



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:31 am GMT

PDB ID : 3Q4F
Title : Crystal structure of xrcc4/xlf-cernunnos complex
Authors : Ropars, V.; Legrand, P.; Charbonnier, J.B.
Deposited on : 2010-12-23
Resolution : 5.50 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
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

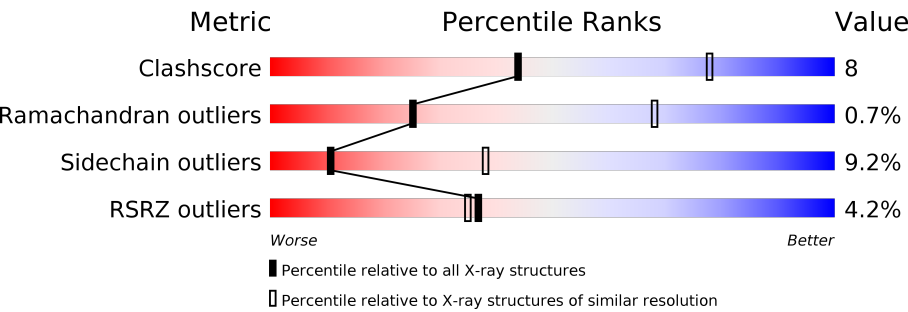
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 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))
Clashscore	112137	1021 (7.20-3.76)
Ramachandran outliers	110173	1082 (7.20-3.70)
Sidechain outliers	110143	1055 (7.20-3.70)
RSRZ outliers	101464	1061 (7.20-3.70)

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. 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	230	
1	B	230	
1	E	230	
1	F	230	
2	C	186	
2	D	186	
2	G	186	

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Mol	Chain	Length	Quality of chain
2	H	186	<div><div></div><div>2%</div><div>73%</div><div>10%</div><div>16%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12296 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	E	227	Total	C	N	O	S	0	0	0
			1807	1153	306	333	15			
1	F	227	Total	C	N	O	S	0	0	0
			1807	1153	306	333	15			
1	A	227	Total	C	N	O	S	0	0	0
			1807	1153	306	333	15			
1	B	227	Total	C	N	O	S	0	0	0
			1807	1153	306	333	15			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	225	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
E	226	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
E	227	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
E	228	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
E	229	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
E	230	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
F	225	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
F	226	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
F	227	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
F	228	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
F	229	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
F	230	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
A	225	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
A	226	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
A	227	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
A	228	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
A	229	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
A	230	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
B	225	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
B	226	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
B	227	HIS	-	EXPRESSION TAG	UNP Q9H9Q4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	228	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
B	229	HIS	-	EXPRESSION TAG	UNP Q9H9Q4
B	230	HIS	-	EXPRESSION TAG	UNP Q9H9Q4

- Molecule 2 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	157	Total 1267	C 800	N 212	O 249	S 6	0	0	0
2	D	157	Total 1267	C 800	N 212	O 249	S 6	0	0	0
2	G	157	Total 1267	C 800	N 212	O 249	S 6	0	0	0
2	H	157	Total 1267	C 800	N 212	O 249	S 6	0	0	0

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-28	MET	-	EXPRESSION TAG	UNP Q13426
C	-27	SER	-	EXPRESSION TAG	UNP Q13426
C	-26	TYR	-	EXPRESSION TAG	UNP Q13426
C	-25	TYR	-	EXPRESSION TAG	UNP Q13426
C	-24	HIS	-	EXPRESSION TAG	UNP Q13426
C	-23	HIS	-	EXPRESSION TAG	UNP Q13426
C	-22	HIS	-	EXPRESSION TAG	UNP Q13426
C	-21	HIS	-	EXPRESSION TAG	UNP Q13426
C	-20	HIS	-	EXPRESSION TAG	UNP Q13426
C	-19	HIS	-	EXPRESSION TAG	UNP Q13426
C	-18	LEU	-	EXPRESSION TAG	UNP Q13426
C	-17	GLU	-	EXPRESSION TAG	UNP Q13426
C	-16	SER	-	EXPRESSION TAG	UNP Q13426
C	-15	THR	-	EXPRESSION TAG	UNP Q13426
C	-14	SER	-	EXPRESSION TAG	UNP Q13426
C	-13	LEU	-	EXPRESSION TAG	UNP Q13426
C	-12	TYR	-	EXPRESSION TAG	UNP Q13426
C	-11	LYS	-	EXPRESSION TAG	UNP Q13426
C	-10	LYS	-	EXPRESSION TAG	UNP Q13426
C	-9	ALA	-	EXPRESSION TAG	UNP Q13426
C	-8	GLY	-	EXPRESSION TAG	UNP Q13426
C	-7	PHE	-	EXPRESSION TAG	UNP Q13426
C	-6	GLU	-	EXPRESSION TAG	UNP Q13426

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	ASN	-	EXPRESSION TAG	UNP Q13426
C	-4	LEU	-	EXPRESSION TAG	UNP Q13426
C	-3	TYR	-	EXPRESSION TAG	UNP Q13426
C	-2	PHE	-	EXPRESSION TAG	UNP Q13426
C	-1	GLN	-	EXPRESSION TAG	UNP Q13426
C	0	GLY	-	EXPRESSION TAG	UNP Q13426
D	-28	MET	-	EXPRESSION TAG	UNP Q13426
D	-27	SER	-	EXPRESSION TAG	UNP Q13426
D	-26	TYR	-	EXPRESSION TAG	UNP Q13426
D	-25	TYR	-	EXPRESSION TAG	UNP Q13426
D	-24	HIS	-	EXPRESSION TAG	UNP Q13426
D	-23	HIS	-	EXPRESSION TAG	UNP Q13426
D	-22	HIS	-	EXPRESSION TAG	UNP Q13426
D	-21	HIS	-	EXPRESSION TAG	UNP Q13426
D	-20	HIS	-	EXPRESSION TAG	UNP Q13426
D	-19	HIS	-	EXPRESSION TAG	UNP Q13426
D	-18	LEU	-	EXPRESSION TAG	UNP Q13426
D	-17	GLU	-	EXPRESSION TAG	UNP Q13426
D	-16	SER	-	EXPRESSION TAG	UNP Q13426
D	-15	THR	-	EXPRESSION TAG	UNP Q13426
D	-14	SER	-	EXPRESSION TAG	UNP Q13426
D	-13	LEU	-	EXPRESSION TAG	UNP Q13426
D	-12	TYR	-	EXPRESSION TAG	UNP Q13426
D	-11	LYS	-	EXPRESSION TAG	UNP Q13426
D	-10	LYS	-	EXPRESSION TAG	UNP Q13426
D	-9	ALA	-	EXPRESSION TAG	UNP Q13426
D	-8	GLY	-	EXPRESSION TAG	UNP Q13426
D	-7	PHE	-	EXPRESSION TAG	UNP Q13426
D	-6	GLU	-	EXPRESSION TAG	UNP Q13426
D	-5	ASN	-	EXPRESSION TAG	UNP Q13426
D	-4	LEU	-	EXPRESSION TAG	UNP Q13426
D	-3	TYR	-	EXPRESSION TAG	UNP Q13426
D	-2	PHE	-	EXPRESSION TAG	UNP Q13426
D	-1	GLN	-	EXPRESSION TAG	UNP Q13426
D	0	GLY	-	EXPRESSION TAG	UNP Q13426
G	-28	MET	-	EXPRESSION TAG	UNP Q13426
G	-27	SER	-	EXPRESSION TAG	UNP Q13426
G	-26	TYR	-	EXPRESSION TAG	UNP Q13426
G	-25	TYR	-	EXPRESSION TAG	UNP Q13426
G	-24	HIS	-	EXPRESSION TAG	UNP Q13426
G	-23	HIS	-	EXPRESSION TAG	UNP Q13426
G	-22	HIS	-	EXPRESSION TAG	UNP Q13426

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-21	HIS	-	EXPRESSION TAG	UNP Q13426
G	-20	HIS	-	EXPRESSION TAG	UNP Q13426
G	-19	HIS	-	EXPRESSION TAG	UNP Q13426
G	-18	LEU	-	EXPRESSION TAG	UNP Q13426
G	-17	GLU	-	EXPRESSION TAG	UNP Q13426
G	-16	SER	-	EXPRESSION TAG	UNP Q13426
G	-15	THR	-	EXPRESSION TAG	UNP Q13426
G	-14	SER	-	EXPRESSION TAG	UNP Q13426
G	-13	LEU	-	EXPRESSION TAG	UNP Q13426
G	-12	TYR	-	EXPRESSION TAG	UNP Q13426
G	-11	LYS	-	EXPRESSION TAG	UNP Q13426
G	-10	LYS	-	EXPRESSION TAG	UNP Q13426
G	-9	ALA	-	EXPRESSION TAG	UNP Q13426
G	-8	GLY	-	EXPRESSION TAG	UNP Q13426
G	-7	PHE	-	EXPRESSION TAG	UNP Q13426
G	-6	GLU	-	EXPRESSION TAG	UNP Q13426
G	-5	ASN	-	EXPRESSION TAG	UNP Q13426
G	-4	LEU	-	EXPRESSION TAG	UNP Q13426
G	-3	TYR	-	EXPRESSION TAG	UNP Q13426
G	-2	PHE	-	EXPRESSION TAG	UNP Q13426
G	-1	GLN	-	EXPRESSION TAG	UNP Q13426
G	0	GLY	-	EXPRESSION TAG	UNP Q13426
H	-28	MET	-	EXPRESSION TAG	UNP Q13426
H	-27	SER	-	EXPRESSION TAG	UNP Q13426
H	-26	TYR	-	EXPRESSION TAG	UNP Q13426
H	-25	TYR	-	EXPRESSION TAG	UNP Q13426
H	-24	HIS	-	EXPRESSION TAG	UNP Q13426
H	-23	HIS	-	EXPRESSION TAG	UNP Q13426
H	-22	HIS	-	EXPRESSION TAG	UNP Q13426
H	-21	HIS	-	EXPRESSION TAG	UNP Q13426
H	-20	HIS	-	EXPRESSION TAG	UNP Q13426
H	-19	HIS	-	EXPRESSION TAG	UNP Q13426
H	-18	LEU	-	EXPRESSION TAG	UNP Q13426
H	-17	GLU	-	EXPRESSION TAG	UNP Q13426
H	-16	SER	-	EXPRESSION TAG	UNP Q13426
H	-15	THR	-	EXPRESSION TAG	UNP Q13426
H	-14	SER	-	EXPRESSION TAG	UNP Q13426
H	-13	LEU	-	EXPRESSION TAG	UNP Q13426
H	-12	TYR	-	EXPRESSION TAG	UNP Q13426
H	-11	LYS	-	EXPRESSION TAG	UNP Q13426
H	-10	LYS	-	EXPRESSION TAG	UNP Q13426
H	-9	ALA	-	EXPRESSION TAG	UNP Q13426

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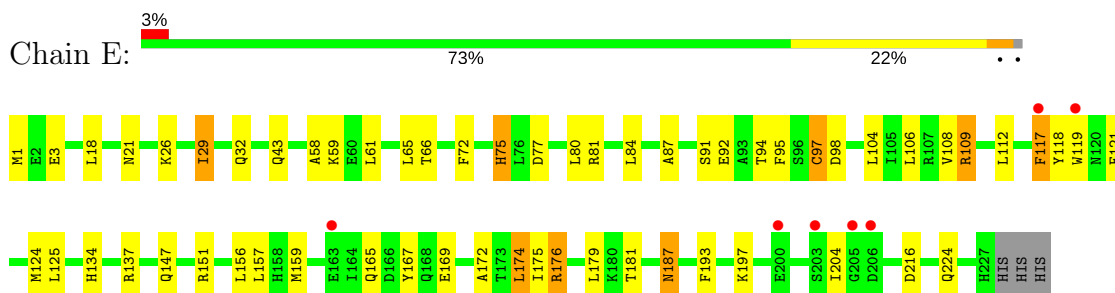
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-8	GLY	-	EXPRESSION TAG	UNP Q13426
H	-7	PHE	-	EXPRESSION TAG	UNP Q13426
H	-6	GLU	-	EXPRESSION TAG	UNP Q13426
H	-5	ASN	-	EXPRESSION TAG	UNP Q13426
H	-4	LEU	-	EXPRESSION TAG	UNP Q13426
H	-3	TYR	-	EXPRESSION TAG	UNP Q13426
H	-2	PHE	-	EXPRESSION TAG	UNP Q13426
H	-1	GLN	-	EXPRESSION TAG	UNP Q13426
H	0	GLY	-	EXPRESSION TAG	UNP Q13426

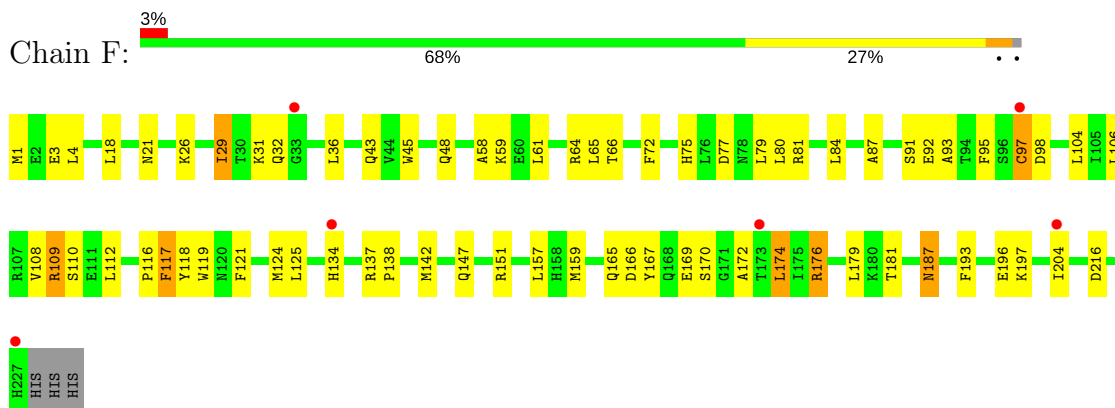
3 Residue-property plots [i](#)

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.

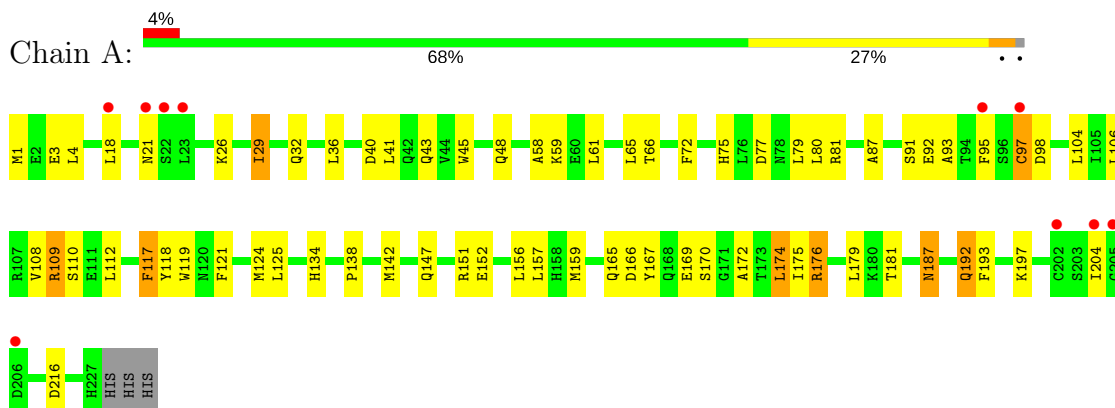
- Molecule 1: Non-homologous end-joining factor 1



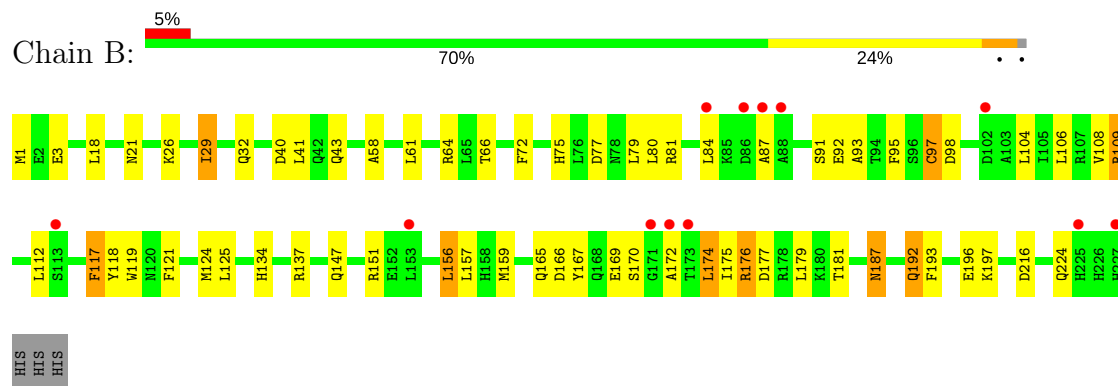
- Molecule 1: Non-homologous end-joining factor 1



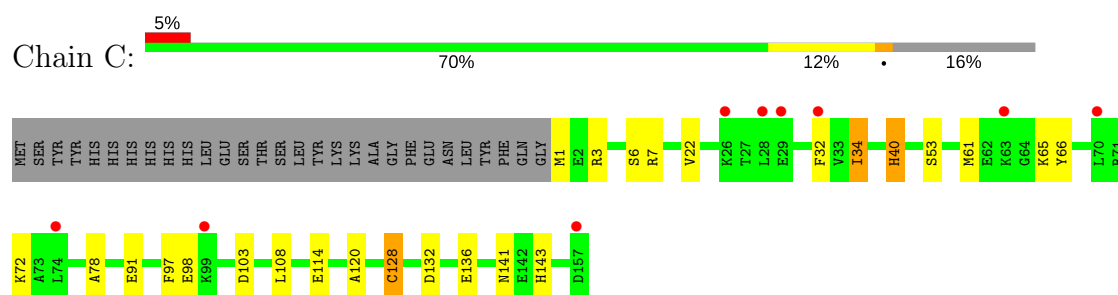
- Molecule 1: Non-homologous end-joining factor 1



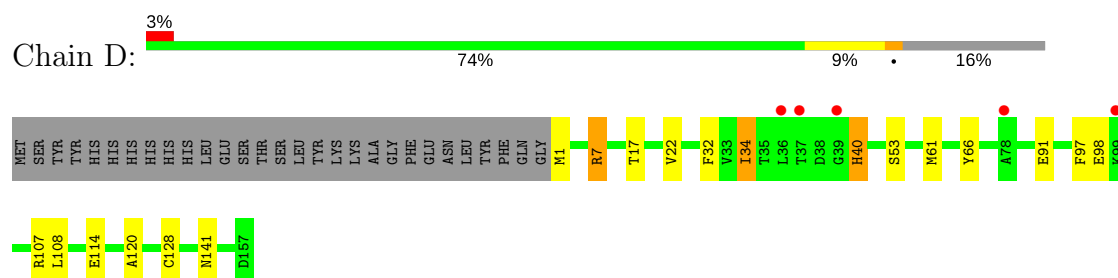
- Molecule 1: Non-homologous end-joining factor 1



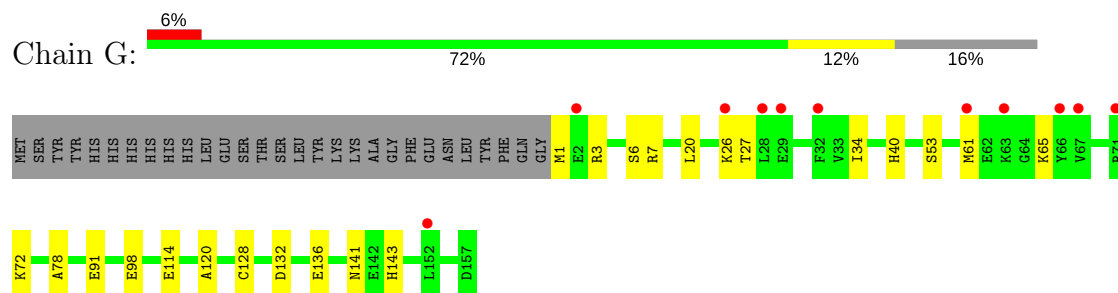
- Molecule 2: DNA repair protein XRCC4



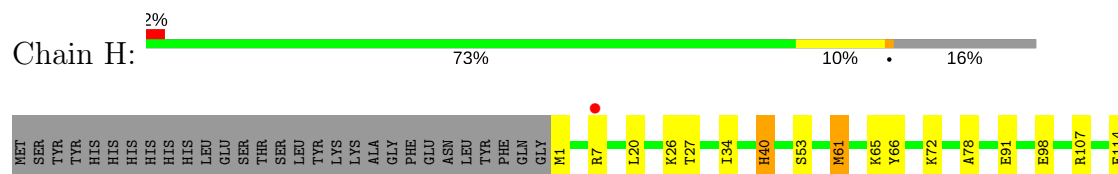
- Molecule 2: DNA repair protein XRCC4

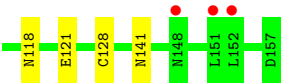


- Molecule 2: DNA repair protein XRCC4



- Molecule 2: DNA repair protein XRCC4





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	103.86Å 103.86Å 855.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.79 – 5.50 47.79 – 5.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.79-5.50) 99.9 (47.79-5.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	0.16	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 5.39Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.249 , 0.309 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	233.9	Xtriage
Anisotropy	0.840	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 231.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	12296	wwPDB-VP
Average B, all atoms (Å ²)	267.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.45	0/1847	0.69	0/2507
1	B	0.46	0/1847	0.72	0/2507
1	E	0.47	0/1847	0.71	0/2507
1	F	0.45	0/1847	0.69	0/2507
2	C	0.43	0/1292	0.56	0/1741
2	D	0.42	0/1292	0.58	0/1741
2	G	0.43	0/1292	0.59	1/1741 (0.1%)
2	H	0.42	0/1292	0.60	1/1741 (0.1%)
All	All	0.44	0/12556	0.66	2/16992 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	26	LYS	C-N-CA	6.95	139.08	121.70
2	G	26	LYS	C-N-CA	6.92	139.00	121.70

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	1807	0	1800	49	0
1	B	1807	0	1800	51	0
1	E	1807	0	1800	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1807	0	1800	49	0
2	C	1267	0	1229	11	0
2	D	1267	0	1229	15	0
2	G	1267	0	1229	5	0
2	H	1267	0	1229	10	0
All	All	12296	0	12116	185	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 (185) 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:72:PHE:CZ	1:A:117:PHE:HE1	1.96	0.84
1:F:72:PHE:CZ	1:F:117:PHE:HE1	1.96	0.84
1:E:72:PHE:CZ	1:E:117:PHE:HE1	1.98	0.81
1:B:72:PHE:CZ	1:B:117:PHE:HE1	1.98	0.80
1:E:193:PHE:HA	1:E:197:LYS:HD2	1.64	0.79
1:B:64:ARG:HH11	2:H:107:ARG:HB2	1.48	0.79
1:A:193:PHE:HA	1:A:197:LYS:HD2	1.65	0.77
1:B:193:PHE:HA	1:B:197:LYS:HD2	1.64	0.77
1:E:159:MET:HG3	1:F:181:THR:HG22	1.68	0.75
1:F:193:PHE:HA	1:F:197:LYS:HD2	1.66	0.75
1:A:165:GLN:O	1:A:169:GLU:HG2	1.88	0.74
1:E:165:GLN:O	1:E:169:GLU:HG2	1.88	0.73
2:D:97:PHE:HE2	2:D:108:LEU:HD23	1.52	0.73
1:B:165:GLN:O	1:B:169:GLU:HG2	1.89	0.72
2:C:97:PHE:HE2	2:C:108:LEU:HD23	1.54	0.72
1:A:175:ILE:CG1	1:B:170:SER:HB3	2.20	0.71
1:F:116:PRO:HG2	2:D:61:MET:HG2	1.72	0.71
1:F:165:GLN:O	1:F:169:GLU:HG2	1.88	0.71
2:D:97:PHE:CE2	2:D:108:LEU:HD23	2.25	0.71
2:C:97:PHE:CE2	2:C:108:LEU:HD23	2.27	0.68
1:E:58:ALA:HB1	1:E:72:PHE:CE2	2.29	0.68
1:A:175:ILE:HG12	1:B:170:SER:HB3	1.74	0.67
1:B:58:ALA:HB1	1:B:72:PHE:CE2	2.29	0.67
1:A:58:ALA:HB1	1:A:72:PHE:CE2	2.29	0.67
1:F:58:ALA:HB1	1:F:72:PHE:CE2	2.30	0.66
2:G:20:LEU:HD11	2:G:34:ILE:HD11	1.77	0.66
2:H:20:LEU:HD11	2:H:34:ILE:HD11	1.79	0.65
1:B:72:PHE:CZ	1:B:117:PHE:CE1	2.84	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:PHE:CZ	1:E:117:PHE:CE1	2.85	0.64
1:E:106:LEU:HB3	1:E:121:PHE:HB2	1.80	0.64
1:A:72:PHE:CZ	1:A:117:PHE:CE1	2.83	0.63
1:B:106:LEU:HB3	1:B:121:PHE:HB2	1.81	0.63
1:A:181:THR:HG22	1:B:159:MET:HG3	1.80	0.63
1:E:137:ARG:CZ	1:F:204:ILE:HD11	2.30	0.62
1:F:72:PHE:CZ	1:F:117:PHE:CE1	2.83	0.61
1:A:106:LEU:HB3	1:A:121:PHE:HB2	1.83	0.61
1:F:64:ARG:HH11	2:D:107:ARG:HB2	1.65	0.61
1:F:106:LEU:HB3	1:F:121:PHE:HB2	1.84	0.59
1:B:40:ASP:C	1:B:41:LEU:HD12	2.24	0.58
1:E:80:LEU:HD21	1:E:95:PHE:HZ	1.69	0.57
1:A:80:LEU:HD21	1:A:95:PHE:HZ	1.70	0.57
1:B:80:LEU:HD21	1:B:95:PHE:HZ	1.69	0.57
1:A:170:SER:HB3	1:B:175:ILE:CG1	2.35	0.57
1:A:61:LEU:HD12	1:A:119:TRP:HA	1.87	0.56
1:E:159:MET:HG3	1:F:181:THR:CG2	2.35	0.56
1:F:61:LEU:HD12	1:F:119:TRP:HA	1.87	0.55
1:B:75:HIS:HD2	1:B:112:LEU:HD13	1.72	0.55
1:B:58:ALA:CB	1:B:72:PHE:CE2	2.90	0.55
1:F:80:LEU:HD21	1:F:95:PHE:HZ	1.71	0.55
1:A:159:MET:HG3	1:B:181:THR:HG22	1.88	0.55
1:B:3:GLU:H	1:B:3:GLU:CD	2.10	0.55
1:F:75:HIS:HD2	1:F:112:LEU:HD13	1.72	0.55
2:D:7:ARG:HD2	1:B:177:ASP:OD2	2.07	0.55
1:A:97:CYS:SG	1:A:104:LEU:HD11	2.46	0.54
1:F:109:ARG:HE	1:F:118:TYR:HE2	1.56	0.54
1:B:64:ARG:HD3	2:H:107:ARG:CB	2.38	0.54
1:F:3:GLU:H	1:F:3:GLU:CD	2.11	0.54
1:E:58:ALA:CB	1:E:72:PHE:CE2	2.91	0.54
1:F:58:ALA:CB	1:F:72:PHE:CE2	2.91	0.54
1:A:179:LEU:HD13	1:B:166:ASP:HB2	1.89	0.53
1:A:109:ARG:HE	1:A:118:TYR:HE2	1.56	0.53
1:A:58:ALA:CB	1:A:72:PHE:CE2	2.91	0.53
1:F:79:LEU:HD11	1:F:93:ALA:HB2	1.89	0.53
1:E:75:HIS:HD2	1:E:112:LEU:HD13	1.73	0.53
1:A:75:HIS:HD2	1:A:112:LEU:HD13	1.74	0.53
1:E:174:LEU:HD13	1:F:167:TYR:CZ	2.44	0.53
1:E:3:GLU:CD	1:E:3:GLU:H	2.11	0.53
1:F:196:GLU:OE2	2:G:143:HIS:CE1	2.62	0.53
1:A:3:GLU:H	1:A:3:GLU:CD	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:143:HIS:CE1	1:B:196:GLU:OE2	2.62	0.53
1:F:26:LYS:NZ	1:F:134:HIS:HD2	2.07	0.52
1:E:176:ARG:HB2	1:E:179:LEU:HD12	1.92	0.52
1:B:176:ARG:HB2	1:B:179:LEU:HD12	1.91	0.52
1:E:61:LEU:HD12	1:E:119:TRP:HA	1.92	0.51
2:D:61:MET:HE3	2:D:66:TYR:HD1	1.76	0.51
1:A:204:ILE:HD11	1:B:137:ARG:CZ	2.40	0.51
1:A:26:LYS:NZ	1:A:134:HIS:HD2	2.08	0.51
1:A:40:ASP:C	1:A:41:LEU:HD12	2.31	0.51
2:D:22:VAL:HG22	2:D:34:ILE:HG23	1.93	0.51
2:C:22:VAL:HG22	2:C:34:ILE:HG23	1.92	0.51
1:A:29:ILE:HD13	1:A:77:ASP:OD1	2.11	0.50
1:E:26:LYS:NZ	1:E:134:HIS:HD2	2.09	0.50
1:F:97:CYS:SG	1:F:104:LEU:HD11	2.51	0.50
1:B:109:ARG:HE	1:B:118:TYR:HE2	1.60	0.50
1:A:181:THR:CG2	1:B:159:MET:HG3	2.40	0.50
1:B:26:LYS:NZ	1:B:134:HIS:HD2	2.09	0.50
1:F:64:ARG:HH11	2:D:107:ARG:CB	2.24	0.50
1:E:97:CYS:SG	1:E:104:LEU:HD11	2.50	0.50
1:A:176:ARG:HB2	1:A:179:LEU:HD12	1.93	0.50
1:E:109:ARG:HE	1:E:118:TYR:HE2	1.59	0.50
1:E:204:ILE:HD11	1:F:137:ARG:CZ	2.42	0.50
1:A:108:VAL:HG12	1:A:119:TRP:HB3	1.94	0.49
1:E:175:ILE:CG1	1:F:170:SER:HB3	2.42	0.49
1:B:108:VAL:HG12	1:B:119:TRP:HB3	1.94	0.49
2:G:120:ALA:HB2	2:H:40:HIS:ND1	2.28	0.49
1:F:43:GLN:OE1	1:F:125:LEU:HD21	2.13	0.49
1:E:108:VAL:HG12	1:E:119:TRP:HB3	1.94	0.49
1:A:157:LEU:HG	1:B:157:LEU:HG	1.95	0.48
2:C:32:PHE:HE1	2:C:34:ILE:HG12	1.78	0.48
1:F:64:ARG:HD3	2:D:107:ARG:HB3	1.95	0.48
1:E:157:LEU:HG	1:F:157:LEU:HG	1.95	0.48
1:E:187:ASN:H	1:E:187:ASN:ND2	2.12	0.48
1:F:108:VAL:HG12	1:F:119:TRP:HB3	1.95	0.48
2:D:32:PHE:HE1	2:D:34:ILE:HG12	1.78	0.48
1:E:181:THR:HG22	1:F:159:MET:HG3	1.94	0.48
1:A:167:TYR:O	1:A:172:ALA:HB3	2.12	0.48
1:A:172:ALA:HB1	1:B:172:ALA:HB1	1.96	0.48
1:B:61:LEU:HD12	1:B:119:TRP:HA	1.95	0.48
1:E:29:ILE:HD13	1:E:77:ASP:OD1	2.14	0.48
1:F:29:ILE:HD13	1:F:77:ASP:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLN:OE1	1:A:125:LEU:HD21	2.13	0.47
1:A:26:LYS:HZ1	1:A:134:HIS:HD2	1.61	0.47
1:B:97:CYS:SG	1:B:104:LEU:HD11	2.54	0.47
1:B:79:LEU:HD11	1:B:93:ALA:HB2	1.97	0.47
1:F:167:TYR:O	1:F:172:ALA:HB3	2.15	0.47
1:E:26:LYS:HZ1	1:E:134:HIS:HD2	1.61	0.46
1:F:176:ARG:HB2	1:F:179:LEU:HD12	1.97	0.46
2:C:40:HIS:ND1	2:D:120:ALA:HB2	2.31	0.46
2:C:61:MET:HE3	2:C:66:TYR:HD1	1.80	0.46
1:E:175:ILE:HD11	1:F:170:SER:HB3	1.97	0.46
1:F:43:GLN:HB2	1:F:45:TRP:CH2	2.50	0.46
1:F:59:LYS:HD3	1:F:65:LEU:HB3	1.98	0.46
1:B:64:ARG:HD3	2:H:107:ARG:HB3	1.96	0.46
1:B:64:ARG:HH11	2:H:107:ARG:CB	2.23	0.46
1:A:43:GLN:HB2	1:A:45:TRP:CH2	2.50	0.46
1:B:167:TYR:O	1:B:172:ALA:HB3	2.16	0.45
1:E:59:LYS:HD3	1:E:65:LEU:HB3	1.97	0.45
1:B:187:ASN:ND2	1:B:187:ASN:H	2.14	0.45
1:B:29:ILE:HD13	1:B:77:ASP:OD1	2.17	0.45
2:H:61:MET:HE2	2:H:66:TYR:HD1	1.82	0.45
1:A:167:TYR:CZ	1:B:174:LEU:HD13	2.52	0.45
1:E:72:PHE:CE2	1:E:117:PHE:HE1	2.34	0.45
1:E:80:LEU:O	1:E:84:LEU:HG	2.17	0.45
1:A:187:ASN:ND2	1:A:187:ASN:H	2.13	0.45
1:F:187:ASN:ND2	1:F:187:ASN:H	2.14	0.44
1:A:72:PHE:CE2	1:A:117:PHE:HE1	2.33	0.44
1:A:174:LEU:HG	1:B:166:ASP:OD2	2.17	0.44
2:D:7:ARG:HD3	2:D:17:THR:HG21	1.99	0.44
2:C:120:ALA:HB2	2:D:40:HIS:ND1	2.33	0.44
1:E:167:TYR:CZ	1:F:174:LEU:HD13	2.53	0.44
1:F:36:LEU:HD22	1:F:121:PHE:CD2	2.53	0.44
1:F:80:LEU:O	1:F:84:LEU:HG	2.17	0.43
1:A:36:LEU:HD22	1:A:121:PHE:CD2	2.53	0.43
1:B:64:ARG:HB3	2:H:107:ARG:HB3	1.99	0.43
1:B:43:GLN:OE1	1:B:125:LEU:HD21	2.18	0.43
1:A:174:LEU:HD13	1:B:167:TYR:CZ	2.53	0.43
1:F:58:ALA:HB1	1:F:72:PHE:HE2	1.83	0.43
1:E:167:TYR:O	1:E:172:ALA:HB3	2.18	0.43
1:A:152:GLU:OE1	1:B:197:LYS:HD3	2.18	0.43
1:A:192:GLN:HG2	1:A:197:LYS:HZ2	1.83	0.43
2:C:72:LYS:O	2:C:78:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:LYS:HZ1	1:B:134:HIS:HD2	1.67	0.43
1:E:147:GLN:HG3	1:E:151:ARG:NH2	2.33	0.43
1:B:72:PHE:CE2	1:B:117:PHE:HE1	2.34	0.43
1:E:58:ALA:HB1	1:E:72:PHE:HE2	1.82	0.43
2:H:72:LYS:O	2:H:78:ALA:HB2	2.19	0.43
1:A:4:LEU:HB2	1:A:48:GLN:HE21	1.84	0.42
1:F:72:PHE:CE2	1:F:117:PHE:HE1	2.33	0.42
1:B:147:GLN:HG3	1:B:151:ARG:NH2	2.35	0.42
1:E:43:GLN:OE1	1:E:125:LEU:HD21	2.19	0.42
2:G:132:ASP:O	2:G:136:GLU:HG3	2.19	0.42
1:A:58:ALA:HB1	1:A:72:PHE:HE2	1.83	0.42
1:B:192:GLN:HG2	1:B:197:LYS:NZ	2.35	0.42
1:F:26:LYS:HZ1	1:F:134:HIS:HD2	1.67	0.42
1:A:192:GLN:HG2	1:A:197:LYS:NZ	2.35	0.42
1:A:59:LYS:HD2	1:A:65:LEU:HB3	2.01	0.42
2:C:132:ASP:O	2:C:136:GLU:HG3	2.20	0.42
1:A:110:SER:O	1:A:117:PHE:N	2.44	0.41
1:A:79:LEU:HD11	1:A:93:ALA:HB2	2.01	0.41
1:F:147:GLN:HG3	1:F:151:ARG:NH2	2.35	0.41
1:A:138:PRO:O	1:A:142:MET:HG3	2.21	0.41
2:H:118:ASN:HD22	2:H:121:GLU:HB3	1.86	0.41
1:F:4:LEU:HB2	1:F:48:GLN:HE21	1.85	0.41
1:E:156:LEU:HB3	1:F:157:LEU:HD21	2.02	0.41
1:E:176:ARG:NH1	1:F:166:ASP:OD1	2.54	0.41
1:A:166:ASP:OD1	1:B:176:ARG:NH1	2.54	0.41
1:B:41:LEU:HD12	1:B:41:LEU:N	2.36	0.41
1:F:138:PRO:O	1:F:142:MET:HG3	2.21	0.41
1:A:147:GLN:HG3	1:A:151:ARG:NH2	2.36	0.41
1:B:80:LEU:O	1:B:84:LEU:HG	2.21	0.40
1:B:156:LEU:HA	1:B:156:LEU:HD12	1.97	0.40
1:F:110:SER:O	1:F:117:PHE:N	2.44	0.40
2:G:72:LYS:O	2:G:78:ALA:HB2	2.21	0.40
2:C:128:CYS:SG	2:D:7:ARG:NH1	2.94	0.40
2:D:97:PHE:N	2:D:97:PHE:CD1	2.89	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	225/230 (98%)	215 (96%)	8 (4%)	2 (1%)	20	63
1	B	225/230 (98%)	215 (96%)	8 (4%)	2 (1%)	20	63
1	E	225/230 (98%)	215 (96%)	8 (4%)	2 (1%)	20	63
1	F	225/230 (98%)	215 (96%)	8 (4%)	2 (1%)	20	63
2	C	155/186 (83%)	146 (94%)	9 (6%)	0	100	100
2	D	155/186 (83%)	147 (95%)	8 (5%)	0	100	100
2	G	155/186 (83%)	145 (94%)	9 (6%)	1 (1%)	28	70
2	H	155/186 (83%)	146 (94%)	8 (5%)	1 (1%)	28	70
All	All	1520/1664 (91%)	1444 (95%)	66 (4%)	10 (1%)	25	68

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	27	THR
2	H	27	THR
1	E	92	GLU
1	F	92	GLU
1	A	92	GLU
1	B	92	GLU
1	E	87	ALA
1	B	87	ALA
1	F	87	ALA
1	A	87	ALA

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	200/204 (98%)	181 (90%)	19 (10%)	10	36
1	B	200/204 (98%)	180 (90%)	20 (10%)	9	34
1	E	200/204 (98%)	180 (90%)	20 (10%)	9	34
1	F	200/204 (98%)	182 (91%)	18 (9%)	11	39
2	C	140/166 (84%)	126 (90%)	14 (10%)	9	34
2	D	140/166 (84%)	130 (93%)	10 (7%)	17	50
2	G	140/166 (84%)	127 (91%)	13 (9%)	10	37
2	H	140/166 (84%)	129 (92%)	11 (8%)	14	46
All	All	1360/1480 (92%)	1235 (91%)	125 (9%)	11	38

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1	MET
1	E	18	LEU
1	E	21	ASN
1	E	29	ILE
1	E	32	GLN
1	E	66	THR
1	E	75	HIS
1	E	81	ARG
1	E	91	SER
1	E	94	THR
1	E	97	CYS
1	E	98	ASP
1	E	109	ARG
1	E	117	PHE
1	E	124	MET
1	E	174	LEU
1	E	176	ARG
1	E	187	ASN
1	E	216	ASP
1	E	224	GLN
1	F	1	MET
1	F	18	LEU
1	F	21	ASN
1	F	29	ILE

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Mol	Chain	Res	Type
1	F	31	LYS
1	F	32	GLN
1	F	66	THR
1	F	81	ARG
1	F	91	SER
1	F	97	CYS
1	F	98	ASP
1	F	109	ARG
1	F	117	PHE
1	F	124	MET
1	F	174	LEU
1	F	176	ARG
1	F	187	ASN
1	F	216	ASP
2	C	1	MET
2	C	3	ARG
2	C	6	SER
2	C	7	ARG
2	C	34	ILE
2	C	40	HIS
2	C	53	SER
2	C	65	LYS
2	C	91	GLU
2	C	98	GLU
2	C	103	ASP
2	C	114	GLU
2	C	128	CYS
2	C	141	ASN
2	D	1	MET
2	D	7	ARG
2	D	34	ILE
2	D	40	HIS
2	D	53	SER
2	D	91	GLU
2	D	98	GLU
2	D	114	GLU
2	D	128	CYS
2	D	141	ASN
1	A	1	MET
1	A	18	LEU
1	A	21	ASN
1	A	29	ILE

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Mol	Chain	Res	Type
1	A	32	GLN
1	A	66	THR
1	A	81	ARG
1	A	91	SER
1	A	97	CYS
1	A	98	ASP
1	A	109	ARG
1	A	117	PHE
1	A	124	MET
1	A	156	LEU
1	A	174	LEU
1	A	176	ARG
1	A	187	ASN
1	A	192	GLN
1	A	216	ASP
1	B	1	MET
1	B	18	LEU
1	B	21	ASN
1	B	29	ILE
1	B	32	GLN
1	B	66	THR
1	B	81	ARG
1	B	91	SER
1	B	97	CYS
1	B	98	ASP
1	B	109	ARG
1	B	117	PHE
1	B	124	MET
1	B	156	LEU
1	B	174	LEU
1	B	176	ARG
1	B	187	ASN
1	B	192	GLN
1	B	216	ASP
1	B	224	GLN
2	G	1	MET
2	G	3	ARG
2	G	6	SER
2	G	7	ARG
2	G	40	HIS
2	G	53	SER
2	G	61	MET

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Mol	Chain	Res	Type
2	G	65	LYS
2	G	91	GLU
2	G	98	GLU
2	G	114	GLU
2	G	128	CYS
2	G	141	ASN
2	H	1	MET
2	H	7	ARG
2	H	40	HIS
2	H	53	SER
2	H	61	MET
2	H	65	LYS
2	H	91	GLU
2	H	98	GLU
2	H	114	GLU
2	H	128	CYS
2	H	141	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	48	GLN
1	E	75	HIS
1	E	134	HIS
1	E	147	GLN
1	E	187	ASN
1	E	226	HIS
1	F	48	GLN
1	F	75	HIS
1	F	134	HIS
1	F	147	GLN
1	F	187	ASN
1	F	226	HIS
2	C	54	GLN
2	C	87	ASN
2	C	143	HIS
2	D	54	GLN
2	D	87	ASN
1	A	48	GLN
1	A	75	HIS
1	A	134	HIS
1	A	147	GLN

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Mol	Chain	Res	Type
1	A	187	ASN
1	A	226	HIS
1	B	48	GLN
1	B	75	HIS
1	B	134	HIS
1	B	147	GLN
1	B	187	ASN
1	B	226	HIS
2	G	54	GLN
2	G	87	ASN
2	G	143	HIS
2	H	54	GLN
2	H	87	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	227/230 (98%)	0.13	10 (4%) 35 33	225, 268, 297, 299	7 (3%)
1	B	227/230 (98%)	0.23	12 (5%) 27 28	229, 277, 298, 299	6 (2%)
1	E	227/230 (98%)	0.22	7 (3%) 49 45	207, 258, 296, 299	7 (3%)
1	F	227/230 (98%)	0.09	6 (2%) 56 52	217, 262, 297, 299	6 (2%)
2	C	157/186 (84%)	0.18	9 (5%) 24 26	233, 262, 294, 299	0
2	D	157/186 (84%)	-0.14	5 (3%) 48 44	223, 267, 290, 299	0
2	G	157/186 (84%)	0.32	11 (7%) 17 20	230, 268, 294, 298	0
2	H	157/186 (84%)	-0.07	4 (2%) 58 53	237, 279, 295, 299	0
All	All	1536/1664 (92%)	0.13	64 (4%) 37 35	207, 269, 297, 299	26 (1%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	HIS	5.8
1	E	203	SER	5.6
1	F	227	HIS	5.4
1	E	205	GLY	4.9
2	G	29	GLU	4.5
1	B	172	ALA	4.4
1	B	171	GLY	4.3
2	C	29	GLU	3.5
1	A	205	GLY	3.5
2	G	28	LEU	3.5
2	G	63	LYS	3.3
2	C	63	LYS	3.3
2	G	67	VAL	3.3
1	E	163	GLU	3.2
2	G	66	TYR	3.2
1	A	202	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	22	SER	3.0
1	B	102	ASP	2.9
2	G	32	PHE	2.9
2	C	26	LYS	2.8
1	A	21	ASN	2.8
1	B	86	ASP	2.8
1	E	206	ASP	2.8
2	C	28	LEU	2.7
1	E	117	PHE	2.6
2	H	151	LEU	2.6
1	B	88	ALA	2.6
1	B	87	ALA	2.5
1	A	97	CYS	2.5
2	G	2	GLU	2.5
1	F	173	THR	2.5
1	B	225	HIS	2.4
1	F	33	GLY	2.4
1	A	206	ASP	2.4
2	C	32	PHE	2.4
1	F	97	CYS	2.4
1	B	173	THR	2.4
1	B	113	SER	2.4
1	B	84	LEU	2.3
1	B	153	LEU	2.3
2	H	152	LEU	2.3
2	C	99	LYS	2.3
2	C	157	ASP	2.3
1	E	119	TRP	2.2
1	F	134	HIS	2.2
1	F	204	ILE	2.2
2	C	70	LEU	2.2
1	A	204	ILE	2.2
1	A	18	LEU	2.2
2	D	37	THR	2.1
1	A	95	PHE	2.1
2	H	148	ASN	2.1
2	H	7	ARG	2.1
2	D	99	LYS	2.1
2	D	78	ALA	2.1
2	G	26	LYS	2.1
2	D	36	LEU	2.1
1	A	23	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	200	GLU	2.1
2	C	74	LEU	2.1
2	G	71	ARG	2.1
2	G	61	MET	2.0
2	G	152	LEU	2.0
2	D	39	GLY	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.