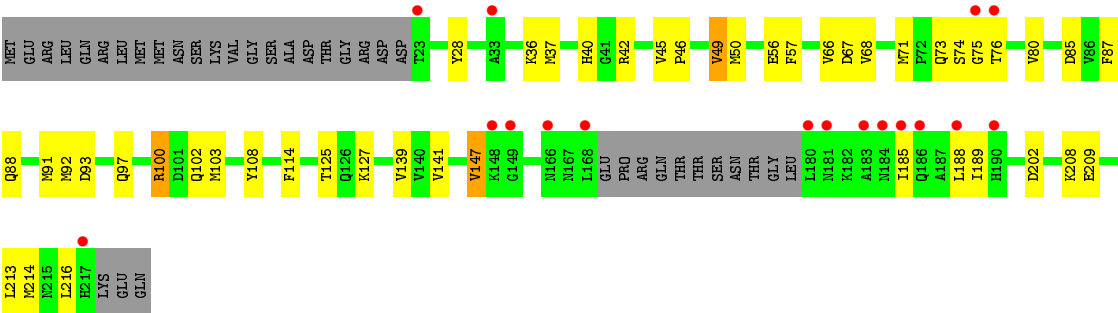


- Molecule 2: 26S proteasome regulatory subunit RPN11

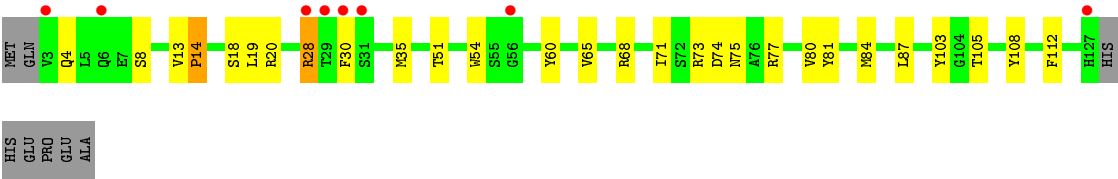


- Molecule 2: 26S proteasome regulatory subunit RPN11

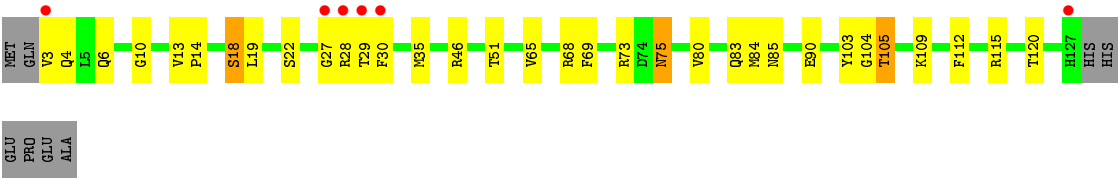




• Molecule 3: Nb1



• Molecule 3: Nb1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.26Å 63.43Å 100.11Å 100.08° 92.75° 90.62°	Depositor
Resolution (Å)	30.00 – 2.40 28.75 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (30.00-2.40) 92.2 (28.75-2.40)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.195 , 0.252 0.190 , 0.244	Depositor DCC
$R_{free}$ test set	2088 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 45.1	EDS
Estimated twinning fraction	0.067 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 41608 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7359	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.46% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.77	0/1275	0.79	0/1734
1	D	0.88	1/1288 (0.1%)	0.86	2/1750 (0.1%)
2	B	0.84	1/1421 (0.1%)	0.85	2/1919 (0.1%)
2	E	0.86	1/1427 (0.1%)	0.83	1/1933 (0.1%)
3	C	0.80	0/999	0.86	1/1354 (0.1%)
3	F	0.83	0/1001	0.88	1/1356 (0.1%)
All	All	0.83	3/7411 (0.0%)	0.84	7/10046 (0.1%)

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
3	F	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	178	GLY	C-O	7.70	1.35	1.23
1	D	108	GLU	CG-CD	6.62	1.61	1.51
2	E	209	GLU	CG-CD	5.33	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	20	ARG	NE-CZ-NH1	-7.81	116.39	120.30
1	D	89	LEU	CA-CB-CG	7.81	133.26	115.30
2	B	153	ILE	CG1-CB-CG2	-5.80	98.63	111.40
2	B	100	ARG	NE-CZ-NH2	-5.39	117.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	10	ILE	CG1-CB-CG2	-5.38	99.57	111.40
3	F	68	ARG	CG-CD-NE	-5.36	100.55	111.80
2	E	100	ARG	NE-CZ-NH2	-5.30	117.65	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	104	GLY	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	1252	0	1216	20	0
1	D	1265	0	1233	34	0
2	B	1396	0	1404	46	0
2	E	1402	0	1383	38	0
3	C	973	0	912	16	0
3	F	975	0	919	20	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
5	A	11	0	0	0	0
5	B	21	0	0	0	0
5	C	14	0	0	0	0
5	D	17	0	0	0	0
5	E	11	0	0	0	0
5	F	20	0	0	0	0
All	All	7359	0	7067	156	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 11.

All (156) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:VAL:HG12	2:B:153:ILE:HD13	1.41	1.02
2:B:151:VAL:CG1	2:B:153:ILE:HD13	1.91	1.00
1:D:70:HIS:HE1	1:D:109:LEU:HD21	1.33	0.94
1:D:70:HIS:CE1	1:D:109:LEU:HD21	2.02	0.93
2:B:59:ASP:O	2:B:135:ARG:NH1	2.08	0.86
2:B:151:VAL:HG12	2:B:153:ILE:CD1	2.08	0.83
3:C:13:VAL:HG21	3:C:19:LEU:HG	1.60	0.83
1:A:26:GLN:HA	1:A:26:GLN:OE1	1.76	0.82
3:C:35:MET:HG3	3:C:80:VAL:HG21	1.63	0.80
2:B:151:VAL:CG1	2:B:153:ILE:CD1	2.59	0.80
2:E:100:ARG:HD3	2:E:102:GLN:NE2	2.00	0.77
2:E:74:SER:O	2:E:76:THR:N	2.19	0.75
2:B:111:HIS:CD2	2:B:115:GLY:O	2.44	0.70
1:A:9:THR:HG23	1:A:162:GLU:HB3	1.73	0.70
1:D:36:VAL:HG13	1:D:89:LEU:HD13	1.74	0.69
1:A:32:ARG:HG2	1:A:58:GLU:OE2	1.92	0.69
3:F:13:VAL:HG21	3:F:19:LEU:HG	1.75	0.68
3:F:4:GLN:NE2	3:F:112:PHE:CE1	2.62	0.68
2:B:148:LYS:HE2	2:E:45:VAL:O	1.94	0.67
2:B:84:ASP:HB3	2:B:87:PHE:HB3	1.77	0.66
2:B:58:VAL:O	2:B:59:ASP:C	2.33	0.66
2:B:100:ARG:HD3	2:B:102:GLN:OE1	1.97	0.65
3:F:35:MET:HG3	3:F:80:VAL:HG21	1.78	0.65
2:B:23:THR:HG22	2:B:24:LYS:H	1.61	0.64
1:A:9:THR:CG2	1:A:162:GLU:HB3	2.27	0.63
2:E:100:ARG:HD3	2:E:102:GLN:HE21	1.63	0.63
2:E:40:HIS:CE1	2:E:49:VAL:HG13	2.34	0.63
1:A:161:ILE:HD13	2:B:216:LEU:HA	1.81	0.63
2:B:56:GLU:OE1	3:C:105:THR:HB	1.99	0.63
1:A:132:LEU:HD23	1:A:134:THR:HG22	1.83	0.61
2:E:49:VAL:HG23	2:E:73:GLN:NE2	2.16	0.60
3:C:4:GLN:HG3	3:C:28:ARG:HD2	1.83	0.60
2:E:49:VAL:HG23	2:E:73:GLN:HE21	1.67	0.59
2:B:181:ASN:CG	2:B:184:ASN:HD22	2.05	0.59
2:B:113:GLY:HA2	2:E:46:PRO:HB2	1.85	0.59
2:E:74:SER:C	2:E:76:THR:H	2.06	0.59
1:D:132:LEU:HD23	1:D:161:ILE:HD11	1.84	0.59
3:F:3:VAL:HG23	3:F:115:ARG:HH21	1.69	0.58
1:D:108:GLU:OE2	1:D:152:LYS:NZ	2.37	0.57
2:E:56:GLU:OE1	3:F:105:THR:HB	2.05	0.56
1:D:127:GLN:NE2	2:E:208:LYS:O	2.38	0.56
2:B:45:VAL:HG12	2:E:114:PHE:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:80:VAL:HG23	2:E:125:THR:HA	1.87	0.55
3:F:19:LEU:HD12	3:F:84:MET:HE3	1.87	0.55
1:D:119:LEU:HD11	1:D:136:ALA:HB1	1.89	0.55
1:D:7:LYS:HB3	1:D:45:THR:HG23	1.86	0.55
1:A:83:ILE:HD12	2:B:70:ALA:HB3	1.87	0.55
3:F:4:GLN:NE2	3:F:112:PHE:CD1	2.75	0.54
3:F:75:ASN:ND2	3:F:75:ASN:H	2.05	0.54
1:D:79:MET:HE1	2:E:91:MET:HB2	1.88	0.54
2:B:37:MET:CE	2:B:68:VAL:HG21	2.37	0.54
1:A:139:ALA:O	1:A:140:ILE:HG23	2.08	0.54
1:D:40:ASP:OD1	1:D:42:ASN:HB2	2.08	0.53
2:E:185:ILE:O	2:E:189:ILE:HG13	2.08	0.53
1:D:32:ARG:NH2	1:D:58:GLU:OE2	2.34	0.53
1:D:22:TYR:CD2	1:D:125:VAL:HG11	2.44	0.53
1:D:79:MET:HE3	2:E:87:PHE:CD1	2.44	0.53
3:C:35:MET:HG3	3:C:80:VAL:CG2	2.36	0.53
3:C:19:LEU:HB2	3:C:84:MET:HE3	1.91	0.52
2:B:111:HIS:HD2	2:B:115:GLY:O	1.89	0.52
2:B:159:ILE:HB	2:B:197:TYR:CD2	2.45	0.52
1:A:9:THR:HG23	1:A:162:GLU:CB	2.39	0.52
3:F:13:VAL:HG12	3:F:14:PRO:HD2	1.91	0.52
2:B:58:VAL:O	2:B:59:ASP:O	2.28	0.51
3:C:74:ASP:CG	3:C:77:ARG:HH11	2.13	0.51
2:B:151:VAL:HG13	2:B:153:ILE:CD1	2.41	0.51
1:D:10:ILE:CD1	1:D:159:CYS:HB2	2.41	0.50
2:B:23:THR:HG22	2:B:24:LYS:N	2.25	0.50
2:E:100:ARG:CD	2:E:102:GLN:HE21	2.23	0.50
3:F:4:GLN:HB2	3:F:28:ARG:HH11	1.75	0.50
3:C:54:TRP:HE3	3:C:75:ASN:HB3	1.77	0.50
1:A:39:GLY:HA3	1:A:47:ARG:O	2.12	0.49
3:C:51:THR:HG22	3:C:60:TYR:HB3	1.94	0.49
1:D:54:LEU:HD21	1:D:73:ILE:HG12	1.95	0.49
2:B:152:VAL:C	2:B:153:ILE:HD12	2.32	0.49
2:B:144:ILE:O	2:B:147:VAL:HG22	2.13	0.49
2:B:69:PHE:HE1	2:B:71:MET:CE	2.26	0.49
1:A:99:LEU:HD23	1:A:122:ILE:HD11	1.94	0.49
2:E:37:MET:HE3	2:E:141:VAL:CG2	2.43	0.49
1:D:20:ASP:OD2	2:E:100:ARG:NH2	2.46	0.48
1:D:38:LEU:HD23	1:D:89:LEU:HA	1.94	0.48
2:E:88:GLN:HG3	2:E:92:MET:HE2	1.95	0.48
2:E:49:VAL:CG2	2:E:73:GLN:HE21	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:TRP:CE3	3:C:75:ASN:HB3	2.48	0.48
2:B:114:PHE:HB3	2:B:117:TRP:CZ3	2.48	0.48
1:D:22:TYR:CG	1:D:125:VAL:HG11	2.48	0.48
1:D:175:LEU:HD22	2:E:214:MET:CE	2.44	0.48
1:D:15:LEU:HD21	1:D:134:THR:CG2	2.44	0.48
1:D:36:VAL:CG1	1:D:89:LEU:HD13	2.43	0.47
2:E:36:LYS:NZ	2:E:67:ASP:OD1	2.38	0.47
1:D:169:ILE:CD1	2:E:147:VAL:HA	2.44	0.47
1:D:7:LYS:NZ	1:D:160:THR:HB	2.30	0.47
1:A:8:VAL:HB	1:A:159:CYS:HB3	1.97	0.47
1:D:68:LEU:HD12	1:D:109:LEU:HD22	1.97	0.47
2:B:159:ILE:HB	2:B:197:TYR:CE2	2.50	0.47
1:D:92:TRP:CE2	1:D:120:LEU:HD13	2.49	0.47
1:A:132:LEU:HD23	1:A:134:THR:CG2	2.43	0.46
2:E:42:ARG:HD2	2:E:42:ARG:HA	1.62	0.46
2:B:111:HIS:CE1	2:B:117:TRP:O	2.68	0.46
2:B:37:MET:HE1	2:B:68:VAL:HG21	1.96	0.46
1:D:12:PRO:HB3	2:E:216:LEU:HD13	1.97	0.46
3:F:13:VAL:HG22	3:F:19:LEU:HD21	1.97	0.46
3:F:4:GLN:HE22	3:F:30:PHE:HB2	1.81	0.46
2:E:49:VAL:CG2	2:E:73:GLN:NE2	2.79	0.46
3:C:51:THR:HG23	3:C:103:TYR:CE1	2.51	0.46
2:E:57:PHE:HE2	2:E:103:MET:HE1	1.79	0.46
2:B:29:ILE:O	2:B:203:TYR:HA	2.16	0.46
2:B:212:MET:O	2:B:216:LEU:HG	2.15	0.46
1:D:35:GLY:HA3	1:D:93:TYR:CE2	2.51	0.46
1:D:56:PHE:HD1	1:D:68:LEU:HD23	1.81	0.45
1:A:35:GLY:HA3	1:A:93:TYR:CE2	2.52	0.45
2:B:25:GLU:OE2	2:B:157:ARG:NH2	2.50	0.45
1:A:26:GLN:CA	1:A:26:GLN:OE1	2.56	0.45
2:B:37:MET:HE2	2:B:108:TYR:HB3	1.97	0.45
2:B:117:TRP:CD1	2:B:118:LEU:N	2.84	0.45
1:D:9:THR:HG23	1:D:162:GLU:HB3	1.98	0.45
2:E:66:VAL:HG22	3:F:109:LYS:HE3	1.98	0.45
3:F:13:VAL:HG12	3:F:14:PRO:CD	2.47	0.44
3:C:71:ILE:HA	3:C:81:TYR:O	2.18	0.44
3:F:69:PHE:HA	3:F:83:GLN:O	2.18	0.44
2:B:25:GLU:OE1	2:B:157:ARG:NH1	2.51	0.44
2:E:57:PHE:CE2	2:E:103:MET:HE1	2.53	0.44
3:C:84:MET:HB3	3:C:87:LEU:HD21	1.98	0.44
1:A:32:ARG:CZ	1:A:100:ARG:HG3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:MET:HE3	2:B:68:VAL:HG21	1.99	0.44
2:B:114:PHE:HB3	2:B:117:TRP:HZ3	1.82	0.44
1:D:12:PRO:HD2	1:D:163:ALA:HB2	1.99	0.44
1:D:15:LEU:HD12	2:E:216:LEU:HD21	2.01	0.43
2:B:25:GLU:OE2	2:B:157:ARG:CZ	2.67	0.43
2:B:135:ARG:HE	2:B:157:ARG:HH22	1.65	0.43
2:E:213:LEU:HA	2:E:216:LEU:HD12	1.99	0.43
3:F:112:PHE:N	3:F:112:PHE:CD2	2.87	0.43
3:F:10:GLY:HA2	3:F:19:LEU:HD13	2.01	0.42
2:B:116:CYS:SG	2:B:152:VAL:HG12	2.59	0.42
3:F:51:THR:HG23	3:F:103:TYR:CE1	2.54	0.42
3:C:30:PHE:CE2	3:C:112:PHE:HB3	2.55	0.42
1:D:28:LYS:O	1:D:29:GLU:C	2.56	0.42
2:E:74:SER:C	2:E:76:THR:N	2.72	0.42
2:B:69:PHE:HE1	2:B:71:MET:HE1	1.84	0.42
2:E:37:MET:HE3	2:E:141:VAL:HG21	2.01	0.42
2:E:28:TYR:CD1	2:E:202:ASP:HB3	2.55	0.42
2:B:78:VAL:O	2:B:78:VAL:HG12	2.19	0.41
3:F:30:PHE:CD2	3:F:112:PHE:CD2	3.08	0.41
2:B:137:VAL:HG12	2:B:138:ALA:N	2.34	0.41
2:B:117:TRP:CG	2:B:118:LEU:N	2.88	0.41
1:A:16:LEU:HD23	2:B:212:MET:HE1	2.02	0.41
1:D:43:SER:OG	1:D:44:SER:N	2.53	0.41
3:F:18:SER:OG	3:F:85:ASN:ND2	2.49	0.41
1:A:71:ASN:O	1:A:75:ASN:ND2	2.52	0.41
3:C:13:VAL:HG12	3:C:14:PRO:O	2.21	0.41
1:D:132:LEU:HA	1:D:133:PRO:HD3	1.92	0.41
2:E:108:TYR:HA	2:E:139:VAL:O	2.21	0.41
1:A:24:ARG:HA	3:C:108:TYR:CD2	2.56	0.40
2:E:93:ASP:O	2:E:97:GLN:HG3	2.21	0.40
2:E:71:MET:HE2	2:E:71:MET:HA	2.02	0.40
1:A:22:TYR:CD1	1:A:125:VAL:HG21	2.56	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	159/187 (85%)	154 (97%)	3 (2%)	2 (1%)	15	21
1	D	160/187 (86%)	153 (96%)	7 (4%)	0	100	100
2	B	177/220 (80%)	170 (96%)	6 (3%)	1 (1%)	30	43
2	E	180/220 (82%)	172 (96%)	7 (4%)	1 (1%)	30	43
3	C	123/133 (92%)	120 (98%)	3 (2%)	0	100	100
3	F	123/133 (92%)	118 (96%)	4 (3%)	1 (1%)	24	35
All	All	922/1080 (85%)	887 (96%)	30 (3%)	5 (0%)	34	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	59	ASP
2	E	75	GLY
1	A	141	GLU
1	A	30	ASN
3	F	27	GLY

### 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	132/162 (82%)	122 (92%)	10 (8%)	16	25
1	D	134/162 (83%)	128 (96%)	6 (4%)	34	52
2	B	152/191 (80%)	142 (93%)	10 (7%)	21	32
2	E	150/191 (78%)	143 (95%)	7 (5%)	32	50
3	C	101/109 (93%)	94 (93%)	7 (7%)	19	30
3	F	101/109 (93%)	90 (89%)	11 (11%)	8	11
All	All	770/924 (83%)	719 (93%)	51 (7%)	21	32

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	71	ASN
1	A	73	ILE
1	A	83	ILE
1	A	108	GLU
1	A	109	LEU
1	A	121	LEU
1	A	127	GLN
1	A	132	LEU
1	A	138	VAL
2	B	24	LYS
2	B	68	VAL
2	B	76	THR
2	B	86	VAL
2	B	96	LYS
2	B	117	TRP
2	B	128	SER
2	B	154	ASP
2	B	198	SER
2	B	214	MET
3	C	8	SER
3	C	14	PRO
3	C	18	SER
3	C	28	ARG
3	C	65	VAL
3	C	68	ARG
3	C	73	ARG
1	D	7	LYS
1	D	9	THR
1	D	43	SER
1	D	64	ASP
1	D	89	LEU
1	D	109	LEU
2	E	49	VAL
2	E	50	MET
2	E	68	VAL
2	E	85	ASP
2	E	127	LYS
2	E	147	VAL
2	E	188	LEU
3	F	6	GLN
3	F	18	SER

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Mol	Chain	Res	Type
3	F	22	SER
3	F	29	THR
3	F	46	ARG
3	F	65	VAL
3	F	73	ARG
3	F	75	ASN
3	F	90	GLU
3	F	105	THR
3	F	120	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	73	GLN
2	B	111	HIS
2	B	184	ASN
2	B	200	ASN
1	D	21	HIS
1	D	70	HIS
2	E	73	GLN
2	E	88	GLN
2	E	102	GLN
2	E	195	HIS
2	E	204	HIS
2	E	217	HIS
3	F	40	GLN
3	F	75	ASN
3	F	85	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 2 ligands modelled in this entry, 2 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, 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	163/187 (87%)	0.19	8 (4%) 33 34	27, 52, 77, 92	0
1	D	164/187 (87%)	0.05	3 (1%) 71 71	24, 46, 66, 82	0
2	B	181/220 (82%)	0.12	7 (3%) 43 44	24, 44, 75, 93	0
2	E	184/220 (83%)	0.31	17 (9%) 11 11	22, 42, 92, 144	0
3	C	125/133 (93%)	0.25	8 (6%) 23 23	24, 45, 74, 98	0
3	F	125/133 (93%)	-0.02	6 (4%) 34 35	21, 41, 71, 88	0
All	All	942/1080 (87%)	0.16	49 (5%) 31 31	21, 45, 76, 144	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	180	LEU	9.4
2	B	163	ALA	8.3
2	E	185	ILE	7.2
2	E	181	ASN	6.8
2	E	184	ASN	6.6
3	C	30	PHE	6.1
3	C	28	ARG	5.8
3	F	29	THR	5.4
3	F	30	PHE	5.0
3	C	29	THR	4.9
2	E	183	ALA	4.8
2	E	75	GLY	4.7
2	E	149	GLY	4.1
3	F	3	VAL	3.9
2	E	76	THR	3.8
1	A	142	GLN	3.8
3	F	28	ARG	3.6
2	E	186	GLN	3.6
2	E	168	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	23	THR	3.5
1	A	42	ASN	3.4
3	C	3	VAL	3.4
1	A	30	ASN	3.2
1	A	153	THR	3.1
2	E	148	LYS	3.0
2	E	217	HIS	3.0
2	B	76	THR	2.9
2	E	166	ASN	2.8
3	C	127	HIS	2.8
1	A	128	GLN	2.6
2	E	188	LEU	2.6
1	D	5	HIS	2.5
1	D	42	ASN	2.5
2	E	190	HIS	2.4
1	A	40	ASP	2.4
1	A	130	VAL	2.4
3	F	127	HIS	2.4
2	B	160	ASP	2.3
2	B	114	PHE	2.3
3	C	31	SER	2.2
2	B	74	SER	2.2
3	F	27	GLY	2.2
2	B	161	THR	2.1
2	E	33	ALA	2.1
2	B	192	LEU	2.1
1	A	6	GLU	2.1
3	C	56	GLY	2.1
3	C	6	GLN	2.0
1	D	30	ASN	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, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ZN	B	401	1/1	0.95	0.06	-3.55	74,74,74,74	0
4	ZN	E	401	1/1	0.99	0.03	-	64,64,64,64	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.