



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:28 AM UTC

PDB ID : 3Q4F / pdb_00003q4f
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

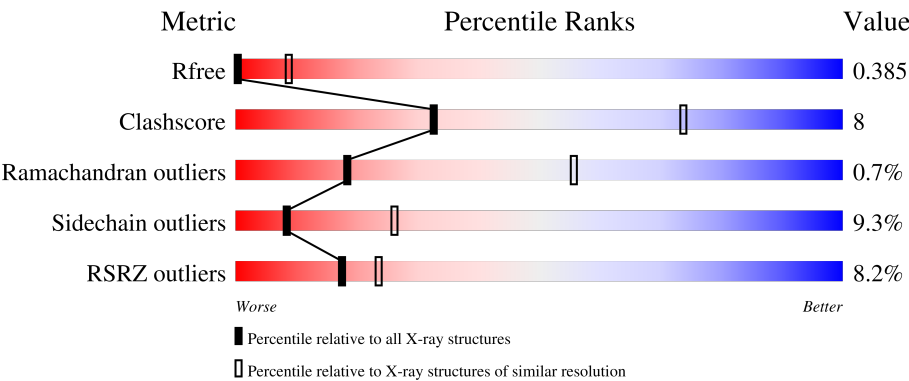
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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))
R _{free}	180053	1088 (7.00-4.00)
Clashscore	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)

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 of 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 $\leq 5\%$. 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	8% 67%28% . .
1	B	230	5% 68%26%5% .
1	E	230	10% 71%23% . .
1	F	230	6% 67%29% . .
2	C	186	4% 69%13% . 16%

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Mol	Chain	Length	Quality of chain
2	D	186	9% 72% 10% • 16%
2	G	186	13% 70% 14% • 16%
2	H	186	6% 72% 12% • 16%

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	C	N	O	S	0	0	0
			1267	800	212	249	6			
2	D	157	Total	C	N	O	S	0	0	0
			1267	800	212	249	6			
2	G	157	Total	C	N	O	S	0	0	0
			1267	800	212	249	6			
2	H	157	Total	C	N	O	S	0	0	0
			1267	800	212	249	6			

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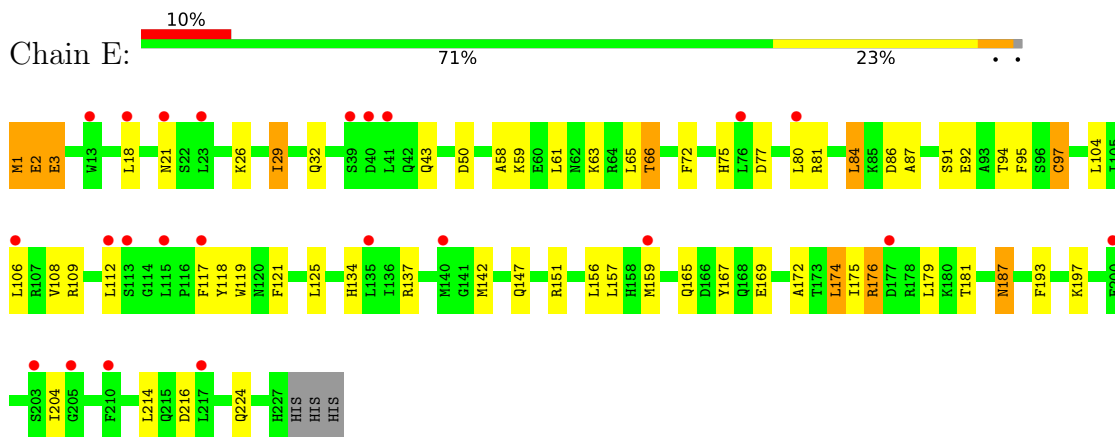
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Chain	Residue	Modelled	Actual	Comment	Reference
H	-8	GLY	-	expression tag	UNP Q13426
H	-7	PHE	-	expression tag	UNP Q13426
H	-6	GLU	-	expression tag	UNP Q13426
H	-5	ASN	-	expression tag	UNP Q13426
H	-4	LEU	-	expression tag	UNP Q13426
H	-3	TYR	-	expression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

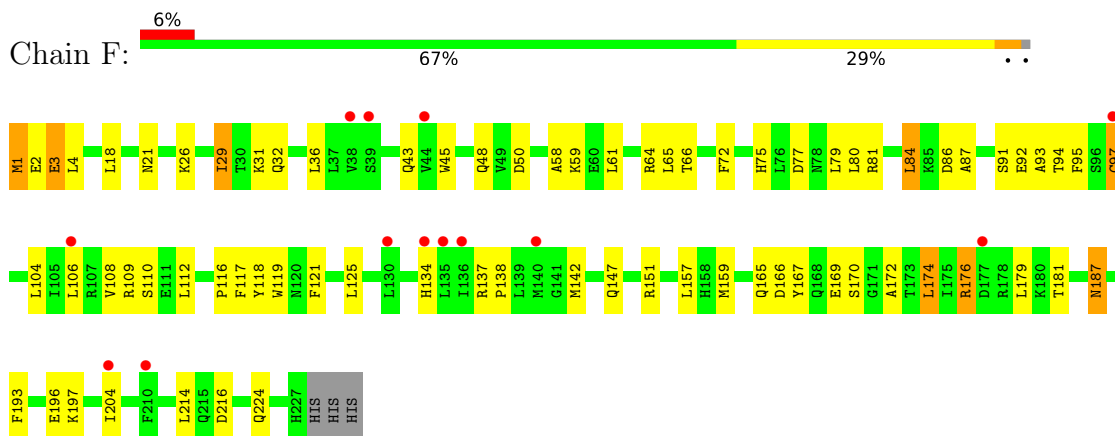
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

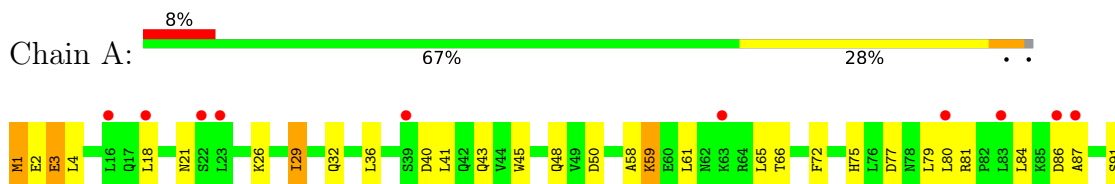
- Molecule 1: Non-homologous end-joining factor 1

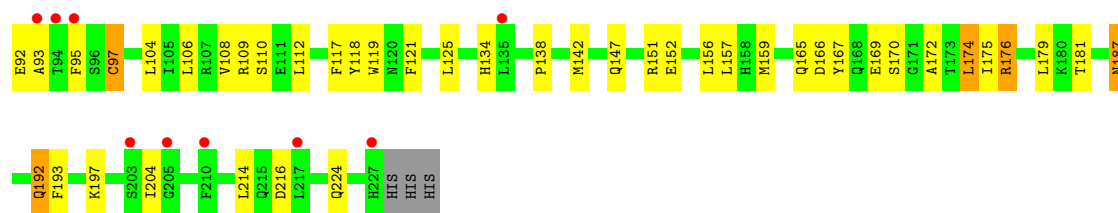


- Molecule 1: Non-homologous end-joining factor 1

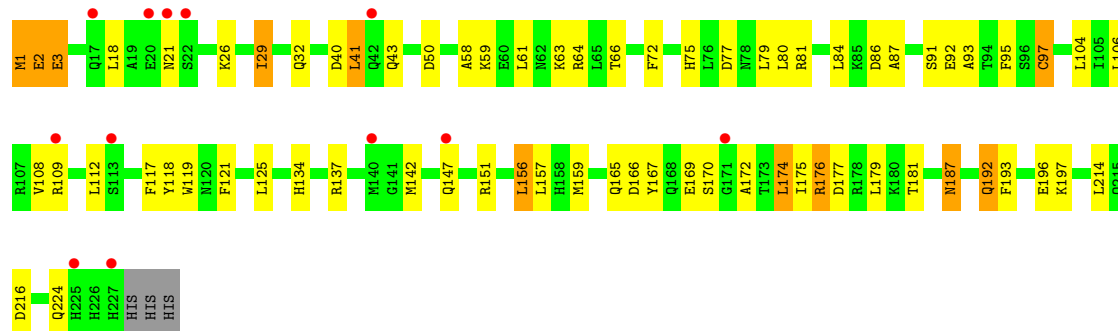


- Molecule 1: Non-homologous end-joining factor 1

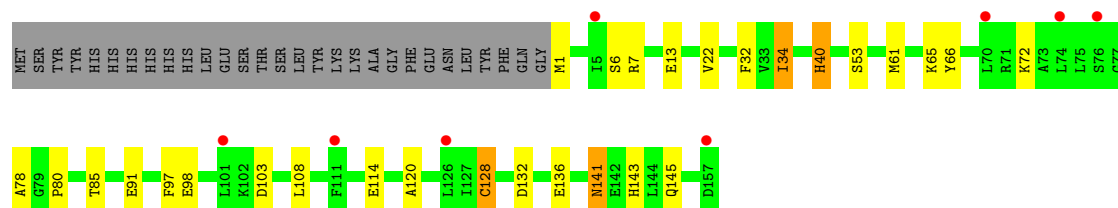




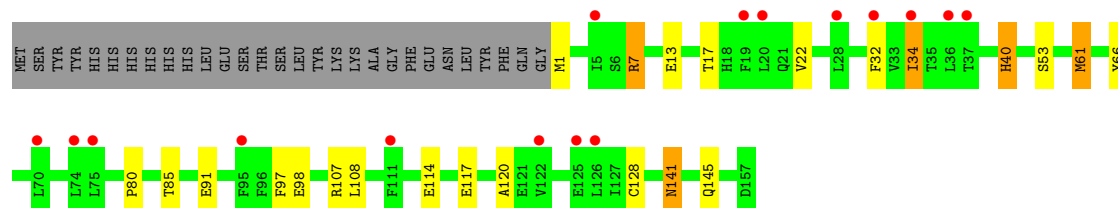
• Molecule 1: Non-homologous end-joining factor 1



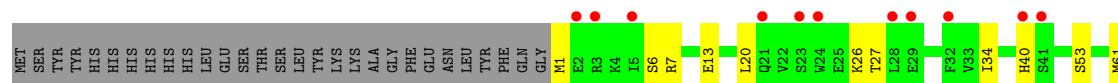
• Molecule 2: DNA repair protein XRCC4

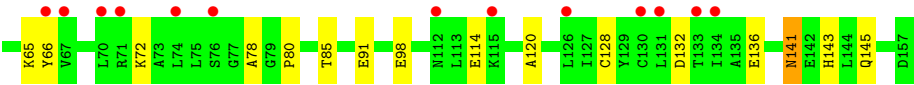


• Molecule 2: DNA repair protein XRCC4

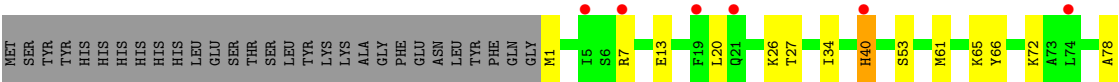


• Molecule 2: DNA repair protein XRCC4





● 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 48.79 – 5.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.79-5.50) 99.7 (48.79-5.50)	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-TNT, BUSTER 2.8.0	Depositor
R, R_{free}	0.249 , 0.309 0.273 , 0.385	Depositor DCC
R_{free} test set	494 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	233.9	Xtriage
Anisotropy	0.840	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 277.2	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	0.72	0/1847	1.20	3/2507 (0.1%)
1	B	0.72	0/1847	1.23	3/2507 (0.1%)
1	E	0.74	0/1847	1.22	7/2507 (0.3%)
1	F	0.71	0/1847	1.20	3/2507 (0.1%)
2	C	0.66	0/1292	1.09	4/1741 (0.2%)
2	D	0.64	0/1292	1.10	5/1741 (0.3%)
2	G	0.66	0/1292	1.14	6/1741 (0.3%)
2	H	0.64	0/1292	1.14	4/1741 (0.2%)
All	All	0.69	0/12556	1.17	35/16992 (0.2%)

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	26	LYS	CA-C-N	9.18	139.08	121.54
2	H	26	LYS	C-N-CA	9.18	139.08	121.54
2	G	26	LYS	CA-C-N	9.14	139.00	121.54
2	G	26	LYS	C-N-CA	9.14	139.00	121.54
1	E	86	ASP	CA-CB-CG	6.93	119.53	112.60
1	F	86	ASP	CA-CB-CG	6.75	119.35	112.60
1	A	86	ASP	CA-CB-CG	6.56	119.16	112.60
1	B	86	ASP	CA-CB-CG	6.39	118.99	112.60
2	G	141	ASN	CA-CB-CG	6.20	118.80	112.60
2	D	145	GLN	CB-CG-CD	-5.72	102.88	112.60
2	C	145	GLN	CB-CG-CD	-5.55	103.16	112.60
2	C	80	PRO	CA-C-N	5.53	129.96	120.72
2	C	80	PRO	C-N-CA	5.53	129.96	120.72
1	F	84	LEU	CA-C-N	5.50	128.41	120.38
1	F	84	LEU	C-N-CA	5.50	128.41	120.38
2	G	145	GLN	CB-CG-CD	-5.49	103.27	112.60
2	D	141	ASN	CA-CB-CG	5.46	118.06	112.60
1	E	66	THR	CB-CA-C	5.46	119.87	111.85
2	H	145	GLN	CB-CG-CD	-5.43	103.37	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	80	PRO	CA-C-N	5.39	129.72	120.72
2	D	80	PRO	C-N-CA	5.39	129.72	120.72
2	G	80	PRO	CA-C-N	5.37	129.69	120.72
2	G	80	PRO	C-N-CA	5.37	129.69	120.72
1	B	63	LYS	N-CA-C	5.36	118.92	112.38
1	A	84	LEU	CA-C-N	5.35	128.19	120.38
1	A	84	LEU	C-N-CA	5.35	128.19	120.38
1	E	63	LYS	N-CA-C	5.30	118.85	112.38
2	D	117	GLU	CB-CG-CD	5.29	121.59	112.60
1	E	84	LEU	CA-C-N	5.28	128.08	120.38
1	E	84	LEU	C-N-CA	5.28	128.08	120.38
2	C	141	ASN	CA-CB-CG	5.15	117.75	112.60
2	H	141	ASN	CA-CB-CG	5.13	117.73	112.60
1	B	41	LEU	CD1-CG-CD2	-5.09	99.61	110.80
1	E	2	GLU	CA-C-N	5.00	126.98	120.28
1	E	2	GLU	C-N-CA	5.00	126.98	120.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1807	0	1800	50	0
1	B	1807	0	1800	54	0
1	E	1807	0	1800	39	0
1	F	1807	0	1800	50	0
2	C	1267	0	1229	11	0
2	D	1267	0	1229	15	0
2	G	1267	0	1229	7	0
2	H	1267	0	1229	11	0
All	All	12296	0	12116	192	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 (192) 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
2:C:97:PHE:HE2	2:C:108:LEU:HD23	1.54	0.72
1:B:165:GLN:O	1:B:169:GLU:HG2	1.89	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
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:A:181:THR:HG22	1:B:159:MET:HG3	1.80	0.63
1:B:106:LEU:HB3	1:B:121:PHE:HB2	1.81	0.63
1:B:40:ASP:C	1:B:41:LEU:HD12	2.24	0.62
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:3:GLU:CD	1:B:3:GLU:H	2.10	0.59
1:F:3:GLU:H	1:F:3:GLU:CD	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:GLU:H	1:E:3:GLU:CD	2.11	0.58
1:E:80:LEU:HD21	1:E:95:PHE:HZ	1.69	0.57
2:G:61:MET:HE3	2:G:66:TYR:HA	1.85	0.57
1:A:3:GLU:H	1:A:3:GLU:CD	2.11	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
2:H:61:MET:HE3	2:H:66:TYR:HA	1.87	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:A:40:ASP:C	1:A:41:LEU:HD12	2.31	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: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: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:58:ALA:CB	1:A:72:PHE:CE2	2.91	0.53
1:A:109:ARG:HE	1:A:118:TYR:HE2	1.56	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:E:174:LEU:HD13	1:F:167:TYR:CZ	2.44	0.53
1:A:75:HIS:HD2	1:A:112:LEU:HD13	1.74	0.53
1:F:196:GLU:OE2	2:G:143:HIS:CE1	2.62	0.53
2:C:143:HIS:CE1	1:B:196:GLU:OE2	2.62	0.53
1:E:1:MET:HE3	1:E:50:ASP:HB3	1.91	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1:MET:HE3	1:F:50:ASP:HB3	1.93	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:A:181:THR:CG2	1:B:159:MET:HG3	2.40	0.50
1:B:109:ARG:HE	1:B:118:TYR:HE2	1.60	0.50
2:D:61:MET:HE3	2:D:66:TYR:HD1	1.76	0.50
1:E:97:CYS:SG	1:E:104:LEU:HD11	2.50	0.50
1:F:64:ARG:HH11	2:D:107:ARG:CB	2.24	0.50
1:B:26:LYS:NZ	1:B:134:HIS:HD2	2.09	0.50
1:E:109:ARG:HE	1:E:118:TYR:HE2	1.59	0.50
1:A:176:ARG:HB2	1:A:179:LEU:HD12	1.93	0.50
1:E:204:ILE:HD11	1:F:137:ARG:CZ	2.42	0.50
1:E:142:MET:HE1	1:E:214:LEU:HB3	1.94	0.49
1:E:175:ILE:CG1	1:F:170:SER:HB3	2.42	0.49
1:A:108:VAL:HG12	1:A:119:TRP:HB3	1.94	0.49
1:B:108:VAL:HG12	1:B:119:TRP:HB3	1.94	0.49
1:B:1:MET:HE3	1:B:50:ASP:HB3	1.93	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:E:157:LEU:HG	1:F:157:LEU:HG	1.95	0.48
1:F:64:ARG:HD3	2:D:107:ARG:HB3	1.95	0.48
2:C:32:PHE:HE1	2:C:34:ILE:HG12	1.78	0.48
1:A:157:LEU:HG	1:B:157:LEU:HG	1.95	0.48
1:B:142:MET:HE1	1:B:214:LEU:HB3	1.95	0.48
1:E:187:ASN:ND2	1:E:187:ASN:H	2.12	0.48
1:F:108:VAL:HG12	1:F:119:TRP:HB3	1.95	0.48
1:E:181:THR:HG22	1:F:159:MET:HG3	1.94	0.48
2:D:32:PHE:HE1	2:D:34:ILE:HG12	1.78	0.48
1:A:167:TYR:O	1:A:172:ALA:HB3	2.12	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
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
2:C:61:MET:HE3	2:C:66:TYR:HD1	1.79	0.48
1:A:43:GLN:OE1	1:A:125:LEU:HD21	2.13	0.47
1:A:1:MET:HE3	1:A:50:ASP:HB3	1.96	0.47
1:B:97:CYS:SG	1:B:104:LEU:HD11	2.54	0.47
1:F:167:TYR:O	1:F:172:ALA:HB3	2.15	0.47
1:B:79:LEU:HD11	1:B:93:ALA:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:176:ARG:HB2	1:F:179:LEU:HD12	1.97	0.46
1:E:175:ILE:HD11	1:F:170:SER:HB3	1.97	0.46
2:C:40:HIS:ND1	2:D:120:ALA:HB2	2.31	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:HH11	2:H:107:ARG:CB	2.23	0.46
1:B:64:ARG:HD3	2:H:107:ARG:HB3	1.96	0.46
1:A:142:MET:HE1	1:A:214:LEU:HB3	1.98	0.46
1:A:43:GLN:HB2	1:A:45:TRP:CH2	2.50	0.46
1:F:142:MET:HE1	1:F:214:LEU:HB3	1.98	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:29:ILE:HD13	1:B:77:ASP:OD1	2.17	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:167:TYR:CZ	1:B:174:LEU:HD13	2.52	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:B:187:ASN:ND2	1:B:187:ASN:H	2.14	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:F:58:ALA:HB1	1:F:72:PHE:HE2	1.83	0.43
1:A:174:LEU:HD13	1:B:167:TYR:CZ	2.53	0.43
1:E:167:TYR:O	1:E:172:ALA:HB3	2.18	0.43
2:C:72:LYS:O	2:C:78:ALA:HB2	2.18	0.43
1:A:152:GLU:OE1	1:B:197:LYS:HD3	2.18	0.43
1:E:147:GLN:HG3	1:E:151:ARG:NH2	2.33	0.43
1:E:58:ALA:HB1	1:E:72:PHE:HE2	1.82	0.43
1:B:72:PHE:CE2	1:B:117:PHE:HE1	2.34	0.43
2:H:72:LYS:O	2:H:78:ALA:HB2	2.19	0.43
1:F:72:PHE:CE2	1:F:117:PHE:HE1	2.33	0.42
1:A:4:LEU:HB2	1:A:48:GLN:HE21	1.84	0.42
1:B:147:GLN:HG3	1:B:151:ARG:NH2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:59:LYS:HD2	1:A:65:LEU:HB3	2.01	0.42
1:A:192:GLN:HG2	1:A:197:LYS:NZ	2.35	0.42
2:G:120:ALA:HB2	2:H:40:HIS:HD1	1.85	0.42
2:C:132:ASP:O	2:C:136:GLU:HG3	2.20	0.42
1:A:79:LEU:HD11	1:A:93:ALA:HB2	2.01	0.41
1:A:110:SER:O	1:A:117:PHE:N	2.44	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:F:138:PRO:O	1:F:142:MET:HG3	2.21	0.41
1:B:41:LEU:HD12	1:B:41:LEU:N	2.36	0.41
1:A:147:GLN:HG3	1:A:151:ARG:NH2	2.36	0.41
1:B:2:GLU:CD	1:B:2:GLU:H	2.28	0.41
1:B:80:LEU:O	1:B:84:LEU:HG	2.21	0.40
1:B:156:LEU:HD12	1:B:156:LEU:HA	1.97	0.40
1:F:110:SER:O	1:F:117:PHE:N	2.44	0.40
1:A:181:THR:HG22	1:B:159:MET:HE3	2.03	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:CD1	2:D:97:PHE:N	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%)	14	50
1	B	225/230 (98%)	215 (96%)	8 (4%)	2 (1%)	14	50
1	E	225/230 (98%)	215 (96%)	8 (4%)	2 (1%)	14	50
1	F	225/230 (98%)	215 (96%)	8 (4%)	2 (1%)	14	50
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%)	21	59
2	H	155/186 (83%)	146 (94%)	8 (5%)	1 (1%)	21	59
All	All	1520/1664 (91%)	1444 (95%)	66 (4%)	10 (1%)	18	56

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%)	8	25
1	B	200/204 (98%)	181 (90%)	19 (10%)	8	25
1	E	200/204 (98%)	183 (92%)	17 (8%)	10	29
1	F	200/204 (98%)	182 (91%)	18 (9%)	9	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	140/166 (84%)	125 (89%)	15 (11%)	6	21
2	D	140/166 (84%)	127 (91%)	13 (9%)	8	26
2	G	140/166 (84%)	127 (91%)	13 (9%)	8	26
2	H	140/166 (84%)	128 (91%)	12 (9%)	10	29
All	All	1360/1480 (92%)	1234 (91%)	126 (9%)	8	26

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1	MET
1	E	2	GLU
1	E	3	GLU
1	E	18	LEU
1	E	21	ASN
1	E	29	ILE
1	E	32	GLN
1	E	66	THR
1	E	81	ARG
1	E	91	SER
1	E	94	THR
1	E	97	CYS
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	2	GLU
1	F	3	GLU
1	F	18	LEU
1	F	21	ASN
1	F	29	ILE
1	F	31	LYS
1	F	32	GLN
1	F	66	THR
1	F	81	ARG
1	F	91	SER
1	F	94	THR
1	F	97	CYS
1	F	174	LEU
1	F	176	ARG

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Mol	Chain	Res	Type
1	F	187	ASN
1	F	216	ASP
1	F	224	GLN
2	C	1	MET
2	C	6	SER
2	C	7	ARG
2	C	13	GLU
2	C	34	ILE
2	C	40	HIS
2	C	53	SER
2	C	65	LYS
2	C	85	THR
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	13	GLU
2	D	34	ILE
2	D	40	HIS
2	D	53	SER
2	D	61	MET
2	D	85	THR
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	2	GLU
1	A	3	GLU
1	A	18	LEU
1	A	21	ASN
1	A	29	ILE
1	A	32	GLN
1	A	59	LYS
1	A	66	THR
1	A	81	ARG
1	A	91	SER

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Mol	Chain	Res	Type
1	A	97	CYS
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	A	224	GLN
1	B	1	MET
1	B	2	GLU
1	B	3	GLU
1	B	18	LEU
1	B	21	ASN
1	B	29	ILE
1	B	32	GLN
1	B	59	LYS
1	B	66	THR
1	B	81	ARG
1	B	91	SER
1	B	97	CYS
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	6	SER
2	G	7	ARG
2	G	13	GLU
2	G	40	HIS
2	G	53	SER
2	G	65	LYS
2	G	85	THR
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

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Mol	Chain	Res	Type
2	H	13	GLU
2	H	40	HIS
2	H	53	SER
2	H	65	LYS
2	H	85	THR
2	H	91	GLU
2	H	98	GLU
2	H	114	GLU
2	H	128	CYS
2	H	141	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	42	GLN
1	E	48	GLN
1	E	75	HIS
1	E	134	HIS
1	E	147	GLN
1	E	187	ASN
1	E	224	GLN
1	E	226	HIS
1	F	42	GLN
1	F	48	GLN
1	F	75	HIS
1	F	134	HIS
1	F	147	GLN
1	F	187	ASN
2	C	54	GLN
2	C	143	HIS
2	D	21	GLN
2	D	40	HIS
2	D	54	GLN
2	D	87	ASN
1	A	42	GLN
1	A	48	GLN
1	A	75	HIS
1	A	134	HIS
1	A	147	GLN
1	A	187	ASN
1	B	42	GLN
1	B	48	GLN

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Mol	Chain	Res	Type
1	B	75	HIS
1	B	134	HIS
1	B	147	GLN
1	B	187	ASN
1	B	226	HIS
2	G	143	HIS
2	H	40	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 oligosaccharides 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%)	0.29	19 (8%)	17	23	143, 265, 297, 299	7 (3%)
1	B	227/230 (98%)	0.07	12 (5%)	32	33	157, 275, 298, 299	6 (2%)
1	E	227/230 (98%)	0.49	23 (10%)	12	19	129, 257, 296, 299	7 (3%)
1	F	227/230 (98%)	0.28	13 (5%)	29	32	134, 260, 297, 299	6 (2%)
2	C	157/186 (84%)	0.29	8 (5%)	33	34	233, 262, 294, 299	0
2	D	157/186 (84%)	0.31	16 (10%)	12	18	223, 267, 290, 299	0
2	G	157/186 (84%)	0.64	24 (15%)	5	12	230, 268, 294, 298	0
2	H	157/186 (84%)	0.33	11 (7%)	22	27	237, 279, 295, 299	0
All	All	1536/1664 (92%)	0.33	126 (8%)	17	23	129, 267, 297, 299	26 (1%)

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	28	LEU	8.0
2	H	5	ILE	7.7
1	E	140	MET	7.1
2	G	67	VAL	5.6
1	E	41	LEU	5.4
2	D	74	LEU	5.2
1	B	140	MET	5.1
2	C	74	LEU	4.8
1	F	140	MET	4.7
2	G	70	LEU	4.7
1	E	23	LEU	4.5
2	G	74	LEU	4.5
1	E	217	LEU	4.4
2	G	32	PHE	4.4
2	H	7	ARG	4.2
2	G	71	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	203	SER	4.2
1	F	135	LEU	4.2
2	D	75	LEU	4.2
1	A	94	THR	4.0
1	F	210	PHE	4.0
1	E	76	LEU	3.9
2	D	5	ILE	3.9
2	H	74	LEU	3.9
2	C	70	LEU	3.9
1	F	134	HIS	3.8
2	D	95	PHE	3.8
2	D	36	LEU	3.8
1	E	106	LEU	3.7
2	G	131	LEU	3.7
1	B	171	GLY	3.7
1	E	40	ASP	3.7
1	A	135	LEU	3.6
2	G	2	GLU	3.6
2	G	130	CYS	3.4
1	E	135	LEU	3.4
1	F	106	LEU	3.4
1	B	113	SER	3.4
1	F	136	ILE	3.4
1	E	80	LEU	3.4
1	A	83	LEU	3.3
1	A	217	LEU	3.3
1	F	177	ASP	3.1
1	A	95	PHE	3.1
1	B	21	ASN	3.1
2	D	111	PHE	3.1
2	G	21	GLN	3.1
2	H	19	PHE	3.1
2	D	20	LEU	3.0
1	E	39	SER	3.0
2	G	24	TRP	3.0
1	E	113	SER	2.9
2	D	32	PHE	2.9
1	B	42	GLN	2.9
2	C	157	ASP	2.9
1	B	227	HIS	2.8
1	A	93	ALA	2.8
1	A	18	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	38	VAL	2.7
1	B	147	GLN	2.7
1	F	130	LEU	2.7
1	A	203	SER	2.7
1	A	210	PHE	2.7
2	D	19	PHE	2.7
2	D	37	THR	2.7
1	E	205	GLY	2.6
1	E	210	PHE	2.6
2	C	76	SER	2.6
2	G	3	ARG	2.6
1	E	13	TRP	2.6
1	A	227	HIS	2.6
1	E	117	PHE	2.6
1	A	22	SER	2.6
2	G	29	GLU	2.5
2	D	126	LEU	2.5
1	E	115	LEU	2.5
1	A	23	LEU	2.5
2	D	34	ILE	2.5
2	H	40	HIS	2.5
2	H	142	GLU	2.5
2	C	5	ILE	2.4
1	E	112	LEU	2.4
2	G	112	ASN	2.4
2	G	41	SER	2.4
1	F	97	CYS	2.4
2	G	66	TYR	2.4
2	G	23	SER	2.3
2	G	5	ILE	2.3
2	G	133	THR	2.3
1	F	39	SER	2.3
2	D	70	LEU	2.3
2	C	101	LEU	2.3
2	H	126	LEU	2.3
2	G	76	SER	2.3
1	B	17	GLN	2.3
1	B	22	SER	2.3
1	B	20	GLU	2.2
1	E	21	ASN	2.2
1	A	16	LEU	2.2
2	D	125	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	H	92	SER	2.2
1	F	44	VAL	2.2
1	A	87	ALA	2.2
2	G	40	HIS	2.2
2	G	134	ILE	2.2
1	E	177	ASP	2.2
2	G	126	LEU	2.2
1	B	109	ARG	2.2
2	C	126	LEU	2.2
1	E	18	LEU	2.1
2	D	122	VAL	2.1
1	E	159	MET	2.1
1	A	39	SER	2.1
2	H	21	GLN	2.1
2	G	115	LYS	2.1
1	A	63	LYS	2.1
2	H	130	CYS	2.1
1	F	204	ILE	2.1
1	A	205	GLY	2.0
2	D	28	LEU	2.0
2	C	111	PHE	2.0
1	A	86	ASP	2.0
1	B	225	HIS	2.0
1	E	200	GLU	2.0
1	A	80	LEU	2.0
2	H	133	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.