Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:27 am BST

PDB ID	:	4LJQ
Title	:	Crystal structure of the catalytic core of E3 ligase HOIP
Authors	:	Stieglitz, B.; Rana, R.R.; Koliopoulos, M.G.; Morris-Davies, A.C.; Christodoulou, E.; Howell, S.; Brown, N.R.; Rittinger, K.
Deposited on	:	2013-07-05
Resolution	:	2.45 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:

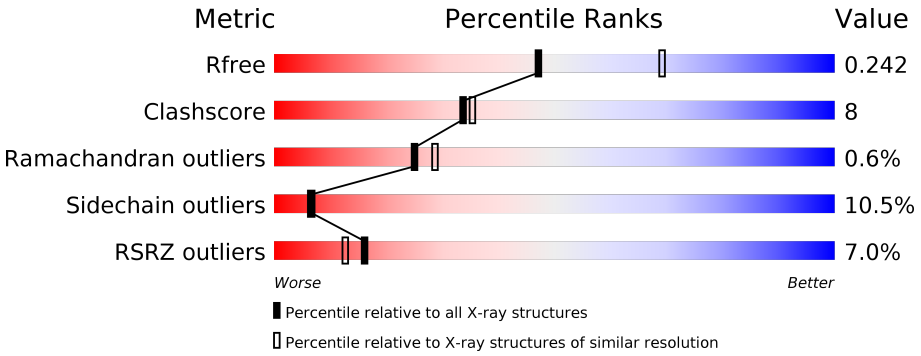
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	223	7% 70% 12% • 15%
1	B	223	3% 70% 13% • 14%
1	C	223	6% 68% 15% • 14%
1	D	223	8% 70% 12% • 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5913 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 E3 ubiquitin-protein ligase RNF31.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	192	Total	C	N	O	S	Se	0	0	0
			1468	939	258	255	13	3			
1	A	190	Total	C	N	O	S	Se	0	0	0
			1448	918	253	261	13	3			
1	C	192	Total	C	N	O	S	Se	0	0	0
			1479	941	254	268	13	3			
1	D	190	Total	C	N	O	S	Se	0	0	0
			1457	925	252	264	13	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	850	GLY	-	EXPRESSION TAG	UNP Q96EP0
B	851	PRO	-	EXPRESSION TAG	UNP Q96EP0
B	852	GLY	-	EXPRESSION TAG	UNP Q96EP0
A	850	GLY	-	EXPRESSION TAG	UNP Q96EP0
A	851	PRO	-	EXPRESSION TAG	UNP Q96EP0
A	852	GLY	-	EXPRESSION TAG	UNP Q96EP0
C	850	GLY	-	EXPRESSION TAG	UNP Q96EP0
C	851	PRO	-	EXPRESSION TAG	UNP Q96EP0
C	852	GLY	-	EXPRESSION TAG	UNP Q96EP0
D	850	GLY	-	EXPRESSION TAG	UNP Q96EP0
D	851	PRO	-	EXPRESSION TAG	UNP Q96EP0
D	852	GLY	-	EXPRESSION TAG	UNP Q96EP0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Zn	0	0
			5	5		
2	A	5	Total	Zn	0	0
			5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	4	Total Zn 4 4	0	0
2	C	4	Total Zn 4 4	0	0

- Molecule 3 is water.

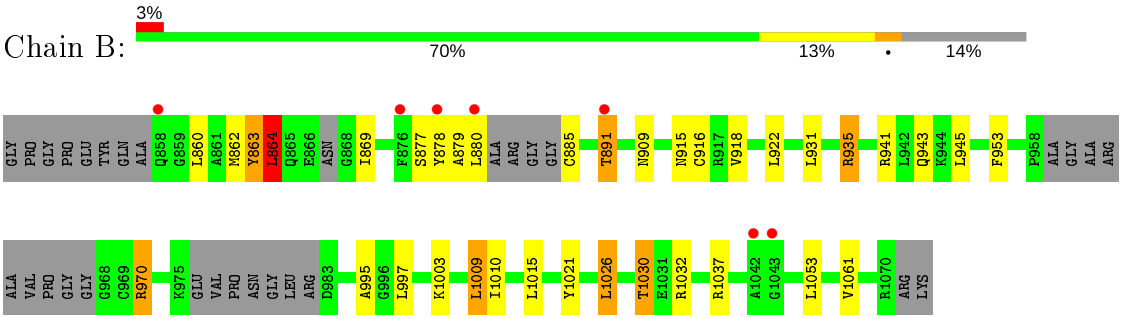
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	21	Total O 21 21	0	0
3	A	9	Total O 9 9	0	0
3	C	7	Total O 7 7	0	0
3	D	6	Total O 6 6	0	0

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.

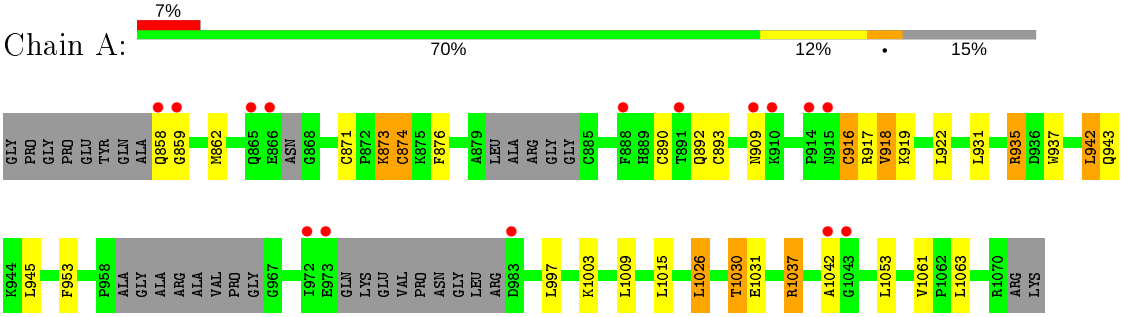
- Molecule 1: E3 ubiquitin-protein ligase RNF31

Chain B:



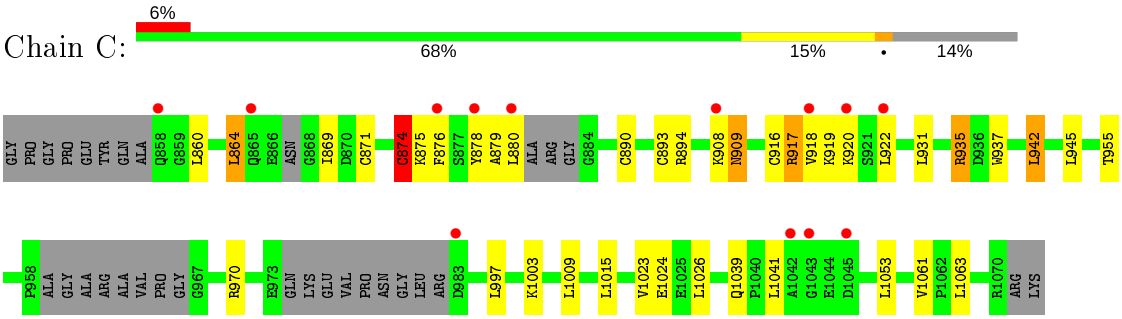
- Molecule 1: E3 ubiquitin-protein ligase RNF31

Chain A:



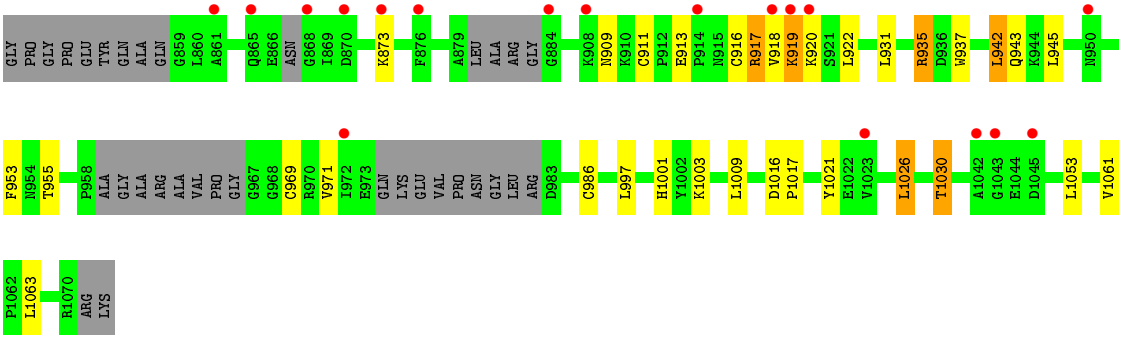
- Molecule 1: E3 ubiquitin-protein ligase RNF31

Chain C:



- Molecule 1: E3 ubiquitin-protein ligase RNF31

Chain D:


GLY PRO GLY PRO GLU TYR GLN ALA GLN G859 L860 A861 Q865 E866 ASN G868 I869 D870 K873 F876 A879 LEU ALA ARG GLY G884 K908 N909 K910 C911 P912 E913 P914 N915 C916 R917 V918 K919 K920 S921 L922 L931 R935 D936 W937 L942 Q943 K944 L945 N950
F953 N954 T955 P958 ALA GLY ALA ARG ALA VAL PRO GLY G967 G968 C969 R970 V971 I972 E973 GLN LYS GLU VAL PRO ASN GLY LEU ARG D983 C986 L997 H1001 Y1002 K1003 L1009 D1016 P1017 Y1021 E1022 V1023 L1026 T1030 A1042 C1043 E1044 D1045 L1053 V1061
P1062 L1063 R1070 ARG LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	44.21Å 47.77Å 111.14Å 101.39° 90.12° 98.92°	Depositor
Resolution (Å)	29.60 – 2.45 29.61 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.60-2.45) 95.1 (29.61-2.45)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.26 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0046	Depositor
R, R_{free}	0.206 , 0.243 0.209 , 0.242	Depositor DCC
R_{free} test set	2008 reflections (6.49%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,k+l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5913	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.06% 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: 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	0.70	1/1481 (0.1%)	0.86	1/2005 (0.0%)
1	B	0.77	0/1500	0.92	8/2028 (0.4%)
1	C	0.67	0/1513	0.83	0/2046
1	D	0.62	0/1491	0.80	0/2017
All	All	0.69	1/5985 (0.0%)	0.85	9/8096 (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
1	A	0	1
1	C	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	874	CYS	CB-SG	-6.30	1.71	1.82

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	874	CYS	CB-CA-C	-9.82	90.76	110.40
1	B	878	TYR	N-CA-C	6.43	128.36	111.00
1	B	863	TYR	N-CA-C	-6.26	94.09	111.00
1	B	864	LEU	N-CA-CB	5.83	122.06	110.40
1	B	941	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	862	MSE	CG-SE-CE	5.25	110.44	98.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	995	ALA	C-N-CA	-5.15	111.49	122.30
1	B	1037	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	885	CYS	CA-CB-SG	5.03	123.05	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	916	CYS	Peptide
1	C	874	CYS	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	1448	0	1339	28	0
1	B	1468	0	1369	21	0
1	C	1479	0	1375	27	0
1	D	1457	0	1347	21	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
3	A	9	0	0	1	0
3	B	21	0	0	1	0
3	C	7	0	0	1	0
3	D	6	0	0	0	0
All	All	5913	0	5430	96	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 (96) 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:A:858:GLN:HB3	1:A:859:GLY:HA2	1.29	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1009:LEU:CA	1:B:1010:ILE:N	2.24	1.00
1:A:858:GLN:CB	1:A:859:GLY:HA2	1.91	1.00
1:B:1009:LEU:O	1:B:1010:ILE:N	1.98	0.97
1:A:874:CYS:HB3	1:A:876:PHE:H	1.32	0.93
1:C:874:CYS:HB3	1:C:876:PHE:H	1.34	0.91
1:D:916:CYS:HA	1:D:917:ARG:CB	2.06	0.85
1:A:1037:ARG:O	1:A:1037:ARG:HG2	1.72	0.84
1:C:916:CYS:HA	1:C:917:ARG:CB	2.05	0.84
1:B:860:LEU:O	1:B:863:TYR:O	1.98	0.82
1:D:969:CYS:SG	1:D:971:VAL:HG22	2.20	0.80
1:A:858:GLN:HB3	1:A:859:GLY:CA	2.13	0.77
1:D:971:VAL:HG21	1:D:1001:HIS:ND1	2.04	0.71
1:A:1042:ALA:O	3:A:1205:HOH:O	2.08	0.71
1:C:874:CYS:HB3	1:C:876:PHE:N	2.04	0.71
1:D:971:VAL:HG21	1:D:1001:HIS:CE1	2.25	0.71
1:B:1009:LEU:O	1:B:1009:LEU:CA	2.39	0.70
1:C:878:TYR:OH	1:C:890:CYS:O	2.09	0.70
1:C:874:CYS:HB3	1:C:875:LYS:CA	2.20	0.69
1:A:917:ARG:C	1:A:919:LYS:H	1.95	0.69
1:A:858:GLN:CG	1:A:859:GLY:HA2	2.22	0.68
1:B:891:THR:HG21	1:C:920:LYS:O	1.95	0.66
1:C:918:VAL:HG12	1:C:918:VAL:O	1.98	0.64
1:B:1030:THR:HG21	1:B:1053:LEU:HD22	1.80	0.63
1:A:871:CYS:HB3	1:A:874:CYS:HB2	1.79	0.63
1:D:918:VAL:HG12	1:D:918:VAL:O	1.99	0.62
1:C:871:CYS:HB3	1:C:874:CYS:HB2	1.80	0.62
1:A:918:VAL:HG12	1:A:918:VAL:O	1.99	0.62
1:A:858:GLN:HG2	1:A:862:MSE:HE3	1.82	0.61
1:A:874:CYS:HB3	1:A:876:PHE:N	2.10	0.61
1:B:879:ALA:O	1:B:880:LEU:C	2.40	0.60
1:A:858:GLN:CB	1:A:859:GLY:CA	2.75	0.59
1:A:890:CYS:O	1:A:893:CYS:O	2.22	0.57
1:D:913:GLU:CG	1:D:916:CYS:HB2	2.36	0.56
1:C:874:CYS:CB	1:C:875:LYS:HA	2.37	0.55
1:C:1023:VAL:HG12	1:C:1024:GLU:OE2	2.06	0.55
1:C:919:LYS:O	1:C:920:LYS:HB2	2.07	0.55
1:C:916:CYS:CA	1:C:917:ARG:CB	2.83	0.54
1:D:971:VAL:HG21	1:D:1001:HIS:CG	2.41	0.54
1:C:874:CYS:CB	1:C:875:LYS:CA	2.86	0.53
1:D:971:VAL:HG23	1:D:986:CYS:HB2	1.90	0.53
1:A:1026:LEU:O	1:A:1030:THR:HG23	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:919:LYS:O	1:D:920:LYS:CB	2.57	0.52
1:D:916:CYS:CA	1:D:917:ARG:CB	2.84	0.52
1:D:937:TRP:CE3	1:D:942:LEU:HD13	2.44	0.52
1:B:880:LEU:HD23	1:B:880:LEU:H	1.75	0.52
1:A:1037:ARG:CG	1:A:1037:ARG:O	2.51	0.50
1:A:874:CYS:CB	1:A:876:PHE:H	2.15	0.50
1:C:937:TRP:CE3	1:C:942:LEU:HD13	2.46	0.50
1:C:874:CYS:CB	1:C:876:PHE:H	2.15	0.50
1:B:1026:LEU:O	1:B:1030:THR:HG23	2.12	0.50
1:D:911:CYS:HB3	1:D:919:LYS:HE2	1.94	0.49
1:D:1026:LEU:O	1:D:1030:THR:HG23	2.12	0.49
1:B:943:GLN:HG2	1:B:953:PHE:CE2	2.49	0.47
1:D:943:GLN:HG2	1:D:953:PHE:CE2	2.49	0.47
1:A:917:ARG:C	1:A:919:LYS:N	2.63	0.47
1:B:1009:LEU:O	1:B:1010:ILE:CA	2.61	0.47
1:C:1003:LYS:HE3	1:C:1003:LYS:HB2	1.75	0.47
1:A:937:TRP:CE3	1:A:942:LEU:HD13	2.50	0.46
1:A:943:GLN:HG2	1:A:953:PHE:CE2	2.50	0.46
1:C:931:LEU:O	1:C:935:ARG:HD2	2.16	0.46
1:B:1026:LEU:O	1:B:1030:THR:CG2	2.64	0.46
1:B:1003:LYS:HB2	1:B:1003:LYS:HE3	1.78	0.46
1:A:917:ARG:O	1:A:919:LYS:N	2.46	0.45
1:C:878:TYR:CZ	1:C:890:CYS:O	2.68	0.45
1:C:893:CYS:O	1:C:894:ARG:CB	2.64	0.45
1:A:876:PHE:CG	1:A:892:GLN:HG3	2.52	0.45
1:C:860:LEU:HD23	1:C:864:LEU:HD22	1.98	0.45
1:D:931:LEU:O	1:D:935:ARG:HD2	2.17	0.45
1:C:970:ARG:CG	3:C:1202:HOH:O	2.65	0.44
1:D:1003:LYS:HE3	1:D:1003:LYS:HB2	1.77	0.44
1:B:863:TYR:O	1:B:864:LEU:CB	2.64	0.44
1:D:971:VAL:HG13	1:D:997:LEU:HD22	1.99	0.44
1:D:1026:LEU:O	1:D:1030:THR:CG2	2.66	0.44
1:C:908:LYS:HG3	1:C:920:LYS:HA	2.00	0.44
1:A:1026:LEU:O	1:A:1030:THR:CG2	2.65	0.44
1:C:919:LYS:O	1:C:920:LYS:CB	2.66	0.44
1:B:1032:ARG:NH1	3:B:1206:HOH:O	2.34	0.43
1:B:869:ILE:HG23	1:B:869:ILE:O	2.18	0.43
1:C:874:CYS:HB3	1:C:875:LYS:HA	1.95	0.43
1:A:1003:LYS:HB2	1:A:1003:LYS:HE3	1.79	0.43
1:A:931:LEU:O	1:A:935:ARG:HD2	2.19	0.43
1:B:931:LEU:O	1:B:935:ARG:HD2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:879:ALA:O	1:C:880:LEU:C	2.56	0.43
1:B:970:ARG:CG	1:B:970:ARG:HH11	2.32	0.43
1:A:873:LYS:HE2	1:A:873:LYS:HB3	1.74	0.43
1:A:858:GLN:HG3	1:A:859:GLY:HA2	1.98	0.43
1:B:916:CYS:SG	1:B:918:VAL:HG22	2.60	0.42
1:A:916:CYS:HB3	1:A:917:ARG:HA	2.02	0.42
1:B:863:TYR:O	1:B:864:LEU:HB2	2.20	0.42
1:B:1021:TYR:HD2	1:B:1026:LEU:HD13	1.86	0.41
1:C:937:TRP:HE3	1:C:942:LEU:HD13	1.85	0.41
1:D:937:TRP:HE3	1:D:942:LEU:HD13	1.85	0.41
1:C:909:ASN:HB2	1:C:919:LYS:HG3	2.02	0.41
1:D:1016:ASP:HA	1:D:1017:PRO:HD3	1.94	0.41
1:D:1021:TYR:HD2	1:D:1026:LEU:HD13	1.87	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	180/223 (81%)	168 (93%)	11 (6%)	1 (1%)	25	29
1	B	180/223 (81%)	173 (96%)	6 (3%)	1 (1%)	25	29
1	C	182/223 (82%)	172 (94%)	9 (5%)	1 (0%)	29	34
1	D	180/223 (81%)	172 (96%)	7 (4%)	1 (1%)	25	29
All	All	722/892 (81%)	685 (95%)	33 (5%)	4 (1%)	25	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	917	ARG
1	D	917	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	864	LEU
1	A	918	VAL

5.3.2 Protein sidechains (i)

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	146/182 (80%)	130 (89%)	16 (11%)	6	5
1	B	145/182 (80%)	131 (90%)	14 (10%)	8	8
1	C	150/182 (82%)	132 (88%)	18 (12%)	5	4
1	D	148/182 (81%)	134 (90%)	14 (10%)	8	9
All	All	589/728 (81%)	527 (90%)	62 (10%)	7	6

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	877	SER
1	B	891	THR
1	B	909	ASN
1	B	915	ASN
1	B	922	LEU
1	B	935	ARG
1	B	945	LEU
1	B	970	ARG
1	B	997	LEU
1	B	1009	LEU
1	B	1015	LEU
1	B	1026	LEU
1	B	1030	THR
1	B	1061	VAL
1	A	873	LYS
1	A	909	ASN
1	A	922	LEU
1	A	935	ARG
1	A	942	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	945	LEU
1	A	997	LEU
1	A	1009	LEU
1	A	1015	LEU
1	A	1026	LEU
1	A	1030	THR
1	A	1031	GLU
1	A	1037	ARG
1	A	1053	LEU
1	A	1061	VAL
1	A	1063	LEU
1	C	864	LEU
1	C	869	ILE
1	C	874	CYS
1	C	909	ASN
1	C	922	LEU
1	C	935	ARG
1	C	942	LEU
1	C	945	LEU
1	C	955	THR
1	C	997	LEU
1	C	1009	LEU
1	C	1015	LEU
1	C	1026	LEU
1	C	1039	GLN
1	C	1041	LEU
1	C	1053	LEU
1	C	1061	VAL
1	C	1063	LEU
1	D	873	LYS
1	D	909	ASN
1	D	919	LYS
1	D	922	LEU
1	D	935	ARG
1	D	942	LEU
1	D	945	LEU
1	D	955	THR
1	D	1009	LEU
1	D	1026	LEU
1	D	1030	THR
1	D	1053	LEU
1	D	1061	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	1063	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	887	HIS
1	A	889	HIS
1	D	949	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 18 ligands modelled in this entry, 18 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^{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	187/223 (83%)	0.25	15 (8%) 12 9	26, 45, 88, 107	0
1	B	189/223 (84%)	0.03	7 (3%) 41 38	17, 36, 72, 95	0
1	C	189/223 (84%)	0.30	13 (6%) 16 13	24, 47, 86, 107	0
1	D	187/223 (83%)	0.42	18 (9%) 8 5	33, 52, 91, 119	0
All	All	752/892 (84%)	0.25	53 (7%) 16 13	17, 45, 87, 119	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	876	PHE	5.6
1	D	861	ALA	4.7
1	D	918	VAL	4.3
1	B	876	PHE	4.2
1	D	873	LYS	4.0
1	A	1043	GLY	3.9
1	C	880	LEU	3.9
1	B	1042	ALA	3.9
1	D	1045	ASP	3.7
1	C	858	GLN	3.5
1	A	915	ASN	3.5
1	D	1042	ALA	3.4
1	A	888	PHE	3.3
1	A	858	GLN	3.3
1	C	865	GLN	3.1
1	B	1043	GLY	3.1
1	D	884	GLY	3.0
1	A	865	GLN	2.9
1	A	914	PRO	2.9
1	D	919	LYS	2.9
1	A	983	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	920	LYS	2.8
1	A	859	GLY	2.8
1	B	880	LEU	2.8
1	D	972	ILE	2.7
1	C	1045	ASP	2.7
1	A	866	GLU	2.6
1	B	858	GLN	2.6
1	A	909	ASN	2.5
1	D	1023	VAL	2.5
1	A	891	THR	2.5
1	D	865	GLN	2.5
1	B	878	TYR	2.4
1	D	1043	GLY	2.4
1	C	1043	GLY	2.3
1	C	918	VAL	2.3
1	C	908	LYS	2.3
1	D	868	GLY	2.3
1	C	983	ASP	2.3
1	A	910	LYS	2.3
1	D	950	ASN	2.3
1	C	878	TYR	2.2
1	B	891	THR	2.2
1	D	908	LYS	2.2
1	A	1042	ALA	2.2
1	C	1042	ALA	2.2
1	A	972	ILE	2.1
1	A	973	GLU	2.1
1	C	920	LYS	2.1
1	C	922	LEU	2.1
1	D	914	PRO	2.1
1	D	870	ASP	2.1
1	C	876	PHE	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

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
2	ZN	A	1101	1/1	0.95	0.06	60,60,60,60	0
2	ZN	A	1103	1/1	0.98	0.07	54,54,54,54	0
2	ZN	B	1101	1/1	0.98	0.04	49,49,49,49	0
2	ZN	C	1101	1/1	0.98	0.06	46,46,46,46	0
2	ZN	D	1101	1/1	0.98	0.04	69,69,69,69	0
2	ZN	B	1103	1/1	0.99	0.10	35,35,35,35	0
2	ZN	A	1105	1/1	0.99	0.16	39,39,39,39	0
2	ZN	C	1102	1/1	0.99	0.16	33,33,33,33	0
2	ZN	D	1103	1/1	0.99	0.09	58,58,58,58	0
2	ZN	C	1103	1/1	0.99	0.06	51,51,51,51	0
2	ZN	D	1102	1/1	1.00	0.14	35,35,35,35	0
2	ZN	B	1105	1/1	1.00	0.16	30,30,30,30	0
2	ZN	D	1104	1/1	1.00	0.10	38,38,38,38	0
2	ZN	A	1102	1/1	1.00	0.13	27,27,27,27	0
2	ZN	B	1102	1/1	1.00	0.15	22,22,22,22	0
2	ZN	C	1104	1/1	1.00	0.11	31,31,31,31	0
2	ZN	A	1104	1/1	1.00	0.10	41,41,41,41	0
2	ZN	B	1104	1/1	1.00	0.11	29,29,29,29	0

6.5 Other polymers

There are no such residues in this entry.