



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:25 AM GMT

PDB ID : 2QM4
Title : Crystal structure of human XLF/Cernunnos, a non-homologous end-joining factor
Authors : Li, Y.; Chirgadze, D.Y.; Sibanda, B.L.; Bolanos-Garcia, V.M.; Davies, O.R.; Blundell, T.L.
Deposited on : 2007-07-14
Resolution : 2.30 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

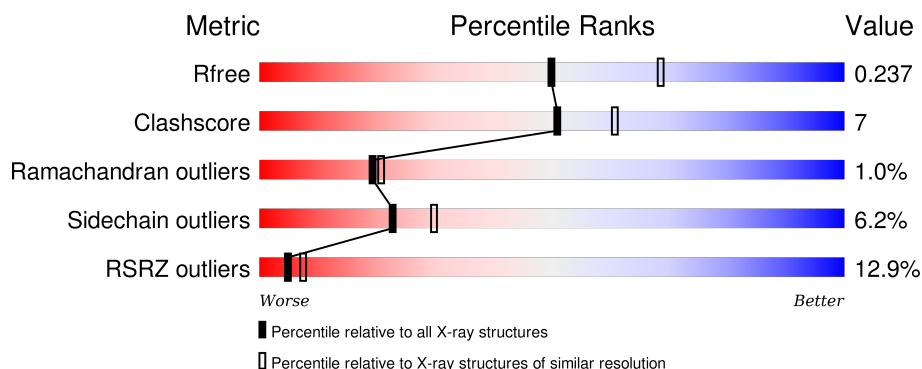
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	235	
1	B	235	
1	C	235	
1	D	235	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7510 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 Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	Se	0	7	0
			1864	1191	312	344	6	11			
1	B	225	Total	C	N	O	S	Se	0	10	0
			1821	1167	304	334	6	10			
1	C	229	Total	C	N	O	S	Se	0	4	0
			1818	1160	305	337	6	10			
1	D	225	Total	C	N	O	S	Se	0	7	0
			1775	1137	292	330	6	10			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	EXPRESSION TAG	UNP Q9H9Q4
A	0	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	10	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	124	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	140	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	142	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	159	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	194	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	212	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
A	219	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	-1	SER	-	EXPRESSION TAG	UNP Q9H9Q4
B	0	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	10	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	124	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	140	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	142	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	159	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	194	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
B	212	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	219	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	-1	SER	-	EXPRESSION TAG	UNP Q9H9Q4
C	0	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	10	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	124	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	140	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	142	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	159	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	194	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	212	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
C	219	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	-1	SER	-	EXPRESSION TAG	UNP Q9H9Q4
D	0	GLY	-	EXPRESSION TAG	UNP Q9H9Q4
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	10	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	124	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	140	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	142	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	159	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	194	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	212	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4
D	219	MSE	MET	MODIFIED RESIDUE	UNP Q9H9Q4

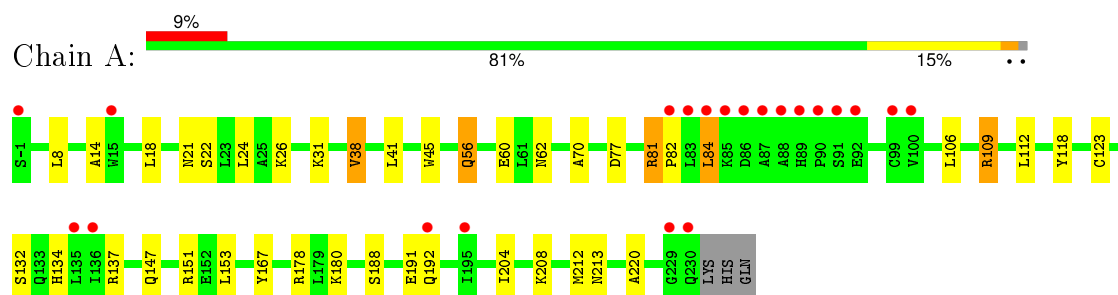
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	73	Total O 73 73	0	0
2	B	49	Total O 49 49	0	0
2	C	47	Total O 47 47	0	0
2	D	63	Total O 63 63	0	0

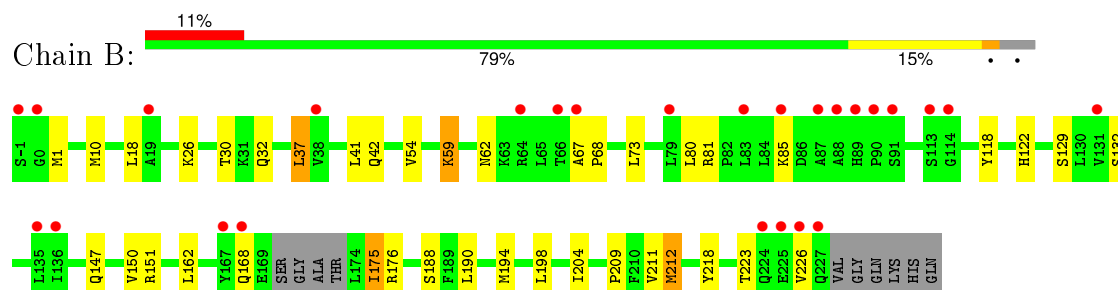
3 Residue-property plots [i](#)

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

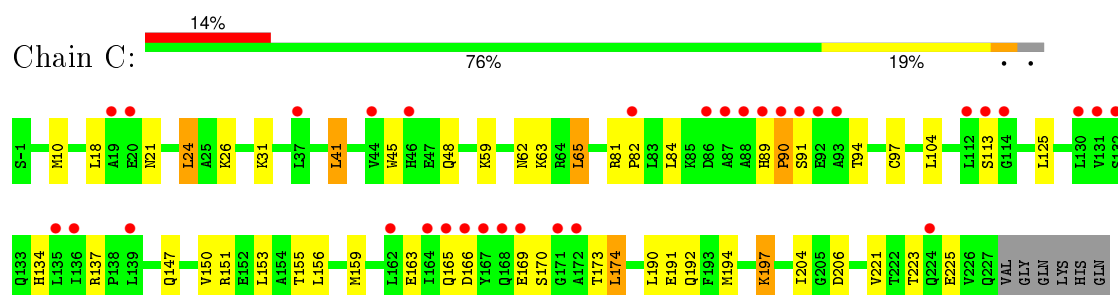
- Molecule 1: Non-homologous end-joining factor 1



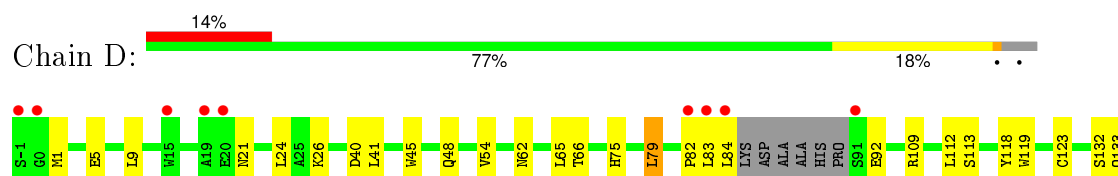
- Molecule 1: Non-homologous end-joining factor 1

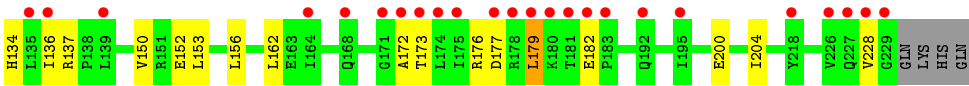


- Molecule 1: Non-homologous end-joining factor 1



- Molecule 1: Non-homologous end-joining factor 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.74Å 92.91Å 103.69Å 90.00° 106.22° 90.00°	Depositor
Resolution (Å)	37.01 – 2.30 37.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.01-2.30) 92.8 (37.00-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.75 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.239 0.180 , 0.237	Depositor DCC
R_{free} test set	2000 reflections (4.35%)	DCC
Wilson B-factor (Å ²)	38.4	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 42.4	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 47931 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7510	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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](#)

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	0.62	0/1909	0.69	0/2570
1	B	0.60	0/1875	0.65	1/2526 (0.0%)
1	C	0.61	2/1856 (0.1%)	0.69	3/2500 (0.1%)
1	D	0.66	0/1821	0.73	0/2454
All	All	0.62	2/7461 (0.0%)	0.69	4/10050 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	163	GLU	CD-OE1	6.90	1.33	1.25
1	C	163	GLU	CD-OE2	6.39	1.32	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	PRO	N-CA-CB	6.40	110.98	103.30
1	B	37	LEU	CA-CB-CG	5.52	127.99	115.30
1	C	174	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	65	LEU	CA-CB-CG	5.09	127.01	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1864	0	1886	36	0
1	B	1821	0	1825	28	0
1	C	1818	0	1821	20	0
1	D	1775	0	1765	31	0
2	A	73	0	0	1	0
2	B	49	0	0	2	0
2	C	47	0	0	1	0
2	D	63	0	0	3	0
All	All	7510	0	7297	100	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 7.

All (100) 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:109:ARG:HG3	1:A:109:ARG:HH11	1.24	1.00
1:A:62:ASN:HD21	1:A:118:TYR:H	1.20	0.89
1:A:208:LYS:NZ	1:A:212[A]:MSE:HE3	1.87	0.89
1:B:211:VAL:HG12	1:B:212[A]:MSE:HE3	1.55	0.87
1:D:62:ASN:HD21	1:D:118:TYR:H	1.28	0.82
1:A:188:SER:O	1:A:192:GLN:HG2	1.81	0.81
1:A:208:LYS:HZ2	1:A:212[A]:MSE:HE3	1.47	0.78
1:D:1:MSE:HE2	2:D:283:HOH:O	1.84	0.77
1:A:109:ARG:HH11	1:A:109:ARG:CG	1.98	0.75
1:B:212[A]:MSE:HA	1:B:212[A]:MSE:HE2	1.69	0.74
1:D:75:HIS:CE1	1:D:79:LEU:HD21	2.26	0.71
1:A:26:LYS:HZ2	1:A:134:HIS:HD2	1.35	0.71
1:B:30:THR:OG1	1:B:32:GLN:HG2	1.91	0.71
1:C:155:THR:O	1:C:159[B]:MSE:HG2	1.91	0.69
1:A:81:ARG:HB3	1:A:82:PRO:HD3	1.77	0.67
1:C:206:ASP:HB2	2:C:266:HOH:O	1.93	0.67
1:C:165:GLN:O	1:C:169:GLU:HG2	1.97	0.65
1:C:18:LEU:HD22	1:C:97:CYS:HB2	1.77	0.64
1:D:228:VAL:HG12	1:D:228:VAL:O	1.98	0.63
1:B:62:ASN:HD21	1:B:118:TYR:H	1.48	0.62
1:A:109:ARG:HG3	1:A:109:ARG:NH1	2.01	0.62
1:B:223:THR:O	1:B:226:VAL:HG22	2.00	0.62
1:C:26:LYS:NZ	1:C:134:HIS:HD2	1.98	0.61
1:A:26:LYS:NZ	1:A:134:HIS:HD2	2.01	0.59
1:A:208:LYS:HZ3	1:A:212[A]:MSE:HE3	1.67	0.57
1:A:21:ASN:CG	1:A:22:SER:H	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ASP:HB2	1:D:179:LEU:HD23	1.85	0.56
1:B:54:VAL:HG21	1:B:73:LEU:HD21	1.88	0.56
1:B:175:ILE:HG23	1:B:176:ARG:H	1.70	0.56
1:B:175:ILE:HG23	1:B:176:ARG:N	2.20	0.56
1:A:153:LEU:HD11	1:B:150:VAL:HG13	1.87	0.56
1:B:10:MSE:HE2	1:B:10:MSE:HA	1.87	0.56
1:C:197:LYS:HG2	1:D:152:GLU:OE2	2.06	0.56
1:C:10:MSE:HE2	1:C:10:MSE:HA	1.88	0.55
1:A:14:ALA:HB2	1:A:84:LEU:HD12	1.89	0.55
1:C:190:LEU:O	1:C:194:MSE:HG2	2.06	0.55
1:A:31[B]:LYS:HE3	1:A:70:ALA:HB1	1.88	0.55
1:B:26:LYS:NZ	1:B:218:TYR:OH	2.41	0.54
1:C:153:LEU:HD11	1:D:150:VAL:HG13	1.90	0.53
1:D:1:MSE:HE3	1:D:48:GLN:OE1	2.09	0.53
1:A:26:LYS:HZ2	1:A:134:HIS:CD2	2.23	0.53
1:C:147:GLN:HE21	1:C:151:ARG:NH1	2.06	0.53
1:B:212[A]:MSE:HA	1:B:212[A]:MSE:CE	2.39	0.53
1:A:8:LEU:HD11	1:A:26:LYS:HG3	1.92	0.51
1:B:59:LYS:HG3	2:B:247:HOH:O	2.10	0.50
1:C:137:ARG:O	1:D:204:ILE:HD11	2.11	0.50
1:D:1:MSE:CE	2:D:283:HOH:O	2.50	0.49
1:A:109:ARG:CG	1:A:109:ARG:NH1	2.68	0.48
1:D:176:ARG:HB2	1:D:179:LEU:HD22	1.94	0.48
1:A:137[B]:ARG:NH1	1:B:42[B]:GLN:NE2	2.60	0.48
1:A:31[B]:LYS:HG3	1:A:70:ALA:HB1	1.95	0.48
1:B:209:PRO:HA	1:B:212[B]:MSE:HE2	1.95	0.48
1:A:41:LEU:HD13	1:A:204:ILE:CG2	2.44	0.48
1:B:1:MSE:CE	1:D:66:THR:HG21	2.45	0.47
1:D:109:ARG:NH2	2:D:287:HOH:O	2.47	0.47
1:B:10:MSE:HB2	2:B:245:HOH:O	2.14	0.46
1:C:26:LYS:HZ2	1:C:134:HIS:HD2	1.63	0.46
1:D:54:VAL:HA	1:D:119:TRP:HH2	1.80	0.46
1:A:147:GLN:O	1:A:151:ARG:HG2	2.14	0.46
1:D:9:LEU:HD21	1:D:133:GLN:HG2	1.97	0.46
1:C:204:ILE:HD11	1:D:137[B]:ARG:CZ	2.45	0.46
1:A:167:TYR:OH	1:B:168:GLN:HG2	2.16	0.46
1:D:26:LYS:HE2	1:D:134:HIS:HD2	1.80	0.45
1:B:190:LEU:O	1:B:194:MSE:HG2	2.16	0.45
1:B:41:LEU:HD13	1:B:204:ILE:HD12	1.99	0.45
1:D:45:TRP:HB3	1:D:123:CYS:HB3	1.99	0.44
1:D:5:GLU:HG2	1:D:48:GLN:NE2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:HIS:HE1	2:A:234:HOH:O	2.01	0.44
1:B:122:HIS:HB3	1:D:113:SER:O	2.16	0.44
1:D:75:HIS:CD2	1:D:112:LEU:HD13	2.52	0.44
1:A:77:ASP:O	1:A:81:ARG:HB2	2.17	0.44
1:D:83:LEU:O	1:D:84:LEU:CB	2.65	0.43
1:D:132:SER:HA	1:D:136:ILE:HB	2.00	0.43
1:D:62:ASN:HD21	1:D:118:TYR:N	2.06	0.43
1:B:175:ILE:CG2	1:B:176:ARG:N	2.82	0.43
1:D:228:VAL:CG1	1:D:228:VAL:O	2.65	0.43
1:A:56:GLN:NE2	1:A:60:GLU:OE2	2.52	0.43
1:C:10:MSE:HE1	1:C:223:THR:HA	2.01	0.42
1:A:45:TRP:HB3	1:A:123:CYS:HB3	2.01	0.42
1:A:18:LEU:HD21	1:A:106:LEU:CD1	2.49	0.42
1:A:178:ARG:HD2	1:A:180:LYS:HE3	2.01	0.42
1:A:38[A]:VAL:HG12	1:A:45:TRP:HB2	2.01	0.42
1:C:81:ARG:N	1:C:82:PRO:HD2	2.34	0.42
1:C:24:LEU:HD22	1:C:41:LEU:CD1	2.48	0.42
1:D:1:MSE:CE	1:D:48:GLN:HG2	2.49	0.42
1:A:213:ASN:HB3	1:B:147[A]:GLN:OE1	2.19	0.42
1:D:24:LEU:HD22	1:D:41:LEU:HD21	2.02	0.42
1:C:45:TRP:CE3	1:C:104:LEU:HD22	2.55	0.42
1:D:176:ARG:CB	1:D:179:LEU:HD22	2.50	0.41
1:A:31[B]:LYS:HG3	1:A:70:ALA:CB	2.51	0.41
1:A:137[A]:ARG:CZ	1:B:204:ILE:HD11	2.51	0.41
1:A:153:LEU:CD1	1:B:150:VAL:HG13	2.50	0.41
1:D:40:ASP:O	1:D:41:LEU:HB2	2.20	0.41
1:A:220:ALA:HB1	1:B:198:LEU:CD2	2.51	0.41
1:C:221:VAL:O	1:C:225:GLU:HG3	2.20	0.41
1:A:109:ARG:HD2	1:A:118:TYR:CE1	2.56	0.40
1:B:80:LEU:HD12	1:B:80:LEU:HA	1.95	0.40
1:B:67:ALA:HB1	1:B:68:PRO:HD2	2.04	0.40
1:C:150:VAL:HG13	1:D:153:LEU:HD11	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	237/235 (101%)	228 (96%)	9 (4%)	0	100	100
1	B	231/235 (98%)	219 (95%)	12 (5%)	0	100	100
1	C	231/235 (98%)	218 (94%)	8 (4%)	5 (2%)	8	6
1	D	228/235 (97%)	214 (94%)	10 (4%)	4 (2%)	11	9
All	All	927/940 (99%)	879 (95%)	39 (4%)	9 (1%)	19	21

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	89	HIS
1	C	90	PRO
1	C	91	SER
1	D	92	GLU
1	D	172	ALA
1	C	113	SER
1	D	82	PRO
1	D	182	GLU
1	C	170	SER

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	208/198 (105%)	198 (95%)	10 (5%)	31	42
1	B	201/198 (102%)	187 (93%)	14 (7%)	19	23
1	C	200/198 (101%)	181 (90%)	19 (10%)	11	12
1	D	195/198 (98%)	185 (95%)	10 (5%)	29	39
All	All	804/792 (102%)	751 (93%)	53 (7%)	23	27

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	38[A]	VAL
1	A	38[B]	VAL
1	A	56	GLN
1	A	81	ARG
1	A	84	LEU
1	A	109	ARG
1	A	112	LEU
1	A	132	SER
1	A	191	GLU
1	B	18	LEU
1	B	37	LEU
1	B	59	LYS
1	B	81	ARG
1	B	85	LYS
1	B	129	SER
1	B	132	SER
1	B	151[A]	ARG
1	B	151[B]	ARG
1	B	162	LEU
1	B	175	ILE
1	B	188	SER
1	B	212[A]	MSE
1	B	212[B]	MSE
1	C	21	ASN
1	C	24	LEU
1	C	31	LYS
1	C	41	LEU
1	C	48	GLN
1	C	59	LYS
1	C	62	ASN
1	C	63	LYS
1	C	65	LEU
1	C	84	LEU
1	C	94	THR
1	C	125	LEU
1	C	156	LEU
1	C	173	THR
1	C	174	LEU
1	C	191	GLU
1	C	192[A]	GLN
1	C	192[B]	GLN
1	C	197	LYS

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Mol	Chain	Res	Type
1	D	21	ASN
1	D	65	LEU
1	D	79	LEU
1	D	156	LEU
1	D	162	LEU
1	D	173	THR
1	D	177	ASP
1	D	179	LEU
1	D	200[A]	GLU
1	D	200[B]	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	56	GLN
1	A	62	ASN
1	A	134	HIS
1	A	227	GLN
1	B	48	GLN
1	B	62	ASN
1	C	32	GLN
1	C	122	HIS
1	C	134	HIS
1	C	147	GLN
1	C	187	ASN
1	D	56	GLN
1	D	62	ASN
1	D	75	HIS
1	D	134	HIS
1	D	165	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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, 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	223/235 (94%)	0.73	21 (9%) 11 16	41, 54, 85, 112	2 (0%)
1	B	216/235 (91%)	0.85	26 (12%) 6 9	44, 57, 89, 106	1 (0%)
1	C	220/235 (93%)	1.09	33 (15%) 3 5	30, 58, 83, 94	3 (1%)
1	D	216/235 (91%)	0.96	33 (15%) 3 5	40, 53, 74, 96	0
All	All	875/940 (93%)	0.91	113 (12%) 5 7	30, 55, 85, 112	6 (0%)

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	ALA	10.3
1	B	88	ALA	8.0
1	B	90	PRO	6.6
1	C	113	SER	6.6
1	C	20	GLU	6.6
1	C	91	SER	6.0
1	D	83	LEU	5.7
1	B	89	HIS	5.5
1	A	82	PRO	5.5
1	C	86	ASP	5.3
1	C	171	GLY	5.1
1	D	175	ILE	5.1
1	D	174	LEU	5.0
1	C	87	ALA	5.0
1	C	131	VAL	4.8
1	D	229	GLY	4.8
1	A	89	HIS	4.7
1	A	92	GLU	4.6
1	A	230	GLN	4.5
1	D	173	THR	4.5
1	D	178	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	-1	SER	4.5
1	C	135	LEU	4.5
1	A	88	ALA	4.5
1	D	228	VAL	4.5
1	C	114	GLY	4.4
1	B	-1	SER	4.4
1	B	91	SER	4.3
1	A	229	GLY	4.2
1	B	66	THR	4.2
1	C	89	HIS	4.2
1	B	0	GLY	4.1
1	D	82	PRO	4.1
1	D	177	ASP	4.1
1	D	226	VAL	4.1
1	D	139	LEU	4.1
1	D	91	SER	4.1
1	A	83	LEU	4.1
1	A	85	LYS	4.0
1	A	195	ILE	4.0
1	B	225[A]	GLU	4.0
1	A	-1	SER	3.9
1	B	136	ILE	3.9
1	C	136	ILE	3.9
1	B	114	GLY	3.9
1	B	113	SER	3.8
1	B	87	ALA	3.8
1	C	167	TYR	3.7
1	D	164	ILE	3.7
1	C	130	LEU	3.6
1	B	135	LEU	3.6
1	C	82	PRO	3.5
1	B	67	ALA	3.5
1	C	112	LEU	3.5
1	D	181	THR	3.5
1	D	172	ALA	3.4
1	A	84	LEU	3.4
1	C	164	ILE	3.3
1	D	136	ILE	3.2
1	A	87	ALA	3.2
1	A	86	ASP	3.2
1	C	19	ALA	3.1
1	A	99	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	183	PRO	2.9
1	A	90	PRO	2.9
1	B	64[A]	ARG	2.9
1	B	131	VAL	2.9
1	C	92	GLU	2.8
1	D	0	GLY	2.8
1	D	19	ALA	2.8
1	C	166	ASP	2.8
1	A	136	ILE	2.7
1	D	192	GLN	2.7
1	C	165	GLN	2.7
1	D	227	GLN	2.7
1	C	37	LEU	2.6
1	C	224	GLN	2.6
1	D	84	LEU	2.6
1	C	90	PRO	2.6
1	D	135	LEU	2.6
1	C	44	VAL	2.6
1	A	91	SER	2.5
1	C	162	LEU	2.4
1	B	224	GLN	2.4
1	D	15	TRP	2.4
1	C	132	SER	2.4
1	C	169	GLU	2.4
1	D	171	GLY	2.3
1	C	46	HIS	2.3
1	D	179	LEU	2.3
1	B	226	VAL	2.3
1	A	100	VAL	2.3
1	C	139	LEU	2.3
1	B	19	ALA	2.2
1	B	167	TYR	2.2
1	B	38	VAL	2.2
1	D	182	GLU	2.2
1	D	168	GLN	2.2
1	D	218	TYR	2.2
1	A	135	LEU	2.2
1	C	168	GLN	2.1
1	D	20	GLU	2.1
1	B	85	LYS	2.1
1	B	83	LEU	2.1
1	D	195	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	180	LYS	2.1
1	B	79	LEU	2.1
1	A	192	GLN	2.1
1	B	168	GLN	2.1
1	C	172	ALA	2.1
1	B	227	GLN	2.0
1	A	15	TRP	2.0
1	C	93	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.