Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 11:05 PM BST

PDB ID	:	4OJ0
Title	:	mCardinal V218E
Authors	:	Ataie, N.; Ng, H.
Deposited on	:	2014-01-20
Resolution	:	1.70 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 following versions of software and data (see references ⓘ) were used in the production of this report:

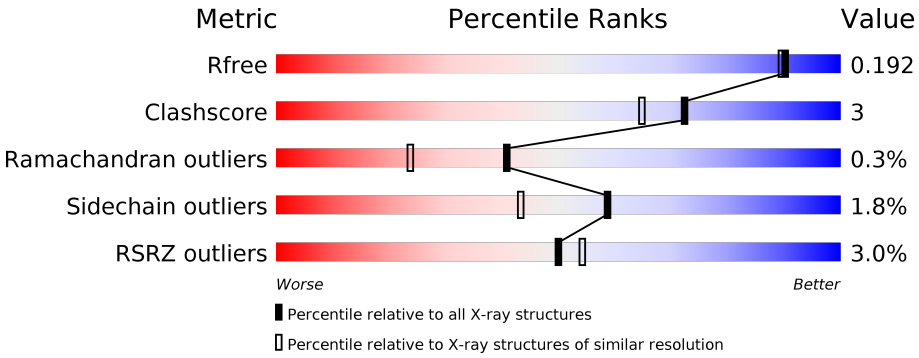
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	244	2% 86% 5% • 8%
1	B	244	% 86% 5% 8%
1	C	244	3% 85% 7% 8%
1	D	244	5% 85% 7% • 8%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14788 atoms, of which 6973 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 Fluorescent protein FP480.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	225	Total	C	H	N	O	S	0	0	0
			3542	1140	1746	303	340	13			
1	B	225	Total	C	H	N	O	S	0	0	0
			3542	1140	1746	303	340	13			
1	C	225	Total	C	H	N	O	S	0	0	0
			3531	1140	1735	303	340	13			
1	D	225	Total	C	H	N	O	S	0	0	0
			3542	1140	1746	303	340	13			

There are 164 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ASP	-	EXPRESSION TAG	UNP D0VX33
A	-4	PRO	-	EXPRESSION TAG	UNP D0VX33
A	-3	MET	-	EXPRESSION TAG	UNP D0VX33
A	-2	VAL	-	EXPRESSION TAG	UNP D0VX33
A	-1	SER	-	EXPRESSION TAG	UNP D0VX33
A	0	LYS	-	EXPRESSION TAG	UNP D0VX33
A	1	GLY	-	EXPRESSION TAG	UNP D0VX33
A	2	GLU	-	EXPRESSION TAG	UNP D0VX33
A	6	LYS	THR	CONFLICT	UNP D0VX33
A	10	PRO	HIS	CONFLICT	UNP D0VX33
A	28	THR	SER	CONFLICT	UNP D0VX33
A	61	CYS	SER	CONFLICT	UNP D0VX33
A	63	NRQ	MET	CHROMOPHORE	UNP D0VX33
A	63	NRQ	TYR	CHROMOPHORE	UNP D0VX33
A	63	NRQ	GLY	CHROMOPHORE	UNP D0VX33
A	67	LYS	HIS	CONFLICT	UNP D0VX33
A	71	LYS	ASN	CONFLICT	UNP D0VX33
A	73	PRO	THR	CONFLICT	UNP D0VX33
A	74	LYS	GLN	CONFLICT	UNP D0VX33
A	80	PHE	TRP	CONFLICT	UNP D0VX33
A	104	VAL	ALA	CONFLICT	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
A	121	LEU	ILE	CONFLICT	UNP D0VX33
A	143	THR	HIS	CONFLICT	UNP D0VX33
A	146	THR	MET	CONFLICT	UNP D0VX33
A	158	CYS	ALA	CONFLICT	UNP D0VX33
A	160	MET	LEU	CONFLICT	UNP D0VX33
A	165	ASP	VAL	CONFLICT	UNP D0VX33
A	171	HIS	ILE	CONFLICT	UNP D0VX33
A	174	LEU	PHE	CONFLICT	UNP D0VX33
A	185	GLY	LYS	CONFLICT	UNP D0VX33
A	194	PHE	TYR	CONFLICT	UNP D0VX33
A	197	ARG	TYR	CONFLICT	UNP D0VX33
A	207	ASN	LYS	CONFLICT	UNP D0VX33
A	218	GLU	VAL	ENGINEERED MUTATION	UNP D0VX33
A	234	GLY	-	EXPRESSION TAG	UNP D0VX33
A	235	MET	-	EXPRESSION TAG	UNP D0VX33
A	236	ASP	-	EXPRESSION TAG	UNP D0VX33
A	237	GLU	-	EXPRESSION TAG	UNP D0VX33
A	238	LEU	-	EXPRESSION TAG	UNP D0VX33
A	239	TYR	-	EXPRESSION TAG	UNP D0VX33
A	240	LYS	-	EXPRESSION TAG	UNP D0VX33
B	-5	ASP	-	EXPRESSION TAG	UNP D0VX33
B	-4	PRO	-	EXPRESSION TAG	UNP D0VX33
B	-3	MET	-	EXPRESSION TAG	UNP D0VX33
B	-2	VAL	-	EXPRESSION TAG	UNP D0VX33
B	-1	SER	-	EXPRESSION TAG	UNP D0VX33
B	0	LYS	-	EXPRESSION TAG	UNP D0VX33
B	1	GLY	-	EXPRESSION TAG	UNP D0VX33
B	2	GLU	-	EXPRESSION TAG	UNP D0VX33
B	6	LYS	THR	CONFLICT	UNP D0VX33
B	10	PRO	HIS	CONFLICT	UNP D0VX33
B	28	THR	SER	CONFLICT	UNP D0VX33
B	61	CYS	SER	CONFLICT	UNP D0VX33
B	63	NRQ	MET	CHROMOPHORE	UNP D0VX33
B	63	NRQ	TYR	CHROMOPHORE	UNP D0VX33
B	63	NRQ	GLY	CHROMOPHORE	UNP D0VX33
B	67	LYS	HIS	CONFLICT	UNP D0VX33
B	71	LYS	ASN	CONFLICT	UNP D0VX33
B	73	PRO	THR	CONFLICT	UNP D0VX33
B	74	LYS	GLN	CONFLICT	UNP D0VX33
B	80	PHE	TRP	CONFLICT	UNP D0VX33
B	104	VAL	ALA	CONFLICT	UNP D0VX33
B	121	LEU	ILE	CONFLICT	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
B	143	THR	HIS	CONFLICT	UNP D0VX33
B	146	THR	MET	CONFLICT	UNP D0VX33
B	158	CYS	ALA	CONFLICT	UNP D0VX33
B	160	MET	LEU	CONFLICT	UNP D0VX33
B	165	ASP	VAL	CONFLICT	UNP D0VX33
B	171	HIS	ILE	CONFLICT	UNP D0VX33
B	174	LEU	PHE	CONFLICT	UNP D0VX33
B	185	GLY	LYS	CONFLICT	UNP D0VX33
B	194	PHE	TYR	CONFLICT	UNP D0VX33
B	197	ARG	TYR	CONFLICT	UNP D0VX33
B	207	ASN	LYS	CONFLICT	UNP D0VX33
B	218	GLU	VAL	ENGINEERED MUTATION	UNP D0VX33
B	234	GLY	-	EXPRESSION TAG	UNP D0VX33
B	235	MET	-	EXPRESSION TAG	UNP D0VX33
B	236	ASP	-	EXPRESSION TAG	UNP D0VX33
B	237	GLU	-	EXPRESSION TAG	UNP D0VX33
B	238	LEU	-	EXPRESSION TAG	UNP D0VX33
B	239	TYR	-	EXPRESSION TAG	UNP D0VX33
B	240	LYS	-	EXPRESSION TAG	UNP D0VX33
C	-5	ASP	-	EXPRESSION TAG	UNP D0VX33
C	-4	PRO	-	EXPRESSION TAG	UNP D0VX33
C	-3	MET	-	EXPRESSION TAG	UNP D0VX33
C	-2	VAL	-	EXPRESSION TAG	UNP D0VX33
C	-1	SER	-	EXPRESSION TAG	UNP D0VX33
C	0	LYS	-	EXPRESSION TAG	UNP D0VX33
C	1	GLY	-	EXPRESSION TAG	UNP D0VX33
C	2	GLU	-	EXPRESSION TAG	UNP D0VX33
C	6	LYS	THR	CONFLICT	UNP D0VX33
C	10	PRO	HIS	CONFLICT	UNP D0VX33
C	28	THR	SER	CONFLICT	UNP D0VX33
C	61	CYS	SER	CONFLICT	UNP D0VX33
C	63	NRQ	MET	CHROMOPHORE	UNP D0VX33
C	63	NRQ	TYR	CHROMOPHORE	UNP D0VX33
C	63	NRQ	GLY	CHROMOPHORE	UNP D0VX33
C	67	LYS	HIS	CONFLICT	UNP D0VX33
C	71	LYS	ASN	CONFLICT	UNP D0VX33
C	73	PRO	THR	CONFLICT	UNP D0VX33
C	74	LYS	GLN	CONFLICT	UNP D0VX33
C	80	PHE	TRP	CONFLICT	UNP D0VX33
C	104	VAL	ALA	CONFLICT	UNP D0VX33
C	121	LEU	ILE	CONFLICT	UNP D0VX33
C	143	THR	HIS	CONFLICT	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
C	146	THR	MET	CONFLICT	UNP D0VX33
C	158	CYS	ALA	CONFLICT	UNP D0VX33
C	160	MET	LEU	CONFLICT	UNP D0VX33
C	165	ASP	VAL	CONFLICT	UNP D0VX33
C	171	HIS	ILE	CONFLICT	UNP D0VX33
C	174	LEU	PHE	CONFLICT	UNP D0VX33
C	185	GLY	LYS	CONFLICT	UNP D0VX33
C	194	PHE	TYR	CONFLICT	UNP D0VX33
C	197	ARG	TYR	CONFLICT	UNP D0VX33
C	207	ASN	LYS	CONFLICT	UNP D0VX33
C	218	GLU	VAL	ENGINEERED MUTATION	UNP D0VX33
C	234	GLY	-	EXPRESSION TAG	UNP D0VX33
C	235	MET	-	EXPRESSION TAG	UNP D0VX33
C	236	ASP	-	EXPRESSION TAG	UNP D0VX33
C	237	GLU	-	EXPRESSION TAG	UNP D0VX33
C	238	LEU	-	EXPRESSION TAG	UNP D0VX33
C	239	TYR	-	EXPRESSION TAG	UNP D0VX33
C	240	LYS	-	EXPRESSION TAG	UNP D0VX33
D	-5	ASP	-	EXPRESSION TAG	UNP D0VX33
D	-4	PRO	-	EXPRESSION TAG	UNP D0VX33
D	-3	MET	-	EXPRESSION TAG	UNP D0VX33
D	-2	VAL	-	EXPRESSION TAG	UNP D0VX33
D	-1	SER	-	EXPRESSION TAG	UNP D0VX33
D	0	LYS	-	EXPRESSION TAG	UNP D0VX33
D	1	GLY	-	EXPRESSION TAG	UNP D0VX33
D	2	GLU	-	EXPRESSION TAG	UNP D0VX33
D	6	LYS	THR	CONFLICT	UNP D0VX33
D	10	PRO	HIS	CONFLICT	UNP D0VX33
D	28	THR	SER	CONFLICT	UNP D0VX33
D	61	CYS	SER	CONFLICT	UNP D0VX33
D	63	NRQ	MET	CHROMOPHORE	UNP D0VX33
D	63	NRQ	TYR	CHROMOPHORE	UNP D0VX33
D	63	NRQ	GLY	CHROMOPHORE	UNP D0VX33
D	67	LYS	HIS	CONFLICT	UNP D0VX33
D	71	LYS	ASN	CONFLICT	UNP D0VX33
D	73	PRO	THR	CONFLICT	UNP D0VX33
D	74	LYS	GLN	CONFLICT	UNP D0VX33
D	80	PHE	TRP	CONFLICT	UNP D0VX33
D	104	VAL	ALA	CONFLICT	UNP D0VX33
D	121	LEU	ILE	CONFLICT	UNP D0VX33
D	143	THR	HIS	CONFLICT	UNP D0VX33
D	146	THR	MET	CONFLICT	UNP D0VX33

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Chain	Residue	Modelled	Actual	Comment	Reference
D	158	CYS	ALA	CONFLICT	UNP D0VX33
D	160	MET	LEU	CONFLICT	UNP D0VX33
D	165	ASP	VAL	CONFLICT	UNP D0VX33
D	171	HIS	ILE	CONFLICT	UNP D0VX33
D	174	LEU	PHE	CONFLICT	UNP D0VX33
D	185	GLY	LYS	CONFLICT	UNP D0VX33
D	194	PHE	TYR	CONFLICT	UNP D0VX33
D	197	ARG	TYR	CONFLICT	UNP D0VX33
D	207	ASN	LYS	CONFLICT	UNP D0VX33
D	218	GLU	VAL	ENGINEERED MUTATION	UNP D0VX33
D	234	GLY	-	EXPRESSION TAG	UNP D0VX33
D	235	MET	-	EXPRESSION TAG	UNP D0VX33
D	236	ASP	-	EXPRESSION TAG	UNP D0VX33
D	237	GLU	-	EXPRESSION TAG	UNP D0VX33
D	238	LEU	-	EXPRESSION TAG	UNP D0VX33
D	239	TYR	-	EXPRESSION TAG	UNP D0VX33
D	240	LYS	-	EXPRESSION TAG	UNP D0VX33

- Molecule 2 is water.

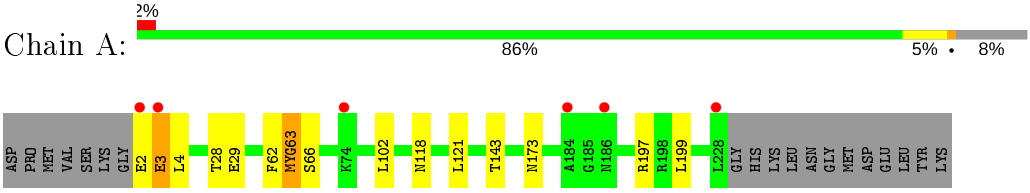
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	151	Total O 151 151	0	0
2	B	154	Total O 154 154	0	0
2	C	163	Total O 163 163	0	0
2	D	163	Total O 163 163	0	0

3 Residue-property plots

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.

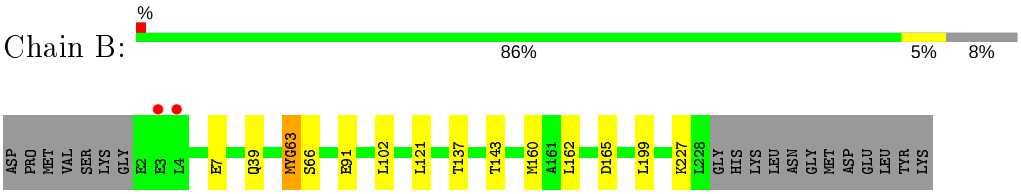
- Molecule 1: Fluorescent protein FP480

Chain A:



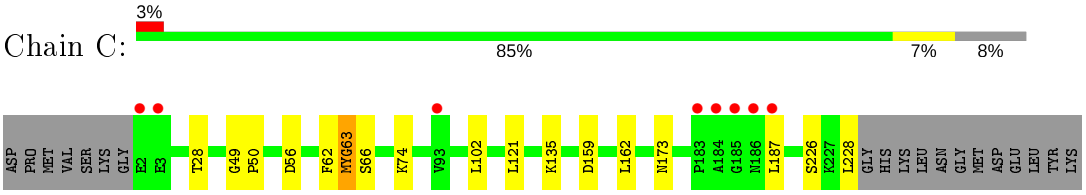
- Molecule 1: Fluorescent protein FP480

Chain B:



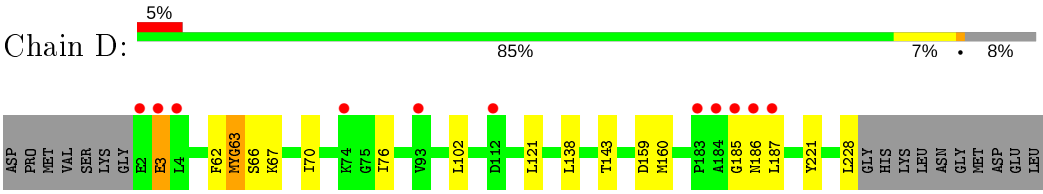
- Molecule 1: Fluorescent protein FP480

Chain C:



- Molecule 1: Fluorescent protein FP480

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.55Å 102.94Å 116.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.44 – 1.70 45.44 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (45.44-1.70) 98.8 (45.44-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.165 , 0.192 0.167 , 0.192	Depositor DCC
R_{free} test set	1190 reflections (1.25%)	wwPDB-VP
Wilson B-factor (Å^2)	22.4	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14788	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.56	0/1814	0.69	0/2448
1	B	0.55	0/1814	0.68	0/2448
1	C	0.57	0/1814	0.68	0/2448
1	D	0.55	0/1814	0.68	0/2448
All	All	0.56	0/7256	0.68	0/9792

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
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	GLU	Peptide
1	D	186	ASN	Peptide

5.2 Too-close contacts (i)

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	1796	1746	1752	11	0
1	B	1796	1746	1752	10	0
1	C	1796	1735	1752	11	0
1	D	1796	1746	1752	10	0
2	A	151	0	0	0	0
2	B	154	0	0	1	0
2	C	163	0	0	0	0
2	D	163	0	0	0	0
All	All	7815	6973	7008	40	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 (40) 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:63:NRQ:O3	1:C:66:SER:N	2.07	0.87
1:A:63:NRQ:O3	1:A:66:SER:N	2.13	0.81
1:A:63:NRQ:HE1	1:A:143:THR:HG21	1.81	0.62
1:C:62:PHE:C	1:C:63:NRQ:CA1	2.70	0.60
1:C:63:NRQ:CA3	1:C:66:SER:N	2.65	0.59
1:B:63:NRQ:O3	1:B:66:SER:N	2.36	0.58
1:B:63:NRQ:CA3	1:B:66:SER:N	2.70	0.54
1:A:63:NRQ:CE1	1:A:143:THR:HG21	2.37	0.54
1:B:63:NRQ:HA31	1:B:63:NRQ:N1	2.23	0.53
1:D:63:NRQ:CA3	1:D:66:SER:N	2.74	0.50
1:B:39:GLN:HE22	1:B:66:SER:CB	2.25	0.50
1:D:63:NRQ:HD2	1:D:63:NRQ:N2	2.27	0.49
1:A:63:NRQ:HE2	1:A:199:LEU:HB2	1.95	0.48
1:A:62:PHE:C	1:A:63:NRQ:CA1	2.81	0.48
1:A:63:NRQ:CA3	1:A:66:SER:N	2.77	0.48
1:C:159:ASP:OD1	1:C:173:ASN:ND2	2.46	0.47
1:D:63:NRQ:HA31	1:D:63:NRQ:N1	2.28	0.47
1:A:63:NRQ:HD2	1:A:63:NRQ:N2	2.29	0.47
1:C:74:LYS:NZ	1:D:221:TYR:H	2.12	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASN:ND2	1:D:159:ASP:OD2	2.46	0.46
1:C:102:LEU:HD11	1:C:121:LEU:HD21	1.98	0.46
1:D:143:THR:HG21	1:D:160:MET:HG2	1.97	0.46
1:B:63:NRQ:HE2	1:B:199:LEU:HB2	2.00	0.44
1:D:102:LEU:HD11	1:D:121:LEU:HD13	1.98	0.44
1:D:76:ILE:HG12	1:D:221:TYR:CE2	2.53	0.44
1:B:227:LYS:NZ	2:B:428:HOH:O	2.50	0.43
1:C:63:NRQ:HD2	1:C:63:NRQ:N2	2.33	0.43
1:D:62:PHE:O	1:D:63:NRQ:N1	2.51	0.43
1:C:49:GLY:HA2	1:C:50:PRO:C	2.40	0.43
1:B:63:NRQ:N2	1:B:63:NRQ:HD2	2.34	0.43
1:C:228:LEU:HD12	1:C:228:LEU:HA	1.82	0.42
1:C:56:ASP:HB3	1:C:162:LEU:HD21	2.01	0.42
1:D:67:LYS:HE3	1:D:70:ILE:HD11	2.03	0.41
1:B:102:LEU:HD11	1:B:121:LEU:HD13	2.03	0.41
1:C:63:NRQ:O3	1:C:66:SER:CA	2.69	0.41
1:A:63:NRQ:CE2	1:A:197:ARG:HD3	2.51	0.41
1:B:137:THR:HG21	1:B:162:LEU:HD13	2.03	0.41
1:A:3:GLU:HG3	1:A:4:LEU:HG	2.03	0.40
1:B:143:THR:HG21	1:B:160:MET:HG2	2.03	0.40
1:A:102:LEU:HD11	1:A:121:LEU:HD13	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	220/244 (90%)	217 (99%)	2 (1%)	1 (0%)	29 13
1	B	220/244 (90%)	218 (99%)	2 (1%)	0	100 100
1	C	220/244 (90%)	217 (99%)	3 (1%)	0	100 100
1	D	220/244 (90%)	211 (96%)	7 (3%)	2 (1%)	17 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	880/976 (90%)	863 (98%)	14 (2%)	3 (0%)	41 24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	D	3	GLU
1	D	185	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	193/209 (92%)	190 (98%)	3 (2%)	62 48
1	B	193/209 (92%)	190 (98%)	3 (2%)	62 48
1	C	193/209 (92%)	189 (98%)	4 (2%)	53 36
1	D	193/209 (92%)	189 (98%)	4 (2%)	53 36
All	All	772/836 (92%)	758 (98%)	14 (2%)	59 43

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	29	GLU
1	A	118	ASN
1	B	7	GLU
1	B	91	GLU
1	B	165	ASP
1	C	28	THR
1	C	135	LYS
1	C	187	LEU
1	C	226	SER
1	D	3	GLU
1	D	138	LEU

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Mol	Chain	Res	Type
1	D	187	LEU
1	D	228	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	NRQ	B	63	1	23,24,25	2.35	4 (17%)	23,32,34	2.53	12 (52%)
1	NRQ	D	63	1	23,24,25	2.50	5 (21%)	23,32,34	2.91	11 (47%)
1	NRQ	A	63	1	23,24,25	2.06	4 (17%)	23,32,34	2.54	13 (56%)
1	NRQ	C	63	1	23,24,25	2.20	4 (17%)	23,32,34	3.28	13 (56%)

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
1	NRQ	B	63	1	-	4/9/31/32	0/2/2/2
1	NRQ	D	63	1	-	2/9/31/32	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NRQ	A	63	1	-	5/9/31/32	0/2/2/2
1	NRQ	C	63	1	-	3/9/31/32	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	NRQ	CA2-C2	9.25	1.57	1.48
1	B	63	NRQ	CA2-C2	8.66	1.57	1.48
1	C	63	NRQ	CA2-C2	7.66	1.56	1.48
1	A	63	NRQ	CA2-C2	7.01	1.55	1.48
1	D	63	NRQ	C2-N3	4.78	1.51	1.39
1	A	63	NRQ	C2-N3	4.29	1.50	1.39
1	B	63	NRQ	C2-N3	4.02	1.49	1.39
1	C	63	NRQ	C2-N3	3.95	1.49	1.39
1	C	63	NRQ	C1-N3	3.91	1.44	1.38
1	B	63	NRQ	C1-N3	3.56	1.44	1.38
1	A	63	NRQ	OH-CZ	3.47	1.45	1.37
1	D	63	NRQ	OH-CZ	3.37	1.44	1.37
1	D	63	NRQ	C1-N3	3.10	1.43	1.38
1	C	63	NRQ	OH-CZ	3.05	1.44	1.37
1	B	63	NRQ	OH-CZ	2.98	1.44	1.37
1	A	63	NRQ	C1-N3	2.44	1.42	1.38
1	D	63	NRQ	CB2-CA2	2.04	1.36	1.35

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	63	NRQ	CA2-C2-N3	7.29	106.82	103.37
1	C	63	NRQ	CA3-N3-C1	7.10	142.13	128.22
1	D	63	NRQ	CA2-C2-N3	6.10	106.26	103.37
1	D	63	NRQ	C2-CA2-N2	-5.56	105.04	108.93
1	D	63	NRQ	O2-C2-CA2	-5.07	128.11	130.96
1	B	63	NRQ	O2-C2-CA2	-4.79	128.27	130.96
1	B	63	NRQ	O3-C3-CA3	-4.75	112.06	126.39
1	A	63	NRQ	CB2-CA2-N2	4.66	135.29	128.83
1	D	63	NRQ	CB2-CA2-N2	4.64	135.26	128.83
1	C	63	NRQ	C2-CA2-N2	-4.50	105.78	108.93
1	C	63	NRQ	O3-C3-CA3	-4.41	113.09	126.39
1	C	63	NRQ	CB2-CA2-N2	4.40	134.93	128.83
1	C	63	NRQ	O2-C2-CA2	-4.34	128.53	130.96
1	A	63	NRQ	O3-C3-CA3	-4.16	113.84	126.39
1	A	63	NRQ	CA2-C2-N3	4.03	105.28	103.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	63	NRQ	CB2-CA2-N2	3.95	134.31	128.83
1	B	63	NRQ	CA2-C2-N3	3.92	105.22	103.37
1	A	63	NRQ	N3-C1-N2	3.85	118.36	113.28
1	A	63	NRQ	CB2-CA2-C2	-3.81	117.73	122.28
1	D	63	NRQ	CA3-N3-C1	3.77	135.60	128.22
1	D	63	NRQ	O3-C3-CA3	-3.68	115.28	126.39
1	B	63	NRQ	C2-CA2-N2	-3.53	106.46	108.93
1	B	63	NRQ	N3-C1-N2	3.44	117.82	113.28
1	C	63	NRQ	N3-C1-N2	3.42	117.79	113.28
1	A	63	NRQ	CD1-CG2-CD2	3.39	122.66	117.64
1	C	63	NRQ	CD1-CG2-CD2	3.37	122.63	117.64
1	D	63	NRQ	N3-C1-N2	3.25	117.57	113.28
1	C	63	NRQ	CA3-N3-C2	-3.23	116.39	123.80
1	D	63	NRQ	CA2-N2-C1	3.16	110.12	104.33
1	A	63	NRQ	CG2-CB2-CA2	-3.00	126.27	129.94
1	B	63	NRQ	CE-SD-CG1	2.99	110.67	100.40
1	B	63	NRQ	CD1-CG2-CD2	2.85	121.85	117.64
1	A	63	NRQ	C2-CA2-N2	-2.80	106.97	108.93
1	D	63	NRQ	CD1-CG2-CD2	2.68	121.61	117.64
1	A	63	NRQ	CE1-CD1-CG2	-2.62	117.83	121.25
1	B	63	NRQ	CB2-CA2-C2	-2.56	119.22	122.28
1	C	63	NRQ	CA2-N2-C1	2.55	108.99	104.33
1	A	63	NRQ	O2-C2-CA2	-2.51	129.55	130.96
1	C	63	NRQ	CE-SD-CG1	2.51	109.03	100.40
1	C	63	NRQ	CB2-CA2-C2	-2.51	119.28	122.28
1	B	63	NRQ	CA2-N2-C1	2.46	108.83	104.33
1	A	63	NRQ	CE-SD-CG1	2.44	108.78	100.40
1	B	63	NRQ	CA3-N3-C1	2.36	132.84	128.22
1	C	63	NRQ	CE2-CD2-CG2	-2.26	118.30	121.25
1	A	63	NRQ	CA3-N3-C1	2.20	132.54	128.22
1	D	63	NRQ	CB2-CA2-C2	-2.16	119.70	122.28
1	D	63	NRQ	CE-SD-CG1	2.06	107.49	100.40
1	B	63	NRQ	CE2-CD2-CG2	-2.03	118.60	121.25
1	A	63	NRQ	CD2-CG2-CB2	-2.00	114.39	121.22

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	63	NRQ	C1-CA1-CB1-CG1
1	C	63	NRQ	C1-CA1-CB1-CG1
1	C	63	NRQ	C3-CA3-N3-C1

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Mol	Chain	Res	Type	Atoms
1	C	63	NRQ	C3-CA3-N3-C2
1	B	63	NRQ	C3-CA3-N3-C2
1	A	63	NRQ	C3-CA3-N3-C2
1	A	63	NRQ	N2-CA2-CB2-CG2
1	B	63	NRQ	CB1-CG1-SD-CE
1	B	63	NRQ	C1-CA1-CB1-CG1
1	A	63	NRQ	C1-CA1-CB1-CG1
1	D	63	NRQ	C3-CA3-N3-C2
1	A	63	NRQ	C2-CA2-CB2-CG2
1	B	63	NRQ	C3-CA3-N3-C1
1	A	63	NRQ	C3-CA3-N3-C1

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	63	NRQ	5	0
1	D	63	NRQ	4	0
1	A	63	NRQ	8	0
1	C	63	NRQ	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	224/244 (91%)	-0.07	6 (2%) 54 58	17, 29, 55, 108	0
1	B	224/244 (91%)	-0.09	2 (0%) 84 87	16, 28, 52, 86	0
1	C	224/244 (91%)	-0.08	8 (3%) 42 47	16, 26, 57, 99	0
1	D	224/244 (91%)	-0.04	11 (4%) 29 33	17, 29, 58, 99	0
All	All	896/976 (91%)	-0.07	27 (3%) 50 54	16, 28, 57, 108	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	184	ALA	5.8
1	A	2	GLU	5.6
1	A	186	ASN	5.5
1	C	184	ALA	5.0
1	D	183	PRO	4.4
1	C	187	LEU	3.5
1	D	3	GLU	3.5
1	A	184	ALA	3.4
1	D	2	GLU	3.3
1	D	185	GLY	3.1
1	A	3	GLU	3.0
1	D	186	ASN	3.0
1	C	183	PRO	2.9
1	A	228	LEU	2.9
1	B	3	GLU	2.8
1	B	4	LEU	2.7
1	D	93	VAL	2.6
1	C	185	GLY	2.5
1	D	4	LEU	2.4
1	C	186	ASN	2.3
1	D	187	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	74	LYS	2.3
1	C	93	VAL	2.2
1	D	112	ASP	2.1
1	C	3	GLU	2.1
1	C	2	GLU	2.1
1	D	74	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	NRQ	A	63	23/24	0.89	0.16	22,35,67,72	0
1	NRQ	D	63	23/24	0.92	0.13	24,38,51,55	0
1	NRQ	C	63	23/24	0.93	0.12	23,33,44,47	0
1	NRQ	B	63	23/24	0.94	0.11	22,31,39,41	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.