



Full wwPDB X-ray Structure Validation Report ⓘ

May 3, 2016 – 04:54 PM EDT

PDB ID : 4WHV
Title : E3 ubiquitin-protein ligase RNF8 in complex with Ubiquitin-conjugating enzyme E2 N and Polyubiquitin-B
Authors : Hodge, C.D.; Edwards, R.A.; Glover, J.N.M.
Deposited on : 2014-09-23
Resolution : 8.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027457

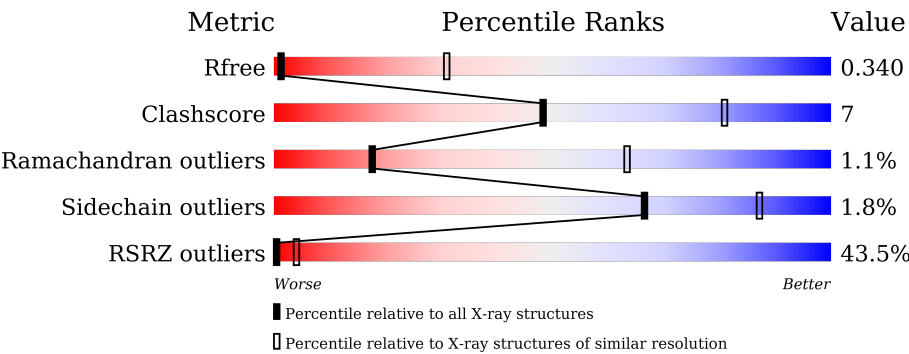
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 8.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1015 (11.50-3.66)
Clashscore	102246	1064 (11.50-3.70)
Ramachandran outliers	100387	1036 (11.50-3.66)
Sidechain outliers	100360	1006 (11.50-3.66)
RSRZ outliers	91569	1014 (11.50-3.66)

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	B	160	<div><div>41%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>76%13%•8%</div></div>
1	E	160	<div><div>43%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>74%15%•8%</div></div>
1	H	160	<div><div>51%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>77%13%•8%</div></div>
1	K	160	<div><div>47%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>79%10%•8%</div></div>
2	C	149	<div><div>36%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>79%11%••9%</div></div>
2	D	149	<div><div>36%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>81%12%•7%</div></div>

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Mol	Chain	Length	Quality of chain
2	I	149	<div><div></div><div>14%56%10%32%</div><div></div></div>
2	J	149	<div><div></div><div>23%58%9%32%</div><div></div></div>
3	A	83	<div><div></div><div>36%81%5%14%</div><div></div></div>
3	F	83	<div><div></div><div>33%76%10%14%</div><div></div></div>
3	G	83	<div><div></div><div>42%83%14%</div><div></div></div>
3	L	83	<div><div></div><div>51%75%11%14%</div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9620 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 N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	147	Total	C	N	O	S	0	0	0
			1123	723	189	209	2			
1	E	147	Total	C	N	O	S	0	0	0
			1123	723	189	209	2			
1	H	147	Total	C	N	O	S	0	0	0
			1123	723	189	209	2			
1	K	147	Total	C	N	O	S	0	0	0
			1123	723	189	209	2			

There are 36 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
B	87	LYS	CYS	engineered mutation	UNP P61088
E	-7	GLY	-	expression tag	UNP P61088
E	-6	PRO	-	expression tag	UNP P61088
E	-5	LEU	-	expression tag	UNP P61088
E	-4	GLY	-	expression tag	UNP P61088
E	-3	SER	-	expression tag	UNP P61088
E	-2	PRO	-	expression tag	UNP P61088
E	-1	GLU	-	expression tag	UNP P61088
E	0	PHE	-	expression tag	UNP P61088
E	87	LYS	CYS	engineered mutation	UNP P61088
H	-7	GLY	-	expression tag	UNP P61088
H	-6	PRO	-	expression tag	UNP P61088
H	-5	LEU	-	expression tag	UNP P61088

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	GLY	-	expression tag	UNP P61088
H	-3	SER	-	expression tag	UNP P61088
H	-2	PRO	-	expression tag	UNP P61088
H	-1	GLU	-	expression tag	UNP P61088
H	0	PHE	-	expression tag	UNP P61088
H	87	LYS	CYS	engineered mutation	UNP P61088
K	-7	GLY	-	expression tag	UNP P61088
K	-6	PRO	-	expression tag	UNP P61088
K	-5	LEU	-	expression tag	UNP P61088
K	-4	GLY	-	expression tag	UNP P61088
K	-3	SER	-	expression tag	UNP P61088
K	-2	PRO	-	expression tag	UNP P61088
K	-1	GLU	-	expression tag	UNP P61088
K	0	PHE	-	expression tag	UNP P61088
K	87	LYS	CYS	engineered mutation	UNP P61088

- Molecule 2 is a protein called E3 ubiquitin-protein ligase RNF8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	136	Total	C	N	O	S	0	0	0
			916	563	166	177	10			
2	D	139	Total	C	N	O	S	0	0	0
			930	571	169	180	10			
2	I	101	Total	C	N	O	S	0	0	0
			741	458	131	142	10			
2	J	101	Total	C	N	O	S	0	0	0
			741	458	131	142	10			

There are 32 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
D	337	GLY	-	expression tag	UNP O76064
D	338	PRO	-	expression tag	UNP O76064
D	339	LEU	-	expression tag	UNP O76064

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

- Molecule 3 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	71	Total	C	N	O	S	0	0	0
			448	292	74	81	1			
3	F	71	Total	C	N	O	S	0	0	0
			448	292	74	81	1			
3	G	71	Total	C	N	O	S	0	0	0
			448	292	74	81	1			
3	L	71	Total	C	N	O	S	0	0	0
			448	292	74	81	1			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP P0CG47
A	-5	PRO	-	expression tag	UNP P0CG47
A	-4	GLY	-	expression tag	UNP P0CG47
A	-3	TYR	-	expression tag	UNP P0CG47
A	-2	GLN	-	expression tag	UNP P0CG47

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASP	-	expression tag	UNP P0CG47
A	0	PRO	-	expression tag	UNP P0CG47
F	-6	GLY	-	expression tag	UNP P0CG47
F	-5	PRO	-	expression tag	UNP P0CG47
F	-4	GLY	-	expression tag	UNP P0CG47
F	-3	TYR	-	expression tag	UNP P0CG47
F	-2	GLN	-	expression tag	UNP P0CG47
F	-1	ASP	-	expression tag	UNP P0CG47
F	0	PRO	-	expression tag	UNP P0CG47
G	-6	GLY	-	expression tag	UNP P0CG47
G	-5	PRO	-	expression tag	UNP P0CG47
G	-4	GLY	-	expression tag	UNP P0CG47
G	-3	TYR	-	expression tag	UNP P0CG47
G	-2	GLN	-	expression tag	UNP P0CG47
G	-1	ASP	-	expression tag	UNP P0CG47
G	0	PRO	-	expression tag	UNP P0CG47
L	-6	GLY	-	expression tag	UNP P0CG47
L	-5	PRO	-	expression tag	UNP P0CG47
L	-4	GLY	-	expression tag	UNP P0CG47
L	-3	TYR	-	expression tag	UNP P0CG47
L	-2	GLN	-	expression tag	UNP P0CG47
L	-1	ASP	-	expression tag	UNP P0CG47
L	0	PRO	-	expression tag	UNP P0CG47

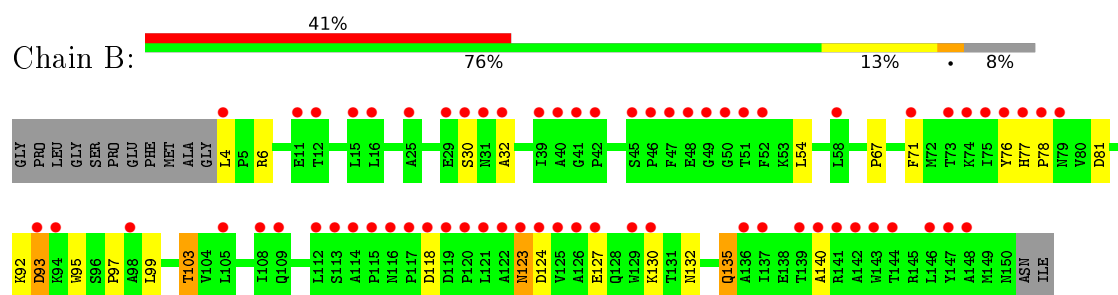
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

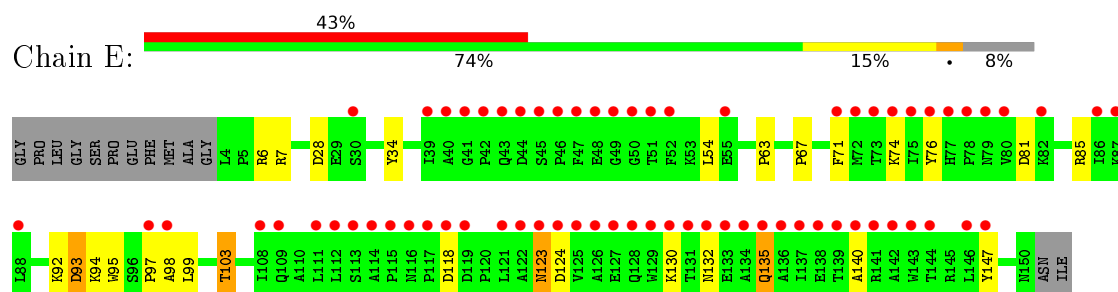
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

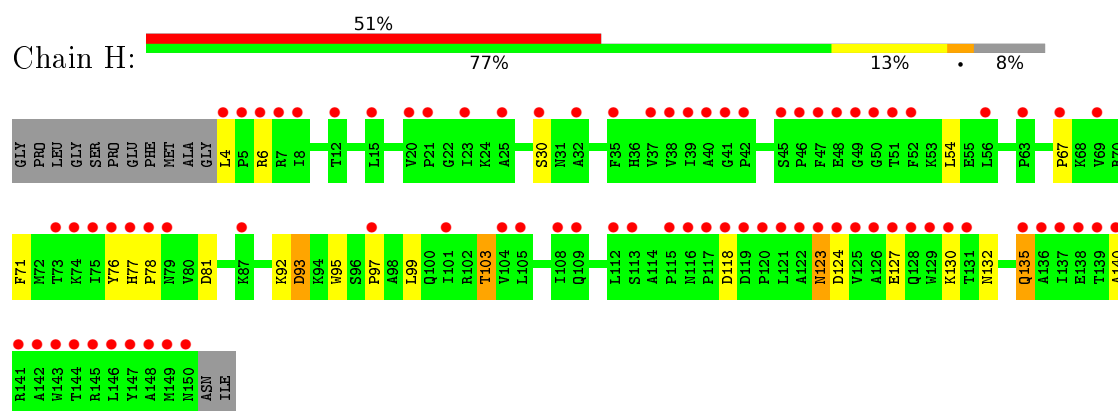
- Molecule 1: Ubiquitin-conjugating enzyme E2 N



- Molecule 1: Ubiquitin-conjugating enzyme E2 N

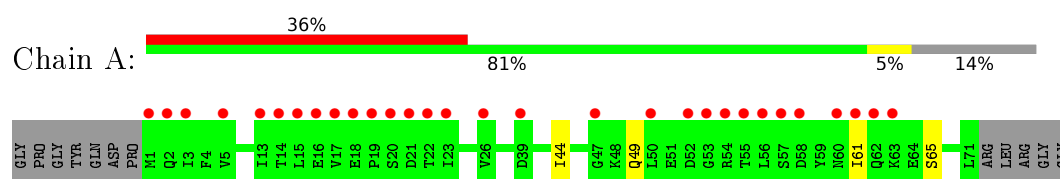


- Molecule 1: Ubiquitin-conjugating enzyme E2 N

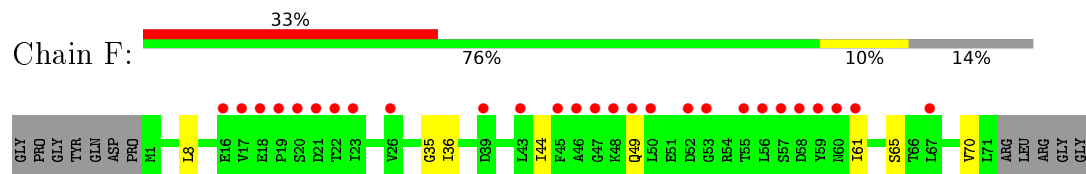


- Molecule 1: Ubiquitin-conjugating enzyme E2 N

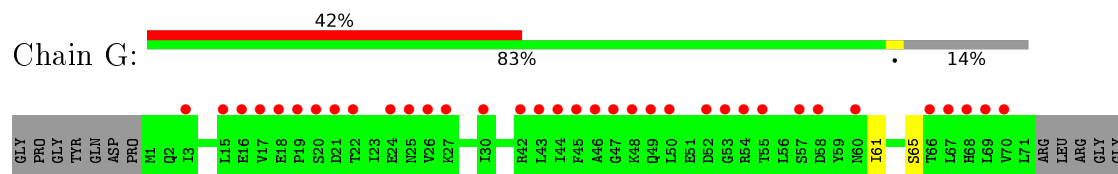




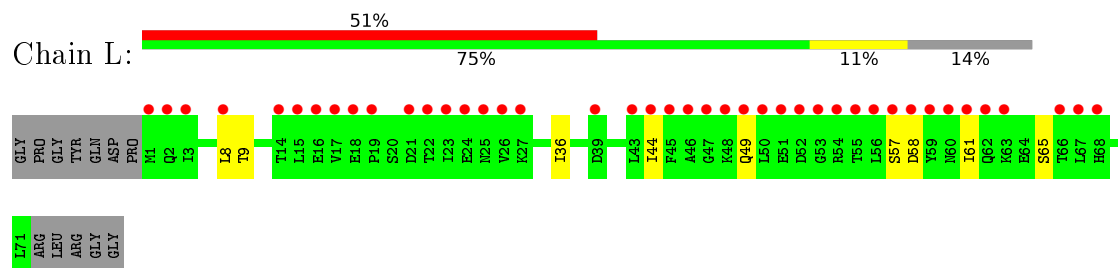
- Molecule 3: Polyubiquitin-B



- Molecule 3: Polyubiquitin-B



- Molecule 3: Polyubiquitin-B



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	341.38Å 341.38Å 113.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.27 – 8.30 49.27 – 8.21	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.27-8.30) 99.8 (49.27-8.21)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.65 (at 8.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.329 , 0.337 0.337 , 0.340	Depositor DCC
R_{free} test set	183 reflections (4.63%)	DCC
Wilson B-factor (Å ²)	468.4	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 824.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.67	EDS
Total number of atoms	9620	wwPDB-VP
Average B, all atoms (Å ²)	522.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	B	0.27	0/1151	0.48	0/1575
1	E	0.27	0/1151	0.48	0/1575
1	H	0.27	0/1151	0.48	0/1575
1	K	0.27	0/1151	0.48	0/1575
2	C	0.48	0/922	0.68	0/1255
2	D	0.48	0/936	0.65	0/1274
2	I	0.49	0/747	0.63	0/1010
2	J	0.49	0/747	0.60	0/1010
3	A	0.37	0/452	0.55	0/624
3	F	0.37	0/452	0.55	0/624
3	G	0.37	0/452	0.55	0/624
3	L	0.37	0/452	0.55	0/624
All	All	0.38	0/9764	0.56	0/13345

There are no bond length outliers.

There are no bond angle outliers.

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	B	1123	0	1090	12	3

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1123	0	1090	32	8
1	H	1123	0	1090	13	3
1	K	1123	0	1090	18	0
2	C	916	0	747	19	0
2	D	930	0	751	39	0
2	I	741	0	668	18	0
2	J	741	0	668	16	0
3	A	448	0	394	2	0
3	F	448	0	394	10	0
3	G	448	0	394	1	0
3	L	448	0	394	10	6
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
All	All	9620	0	8770	134	19

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (134) 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:K:98:ALA:O	3:L:9:THR:HA	1.22	1.27
2:D:438:PRO:O	1:E:98:ALA:HB3	1.49	1.13
2:D:408:GLU:OE2	1:E:6:ARG:CB	2.01	1.08
1:K:98:ALA:O	3:L:9:THR:CA	2.03	1.05
2:C:446:SER:HA	2:I:445:LYS:O	1.58	1.04
2:D:407:SER:OG	1:E:7:ARG:HA	1.62	1.00
1:H:99:LEU:O	1:H:103:THR:OG1	1.91	0.89
1:E:99:LEU:O	1:E:103:THR:OG1	1.91	0.89
1:K:99:LEU:O	1:K:103:THR:OG1	1.91	0.87
1:B:99:LEU:O	1:B:103:THR:OG1	1.91	0.87
2:C:451:LEU:HD11	3:F:35:GLY:HA3	1.56	0.87
2:I:400:GLU:O	2:I:402:GLN:N	2.07	0.86
2:C:400:GLU:O	2:C:402:GLN:N	2.07	0.86
2:D:407:SER:CB	1:E:7:ARG:HA	2.05	0.85
1:B:6:ARG:CB	2:C:471:ARG:HH22	1.89	0.84
1:K:99:LEU:HA	3:L:8:LEU:O	1.76	0.84
2:J:407:SER:OG	1:K:7:ARG:CB	2.25	0.84
1:H:6:ARG:CB	2:I:408:GLU:OE2	2.27	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:438:PRO:C	1:E:98:ALA:CB	2.49	0.81
2:D:438:PRO:C	1:E:98:ALA:HB3	2.02	0.80
2:D:438:PRO:HB2	1:E:98:ALA:HB2	1.69	0.74
2:C:445:LYS:O	2:I:446:SER:HA	1.88	0.73
2:D:438:PRO:O	1:E:98:ALA:CB	2.35	0.73
1:H:6:ARG:CB	2:I:471:ARG:HH22	2.06	0.69
2:J:397:LEU:O	2:J:409:TYR:OH	2.05	0.69
2:C:445:LYS:O	2:I:446:SER:CB	2.41	0.68
2:D:407:SER:HB2	1:E:7:ARG:HA	1.77	0.66
2:C:432:LYS:O	2:I:432:LYS:HA	1.96	0.66
2:D:438:PRO:CB	1:E:98:ALA:HB2	2.24	0.65
1:H:97:PRO:CB	2:I:405:ILE:HG12	2.26	0.65
2:C:459:LYS:NZ	2:D:400:GLU:OE2	2.29	0.63
2:D:438:PRO:C	1:E:98:ALA:HB2	2.19	0.62
2:D:434:LYS:HE2	1:E:95:TRP:O	1.99	0.62
2:D:414:VAL:HG21	2:D:427:ILE:HG21	1.81	0.61
2:I:459:LYS:NZ	2:J:400:GLU:OE2	2.29	0.61
2:J:414:VAL:HG21	2:J:427:ILE:HG21	1.81	0.61
1:E:103:THR:HG23	3:F:70:VAL:HG12	1.83	0.60
2:J:435:ILE:O	2:J:435:ILE:HG22	2.03	0.59
2:D:435:ILE:HG22	2:D:435:ILE:O	2.03	0.58
2:D:434:LYS:HE2	2:D:441:ARG:HH22	1.67	0.58
1:K:99:LEU:CA	3:L:8:LEU:O	2.49	0.58
2:D:441:ARG:HH12	1:E:95:TRP:C	2.03	0.58
2:J:440:CYS:HA	3:L:36:ILE:HG12	1.86	0.58
2:J:434:LYS:HE2	2:J:441:ARG:HH22	1.67	0.57
1:E:103:THR:CG2	3:F:70:VAL:HG12	2.35	0.56
2:J:401:LEU:O	2:J:409:TYR:HA	2.06	0.56
1:B:6:ARG:CB	2:C:471:ARG:NH2	2.65	0.56
2:D:407:SER:OG	1:E:7:ARG:CA	2.46	0.56
2:C:445:LYS:O	2:I:446:SER:CA	2.52	0.55
2:C:396:VAL:O	2:C:400:GLU:HB2	2.07	0.55
2:I:396:VAL:O	2:I:400:GLU:HB2	2.07	0.55
2:J:441:ARG:NH1	1:K:95:TRP:O	2.40	0.55
2:D:405:ILE:HG23	1:E:63:PRO:HG2	1.88	0.55
2:D:401:LEU:O	2:D:409:TYR:HA	2.06	0.55
2:D:408:GLU:CD	1:E:6:ARG:CB	2.74	0.54
2:C:401:LEU:O	2:C:409:TYR:HA	2.08	0.54
2:D:439:ILE:HG23	3:F:8:LEU:HD12	1.91	0.53
2:I:408:GLU:OE2	2:I:471:ARG:NH2	2.42	0.52
2:D:439:ILE:HG22	3:F:36:ILE:HD11	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:401:LEU:O	2:I:409:TYR:HA	2.08	0.52
2:C:408:GLU:OE2	2:C:471:ARG:NH2	2.42	0.52
2:J:397:LEU:O	2:J:398:GLU:HG3	2.10	0.52
2:D:439:ILE:O	3:F:8:LEU:HD11	2.10	0.51
1:H:76:TYR:HB3	1:H:140:ALA:HA	1.93	0.51
2:D:397:LEU:O	2:D:398:GLU:HG3	2.10	0.51
2:J:401:LEU:HD11	2:J:460:MET:HE3	1.92	0.51
2:D:434:LYS:CE	1:E:95:TRP:O	2.59	0.50
2:J:401:LEU:HD22	2:J:457:ILE:CG1	2.42	0.50
1:K:76:TYR:HB3	1:K:140:ALA:HA	1.93	0.50
1:B:76:TYR:HB3	1:B:140:ALA:HA	1.93	0.50
2:D:401:LEU:HD22	2:D:457:ILE:CG1	2.41	0.50
1:E:76:TYR:HB3	1:E:140:ALA:HA	1.93	0.50
2:J:431:MET:HA	2:J:434:LYS:O	2.13	0.49
2:D:407:SER:HB2	1:E:7:ARG:CA	2.42	0.48
2:D:431:MET:HA	2:D:434:LYS:O	2.13	0.48
1:B:97:PRO:CB	2:C:405:ILE:HG12	2.42	0.48
2:D:434:LYS:HD2	1:E:95:TRP:O	2.13	0.47
2:D:440:CYS:HB3	3:F:36:ILE:HG12	1.97	0.47
2:D:397:LEU:O	2:D:409:TYR:OH	2.05	0.46
2:C:425:TYR:CG	2:C:479:ARG:HG2	2.51	0.46
1:H:92:LYS:HG3	1:H:93:ASP:H	1.80	0.46
2:I:425:TYR:CG	2:I:479:ARG:HG2	2.51	0.46
1:E:92:LYS:HG3	1:E:93:ASP:H	1.80	0.46
1:K:92:LYS:HG3	1:K:93:ASP:H	1.80	0.46
1:K:99:LEU:O	3:L:8:LEU:O	2.34	0.45
1:B:92:LYS:HG3	1:B:93:ASP:H	1.80	0.44
1:H:81:ASP:HA	1:H:123:ASN:OD1	2.18	0.44
1:E:118:ASP:HA	1:E:130:LYS:HE3	2.00	0.44
1:K:132:ASN:CG	1:K:135:GLN:HB3	2.38	0.44
1:K:81:ASP:HA	1:K:123:ASN:OD1	2.18	0.44
1:H:118:ASP:HA	1:H:130:LYS:HE3	2.00	0.44
1:B:118:ASP:HA	1:B:130:LYS:HE3	2.00	0.44
1:B:81:ASP:HA	1:B:123:ASN:OD1	2.18	0.44
2:C:396:VAL:HA	2:C:400:GLU:HG3	2.00	0.44
2:D:441:ARG:NH2	1:E:94:LYS:C	2.71	0.44
1:E:132:ASN:CG	1:E:135:GLN:HB3	2.38	0.43
2:D:401:LEU:HD11	2:D:460:MET:HE3	1.99	0.43
1:H:132:ASN:CG	1:H:135:GLN:HB3	2.38	0.43
2:C:418:CYS:O	2:C:419:ALA:HB3	2.19	0.43
2:D:398:GLU:HG3	2:D:409:TYR:OH	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:81:ASP:HA	1:E:123:ASN:OD1	2.18	0.43
1:E:67:PRO:HD3	1:E:95:TRP:CH2	2.54	0.43
2:I:396:VAL:HA	2:I:400:GLU:HG3	2.00	0.43
1:K:67:PRO:HD3	1:K:95:TRP:CH2	2.54	0.43
1:H:67:PRO:HD3	1:H:95:TRP:CH2	2.54	0.43
1:B:132:ASN:CG	1:B:135:GLN:HB3	2.38	0.43
1:K:98:ALA:O	3:L:8:LEU:O	2.37	0.43
1:B:67:PRO:HD3	1:B:95:TRP:CH2	2.54	0.43
2:I:418:CYS:O	2:I:419:ALA:HB3	2.19	0.42
2:C:446:SER:CA	2:I:445:LYS:O	2.46	0.42
2:J:398:GLU:HG3	2:J:409:TYR:OH	2.19	0.42
1:K:98:ALA:O	3:L:9:THR:N	2.48	0.42
3:A:61:ILE:HG23	3:A:65:SER:HB2	2.01	0.42
3:G:61:ILE:HG23	3:G:65:SER:HB2	2.01	0.42
2:D:405:ILE:HG12	1:E:97:PRO:CB	2.50	0.42
1:E:54:LEU:HD11	1:E:71:PHE:CE1	2.55	0.42
1:H:6:ARG:CB	2:I:471:ARG:NH2	2.78	0.42
1:B:54:LEU:HD11	1:B:71:PHE:CE1	2.55	0.42
1:H:77:HIS:HA	1:H:78:PRO:HD3	1.93	0.42
1:K:118:ASP:HA	1:K:130:LYS:HE3	2.00	0.42
3:L:61:ILE:HG23	3:L:65:SER:HB2	2.02	0.42
1:H:54:LEU:HD11	1:H:71:PHE:CE1	2.55	0.42
3:A:44:ILE:HD13	3:A:49:GLN:HA	2.02	0.41
3:F:61:ILE:HG23	3:F:65:SER:HB2	2.01	0.41
1:K:54:LEU:HD11	1:K:71:PHE:CE1	2.55	0.41
3:F:44:ILE:HD13	3:F:49:GLN:HA	2.02	0.41
2:D:407:SER:CB	1:E:7:ARG:CA	2.89	0.41
2:J:401:LEU:HD22	2:J:457:ILE:HG12	2.02	0.41
2:C:400:GLU:C	2:C:402:GLN:N	2.72	0.41
2:D:439:ILE:O	3:F:8:LEU:CD1	2.69	0.41
2:D:401:LEU:HD22	2:D:457:ILE:HG12	2.01	0.40
3:L:44:ILE:HD13	3:L:49:GLN:HA	2.02	0.40
1:B:77:HIS:HA	1:B:78:PRO:HD3	1.93	0.40
2:J:441:ARG:HD3	1:K:96:SER:CB	2.52	0.40

All (19) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:4:LEU:N	1:H:30:SER:O[7_555]	1.16	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:58:ASP:CA	3:L:58:ASP:CA[7_554]	1.24	0.96
1:E:34:TYR:CD2	1:E:74:LYS:NZ[12_554]	1.31	0.89
1:H:4:LEU:N	1:H:30:SER:C[7_555]	1.54	0.66
3:L:57:SER:O	3:L:57:SER:O[7_554]	1.55	0.65
1:E:28:ASP:OD2	1:E:147:TYR:OH[12_554]	1.67	0.53
1:E:34:TYR:CE2	1:E:74:LYS:CD[12_554]	1.67	0.53
3:L:58:ASP:CB	3:L:58:ASP:CB[7_554]	1.69	0.51
1:B:30:SER:O	1:B:32:ALA:CB[7_555]	1.70	0.50
1:B:127:GLU:CG	1:H:127:GLU:CG[7_555]	1.88	0.32
1:E:85:ARG:CD	1:E:85:ARG:CD[12_554]	1.94	0.26
3:L:58:ASP:N	3:L:58:ASP:O[7_554]	2.05	0.15
1:B:4:LEU:CD2	1:B:30:SER:CB[7_555]	2.08	0.12
3:L:58:ASP:CA	3:L:58:ASP:CB[7_554]	2.10	0.10
1:E:34:TYR:CE2	1:E:74:LYS:NZ[12_554]	2.14	0.06
1:E:28:ASP:CG	1:E:147:TYR:OH[12_554]	2.15	0.05
1:E:34:TYR:CE2	1:E:74:LYS:CE[12_554]	2.15	0.05
1:E:34:TYR:CG	1:E:74:LYS:NZ[12_554]	2.16	0.04
3:L:58:ASP:CA	3:L:58:ASP:C[7_554]	2.19	0.01

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	B	145/160 (91%)	136 (94%)	7 (5%)	2 (1%)	14	58
1	E	145/160 (91%)	136 (94%)	7 (5%)	2 (1%)	14	58
1	H	145/160 (91%)	136 (94%)	7 (5%)	2 (1%)	14	58
1	K	145/160 (91%)	136 (94%)	7 (5%)	2 (1%)	14	58
2	C	134/149 (90%)	128 (96%)	4 (3%)	2 (2%)	13	57
2	D	137/149 (92%)	131 (96%)	5 (4%)	1 (1%)	26	71
2	I	99/149 (66%)	93 (94%)	4 (4%)	2 (2%)	9	51
2	J	99/149 (66%)	94 (95%)	4 (4%)	1 (1%)	19	65

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	69/83 (83%)	68 (99%)	1 (1%)	0	100	100
3	F	69/83 (83%)	68 (99%)	1 (1%)	0	100	100
3	G	69/83 (83%)	68 (99%)	1 (1%)	0	100	100
3	L	69/83 (83%)	68 (99%)	1 (1%)	0	100	100
All	All	1325/1568 (84%)	1262 (95%)	49 (4%)	14 (1%)	17	63

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	123	ASN
1	B	124	ASP
2	C	401	LEU
1	E	123	ASN
1	E	124	ASP
1	H	123	ASN
1	H	124	ASP
2	I	401	LEU
1	K	123	ASN
1	K	124	ASP
2	D	398	GLU
2	J	398	GLU
2	I	400	GLU
2	C	400	GLU

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	B	113/135 (84%)	110 (97%)	3 (3%)	52	79
1	E	113/135 (84%)	110 (97%)	3 (3%)	52	79
1	H	113/135 (84%)	110 (97%)	3 (3%)	52	79
1	K	113/135 (84%)	110 (97%)	3 (3%)	52	79
2	C	74/140 (53%)	72 (97%)	2 (3%)	52	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	74/140 (53%)	74 (100%)	0	100	100
2	I	74/140 (53%)	72 (97%)	2 (3%)	52	79
2	J	74/140 (53%)	74 (100%)	0	100	100
3	A	33/73 (45%)	33 (100%)	0	100	100
3	F	33/73 (45%)	33 (100%)	0	100	100
3	G	33/73 (45%)	33 (100%)	0	100	100
3	L	33/73 (45%)	33 (100%)	0	100	100
All	All	880/1392 (63%)	864 (98%)	16 (2%)	66	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	93	ASP
1	B	103	THR
1	B	135	GLN
2	C	401	LEU
2	C	429	GLU
1	E	93	ASP
1	E	103	THR
1	E	135	GLN
1	H	93	ASP
1	H	103	THR
1	H	135	GLN
2	I	401	LEU
2	I	429	GLU
1	K	93	ASP
1	K	103	THR
1	K	135	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

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](#)

Of 8 ligands modelled in this entry, 8 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	B	147/160 (91%)	2.32	66 (44%) 0 4	484, 536, 566, 570	0
1	E	147/160 (91%)	2.94	69 (46%) 0 4	501, 515, 526, 531	0
1	H	147/160 (91%)	2.93	81 (55%) 0 3	498, 539, 553, 556	0
1	K	147/160 (91%)	2.41	75 (51%) 0 4	519, 523, 525, 526	0
2	C	136/149 (91%)	2.02	53 (38%) 0 4	457, 498, 560, 569	0
2	D	139/149 (93%)	2.10	53 (38%) 0 4	439, 547, 599, 608	0
2	I	101/149 (67%)	1.48	21 (20%) 1 7	459, 496, 537, 552	0
2	J	101/149 (67%)	1.65	35 (34%) 0 4	479, 493, 509, 516	0
3	A	71/83 (85%)	1.97	30 (42%) 0 4	544, 554, 561, 564	0
3	F	71/83 (85%)	1.63	27 (38%) 0 4	503, 518, 529, 533	0
3	G	71/83 (85%)	2.20	35 (49%) 0 4	530, 539, 547, 548	0
3	L	71/83 (85%)	2.86	42 (59%) 0 3	547, 550, 554, 556	0
All	All	1349/1568 (86%)	2.27	587 (43%) 0 4	439, 524, 562, 608	0

All (587) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	122	ALA	12.2
1	K	139	THR	12.2
1	E	77	HIS	11.4
1	H	124	ASP	11.3
1	K	142	ALA	10.8
1	E	48	GLU	10.5
1	E	47	PHE	10.4
1	H	117	PRO	9.9
1	E	46	PRO	9.9
1	E	41	GLY	9.9
1	E	129	TRP	9.9

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Mol	Chain	Res	Type	RSRZ
1	E	42	PRO	9.8
1	E	45	SER	9.6
1	H	142	ALA	9.6
1	H	139	THR	9.6
2	I	380	GLU	9.5
2	C	375	THR	9.5
3	L	48	LYS	9.2
3	L	17	VAL	9.2
2	D	368	LYS	9.1
1	E	78	PRO	9.1
2	D	372	LEU	8.9
1	B	124	ASP	8.8
2	D	369	ASN	8.8
1	K	75	ILE	8.7
1	E	115	PRO	8.6
1	E	75	ILE	8.5
1	K	143	TRP	8.5
2	D	375	THR	8.4
1	K	76	TYR	8.3
1	H	123	ASN	8.2
1	E	125	VAL	8.2
1	E	136	ALA	8.1
3	L	45	PHE	8.1
2	C	379	LYS	8.0
1	K	77	HIS	7.9
1	H	51	THR	7.9
2	D	378	GLU	7.9
1	H	126	ALA	7.9
2	C	378	GLU	7.8
1	E	76	TYR	7.8
1	B	47	PHE	7.7
1	E	131	THR	7.7
2	I	480	LYS	7.7
1	E	40	ALA	7.7
1	E	74	LYS	7.6
2	D	365	ILE	7.5
1	H	119	ASP	7.5
2	C	376	LYS	7.5
1	E	126	ALA	7.5
2	I	382	MET	7.4
2	I	381	LYS	7.4
2	J	381	LYS	7.3

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Mol	Chain	Res	Type	RSRZ
2	D	379	LYS	7.3
1	H	76	TYR	7.2
1	B	76	TYR	7.2
3	G	46	ALA	7.1
3	L	49	GLN	7.1
3	L	46	ALA	7.1
1	B	123	ASN	7.0
1	H	47	PHE	7.0
1	H	150	ASN	7.0
2	J	382	MET	7.0
1	H	121	LEU	7.0
2	D	371	GLU	7.0
1	E	112	LEU	6.9
1	E	133	GLU	6.9
3	L	47	GLY	6.9
3	G	43	LEU	6.8
2	D	374	GLN	6.8
3	G	47	GLY	6.8
1	E	44	ASP	6.8
1	H	125	VAL	6.8
1	H	120	PRO	6.7
1	E	130	LYS	6.7
3	A	17	VAL	6.6
1	H	127	GLU	6.6
1	B	32	ALA	6.6
1	E	117	PRO	6.6
1	H	118	ASP	6.5
1	H	50	GLY	6.5
1	E	132	ASN	6.5
1	E	43	GLN	6.4
2	C	377	GLU	6.4
1	E	128	GLN	6.4
3	L	50	LEU	6.4
1	K	140	ALA	6.3
2	I	383	GLN	6.2
1	B	122	ALA	6.2
1	B	46	PRO	6.1
2	D	382	MET	6.1
1	E	113	SER	6.1
1	B	77	HIS	6.1
2	J	380	GLU	6.1
1	H	143	TRP	6.0

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Mol	Chain	Res	Type	RSRZ
1	K	117	PRO	6.0
2	J	421	SER	6.0
1	B	75	ILE	6.0
2	D	376	LYS	5.9
3	A	15	LEU	5.9
2	D	415	THR	5.9
1	H	41	GLY	5.9
1	K	78	PRO	5.8
3	A	16	GLU	5.8
2	J	385	GLN	5.8
1	H	146	LEU	5.8
1	B	30	SER	5.8
1	B	41	GLY	5.8
2	C	372	LEU	5.8
2	J	438	PRO	5.7
1	B	42	PRO	5.7
3	A	1	MET	5.7
1	K	138	GLU	5.6
2	C	369	ASN	5.6
1	B	112	LEU	5.6
1	K	112	LEU	5.6
1	E	49	GLY	5.6
2	J	415	THR	5.6
2	C	415	THR	5.5
1	H	78	PRO	5.5
2	D	377	GLU	5.5
1	H	40	ALA	5.5
1	B	126	ALA	5.5
2	I	386	LYS	5.5
1	B	40	ALA	5.5
1	H	130	LYS	5.5
1	K	123	ASN	5.5
3	F	47	GLY	5.4
1	K	96	SER	5.4
3	L	60	ASN	5.4
2	J	383	GLN	5.4
1	K	118	ASP	5.4
2	C	368	LYS	5.4
1	K	150	ASN	5.4
3	A	20	SER	5.3
3	L	44	ILE	5.3
1	E	50	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	H	135	GLN	5.2
2	D	373	GLU	5.2
1	B	115	PRO	5.1
1	B	127	GLU	5.1
3	G	68	HIS	5.1
1	B	78	PRO	5.1
2	D	381	LYS	5.1
3	L	67	LEU	5.0
2	D	361	PHE	5.0
1	B	52	PHE	5.0
1	E	123	ASN	5.0
2	J	448	THR	5.0
3	G	67	LEU	5.0
1	B	39	ILE	5.0
1	E	135	GLN	5.0
1	K	47	PHE	5.0
1	K	125	VAL	4.9
1	K	74	LYS	4.9
1	E	73	THR	4.9
3	F	58	ASP	4.9
1	H	148	ALA	4.9
1	E	137	ILE	4.9
3	G	48	LYS	4.9
1	H	52	PHE	4.9
2	C	365	ILE	4.9
3	A	21	ASP	4.8
1	E	127	GLU	4.8
2	C	381	LYS	4.8
1	H	140	ALA	4.8
1	E	141	ARG	4.8
2	D	380	GLU	4.8
3	A	2	GLN	4.8
1	E	52	PHE	4.8
1	B	140	ALA	4.7
2	I	385	GLN	4.7
1	H	144	THR	4.7
1	H	46	PRO	4.7
1	B	120	PRO	4.7
2	C	361	PHE	4.7
2	D	448	THR	4.7
1	E	140	ALA	4.7
1	H	116	ASN	4.7

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Mol	Chain	Res	Type	RSRZ
3	G	53	GLY	4.7
2	C	360	ASP	4.7
1	B	125	VAL	4.7
1	E	124	ASP	4.6
3	L	59	TYR	4.6
2	J	414	VAL	4.6
2	C	357	SER	4.6
1	K	4	LEU	4.6
1	B	139	THR	4.6
1	K	144	THR	4.6
3	A	19	PRO	4.6
2	D	366	GLN	4.6
3	L	52	ASP	4.5
1	H	75	ILE	4.5
3	G	44	ILE	4.5
1	E	134	ALA	4.5
2	C	364	ILE	4.5
2	C	371	GLU	4.5
1	H	129	TRP	4.5
1	H	136	ALA	4.5
2	C	350	LEU	4.5
2	J	480	LYS	4.5
1	K	124	ASP	4.5
2	C	349	ALA	4.5
2	D	362	GLU	4.4
1	B	50	GLY	4.4
1	H	128	GLN	4.4
1	E	143	TRP	4.4
1	H	138	GLU	4.4
1	B	74	LYS	4.4
1	H	49	GLY	4.4
3	A	18	GLU	4.4
3	A	39	ASP	4.4
1	H	112	LEU	4.4
3	L	16	GLU	4.3
2	D	358	LYS	4.3
2	D	386	LYS	4.3
3	F	60	ASN	4.3
1	E	111	LEU	4.3
1	K	122	ALA	4.2
2	C	414	VAL	4.2
1	B	117	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
2	D	342	PRO	4.2
1	E	139	THR	4.2
2	D	461	VAL	4.2
3	G	50	LEU	4.2
3	L	61	ILE	4.2
2	C	380	GLU	4.2
2	D	383	GLN	4.1
1	K	126	ALA	4.1
2	J	441	ARG	4.1
2	C	367	ALA	4.1
1	E	138	GLU	4.1
1	E	114	ALA	4.1
2	J	384	ALA	4.1
2	D	385	GLN	4.1
1	K	93	ASP	4.1
2	C	421	SER	4.1
1	K	147	TYR	4.1
1	K	115	PRO	4.1
1	E	55	GLU	4.1
1	E	116	ASN	4.0
1	K	97	PRO	4.0
1	K	141	ARG	4.0
1	H	115	PRO	4.0
3	F	17	VAL	4.0
2	I	421	SER	4.0
3	F	26	VAL	4.0
1	B	143	TRP	4.0
3	L	43	LEU	4.0
1	H	147	TYR	4.0
2	C	358	LYS	3.9
3	G	17	VAL	3.9
3	G	69	LEU	3.9
3	L	27	LYS	3.9
2	D	367	ALA	3.9
1	K	129	TRP	3.9
1	K	94	LYS	3.8
1	B	118	ASP	3.8
2	C	346	GLU	3.8
2	I	415	THR	3.8
1	B	144	THR	3.8
1	E	79	ASN	3.8
1	B	51	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	K	108	ILE	3.8
2	C	374	GLN	3.8
3	L	23	ILE	3.8
1	H	12	THR	3.8
1	K	145	ARG	3.8
2	I	384	ALA	3.8
2	C	373	GLU	3.8
1	B	109	GLN	3.8
3	L	25	ASN	3.8
1	H	77	HIS	3.8
2	D	364	ILE	3.8
1	K	86	ILE	3.8
1	H	131	THR	3.8
3	A	57	SER	3.7
2	C	447	LYS	3.7
1	H	145	ARG	3.7
1	H	45	SER	3.7
3	A	3	ILE	3.7
1	K	46	PRO	3.7
2	D	370	LYS	3.7
3	G	26	VAL	3.7
1	K	80	VAL	3.7
1	B	113	SER	3.7
3	G	45	PHE	3.7
2	C	366	GLN	3.7
1	B	121	LEU	3.7
2	D	357	SER	3.7
1	K	69	VAL	3.6
3	A	56	LEU	3.6
2	C	480	LYS	3.6
3	A	22	THR	3.6
3	L	18	GLU	3.6
3	L	1	MET	3.6
1	H	39	ILE	3.6
1	B	93	ASP	3.6
3	L	26	VAL	3.6
2	C	359	LYS	3.6
1	E	144	THR	3.5
3	G	21	ASP	3.5
2	C	411	ILE	3.5
3	F	18	GLU	3.5
1	K	135	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	25	ALA	3.5
3	L	39	ASP	3.5
1	B	129	TRP	3.5
1	B	137	ILE	3.5
1	K	79	ASN	3.5
3	F	61	ILE	3.5
2	J	405	ILE	3.5
3	F	50	LEU	3.5
3	G	49	GLN	3.5
3	L	21	ASP	3.5
3	G	25	ASN	3.4
1	B	45	SER	3.4
1	B	73	THR	3.4
1	B	136	ALA	3.4
2	D	421	SER	3.4
3	G	20	SER	3.4
1	B	48	GLU	3.4
2	J	447	LYS	3.4
2	D	460	MET	3.4
3	A	55	THR	3.4
3	L	8	LEU	3.4
1	E	147	TYR	3.4
1	K	148	ALA	3.4
3	F	46	ALA	3.3
2	C	353	GLU	3.3
2	C	356	ARG	3.3
2	J	450	SER	3.3
1	B	141	ARG	3.3
1	K	113	SER	3.3
3	A	58	ASP	3.3
1	B	4	LEU	3.3
1	K	146	LEU	3.3
3	F	48	LYS	3.3
1	E	71	PHE	3.3
2	D	409	TYR	3.3
1	K	98	ALA	3.3
1	B	79	ASN	3.3
1	H	74	LYS	3.3
2	C	370	LYS	3.3
2	C	448	THR	3.2
1	E	51	THR	3.2
3	G	52	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	I	405	ILE	3.2
3	L	62	GLN	3.2
3	L	24	GLU	3.2
2	C	363	ALA	3.2
1	K	88	LEU	3.2
2	I	389	VAL	3.2
1	B	58	LEU	3.2
2	J	446	SER	3.2
1	K	95	TRP	3.2
3	A	5	VAL	3.2
1	H	108	ILE	3.1
1	K	87	LYS	3.1
2	D	438	PRO	3.1
3	L	58	ASP	3.1
1	K	82	LYS	3.1
2	C	354	LEU	3.1
1	E	97	PRO	3.1
3	G	55	THR	3.1
3	L	22	THR	3.1
1	K	136	ALA	3.1
1	H	87	LYS	3.1
3	G	24	GLU	3.1
2	C	345	GLN	3.1
1	B	147	TYR	3.1
3	L	63	LYS	3.1
1	H	137	ILE	3.1
3	A	63	LYS	3.1
1	E	109	GLN	3.1
2	D	479	ARG	3.1
3	A	53	GLY	3.1
1	B	31	ASN	3.1
3	L	56	LEU	3.0
1	H	15	LEU	3.0
3	L	57	SER	3.0
1	E	72	MET	3.0
1	E	98	ALA	3.0
1	H	105	LEU	3.0
1	B	116	ASN	3.0
3	G	58	ASP	3.0
2	J	386	LYS	3.0
2	D	450	SER	3.0
2	D	447	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	L	51	GLU	3.0
2	C	355	ASN	3.0
1	E	118	ASP	3.0
1	H	7	ARG	2.9
3	F	56	LEU	2.9
1	K	41	GLY	2.9
3	F	16	GLU	2.9
2	C	383	GLN	2.9
3	G	54	ARG	2.9
3	L	15	LEU	2.9
2	D	354	LEU	2.9
1	K	5	PRO	2.9
2	C	382	MET	2.9
3	A	61	ILE	2.9
1	H	42	PRO	2.9
2	C	362	GLU	2.9
3	F	19	PRO	2.9
2	J	416	LEU	2.9
1	H	56	LEU	2.9
1	K	71	PHE	2.9
3	A	54	ARG	2.8
1	K	32	ALA	2.8
1	H	141	ARG	2.8
1	H	48	GLU	2.8
3	F	43	LEU	2.8
1	H	20	VAL	2.8
3	G	22	THR	2.8
3	A	62	GLN	2.8
1	B	49	GLY	2.8
2	I	387	GLU	2.8
3	F	49	GLN	2.8
3	L	55	THR	2.8
3	F	59	TYR	2.8
1	E	39	ILE	2.8
2	J	460	MET	2.8
2	D	446	SER	2.8
1	K	111	LEU	2.8
1	K	51	THR	2.7
3	L	68	HIS	2.7
2	I	438	PRO	2.7
1	H	8	ILE	2.7
3	L	3	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	463	ASN	2.7
2	J	413	ALA	2.7
1	H	4	LEU	2.7
1	K	149	MET	2.7
3	F	39	ASP	2.7
1	K	42	PRO	2.7
3	L	66	THR	2.7
1	K	116	ASN	2.7
3	L	14	THR	2.7
1	E	142	ALA	2.7
1	H	63	PRO	2.7
2	D	397	LEU	2.6
2	J	439	ILE	2.6
2	D	464	LEU	2.6
2	D	363	ALA	2.6
1	B	142	ALA	2.6
2	I	479	ARG	2.6
3	G	19	PRO	2.6
1	K	91	LEU	2.6
2	J	406	CYS	2.6
1	K	8	ILE	2.6
1	B	114	ALA	2.6
2	J	422	PHE	2.6
1	H	149	MET	2.6
2	I	444	ILE	2.6
3	G	15	LEU	2.6
1	E	87	LYS	2.6
1	H	97	PRO	2.6
3	F	57	SER	2.6
1	H	23	ILE	2.5
1	E	122	ALA	2.5
1	H	109	GLN	2.5
2	D	384	ALA	2.5
1	B	15	LEU	2.5
1	H	73	THR	2.5
3	F	21	ASP	2.5
1	E	30	SER	2.5
2	J	479	ARG	2.5
3	F	23	ILE	2.5
1	H	35	PHE	2.5
1	K	33	ARG	2.5
1	E	108	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
2	J	461	VAL	2.5
1	H	79	ASN	2.5
2	I	447	LYS	2.5
3	F	55	THR	2.5
1	H	5	PRO	2.4
2	C	450	SER	2.4
3	F	53	GLY	2.4
2	D	355	ASN	2.4
2	J	412	GLU	2.4
1	K	81	ASP	2.4
3	A	14	THR	2.4
1	B	71	PHE	2.4
1	H	25	ALA	2.4
1	E	121	LEU	2.4
2	C	409	TYR	2.4
2	C	408	GLU	2.4
1	E	146	LEU	2.4
3	G	3	ILE	2.4
3	L	54	ARG	2.4
1	B	130	LYS	2.4
1	H	6	ARG	2.4
1	K	50	GLY	2.4
3	L	53	GLY	2.4
1	K	49	GLY	2.4
1	K	6	ARG	2.3
1	K	67	PRO	2.3
3	A	23	ILE	2.3
1	K	66	ALA	2.3
2	J	464	LEU	2.3
1	E	82	LYS	2.3
3	A	60	ASN	2.3
3	F	20	SER	2.3
3	F	22	THR	2.3
1	H	37	VAL	2.3
2	C	405	ILE	2.3
1	K	130	LYS	2.3
3	G	60	ASN	2.3
2	C	443	ASP	2.3
3	A	47	GLY	2.3
3	F	67	LEU	2.3
3	F	45	PHE	2.3
2	D	405	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	453	LEU	2.3
3	L	19	PRO	2.3
1	K	121	LEU	2.3
1	H	32	ALA	2.3
2	D	468	VAL	2.2
2	I	477	ARG	2.2
2	D	475	LEU	2.2
1	B	94	LYS	2.2
1	K	58	LEU	2.2
2	J	404	ILE	2.2
3	G	16	GLU	2.2
3	G	27	LYS	2.2
3	G	70	VAL	2.2
3	G	18	GLU	2.2
2	J	457	ILE	2.2
1	K	119	ASP	2.2
3	A	52	ASP	2.2
3	G	57	SER	2.2
1	H	30	SER	2.2
2	C	438	PRO	2.2
2	C	347	HIS	2.2
1	H	101	ILE	2.2
1	E	80	VAL	2.2
1	B	16	LEU	2.2
1	K	109	GLN	2.2
1	H	38	VAL	2.2
1	E	88	LEU	2.2
1	B	12	THR	2.2
1	E	119	ASP	2.2
2	I	414	VAL	2.2
3	A	26	VAL	2.2
1	H	113	SER	2.2
1	H	67	PRO	2.1
2	D	356	ARG	2.1
2	D	411	ILE	2.2
2	I	409	TYR	2.1
2	J	434	LYS	2.1
1	K	90	ILE	2.1
2	C	351	MET	2.1
1	H	69	VAL	2.1
1	E	86	ILE	2.1
2	D	439	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	21	PRO	2.1
2	C	422	PHE	2.1
3	G	66	THR	2.1
1	B	148	ALA	2.1
1	B	98	ALA	2.1
2	J	463	ASN	2.1
2	I	388	GLU	2.1
1	B	105	LEU	2.1
2	C	413	ALA	2.1
3	G	42	ARG	2.1
2	C	453	LEU	2.1
2	J	449	TYR	2.1
3	L	2	GLN	2.1
1	K	92	LYS	2.1
1	B	146	LEU	2.0
1	K	35	PHE	2.0
2	J	427	ILE	2.0
1	K	89	ASP	2.0
3	A	50	LEU	2.0
1	B	29	GLU	2.0
1	B	11	GLU	2.0
1	B	108	ILE	2.0
3	F	52	ASP	2.0
1	K	120	PRO	2.0
2	J	453	LEU	2.0
1	B	119	ASP	2.0
3	A	13	ILE	2.0
1	H	104	VAL	2.0
3	G	30	ILE	2.0
2	D	478	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	ZN	D	502	1/1	0.80	0.24	-1.13	517,517,517,517	0
4	ZN	J	502	1/1	0.98	0.26	-1.23	496,496,496,496	0
4	ZN	D	501	1/1	0.78	0.18	-1.36	517,517,517,517	0
4	ZN	I	502	1/1	0.95	0.19	-1.50	454,454,454,454	0
4	ZN	J	501	1/1	0.83	0.26	-1.56	496,496,496,496	0
4	ZN	I	501	1/1	0.69	0.14	-2.22	454,454,454,454	0
4	ZN	C	502	1/1	0.86	0.17	-2.35	527,527,527,527	0
4	ZN	C	501	1/1	0.82	0.23	-2.40	527,527,527,527	0

6.5 Other polymers [i](#)

There are no such residues in this entry.