



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 02:03 AM UTC

PDB ID : 4ORH / pdb_00004orh
Title : Crystal structure of RNF8 bound to the UBC13/MMS2 heterodimer
Authors : Campbell, S.J.; Edwards, R.A.; Glover, J.N.M.
Deposited on : 2014-02-11
Resolution : 4.80 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

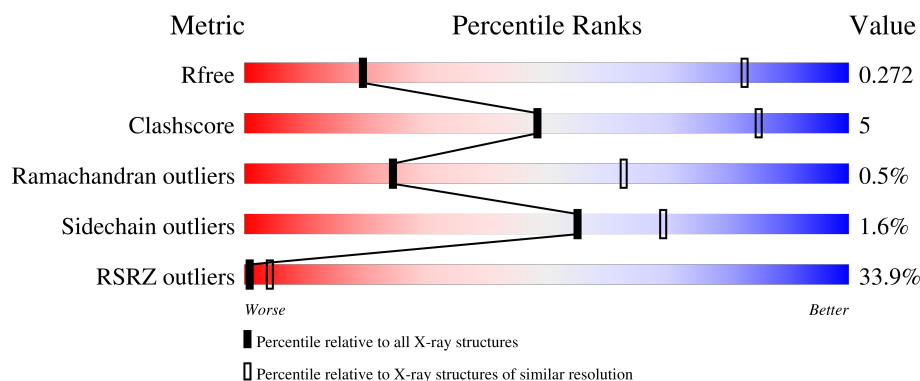
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.80 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	1018 (5.66-3.94)
Clashscore	190562	1001 (5.60-3.98)
Ramachandran outliers	187476	1104 (5.70-3.90)
Sidechain outliers	187428	1085 (5.70-3.90)
RSRZ outliers	180081	1013 (5.66-3.94)

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	153	31% 86% 5% 9%
1	E	153	27% 85% 5% 10%
1	I	153	44% 85% 5% 10%
2	B	160	31% 73% 16% • 8%
2	F	160	34% 72% 17% • 8%

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Mol	Chain	Length	Quality of chain
2	J	160	26% 76% 15% • 8%
3	C	149	23% 53% 8% • 38%
3	G	149	18% 83% 8% • 7%
3	H	149	33% 88% 7% • 5%
3	K	149	32% 81% 11% • 7%
3	L	149	35% 89% 5% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11524 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 Ubiquitin-conjugating enzyme E2 variant 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	139	Total	C	N	O	S	0	3	0
			1121	702	196	215	8			
1	E	138	Total	C	N	O	S	0	3	0
			1117	700	195	214	8			
1	I	138	Total	C	N	O	S	0	3	0
			1117	700	195	214	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP Q15819
A	-6	PRO	-	expression tag	UNP Q15819
A	-5	LEU	-	expression tag	UNP Q15819
A	-4	GLY	-	expression tag	UNP Q15819
A	-3	SER	-	expression tag	UNP Q15819
A	-2	PRO	-	expression tag	UNP Q15819
A	-1	GLU	-	expression tag	UNP Q15819
A	0	PHE	-	expression tag	UNP Q15819
E	-7	GLY	-	expression tag	UNP Q15819
E	-6	PRO	-	expression tag	UNP Q15819
E	-5	LEU	-	expression tag	UNP Q15819
E	-4	GLY	-	expression tag	UNP Q15819
E	-3	SER	-	expression tag	UNP Q15819
E	-2	PRO	-	expression tag	UNP Q15819
E	-1	GLU	-	expression tag	UNP Q15819
E	0	PHE	-	expression tag	UNP Q15819
I	-7	GLY	-	expression tag	UNP Q15819
I	-6	PRO	-	expression tag	UNP Q15819
I	-5	LEU	-	expression tag	UNP Q15819
I	-4	GLY	-	expression tag	UNP Q15819
I	-3	SER	-	expression tag	UNP Q15819
I	-2	PRO	-	expression tag	UNP Q15819
I	-1	GLU	-	expression tag	UNP Q15819

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Chain	Residue	Modelled	Actual	Comment	Reference
I	0	PHE	-	expression tag	UNP Q15819

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	148	Total	C	N	O	S	0	2	0
			1192	767	205	215	5			
2	F	148	Total	C	N	O	S	0	2	0
			1192	767	205	215	5			
2	J	148	Total	C	N	O	S	0	2	0
			1192	767	205	215	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLY	-	expression tag	UNP P61088
B	-6	PRO	-	expression tag	UNP P61088
B	-5	LEU	-	expression tag	UNP P61088
B	-4	GLY	-	expression tag	UNP P61088
B	-3	SER	-	expression tag	UNP P61088
B	-2	PRO	-	expression tag	UNP P61088
B	-1	GLU	-	expression tag	UNP P61088
B	0	PHE	-	expression tag	UNP P61088
F	-7	GLY	-	expression tag	UNP P61088
F	-6	PRO	-	expression tag	UNP P61088
F	-5	LEU	-	expression tag	UNP P61088
F	-4	GLY	-	expression tag	UNP P61088
F	-3	SER	-	expression tag	UNP P61088
F	-2	PRO	-	expression tag	UNP P61088
F	-1	GLU	-	expression tag	UNP P61088
F	0	PHE	-	expression tag	UNP P61088
J	-7	GLY	-	expression tag	UNP P61088
J	-6	PRO	-	expression tag	UNP P61088
J	-5	LEU	-	expression tag	UNP P61088
J	-4	GLY	-	expression tag	UNP P61088
J	-3	SER	-	expression tag	UNP P61088
J	-2	PRO	-	expression tag	UNP P61088
J	-1	GLU	-	expression tag	UNP P61088
J	0	PHE	-	expression tag	UNP P61088

- Molecule 3 is a protein called E3 ubiquitin-protein ligase RNF8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	92	Total	C	N	O	S	0	0	0
			723	451	128	134	10			
3	G	139	Total	C	N	O	S	0	0	0
			958	592	175	181	10			
3	H	142	Total	C	N	O	S	0	0	0
			972	600	178	184	10			
3	K	139	Total	C	N	O	S	0	0	0
			958	592	175	181	10			
3	L	142	Total	C	N	O	S	0	0	0
			972	600	178	184	10			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	337	GLY	-	expression tag	UNP O76064
C	338	PRO	-	expression tag	UNP O76064
C	339	LEU	-	expression tag	UNP O76064
C	340	GLY	-	expression tag	UNP O76064
C	341	SER	-	expression tag	UNP O76064
C	342	PRO	-	expression tag	UNP O76064
C	343	GLU	-	expression tag	UNP O76064
C	344	PHE	-	expression tag	UNP O76064
G	337	GLY	-	expression tag	UNP O76064
G	338	PRO	-	expression tag	UNP O76064
G	339	LEU	-	expression tag	UNP O76064
G	340	GLY	-	expression tag	UNP O76064
G	341	SER	-	expression tag	UNP O76064
G	342	PRO	-	expression tag	UNP O76064
G	343	GLU	-	expression tag	UNP O76064
G	344	PHE	-	expression tag	UNP O76064
H	337	GLY	-	expression tag	UNP O76064
H	338	PRO	-	expression tag	UNP O76064
H	339	LEU	-	expression tag	UNP O76064
H	340	GLY	-	expression tag	UNP O76064
H	341	SER	-	expression tag	UNP O76064
H	342	PRO	-	expression tag	UNP O76064
H	343	GLU	-	expression tag	UNP O76064
H	344	PHE	-	expression tag	UNP O76064
K	337	GLY	-	expression tag	UNP O76064
K	338	PRO	-	expression tag	UNP O76064
K	339	LEU	-	expression tag	UNP O76064
K	340	GLY	-	expression tag	UNP O76064
K	341	SER	-	expression tag	UNP O76064
K	342	PRO	-	expression tag	UNP O76064

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Chain	Residue	Modelled	Actual	Comment	Reference
K	343	GLU	-	expression tag	UNP O76064
K	344	PHE	-	expression tag	UNP O76064
L	337	GLY	-	expression tag	UNP O76064
L	338	PRO	-	expression tag	UNP O76064
L	339	LEU	-	expression tag	UNP O76064
L	340	GLY	-	expression tag	UNP O76064
L	341	SER	-	expression tag	UNP O76064
L	342	PRO	-	expression tag	UNP O76064
L	343	GLU	-	expression tag	UNP O76064
L	344	PHE	-	expression tag	UNP O76064

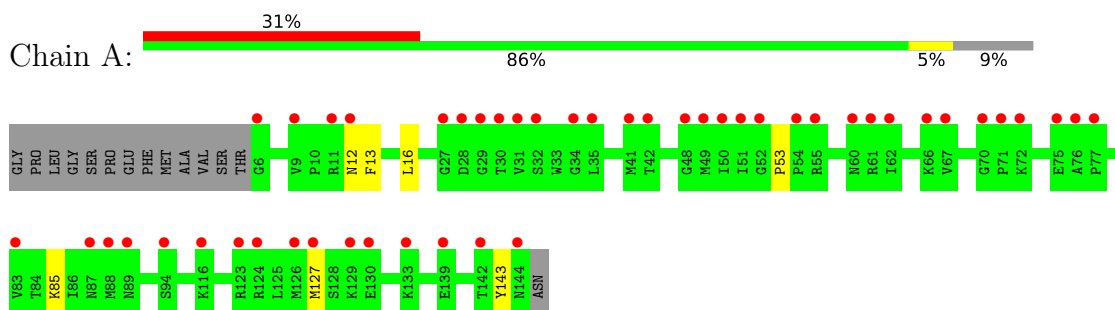
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total 2	Zn 2	0	0
4	G	2	Total 2	Zn 2	0	0
4	H	2	Total 2	Zn 2	0	0
4	K	2	Total 2	Zn 2	0	0
4	L	2	Total 2	Zn 2	0	0

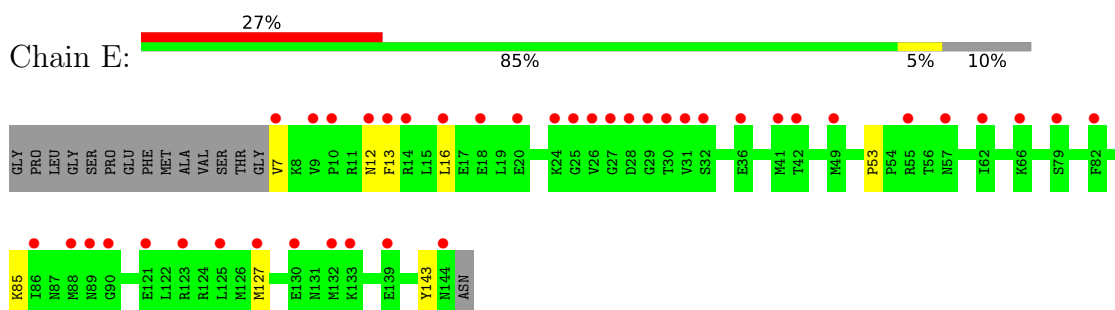
3 Residue-property plots [i](#)

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.

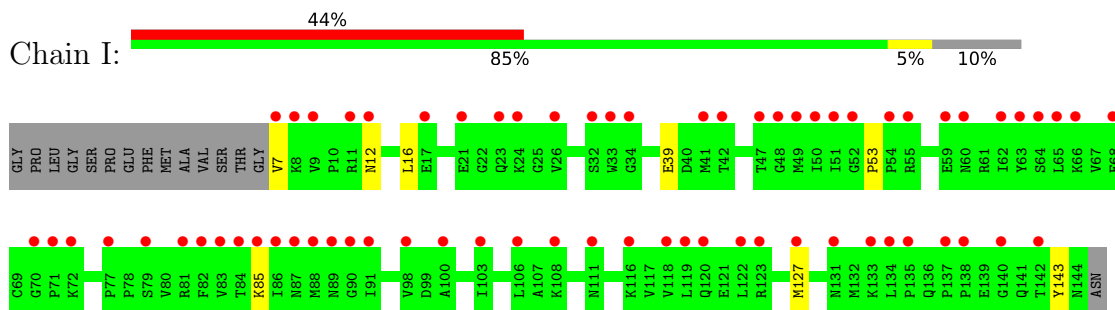
- Molecule 1: Ubiquitin-conjugating enzyme E2 variant 2



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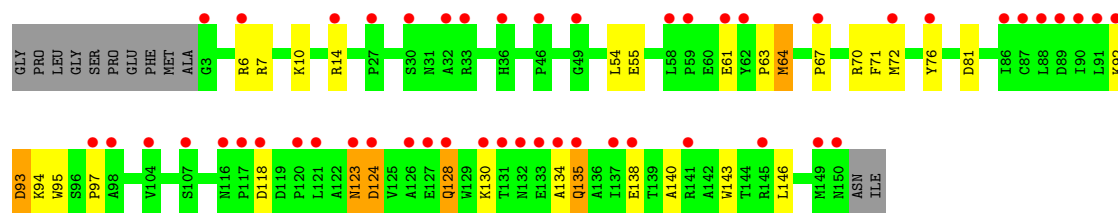


- Molecule 1: Ubiquitin-conjugating enzyme E2 variant 2

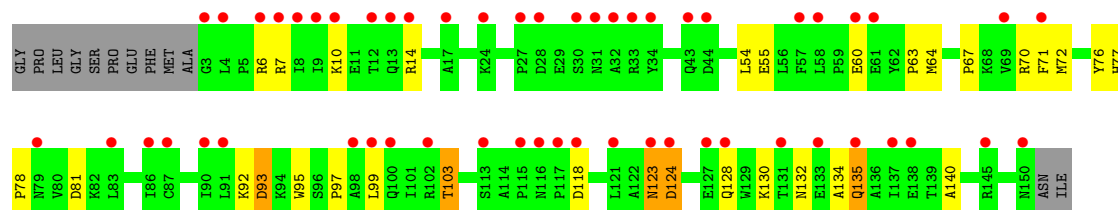


- Molecule 2: Ubiquitin-conjugating enzyme E2 N

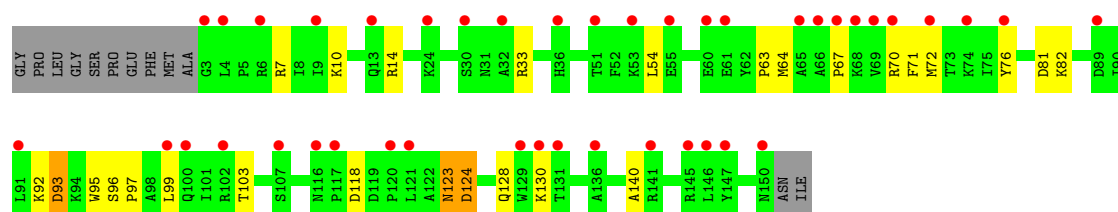
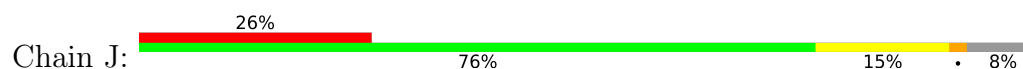




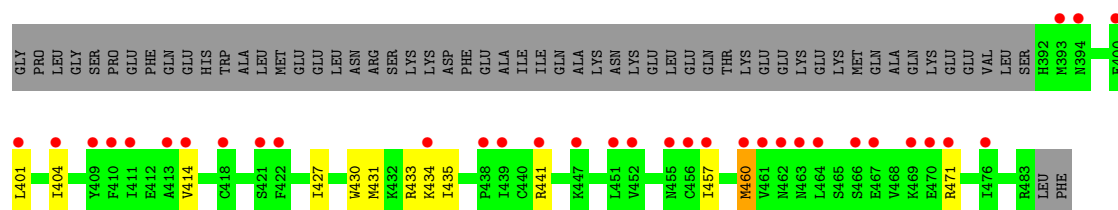
• Molecule 2: Ubiquitin-conjugating enzyme E2 N



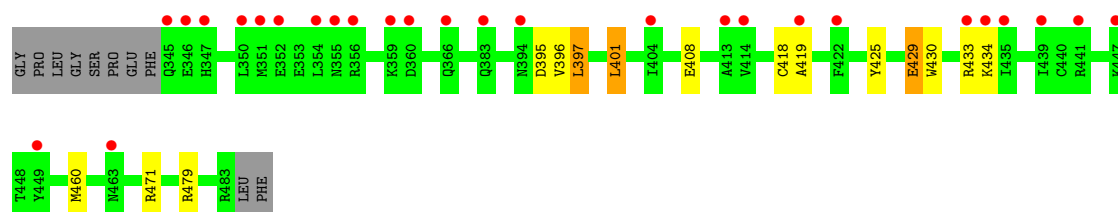
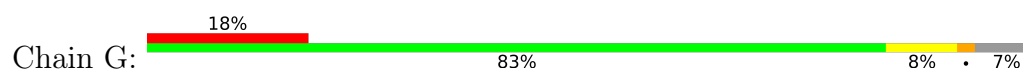
• Molecule 2: Ubiquitin-conjugating enzyme E2 N



• Molecule 3: E3 ubiquitin-protein ligase RNF8

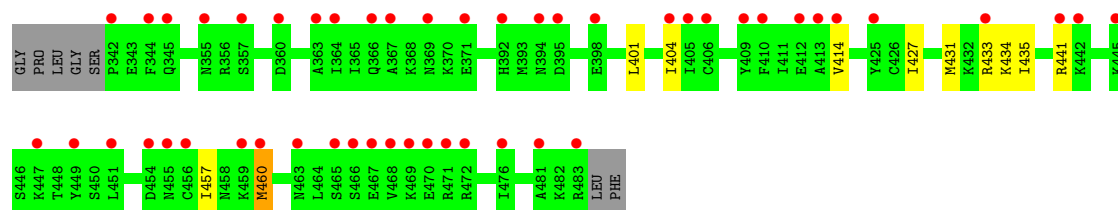


• Molecule 3: E3 ubiquitin-protein ligase RNF8



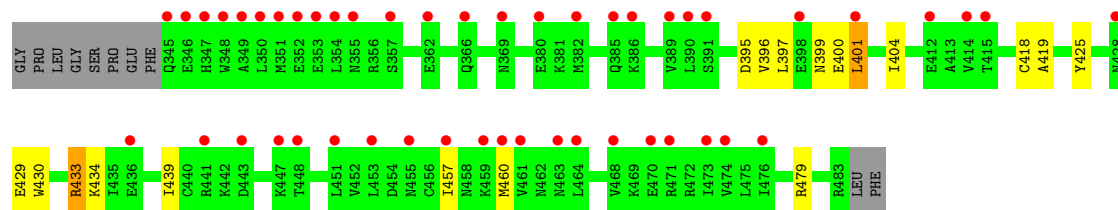
- Molecule 3: E3 ubiquitin-protein ligase RNF8

Chain H: 



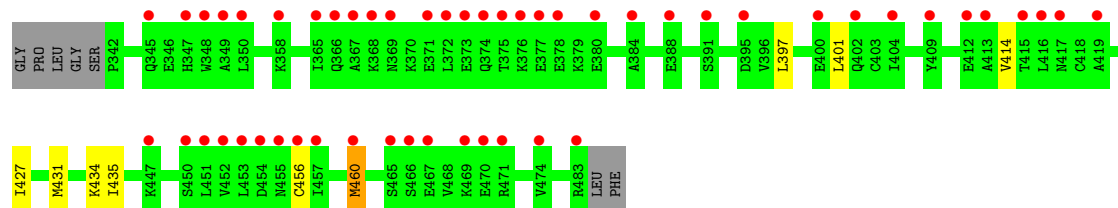
- Molecule 3: E3 ubiquitin-protein ligase RNF8

Chain K: 



- Molecule 3: E3 ubiquitin-protein ligase RNF8

Chain L: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	205.26 Å 205.26 Å 235.37 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	123.54 – 4.80 123.54 – 4.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (123.54-4.80) 98.2 (123.54-4.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 4.88 Å)	Xtriage
Refinement program	PHENIX 1.8.3_1479	Depositor
R, R_{free}	0.276 , 0.282 0.281 , 0.272	Depositor DCC
R_{free} test set	1259 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	178.1	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 499.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	11524	wwPDB-VP
Average B, all atoms (Å ²)	258.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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

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	0.36	0/1144	0.68	0/1547
1	E	0.36	0/1140	0.68	0/1542
1	I	0.36	0/1140	0.68	0/1542
2	B	0.38	0/1225	0.80	1/1666 (0.1%)
2	F	0.39	0/1225	0.80	1/1666 (0.1%)
2	J	0.35	0/1225	0.79	1/1666 (0.1%)
3	C	0.62	0/731	0.83	0/983
3	G	0.69	0/966	1.01	3/1312 (0.2%)
3	H	0.62	0/980	0.93	0/1331
3	K	0.72	0/966	1.02	5/1312 (0.4%)
3	L	0.64	0/980	0.95	0/1331
All	All	0.50	0/11722	0.83	11/15898 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	395	ASP	N-CA-C	6.08	117.58	111.07
3	K	395	ASP	N-CA-C	6.07	117.56	111.07
3	K	401	LEU	CA-C-N	-5.98	113.76	122.19
3	K	401	LEU	C-N-CA	-5.98	113.76	122.19
3	G	401	LEU	CA-C-N	-5.12	115.65	122.72
3	G	401	LEU	C-N-CA	-5.12	115.65	122.72
3	K	396	VAL	O-C-N	5.02	128.70	121.82
2	F	124	ASP	N-CA-C	-5.02	100.11	110.80
2	J	124	ASP	N-CA-C	-5.02	100.12	110.80
2	B	124	ASP	N-CA-C	-5.01	100.12	110.80
3	K	399	ASN	N-CA-C	5.01	119.40	113.28

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	1121	0	1117	5	0
1	E	1117	0	1114	8	0
1	I	1117	0	1114	6	0
2	B	1192	0	1212	29	0
2	F	1192	0	1212	33	0
2	J	1192	0	1212	23	0
3	C	723	0	703	15	0
3	G	958	0	809	17	0
3	H	972	0	814	8	0
3	K	958	0	809	15	0
3	L	972	0	814	7	0
4	C	2	0	0	0	0
4	G	2	0	0	0	0
4	H	2	0	0	0	0
4	K	2	0	0	0	0
4	L	2	0	0	0	0
All	All	11524	0	10930	123	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 5.

All (123) 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)
2:B:64:MET:HE1	3:C:430:TRP:HA	1.29	1.15
2:F:64:MET:O	3:G:433:ARG:NH2	1.97	0.97
1:E:16:LEU:HD11	2:F:70:ARG:HD3	1.44	0.96
3:K:401:LEU:HD13	3:K:457:ILE:HG12	1.48	0.93
2:F:99:LEU:O	2:F:103:THR:OG1	1.91	0.89
3:K:430:TRP:CH2	3:K:434:LYS:HD2	2.11	0.85
3:L:397:LEU:HA	3:L:401:LEU:HD12	1.61	0.83
2:J:64:MET:O	3:K:433:ARG:NH2	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:135:GLN:NE2	2:J:103:THR:OG1	2.13	0.81
1:A:16:LEU:HD11	2:B:70:ARG:HD3	1.61	0.80
1:I:16:LEU:HD11	2:J:70:ARG:HD3	1.64	0.79
3:K:401:LEU:HD13	3:K:457:ILE:CG1	2.13	0.78
3:G:430:TRP:CZ2	3:G:434:LYS:HD2	2.24	0.73
2:B:64:MET:HE2	3:C:433:ARG:HD2	1.72	0.70
2:F:134:ALA:HB2	3:K:439:ILE:O	1.92	0.70
1:E:13:PHE:CZ	2:F:55:GLU:HG3	2.26	0.69
1:I:12:ASN:HB3	2:J:70:ARG:HH21	1.58	0.69
2:F:64:MET:HE1	3:G:430:TRP:HA	1.76	0.68
2:J:7:ARG:NH1	2:J:97:PRO:O	2.29	0.64
3:H:401:LEU:HD22	3:H:457:ILE:CG1	2.28	0.64
3:C:401:LEU:HD22	3:C:457:ILE:CG1	2.28	0.63
2:J:10:LYS:HE3	2:J:14:ARG:HH12	1.64	0.62
3:C:414:VAL:HG21	3:C:427:ILE:HG21	1.81	0.62
1:A:12:ASN:HB3	2:B:70:ARG:HH21	1.64	0.62
2:B:10:LYS:HE3	2:B:14:ARG:HH12	1.64	0.62
3:L:414:VAL:HG21	3:L:427:ILE:HG21	1.81	0.62
1:E:16:LEU:HD11	2:F:70:ARG:CD	2.25	0.62
2:F:6:ARG:HB2	3:G:471:ARG:HH22	1.65	0.61
2:F:10:LYS:HE3	2:F:14:ARG:HH12	1.64	0.61
2:B:94:LYS:HA	3:C:441:ARG:NH2	2.16	0.61
3:H:414:VAL:HG21	3:H:427:ILE:HG21	1.81	0.61
2:J:99:LEU:O	2:J:103:THR:OG1	2.16	0.60
3:C:401:LEU:HD22	3:C:457:ILE:HG12	1.84	0.60
3:H:401:LEU:HD22	3:H:457:ILE:HG12	1.84	0.60
2:F:7:ARG:NH1	2:F:97:PRO:O	2.29	0.59
3:L:435:ILE:O	3:L:435:ILE:HG22	2.03	0.59
3:C:435:ILE:HG22	3:C:435:ILE:O	2.03	0.59
3:H:434:LYS:HE2	3:H:441:ARG:HH22	1.67	0.58
3:H:435:ILE:HG22	3:H:435:ILE:O	2.03	0.58
2:B:143:TRP:HA	2:B:146:LEU:HD12	1.86	0.57
2:B:97:PRO:HD3	3:C:430:TRP:CZ3	2.40	0.56
2:B:135:GLN:NE2	2:F:103:THR:OG1	2.38	0.56
2:B:7:ARG:NH1	2:B:97:PRO:O	2.29	0.55
2:B:70:ARG:NH2	2:B:72[A]:MET:SD	2.79	0.55
2:F:70:ARG:NH2	2:F:72[A]:MET:SD	2.79	0.55
2:J:70:ARG:NH2	2:J:72[A]:MET:SD	2.79	0.55
2:F:7:ARG:HD3	2:F:63:PRO:HG3	1.89	0.55
3:G:430:TRP:CH2	3:G:434:LYS:HD2	2.41	0.55
2:B:94:LYS:HA	3:C:441:ARG:HH21	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:7:ARG:HD3	2:J:63:PRO:HG3	1.89	0.54
2:B:6:ARG:HB2	3:C:471:ARG:HH21	1.72	0.54
2:B:7:ARG:HD3	2:B:63:PRO:HG3	1.89	0.54
2:J:64:MET:HE3	3:K:433:ARG:HH21	1.72	0.53
1:E:13:PHE:HZ	2:F:55:GLU:HG3	1.72	0.53
2:B:61:GLU:CD	3:C:433:ARG:HH22	2.16	0.52
3:G:408:GLU:OE2	3:G:471:ARG:NH2	2.42	0.52
2:F:76:TYR:HB3	2:F:140:ALA:HA	1.93	0.51
2:J:76:TYR:HB3	2:J:140:ALA:HA	1.93	0.51
3:C:401:LEU:HD11	3:C:460:MET:HE3	1.94	0.50
2:F:6:ARG:CB	3:G:471:ARG:HH22	2.24	0.50
2:B:76:TYR:HB3	2:B:140:ALA:HA	1.93	0.50
3:L:401:LEU:HD11	3:L:460:MET:HE3	1.93	0.50
1:E:85:LYS:HA	1:E:143:TYR:CE2	2.47	0.50
1:A:85:LYS:HA	1:A:143:TYR:CE2	2.47	0.50
3:H:401:LEU:HD11	3:H:460:MET:HE3	1.94	0.50
1:I:85:LYS:HA	1:I:143:TYR:CE2	2.47	0.49
2:J:97:PRO:HD3	3:K:430:TRP:CZ3	2.48	0.49
2:J:64:MET:HE1	3:K:430:TRP:HA	1.95	0.48
3:K:430:TRP:CZ2	3:K:434:LYS:HD2	2.47	0.48
3:H:431:MET:HA	3:H:434:LYS:O	2.13	0.48
2:B:64:MET:CE	3:C:433:ARG:HD2	2.42	0.48
3:G:396:VAL:O	3:G:401:LEU:HG	2.13	0.48
2:F:132:ASN:CG	2:F:135:GLN:HB3	2.38	0.48
3:G:397:LEU:HA	3:G:401:LEU:HD12	1.96	0.48
3:L:431:MET:HA	3:L:434:LYS:O	2.13	0.48
3:C:431:MET:HA	3:C:434:LYS:O	2.13	0.48
2:B:134:ALA:O	2:B:138:GLU:HG3	2.13	0.48
2:J:92:LYS:HG3	2:J:93:ASP:H	1.80	0.46
2:F:64:MET:HE1	3:G:430:TRP:CA	2.45	0.46
2:F:92:LYS:HG3	2:F:93:ASP:H	1.80	0.46
3:K:425:TYR:CG	3:K:479:ARG:HG2	2.51	0.45
2:F:97:PRO:HD3	3:G:430:TRP:CH2	2.52	0.45
2:J:96:SER:O	2:J:99:LEU:HG	2.15	0.45
1:I:7:VAL:HG13	2:J:33:ARG:HD2	1.98	0.45
3:G:425:TYR:CG	3:G:479:ARG:HG2	2.51	0.45
2:B:92:LYS:HG3	2:B:93:ASP:H	1.80	0.45
2:J:64:MET:HG3	3:K:429:GLU:OE1	2.17	0.44
2:B:81:ASP:HA	2:B:123:ASN:OD1	2.18	0.44
2:B:6:ARG:NH2	2:B:10:LYS:HD3	2.33	0.44
2:J:81:ASP:HA	2:J:123:ASN:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:118:ASP:HA	2:F:130:LYS:HE3	2.00	0.44
2:B:64:MET:HE1	3:C:430:TRP:CA	2.21	0.44
1:E:7:VAL:HB	2:F:60:GLU:HG2	1.99	0.44
2:F:81:ASP:HA	2:F:123:ASN:OD1	2.18	0.44
1:I:39:GLU:HG2	2:J:82:LYS:HD3	1.99	0.44
2:B:118:ASP:HA	2:B:130:LYS:HE3	2.00	0.43
2:J:118:ASP:HA	2:J:130:LYS:HE3	2.00	0.43
1:E:53:PRO:HB3	1:E:127:MET:HE2	2.01	0.43
2:F:132:ASN:ND2	3:K:404:ILE:HD11	2.33	0.43
1:A:53:PRO:HB3	1:A:127:MET:HE2	2.01	0.43
2:B:128:GLN:OE1	2:B:135:GLN:HG2	2.19	0.43
3:G:396:VAL:O	3:G:397:LEU:O	2.36	0.43
2:B:67:PRO:HD3	2:B:95:TRP:CH2	2.54	0.43
2:F:6:ARG:CG	3:G:471:ARG:HH22	2.32	0.43
2:F:67:PRO:HD3	2:F:95:TRP:CH2	2.54	0.43
2:J:67:PRO:HD3	2:J:95:TRP:CH2	2.54	0.43
3:G:418:CYS:O	3:G:419:ALA:HB3	2.19	0.42
2:J:54:LEU:HD11	2:J:71:PHE:CE1	2.55	0.42
3:K:418:CYS:O	3:K:419:ALA:HB3	2.19	0.42
1:E:12:ASN:HB3	2:F:70:ARG:HH21	1.84	0.42
1:I:53:PRO:HB3	1:I:127:MET:HE2	2.01	0.42
2:B:54:LEU:HD11	2:B:71:PHE:CE1	2.55	0.42
2:F:54:LEU:HD11	2:F:71:PHE:CE1	2.55	0.42
3:K:400:GLU:HB3	3:L:456:CYS:SG	2.60	0.42
2:F:135:GLN:NE2	2:J:99:LEU:O	2.53	0.42
2:F:77:HIS:HA	2:F:78:PRO:HD3	1.93	0.41
1:A:13:PHE:CZ	2:B:55:GLU:HG3	2.55	0.41
2:F:64:MET:HE3	2:F:64:MET:HB3	1.37	0.41
2:F:64:MET:HE1	3:G:429:GLU:C	2.46	0.40
2:B:64:MET:HE2	2:B:64:MET:HB3	1.80	0.40
2:B:128:GLN:OE1	2:B:135:GLN:CG	2.70	0.40
3:K:460:MET:CE	3:L:460:MET:HE1	2.52	0.40
3:G:460:MET:CE	3:H:460:MET:HE1	2.52	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	140/153 (92%)	140 (100%)	0	0	100	100
1	E	139/153 (91%)	139 (100%)	0	0	100	100
1	I	139/153 (91%)	139 (100%)	0	0	100	100
2	B	148/160 (92%)	139 (94%)	7 (5%)	2 (1%)	9	39
2	F	148/160 (92%)	139 (94%)	7 (5%)	2 (1%)	9	39
2	J	148/160 (92%)	139 (94%)	7 (5%)	2 (1%)	9	39
3	C	90/149 (60%)	85 (94%)	5 (6%)	0	100	100
3	G	137/149 (92%)	132 (96%)	4 (3%)	1 (1%)	18	55
3	H	140/149 (94%)	134 (96%)	6 (4%)	0	100	100
3	K	137/149 (92%)	132 (96%)	4 (3%)	1 (1%)	18	55
3	L	140/149 (94%)	135 (96%)	5 (4%)	0	100	100
All	All	1506/1684 (89%)	1453 (96%)	45 (3%)	8 (0%)	24	63

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	123	ASN
2	B	124	ASP
2	F	123	ASN
2	F	124	ASP
3	G	397	LEU
2	J	123	ASN
2	J	124	ASP
3	K	397	LEU

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	127/135 (94%)	127 (100%)	0	100	100
1	E	127/135 (94%)	127 (100%)	0	100	100
1	I	127/135 (94%)	127 (100%)	0	100	100
2	B	128/135 (95%)	124 (97%)	4 (3%)	35	56
2	F	128/135 (95%)	124 (97%)	4 (3%)	35	56
2	J	128/135 (95%)	126 (98%)	2 (2%)	55	69
3	C	80/140 (57%)	78 (98%)	2 (2%)	42	62
3	G	80/140 (57%)	79 (99%)	1 (1%)	61	72
3	H	80/140 (57%)	77 (96%)	3 (4%)	29	51
3	K	80/140 (57%)	79 (99%)	1 (1%)	61	72
3	L	80/140 (57%)	79 (99%)	1 (1%)	61	72
All	All	1165/1510 (77%)	1147 (98%)	18 (2%)	55	71

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	64	MET
2	B	93	ASP
2	B	128	GLN
2	B	135	GLN
3	C	404	ILE
3	C	460	MET
2	F	93	ASP
2	F	103	THR
2	F	128	GLN
2	F	135	GLN
3	G	429	GLU
3	H	404	ILE
3	H	433	ARG
3	H	460	MET
2	J	93	ASP
2	J	128	GLN
3	K	433	ARG
3	L	460	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	J	128	GLN
2	J	135	GLN

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](#)

Of 10 ligands modelled in this entry, 10 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 [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	139/153 (90%)	1.80	48 (34%) 1 4	108, 231, 265, 282	3 (2%)
1	E	138/153 (90%)	1.56	41 (29%) 1 5	108, 220, 271, 291	3 (2%)
1	I	138/153 (90%)	2.28	68 (49%) 0 2	188, 393, 445, 455	3 (2%)
2	B	148/160 (92%)	1.62	50 (33%) 1 4	96, 217, 286, 318	2 (1%)
2	F	148/160 (92%)	1.63	54 (36%) 1 3	97, 209, 260, 299	2 (1%)
2	J	148/160 (92%)	1.49	42 (28%) 1 5	119, 244, 290, 314	2 (1%)
3	C	92/149 (61%)	1.69	34 (36%) 1 3	227, 244, 285, 304	0
3	G	139/149 (93%)	1.32	27 (19%) 3 8	199, 216, 278, 306	0
3	H	142/149 (95%)	1.48	49 (34%) 1 4	207, 228, 256, 288	0
3	K	139/149 (93%)	1.73	48 (34%) 1 4	256, 295, 359, 371	0
3	L	142/149 (95%)	1.74	52 (36%) 1 3	275, 314, 350, 357	0
All	All	1513/1684 (89%)	1.67	513 (33%) 1 4	96, 241, 382, 455	15 (0%)

All (513) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	48	GLY	9.2
1	A	55	ARG	7.5
1	I	86	ILE	7.4
1	A	129	LYS	7.3
1	A	28	ASP	7.2
1	I	63	TYR	7.1
3	K	350	LEU	6.9
1	I	50	ILE	6.5
1	I	65	LEU	6.1
3	K	354	LEU	6.1
1	A	32[A]	SER	6.1
3	L	349	ALA	6.1

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Mol	Chain	Res	Type	RSRZ
3	K	347	HIS	6.1
2	B	118	ASP	6.1
2	B	117	PRO	6.0
1	A	60	ASN	6.0
3	L	345	GLN	6.0
3	G	447	LYS	5.6
2	B	133	GLU	5.5
3	L	451	LEU	5.4
2	J	145	ARG	5.4
3	H	466	SER	5.3
3	C	400	GLU	5.3
1	A	61	ARG	5.3
2	F	131	THR	5.3
1	E	32[A]	SER	5.2
1	A	54	PRO	5.2
3	G	351	MET	5.1
2	J	150	ASN	5.1
1	I	64[A]	SER	5.1
1	I	122	LEU	5.0
1	I	82	PHE	5.0
2	B	138	GLU	4.9
1	A	139	GLU	4.8
1	I	47	THR	4.8
3	K	345	GLN	4.7
3	K	351	MET	4.7
1	A	50	ILE	4.7
3	K	357	SER	4.7
1	I	32[A]	SER	4.6
3	K	390	LEU	4.6
3	L	456	CYS	4.6
2	B	127	GLU	4.5
3	K	353	GLU	4.5
3	L	419	ALA	4.5
3	L	460	MET	4.5
1	I	49	MET	4.4
1	A	49	MET	4.4
3	K	346	GLU	4.4
2	B	141	ARG	4.4
3	K	386	LYS	4.4
1	E	144	ASN	4.3
1	E	12	ASN	4.3
1	E	89	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	31	VAL	4.3
1	I	88	MET	4.3
3	H	342	PRO	4.3
3	G	347	HIS	4.2
1	E	139	GLU	4.2
3	G	345	GLN	4.2
2	F	118	ASP	4.2
1	I	9	VAL	4.2
2	F	99	LEU	4.2
3	L	466	SER	4.2
3	C	447	LYS	4.2
1	A	75	GLU	4.1
2	B	6	ARG	4.1
2	B	67	PRO	4.1
1	I	83	VAL	4.1
1	E	28	ASP	4.0
2	F	60	GLU	4.0
3	L	452	VAL	4.0
2	J	51	THR	4.0
3	K	436	GLU	4.0
3	K	453	LEU	4.0
2	F	116	ASN	4.0
1	I	54	PRO	4.0
1	A	127	MET	3.9
2	F	121	LEU	3.9
2	J	32	ALA	3.9
1	A	144	ASN	3.9
2	F	150	ASN	3.9
3	K	349	ALA	3.9
3	C	466	SER	3.9
3	H	483	ARG	3.8
3	L	350	LEU	3.8
1	I	51	ILE	3.8
1	I	84	THR	3.8
1	I	71	PRO	3.8
3	H	409	TYR	3.8
2	B	150	ASN	3.8
1	E	31	VAL	3.8
3	G	449	TYR	3.8
2	J	66	ALA	3.8
1	I	91	ILE	3.8
1	A	30	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	49	MET	3.7
1	I	8	LYS	3.7
3	H	472	ARG	3.7
1	I	42	THR	3.7
2	F	87	CYS	3.7
2	J	116	ASN	3.7
1	E	130	GLU	3.6
2	J	76	TYR	3.6
2	B	131	THR	3.6
3	L	375	THR	3.6
3	C	414	VAL	3.6
3	C	393	MET	3.6
2	B	120	PRO	3.5
2	J	146	LEU	3.5
3	H	360	ASP	3.5
3	K	348	TRP	3.5
1	I	12	ASN	3.5
2	J	65	ALA	3.5
1	I	111	ASN	3.5
3	H	447	LYS	3.5
3	G	463	ASN	3.5
3	K	455	ASN	3.5
2	J	129	TRP	3.5
1	A	71	PRO	3.4
1	I	119	LEU	3.4
2	B	145	ARG	3.4
1	A	12	ASN	3.4
3	K	463	ASN	3.4
1	E	30	THR	3.4
3	H	476	ILE	3.4
3	K	461	VAL	3.4
1	E	133	LYS	3.4
3	K	460	MET	3.4
2	F	86	ILE	3.4
1	I	98	VAL	3.3
1	I	142	THR	3.3
3	C	455	ASN	3.3
1	A	41	MET	3.3
3	G	413	ALA	3.3
3	L	400	GLU	3.3
3	L	455	ASN	3.3
1	A	42	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	J	55	GLU	3.2
3	L	371	GLU	3.2
3	L	453	LEU	3.2
3	L	409	TYR	3.2
3	H	369	ASN	3.2
3	K	468	VAL	3.2
3	L	483	ARG	3.2
3	H	366	GLN	3.2
3	C	476	ILE	3.2
3	G	435	ILE	3.2
2	F	27	PRO	3.2
2	J	141	ARG	3.2
3	L	474	VAL	3.2
1	I	68	GLU	3.2
1	E	88	MET	3.2
2	J	121	LEU	3.2
2	F	33	ARG	3.2
3	C	439	ILE	3.2
1	E	10	PRO	3.1
2	J	102	ARG	3.1
3	H	469	LYS	3.1
3	G	433	ARG	3.1
2	B	137	ILE	3.1
1	I	79	SER	3.1
3	G	422	PHE	3.1
3	C	461	VAL	3.1
1	E	24	LYS	3.1
2	F	98	ALA	3.1
1	I	118	VAL	3.1
3	G	441	ARG	3.1
2	J	131	THR	3.1
2	B	32	ALA	3.0
3	K	441	ARG	3.0
2	B	72[A]	MET	3.0
2	B	27	PRO	3.0
2	B	76	TYR	3.0
3	L	372	LEU	3.0
3	L	412	GLU	3.0
1	I	60	ASN	3.0
3	C	401	LEU	3.0
1	A	76	ALA	3.0
1	I	103	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
3	C	409	TYR	3.0
1	I	106	LEU	3.0
1	I	85	LYS	3.0
2	B	130	LYS	3.0
2	J	68	LYS	3.0
3	G	414	VAL	3.0
3	C	411	ILE	2.9
3	G	354	LEU	2.9
3	L	416	LEU	2.9
1	A	52	GLY	2.9
3	L	447	LYS	2.9
3	H	413	ALA	2.9
1	E	86	ILE	2.9
3	K	398	GLU	2.9
3	L	374	GLN	2.9
1	E	29	GLY	2.9
1	I	34	GLY	2.9
3	L	376	LYS	2.9
2	J	120	PRO	2.9
2	F	6	ARG	2.9
3	C	421	SER	2.9
3	L	348	TRP	2.9
1	I	62	ILE	2.9
3	K	362	GLU	2.9
2	J	3	GLY	2.9
2	J	89	ASP	2.9
3	G	355	ASN	2.9
3	K	355	ASN	2.9
3	K	476	ILE	2.8
3	L	465	SER	2.8
3	H	451	LEU	2.8
1	A	6	GLY	2.8
1	E	26	VAL	2.8
1	I	55	ARG	2.8
1	I	123	ARG	2.8
1	I	100	ALA	2.8
1	I	135	PRO	2.8
1	I	138	PRO	2.8
2	B	97	PRO	2.8
1	I	66	LYS	2.8
3	H	442	LYS	2.8
3	C	464	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
3	L	373	GLU	2.8
1	I	90	GLY	2.8
3	H	364	ILE	2.8
3	K	473	ILE	2.8
2	F	34	TYR	2.8
1	E	82	PHE	2.8
2	F	102	ARG	2.8
2	F	124	ASP	2.8
3	G	360	ASP	2.8
3	H	414	VAL	2.8
3	C	410	PHE	2.8
3	C	452	VAL	2.8
3	K	471	ARG	2.8
1	I	17	GLU	2.8
2	F	133	GLU	2.8
2	J	100	GLN	2.8
3	L	377	GLU	2.8
3	H	425	TYR	2.8
3	H	394	ASN	2.8
1	A	62	ILE	2.8
3	L	378	GLU	2.8
1	E	14	ARG	2.8
2	F	137	ILE	2.8
3	K	389	VAL	2.8
1	A	66	LYS	2.8
1	I	59	GLU	2.8
1	A	94	SER	2.8
1	I	120	GLN	2.8
3	L	380	GLU	2.8
2	J	30	SER	2.8
1	A	87	ASN	2.7
3	H	460	MET	2.7
1	I	133	LYS	2.7
2	F	43	GLN	2.7
3	G	350	LEU	2.7
2	F	24	LYS	2.7
3	C	467	GLU	2.7
3	G	346	GLU	2.7
1	A	9	VAL	2.7
3	K	443	ASP	2.7
1	I	72	LYS	2.7
1	A	27	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	366	GLN	2.7
1	E	55	ARG	2.7
3	L	391	SER	2.7
1	A	89	ASN	2.7
3	K	369	ASN	2.7
2	J	117	PRO	2.7
3	K	380	GLU	2.7
2	B	33	ARG	2.7
3	L	454	ASP	2.7
1	E	66	LYS	2.7
1	I	7	VAL	2.7
2	J	60	GLU	2.7
2	B	121	LEU	2.7
3	L	367	ALA	2.7
2	B	62	TYR	2.7
1	A	51	ILE	2.7
2	B	132	ASN	2.7
3	C	394	ASN	2.7
3	G	356	ARG	2.7
3	L	415	THR	2.7
3	H	367	ALA	2.6
3	H	410	PHE	2.7
2	B	61	GLU	2.6
2	F	135	GLN	2.6
3	G	404	ILE	2.6
3	H	395	ASP	2.6
3	K	457	ILE	2.6
1	E	41	MET	2.6
3	K	382	MET	2.6
1	I	87	ASN	2.6
2	J	13	GLN	2.6
2	B	30	SER	2.6
3	K	391	SER	2.6
2	F	44	ASP	2.6
2	F	61	GLU	2.6
3	H	344	PHE	2.6
2	J	4	LEU	2.6
2	J	70	ARG	2.6
2	F	28	ASP	2.6
1	E	18	GLU	2.6
2	B	149	MET	2.6
1	A	88	MET	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	87	CYS	2.6
2	F	127	GLU	2.6
3	C	451	LEU	2.6
3	K	366	GLN	2.6
2	J	99	LEU	2.5
1	A	130	GLU	2.5
3	L	384	ALA	2.5
1	E	7	VAL	2.5
1	I	21	GLU	2.5
1	I	23	GLN	2.5
1	I	77	PRO	2.5
3	C	462	ASN	2.5
2	F	7	ARG	2.5
2	B	135	GLN	2.5
2	B	123	ASN	2.5
3	L	404	ILE	2.5
1	A	83	VAL	2.5
2	F	17	ALA	2.5
1	E	121	GLU	2.5
1	I	116	LYS	2.5
2	B	86	ILE	2.5
1	A	70	GLY	2.5
3	H	456	CYS	2.5
3	C	441	ARG	2.5
1	I	33	TRP	2.5
3	H	398	GLU	2.4
3	K	352	GLU	2.4
2	B	46	PRO	2.4
1	A	126	MET	2.4
3	L	395	ASP	2.4
1	I	89	ASN	2.4
2	B	98	ALA	2.4
3	H	392	HIS	2.4
3	C	404	ILE	2.4
3	G	366	GLN	2.4
3	L	467	GLU	2.4
3	C	438	PRO	2.4
1	E	27	GLY	2.4
2	J	24	LYS	2.4
3	K	447	LYS	2.4
2	B	126	ALA	2.4
3	L	365	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	J	107	SER	2.4
2	F	10	LYS	2.4
3	H	449	TYR	2.4
1	A	124	ARG	2.4
2	B	128	GLN	2.4
2	F	14	ARG	2.4
3	H	371	GLU	2.4
3	H	357	SER	2.4
3	G	419	ALA	2.4
2	J	36	HIS	2.4
3	H	412	GLU	2.4
3	K	459	LYS	2.4
2	F	4	LEU	2.4
1	I	140	GLY	2.4
1	A	11	ARG	2.4
2	J	6	ARG	2.4
1	I	108	LYS	2.4
2	F	91	LEU	2.4
3	L	413	ALA	2.4
2	F	90	ILE	2.4
3	L	358	LYS	2.4
2	F	145	ARG	2.3
1	A	34	GLY	2.3
3	L	457	ILE	2.3
1	E	9	VAL	2.3
3	H	465	SER	2.3
3	H	471	ARG	2.3
2	B	58	LEU	2.3
2	B	36	HIS	2.3
1	I	11	ARG	2.3
3	L	450	SER	2.3
1	A	77	PRO	2.3
1	I	131	ASN	2.3
2	B	116	ASN	2.3
2	F	100	GLN	2.3
2	F	138	GLU	2.3
3	H	345	GLN	2.3
3	H	455	ASN	2.3
3	L	368	LYS	2.3
1	A	142	THR	2.3
1	E	132	MET	2.3
1	A	48	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	67	VAL	2.3
1	E	20	GLU	2.3
2	B	92	LYS	2.3
3	L	471	ARG	2.3
1	I	52	GLY	2.3
3	C	413	ALA	2.3
2	F	83	LEU	2.3
3	H	468	VAL	2.3
3	H	467	GLU	2.3
3	L	369	ASN	2.3
2	F	30	SER	2.3
1	I	26	VAL	2.3
2	F	58	LEU	2.3
3	C	460	MET	2.3
3	H	463	ASN	2.2
2	F	71	PHE	2.2
3	C	422	PHE	2.2
2	J	53	LYS	2.2
3	G	359	LYS	2.2
1	E	123	ARG	2.2
1	E	57	ASN	2.2
1	I	24	LYS	2.2
3	C	469	LYS	2.2
1	E	25	GLY	2.2
2	B	90	ILE	2.2
2	F	57	PHE	2.2
3	C	470	GLU	2.2
3	L	470	GLU	2.2
3	H	405	ILE	2.2
3	H	459	LYS	2.2
2	B	88	LEU	2.2
1	I	81	ARG	2.2
2	B	59	PRO	2.2
2	F	117	PRO	2.2
2	J	72[A]	MET	2.2
3	H	355	ASN	2.2
3	H	441	ARG	2.2
2	F	9	ILE	2.2
1	A	133	LYS	2.2
2	F	13	GLN	2.2
2	F	69	VAL	2.2
1	A	29	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	J	136	ALA	2.2
1	E	79	SER	2.2
3	H	406	CYS	2.2
3	H	445	LYS	2.2
2	J	147	TYR	2.2
3	G	352	GLU	2.2
2	B	49	GLY	2.2
2	F	115	PRO	2.2
3	G	394	ASN	2.2
3	G	434	LYS	2.1
3	L	417	ASN	2.1
2	F	12	THR	2.1
2	J	69	VAL	2.1
3	G	383	GLN	2.1
1	E	36	GLU	2.1
1	E	90	GLY	2.1
2	F	32	ALA	2.1
1	A	35	LEU	2.1
3	H	404	ILE	2.1
3	K	401	LEU	2.1
3	K	415	THR	2.1
3	K	448	THR	2.1
2	B	107	SER	2.1
3	K	412	GLU	2.1
1	I	137	PRO	2.1
2	J	9	ILE	2.1
2	J	130	LYS	2.1
2	F	3	GLY	2.1
2	F	113	SER	2.1
1	A	72	LYS	2.1
2	F	8	ILE	2.1
2	J	67	PRO	2.1
3	G	439	ILE	2.1
3	K	474	VAL	2.1
3	C	471	ARG	2.1
3	K	428	ASN	2.1
3	H	481	ALA	2.1
1	E	13	PHE	2.1
3	C	457	ILE	2.1
3	L	388	GLU	2.1
1	I	41	MET	2.1
2	F	31	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
3	C	434	LYS	2.1
3	C	463	ASN	2.1
3	L	347	HIS	2.1
1	I	70	GLY	2.1
3	K	451	LEU	2.1
1	E	127	MET	2.1
3	H	433	ARG	2.1
3	C	456	CYS	2.1
2	B	104	VAL	2.1
1	E	125	LEU	2.0
3	H	454	ASP	2.0
3	C	418	CYS	2.0
1	E	42	THR	2.0
2	F	128	GLN	2.0
3	K	385	GLN	2.0
3	H	470	GLU	2.0
1	A	116	LYS	2.0
1	E	16	LEU	2.0
3	K	464	LEU	2.0
2	B	134	ALA	2.0
3	H	363	ALA	2.0
2	F	79	ASN	2.0
2	F	123	ASN	2.0
3	L	402	GLN	2.0
3	K	414	VAL	2.0
1	I	127	MET	2.0
3	K	470	GLU	2.0
2	J	74[A]	LYS	2.0
3	L	469	LYS	2.0
1	E	62	ILE	2.0
2	B	3	GLY	2.0
2	B	89	ASP	2.0
2	B	124	ASP	2.0
1	A	123	ARG	2.0
2	B	14	ARG	2.0
1	I	134	LEU	2.0
2	B	91	LEU	2.0
2	J	61	GLU	2.0
2	J	91	LEU	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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($\text{\AA}^2$)	Q<0.9
4	ZN	C	501	1/1	0.95	0.09	193,193,193,193	0
4	ZN	C	502	1/1	0.96	0.07	193,193,193,193	0
4	ZN	K	502	1/1	0.97	0.06	203,203,203,203	0
4	ZN	L	501	1/1	0.97	0.10	206,206,206,206	0
4	ZN	H	502	1/1	0.98	0.05	195,195,195,195	0
4	ZN	K	501	1/1	0.98	0.06	203,203,203,203	0
4	ZN	L	502	1/1	0.98	0.04	206,206,206,206	0
4	ZN	G	502	1/1	0.99	0.10	187,187,187,187	0
4	ZN	G	501	1/1	0.99	0.07	187,187,187,187	0
4	ZN	H	501	1/1	1.00	0.02	195,195,195,195	0

6.5 Other polymers [i](#)

There are no such residues in this entry.