



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:12 PM UTC

PDB ID : 4HD0 / pdb_00004hd0
Title : Mre11 ATLD17/18 mutation retains Tel1/ATM activity but blocks DNA double-strand break repair
Authors : Limbo, O.; Moiani, D.; Kertokallio, A.; Wyman, C.; Tainer, J.A.; Russell, P.
Deposited on : 2012-10-01
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

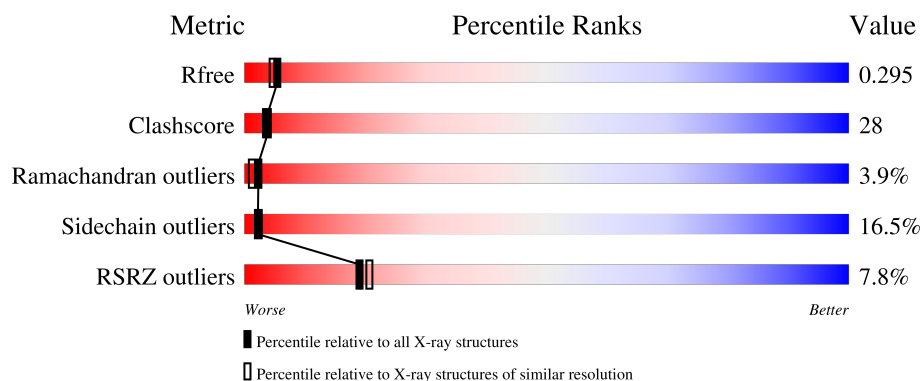
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	339	5% 60% 27% 9% . .
1	B	339	10% 55% 27% 9% . 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5500 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 DNA double-strand break repair protein Mre11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	S	48	3	0
			2765	1792	471	497	5			
1	B	319	Total	C	N	O	S	96	2	0
			2667	1734	456	472	5			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q8U1N9
A	-4	HIS	-	expression tag	UNP Q8U1N9
A	-3	HIS	-	expression tag	UNP Q8U1N9
A	-2	HIS	-	expression tag	UNP Q8U1N9
A	-1	HIS	-	expression tag	UNP Q8U1N9
A	0	HIS	-	expression tag	UNP Q8U1N9
A	204	ARG	LEU	engineered mutation	UNP Q8U1N9
B	-5	HIS	-	expression tag	UNP Q8U1N9
B	-4	HIS	-	expression tag	UNP Q8U1N9
B	-3	HIS	-	expression tag	UNP Q8U1N9
B	-2	HIS	-	expression tag	UNP Q8U1N9
B	-1	HIS	-	expression tag	UNP Q8U1N9
B	0	HIS	-	expression tag	UNP Q8U1N9
B	204	ARG	LEU	engineered mutation	UNP Q8U1N9

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

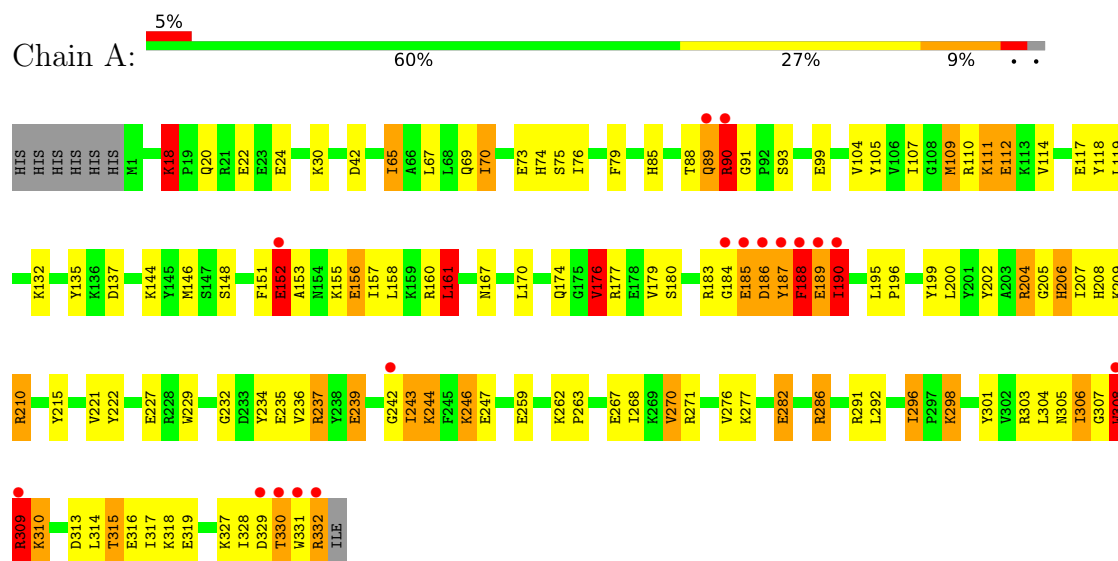
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total 40	O 40	0	0
3	B	24	Total 24	O 24	0	0

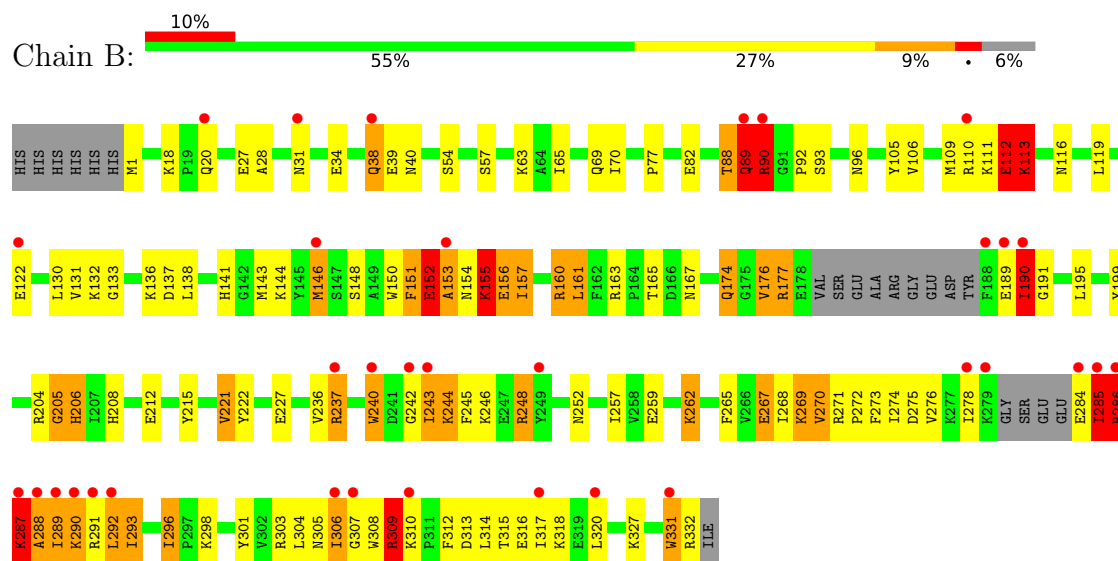
3 Residue-property plots

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: DNA double-strand break repair protein Mre11



- Molecule 1: DNA double-strand break repair protein Mre11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.04Å 70.19Å 81.49Å 90.00° 109.31° 90.00°	Depositor
Resolution (Å)	45.00 – 2.30 45.00 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.00-2.30) 99.5 (45.00-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.223 , 0.277 (Not available) , 0.295	Depositor DCC
R_{free} test set	1633 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	38.5	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5500	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	1.30	6/2845 (0.2%)	1.26	19/3836 (0.5%)
1	B	1.31	15/2735 (0.5%)	1.26	23/3685 (0.6%)
All	All	1.30	21/5580 (0.4%)	1.26	42/7521 (0.6%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	90	ARG	CA-CB	-27.25	1.14	1.54
1	A	152	GLU	CG-CD	15.64	1.91	1.52
1	B	113	LYS	CD-CE	-15.11	1.07	1.52
1	B	331	TRP	CA-CB	-13.91	1.29	1.53
1	B	177	ARG	CD-NE	-11.66	1.29	1.46
1	B	243	ILE	CB-CG1	11.66	1.76	1.53
1	B	287	LYS	CB-CG	-10.57	1.20	1.52
1	B	248	ARG	CG-CD	-10.22	1.21	1.52
1	A	298	LYS	CB-CG	-9.04	1.25	1.52
1	B	243	ILE	CG1-CD1	8.59	1.85	1.51
1	B	112	GLU	CB-CG	8.46	1.77	1.52
1	B	309	ARG	CA-CB	7.21	1.62	1.53
1	A	246	LYS	CB-CG	-6.84	1.31	1.52
1	B	116	ASN	CA-C	-5.68	1.45	1.52
1	B	290	LYS	CB-CG	-5.66	1.35	1.52
1	B	286	ARG	CB-CG	-5.63	1.35	1.52
1	B	205	GLY	N-CA	5.43	1.50	1.45
1	A	188	PHE	CG-CD2	-5.35	1.27	1.38
1	B	106	VAL	C-O	-5.12	1.18	1.24
1	A	65	ILE	C-O	-5.03	1.18	1.24
1	B	77	PRO	C-O	-5.01	1.18	1.23

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	ARG	CA-CB-CG	-10.27	93.57	114.10
1	B	177	ARG	CD-NE-CZ	-10.25	110.05	124.40
1	A	310	LYS	CB-CG-CD	10.17	134.69	111.30
1	A	298	LYS	CB-CG-CD	10.06	134.43	111.30
1	B	237	ARG	CD-NE-CZ	-10.03	110.35	124.40
1	B	331	TRP	CB-CA-C	-9.65	91.21	110.42
1	A	152	GLU	CB-CG-CD	-9.17	97.01	112.60
1	A	153	ALA	N-CA-C	-7.29	103.99	113.17
1	B	287	LYS	CB-CG-CD	7.22	127.90	111.30
1	A	76	ILE	CA-C-N	-7.17	113.28	120.31
1	A	76	ILE	C-N-CA	-7.17	113.28	120.31
1	B	112	GLU	CA-CB-CG	-6.92	100.26	114.10
1	B	151	PHE	N-CA-C	6.85	118.63	111.03
1	B	248	ARG	CB-CG-CD	6.63	126.55	111.30
1	B	155	LYS	N-CA-C	-6.27	101.40	110.24
1	A	176	VAL	CB-CA-C	-6.16	99.90	111.30
1	A	70	ILE	CA-C-N	-6.14	112.68	119.19
1	A	70	ILE	C-N-CA	-6.14	112.68	119.19
1	B	28	ALA	N-CA-C	-6.07	104.23	111.69
1	B	293	ILE	CA-C-N	-6.01	113.93	119.82
1	B	293	ILE	C-N-CA	-6.01	113.93	119.82
1	B	57	SER	CA-C-N	5.91	125.61	119.05
1	B	57	SER	C-N-CA	5.91	125.61	119.05
1	B	244	LYS	N-CA-C	5.74	115.86	108.34
1	A	232	GLY	N-CA-C	-5.67	107.89	115.32
1	A	204	ARG	CG-CD-NE	-5.66	99.56	112.00
1	B	152	GLU	N-CA-C	-5.62	102.08	110.23
1	A	309	ARG	CB-CG-CD	-5.54	98.56	111.30
1	A	18	LYS	CA-C-N	5.46	125.54	119.32
1	A	18	LYS	C-N-CA	5.46	125.54	119.32
1	A	85	HIS	N-CA-C	5.46	118.15	111.82
1	B	165	THR	CA-C-N	-5.45	111.05	121.94
1	B	165	THR	C-N-CA	-5.45	111.05	121.94
1	B	221	VAL	N-CA-C	5.43	115.72	108.11
1	B	309	ARG	N-CA-CB	-5.39	101.47	110.37
1	A	296	ILE	N-CA-C	5.26	113.23	107.60
1	A	309	ARG	CA-CB-CG	5.11	124.33	114.10
1	B	165	THR	N-CA-C	-5.05	103.38	110.35
1	A	308	TRP	CA-CB-CG	5.04	123.17	113.60
1	A	161	LEU	N-CA-C	5.03	116.45	111.07
1	B	70	ILE	CA-C-N	-5.02	113.87	119.19
1	B	70	ILE	C-N-CA	-5.02	113.87	119.19

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	2765	0	2757	145	2
1	B	2667	0	2667	153	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	40	0	0	5	0
3	B	24	0	0	0	0
All	All	5500	0	5424	298	2

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 28.

All (298) 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:B:110:ARG:NE	1:B:131:VAL:HG21	1.30	1.39
1:B:110:ARG:CD	1:B:131:VAL:HG21	1.50	1.38
1:A:177:ARG:NH2	1:A:188:PHE:HB3	1.43	1.33
1:B:110:ARG:HD2	1:B:131:VAL:CG2	1.59	1.31
1:A:186:ASP:CG	1:A:187:TYR:HA	1.57	1.27
1:B:286:ARG:HA	1:B:287:LYS:CB	1.63	1.26
1:B:286:ARG:CA	1:B:287:LYS:HB3	1.66	1.23
1:B:287:LYS:N	1:B:288:ALA:HB2	1.49	1.23
1:B:110:ARG:CD	1:B:131:VAL:CG2	2.17	1.15
1:B:269:LYS:HZ1	1:B:270:VAL:N	1.43	1.15
1:A:180:SER:OG	1:A:186:ASP:O	1.64	1.14
1:B:160:ARG:HH21	1:B:160:ARG:HG3	1.00	1.13
1:B:155:LYS:O	1:B:156:GLU:HG2	1.48	1.11
1:B:262:LYS:C	1:B:262:LYS:HD2	1.76	1.10
1:B:269:LYS:NZ	1:B:270:VAL:H	1.51	1.09
1:B:287:LYS:CA	1:B:288:ALA:HB2	1.81	1.09
1:B:284:GLU:HG2	1:B:285:ILE:HD13	1.33	1.08
1:B:287:LYS:HA	1:B:288:ALA:CB	1.82	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:HH11	1:A:332:ARG:HB3	1.17	1.08
1:B:31:ASN:ND2	1:B:268:ILE:HD13	1.68	1.08
1:A:151:PHE:O	1:A:152:GLU:HB3	1.52	1.07
1:B:88:THR:HG22	1:B:89:GLN:HB2	1.32	1.07
1:B:154:ASN:O	1:B:157:ILE:HG22	1.55	1.06
1:B:289:ILE:HG23	1:B:293:ILE:CD1	1.84	1.06
1:B:287:LYS:CA	1:B:288:ALA:CB	2.35	1.05
1:B:289:ILE:HG23	1:B:293:ILE:HD11	1.39	1.04
1:A:180:SER:CB	1:A:186:ASP:O	2.06	1.04
1:A:111:LYS:HE3	1:A:111:LYS:H	1.19	1.03
1:A:73:GLU:HG3	1:A:74:HIS:CD2	1.93	1.03
1:A:187:TYR:O	1:A:189:GLU:N	1.92	1.03
1:B:88:THR:CG2	1:B:89:GLN:HB2	1.89	1.02
1:A:187:TYR:C	1:A:189:GLU:H	1.64	1.02
1:B:88:THR:HG22	1:B:89:GLN:CB	1.93	0.98
1:B:269:LYS:HZ2	1:B:269:LYS:HA	1.27	0.97
1:B:110:ARG:NE	1:B:131:VAL:CG2	2.26	0.96
1:B:110:ARG:HD2	1:B:131:VAL:HG22	1.47	0.95
1:B:110:ARG:HE	1:B:131:VAL:HG21	1.18	0.94
1:A:177:ARG:CZ	1:A:188:PHE:HB3	1.96	0.94
1:B:88:THR:HA	1:B:89:GLN:HB2	1.50	0.94
1:A:177:ARG:NH2	1:A:188:PHE:CB	2.31	0.93
1:A:177:ARG:HH21	1:A:188:PHE:HB3	1.20	0.93
1:A:186:ASP:CB	1:A:187:TYR:HA	1.99	0.93
1:A:307:GLY:O	1:A:308:TRP:HB2	1.66	0.93
1:B:88:THR:CA	1:B:89:GLN:HB2	2.01	0.91
1:B:262:LYS:HD2	1:B:262:LYS:O	1.69	0.91
1:B:287:LYS:H	1:B:288:ALA:HB2	1.10	0.90
1:B:269:LYS:NZ	1:B:269:LYS:HA	1.86	0.90
1:B:160:ARG:HG3	1:B:160:ARG:NH2	1.77	0.90
1:B:122:GLU:OE2	1:B:132:LYS:HE3	1.71	0.89
1:A:88:THR:HB	1:A:90:ARG:O	1.72	0.88
1:A:186:ASP:OD1	1:A:187:TYR:HA	1.73	0.88
1:B:285:ILE:HA	1:B:286:ARG:HB2	1.56	0.88
1:B:244:LYS:CG	1:B:245:PHE:H	1.86	0.88
1:B:287:LYS:HA	1:B:288:ALA:HB3	1.52	0.88
1:A:332:ARG:HB3	1:A:332:ARG:NH1	1.90	0.87
1:A:329:ASP:O	1:A:330:THR:HG23	1.73	0.86
1:A:111:LYS:H	1:A:111:LYS:CE	1.87	0.86
1:A:313:ASP:OD1	1:A:315:THR:HG23	1.73	0.86
1:A:189:GLU:O	1:A:190:ILE:HG12	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:HIS:HD1	1:A:229:TRP:CG	1.93	0.86
1:B:189:GLU:O	1:B:190:ILE:HG13	1.74	0.86
1:A:184:GLY:O	1:A:185:GLU:HG2	1.76	0.85
1:A:204:ARG:HG2	1:A:222:TYR:CZ	2.11	0.85
1:B:155:LYS:O	1:B:156:GLU:CG	2.24	0.85
1:A:180:SER:HB3	1:A:186:ASP:O	1.78	0.84
1:B:244:LYS:HE3	1:B:291:ARG:HG3	1.60	0.84
1:B:285:ILE:CA	1:B:286:ARG:HB2	2.09	0.83
1:B:287:LYS:H	1:B:288:ALA:CB	1.91	0.83
1:A:70:ILE:O	1:A:73:GLU:HG2	1.77	0.83
1:A:187:TYR:C	1:A:189:GLU:N	2.35	0.83
1:A:243:ILE:HG22	1:A:244:LYS:CG	2.10	0.82
1:A:176:VAL:HG22	1:A:222:TYR:OH	1.78	0.82
1:A:177:ARG:HD3	1:A:188:PHE:HA	1.61	0.82
1:A:190:ILE:HG22	1:A:190:ILE:O	1.78	0.81
1:B:287:LYS:N	1:B:288:ALA:CB	2.40	0.81
1:B:31:ASN:ND2	1:B:268:ILE:CD1	2.44	0.80
1:B:89:GLN:OE1	1:B:89:GLN:HA	1.80	0.80
1:B:269:LYS:NZ	1:B:270:VAL:N	2.19	0.80
1:B:285:ILE:HB	1:B:312:PHE:CE1	2.17	0.79
1:B:31:ASN:HD21	1:B:268:ILE:CD1	1.95	0.79
1:B:204:ARG:HG2	1:B:222:TYR:CZ	2.17	0.79
1:B:155:LYS:C	1:B:156:GLU:HG2	2.08	0.79
1:B:285:ILE:HD12	1:B:309:ARG:O	1.84	0.78
1:B:289:ILE:HG23	1:B:293:ILE:HD13	1.66	0.78
1:A:177:ARG:HH21	1:A:188:PHE:CB	1.96	0.77
1:B:284:GLU:HG2	1:B:285:ILE:CD1	2.14	0.77
1:B:152:GLU:O	1:B:153:ALA:HB3	1.84	0.77
1:B:31:ASN:HD21	1:B:268:ILE:HD13	1.46	0.77
1:B:313:ASP:OD1	1:B:315:THR:HG22	1.85	0.77
1:A:187:TYR:OH	1:A:207:ILE:CD1	2.33	0.76
1:A:243:ILE:HG22	1:A:244:LYS:HG3	1.66	0.76
1:A:151:PHE:O	1:A:152:GLU:CB	2.28	0.75
1:A:186:ASP:OD1	1:A:188:PHE:CE2	2.40	0.74
1:A:209:LYS:NZ	3:A:538:HOH:O	2.17	0.74
1:A:189:GLU:O	1:A:190:ILE:CG1	2.35	0.74
1:A:187:TYR:OH	1:A:207:ILE:HD11	1.87	0.74
1:B:31:ASN:HD22	1:B:268:ILE:HD13	1.48	0.74
1:B:110:ARG:HE	1:B:131:VAL:CG2	1.95	0.74
1:B:287:LYS:HA	1:B:288:ALA:HB2	1.54	0.73
1:B:88:THR:HA	1:B:89:GLN:CB	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:VAL:HG23	1:B:222:TYR:OH	1.88	0.73
1:B:285:ILE:CA	1:B:286:ARG:CB	2.68	0.72
1:A:111:LYS:HE3	1:A:111:LYS:N	2.01	0.71
1:A:286:ARG:HH21	1:A:316:GLU:CG	2.04	0.71
1:B:96[A]:ASN:C	1:B:96[A]:ASN:HD22	1.95	0.70
1:B:174:GLN:OE1	1:B:190:ILE:HD11	1.91	0.70
1:B:284:GLU:CG	1:B:285:ILE:HD13	2.16	0.70
1:B:152:GLU:O	1:B:153:ALA:CB	2.37	0.70
1:B:252:ASN:HB3	1:B:267:GLU:HG3	1.73	0.70
1:A:189:GLU:O	1:A:190:ILE:CB	2.39	0.70
1:A:237:ARG:NH2	3:A:540:HOH:O	2.24	0.70
1:A:286:ARG:HH21	1:A:316:GLU:CD	2.00	0.70
1:A:186:ASP:CB	1:A:187:TYR:CA	2.69	0.69
1:B:88:THR:CB	1:B:89:GLN:HB2	2.22	0.69
1:B:151:PHE:CE2	1:B:189:GLU:OE1	2.46	0.69
1:A:286:ARG:HD3	1:A:317:ILE:CG1	2.23	0.69
1:B:278:ILE:O	1:B:306:ILE:O	2.10	0.68
1:B:244:LYS:CG	1:B:245:PHE:N	2.57	0.68
1:A:70:ILE:O	1:A:73:GLU:CG	2.42	0.67
1:A:185:GLU:OE2	1:A:185:GLU:HA	1.93	0.67
1:B:244:LYS:HG2	1:B:245:PHE:H	1.57	0.67
1:A:180:SER:OG	1:A:186:ASP:C	2.39	0.66
1:A:187:TYR:N	1:A:187:TYR:CD2	2.61	0.65
1:A:286:ARG:NH2	1:A:316:GLU:CD	2.55	0.65
1:B:244:LYS:HG3	1:B:245:PHE:H	1.60	0.65
1:A:243:ILE:HG22	1:A:244:LYS:HG2	1.78	0.64
1:B:96[A]:ASN:O	1:B:96[A]:ASN:ND2	2.28	0.64
1:B:285:ILE:N	1:B:286:ARG:CB	2.60	0.64
1:A:88:THR:CB	1:A:90:ARG:O	2.46	0.64
1:B:151:PHE:O	1:B:155:LYS:N	2.30	0.64
1:B:34:GLU:O	1:B:38:GLN:HG2	1.98	0.64
1:A:210:ARG:CZ	3:A:527:HOH:O	2.46	0.63
1:A:282:GLU:OE1	1:A:286:ARG:NH1	2.31	0.63
1:B:160:ARG:HH21	1:B:160:ARG:CG	1.91	0.63
1:B:285:ILE:N	1:B:286:ARG:HB2	2.14	0.63
1:A:117:GLU:O	1:A:118:TYR:CG	2.52	0.63
1:A:190:ILE:O	1:A:190:ILE:CG2	2.47	0.63
1:B:96[A]:ASN:C	1:B:96[A]:ASN:ND2	2.57	0.62
1:A:109:MET:HE1	1:A:161:LEU:HD11	1.80	0.62
1:A:242:GLY:O	1:A:243:ILE:HB	1.99	0.62
1:B:156:GLU:O	1:B:160:ARG:HG2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:GLU:O	1:A:190:ILE:HB	2.00	0.61
1:A:111:LYS:N	1:A:111:LYS:CD	2.63	0.61
1:A:186:ASP:CG	1:A:187:TYR:CA	2.53	0.61
1:A:184:GLY:O	1:A:185:GLU:CG	2.48	0.61
1:A:20:GLN:O	1:A:24:GLU:HG3	2.01	0.61
1:A:177:ARG:HD3	1:A:188:PHE:CA	2.30	0.61
1:B:262:LYS:O	1:B:262:LYS:CD	2.45	0.61
1:B:289:ILE:CG2	1:B:293:ILE:HD11	2.24	0.61
1:B:89:GLN:O	1:B:90:ARG:O	2.18	0.61
1:B:93:SER:H	1:B:96[B]:ASN:HD22	1.48	0.61
1:A:111:LYS:HE3	1:A:112:GLU:OE2	2.01	0.60
1:A:73:GLU:HG3	1:A:74:HIS:HD2	1.58	0.60
1:A:239:GLU:HG2	1:A:277:LYS:HB3	1.83	0.60
1:A:180:SER:HG	1:A:186:ASP:C	2.06	0.60
1:A:304:LEU:HB3	1:A:306:ILE:HD11	1.83	0.59
1:B:138:LEU:HD12	1:B:167:ASN:O	2.02	0.59
1:B:88:THR:CA	1:B:89:GLN:CB	2.78	0.59
1:B:93:SER:H	1:B:96[B]:ASN:ND2	2.01	0.59
1:A:180:SER:O	1:A:183:ARG:O	2.21	0.58
1:B:286:ARG:HA	1:B:287:LYS:HB3	0.73	0.58
1:A:307:GLY:O	1:A:308:TRP:CB	2.49	0.58
1:A:111:LYS:H	1:A:111:LYS:CD	2.17	0.58
1:B:285:ILE:HB	1:B:312:PHE:HE1	1.65	0.57
1:B:141:HIS:HD2	1:B:199:TYR:OH	1.86	0.57
1:A:208:HIS:ND1	1:A:229:TRP:CD2	2.72	0.57
1:A:188:PHE:C	1:A:190:ILE:H	2.12	0.57
1:B:204:ARG:HG2	1:B:222:TYR:CE2	2.39	0.57
1:B:88:THR:HG22	1:B:89:GLN:HB3	1.83	0.57
1:A:177:ARG:CZ	1:A:188:PHE:HD1	2.18	0.56
1:B:155:LYS:O	1:B:156:GLU:CB	2.52	0.56
1:A:204:ARG:HG2	1:A:222:TYR:CE1	2.40	0.56
1:A:111:LYS:CE	1:A:111:LYS:N	2.63	0.56
1:A:187:TYR:C	1:A:188:PHE:CD2	2.84	0.56
1:A:18:LYS:HZ2	1:A:20:GLN:HB3	1.70	0.55
1:A:188:PHE:O	1:A:190:ILE:N	2.39	0.55
1:B:292:LEU:HD22	1:B:296:ILE:HD11	1.87	0.55
1:A:22:GLU:OE1	3:A:514:HOH:O	2.18	0.55
1:A:79:PHE:HB3	1:A:107:ILE:HD12	1.87	0.55
1:B:89:GLN:OE1	1:B:89:GLN:CA	2.54	0.55
1:A:65:ILE:O	1:A:69[B]:GLN:NE2	2.39	0.55
1:A:204:ARG:CG	1:A:222:TYR:CZ	2.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:VAL:HG21	1:A:292:LEU:HD21	1.87	0.54
1:A:306:ILE:O	1:A:330:THR:HA	2.08	0.54
1:B:155:LYS:C	1:B:156:GLU:CG	2.75	0.54
1:B:276:VAL:HB	1:B:304:LEU:HD23	1.89	0.53
1:B:269:LYS:HA	1:B:269:LYS:CE	2.34	0.53
1:A:186:ASP:HB3	1:A:187:TYR:CA	2.37	0.53
1:A:188:PHE:C	1:A:190:ILE:N	2.66	0.53
1:B:109:MET:HE1	1:B:130:LEU:HD13	1.91	0.53
1:A:271:ARG:HD3	1:A:301:TYR:CD1	2.44	0.53
1:B:252:ASN:CB	1:B:267:GLU:HG3	2.39	0.53
1:A:286:ARG:NH2	1:A:316:GLU:CG	2.71	0.52
1:B:274:ILE:HD13	1:B:296:ILE:HG23	1.91	0.52
1:A:187:TYR:O	1:A:188:PHE:HD2	1.93	0.52
1:B:284:GLU:C	1:B:286:ARG:HB2	2.34	0.52
1:A:208:HIS:CE1	1:A:229:TRP:CD2	2.98	0.52
1:B:262:LYS:C	1:B:262:LYS:CD	2.59	0.51
1:A:187:TYR:O	1:A:188:PHE:C	2.54	0.51
1:B:136:LYS:HB2	1:B:137:ASP:OD2	2.11	0.51
1:A:20:GLN:NE2	1:A:301:TYR:OH	2.43	0.51
1:B:54:SER:OG	1:B:89:GLN:HG2	2.09	0.51
1:B:269:LYS:NZ	1:B:269:LYS:CA	2.67	0.51
1:A:329:ASP:O	1:A:330:THR:CG2	2.53	0.50
1:A:179:VAL:HG11	1:A:207:ILE:HD13	1.92	0.50
1:B:148:SER:HA	1:B:189:GLU:HG3	1.93	0.50
1:A:242:GLY:O	1:A:243:ILE:CB	2.58	0.50
1:B:273:PHE:C	1:B:274:ILE:HG13	2.37	0.50
1:A:111:LYS:NZ	1:A:112:GLU:OE2	2.45	0.49
1:A:331:TRP:C	1:A:332:ARG:HG2	2.37	0.49
1:A:186:ASP:HB3	1:A:187:TYR:CB	2.42	0.49
1:A:286:ARG:HD3	1:A:317:ILE:HG12	1.92	0.49
1:A:286:ARG:HD3	1:A:317:ILE:HG13	1.94	0.49
1:B:206:HIS:O	1:B:208:HIS:HD2	1.95	0.49
1:B:227:GLU:CD	1:B:270:VAL:HG22	2.38	0.49
1:A:73:GLU:CG	1:A:74:HIS:CD2	2.82	0.48
1:B:195:LEU:HB2	1:B:215:TYR:CE2	2.48	0.48
1:A:144:LYS:HE3	1:A:146:MET:CE	2.43	0.48
1:B:152:GLU:O	1:B:152:GLU:HG2	2.12	0.48
1:A:204:ARG:HB2	1:A:221:VAL:O	2.14	0.48
1:B:146:MET:SD	1:B:150:TRP:CD2	3.07	0.48
1:B:92:PRO:HA	1:B:96[B]:ASN:HD22	1.79	0.47
1:B:289:ILE:O	1:B:290:LYS:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:CZ	1:A:188:PHE:CD1	2.97	0.47
1:A:111:LYS:CE	1:A:112:GLU:OE2	2.62	0.47
1:A:110:ARG:HA	1:A:111:LYS:HE2	1.96	0.47
1:A:105:TYR:HB3	1:A:119:LEU:HD21	1.97	0.47
1:A:306:ILE:HD13	1:A:306:ILE:N	2.29	0.47
1:B:151:PHE:CD2	1:B:189:GLU:CD	2.93	0.47
1:B:227:GLU:OE1	1:B:270:VAL:HG22	2.15	0.46
1:A:187:TYR:HB2	1:A:189:GLU:HB2	1.96	0.46
1:B:271:ARG:HD3	1:B:301:TYR:CE1	2.50	0.46
1:A:205:GLY:O	1:A:206:HIS:CB	2.63	0.46
1:A:303:ARG:NH2	1:A:305[B]:ASN:OD1	2.49	0.46
1:B:109:MET:CE	1:B:130:LEU:HD13	2.47	0.45
1:B:65:ILE:O	1:B:69:GLN:HG2	2.15	0.45
1:B:174:GLN:HB2	1:B:189:GLU:OE2	2.16	0.45
1:B:212:GLU:HG3	1:B:221:VAL:HG22	1.97	0.45
1:B:275:ASP:CG	1:B:303:ARG:HH11	2.25	0.45
1:B:105:TYR:HB3	1:B:119:LEU:HD21	1.99	0.45
1:B:289:ILE:O	1:B:293:ILE:HD13	2.17	0.45
1:A:156:GLU:O	1:A:160:ARG:HD2	2.17	0.44
1:A:234:TYR:HE2	1:A:237:ARG:HH11	1.65	0.44
1:A:286:ARG:CD	1:A:317:ILE:HG13	2.47	0.44
1:A:282:GLU:CG	1:A:286:ARG:HH11	2.30	0.44
1:B:38:GLN:O	1:B:40:ASN:N	2.50	0.44
1:A:111:LYS:N	1:A:111:LYS:HD3	2.32	0.44
1:B:151:PHE:CE2	1:B:189:GLU:CD	2.95	0.44
1:B:240:TRP:CZ3	1:B:242:GLY:HA2	2.52	0.44
1:A:110:ARG:HB2	1:A:111:LYS:HE3	1.99	0.44
1:A:204:ARG:CB	1:A:221:VAL:O	2.66	0.44
1:B:82:GLU:HB2	1:B:144:LYS:HB2	1.99	0.44
1:A:42:ASP:HB3	1:A:135:TYR:CZ	2.52	0.44
1:A:286:ARG:NH2	1:A:316:GLU:OE2	2.50	0.44
1:A:292:LEU:HG	1:A:296:ILE:HD11	1.99	0.43
1:A:314:LEU:CD2	1:A:328:ILE:HD13	2.47	0.43
1:B:314:LEU:O	1:B:315:THR:C	2.61	0.43
1:B:284:GLU:C	1:B:286:ARG:CB	2.91	0.43
1:A:177:ARG:NE	1:A:188:PHE:HD1	2.15	0.43
1:B:122:GLU:CD	1:B:132:LYS:HE3	2.42	0.43
1:B:252:ASN:HB2	1:B:265:PHE:HE2	1.84	0.43
1:B:269:LYS:HZ1	1:B:270:VAL:H	0.64	0.43
1:B:271:ARG:HA	1:B:272:PRO:HD2	1.79	0.43
1:A:199:TYR:HB2	1:A:202:TYR:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LYS:HB2	1:B:137:ASP:H	1.47	0.42
1:B:244:LYS:HG2	1:B:245:PHE:N	2.29	0.42
1:B:38:GLN:C	1:B:40:ASN:H	2.27	0.42
1:B:285:ILE:HG12	1:B:285:ILE:O	2.19	0.42
1:A:88:THR:O	1:A:89:GLN:C	2.63	0.42
1:A:137:ASP:OD1	1:A:137:ASP:N	2.39	0.42
1:B:151:PHE:O	1:B:154:ASN:C	2.62	0.42
1:A:195:LEU:HB2	1:A:215:TYR:CE2	2.55	0.42
1:A:262:LYS:HA	1:A:263:PRO:HD2	1.86	0.42
1:A:210:ARG:NH2	3:A:527:HOH:O	2.52	0.41
1:A:65:ILE:HG22	1:A:69[B]:GLN:HE22	1.85	0.41
1:B:1:MET:HE3	1:B:138:LEU:HB2	2.02	0.41
1:B:119:LEU:HD23	1:B:133:GLY:HA2	2.03	0.41
1:B:317:ILE:HD12	1:B:317:ILE:C	2.45	0.41
1:A:167:ASN:HA	1:A:200:LEU:HD11	2.02	0.41
1:A:208:HIS:CE1	1:A:229:TRP:CE3	3.09	0.41
1:B:150:TRP:O	1:B:154:ASN:HB2	2.21	0.41
1:A:227:GLU:CD	1:A:270:VAL:HG22	2.45	0.41
1:B:205:GLY:O	1:B:206:HIS:CB	2.68	0.41
1:B:315:THR:O	1:B:318:LYS:HB2	2.21	0.41
1:B:176:VAL:HG12	1:B:191:GLY:HA2	2.03	0.41
1:A:30:LYS:HB2	1:A:67:LEU:HD22	2.02	0.40
1:A:67:LEU:HD23	1:A:67:LEU:HA	1.88	0.40
1:A:88:THR:CG2	1:A:93:SER:HA	2.51	0.40
1:A:99:GLU:HG3	1:A:104:VAL:O	2.21	0.40
1:A:170:LEU:HD22	1:A:196:PRO:HG2	2.04	0.40
1:B:313:ASP:CG	1:B:315:THR:HG22	2.43	0.40
1:A:158:LEU:HD11	1:A:190:ILE:HG13	2.02	0.40
1:A:180:SER:OG	1:A:187:TYR:N	2.54	0.40
1:B:157:ILE:HD11	1:B:161:LEU:HD12	2.02	0.40
1:B:110:ARG:HH21	1:B:110:ARG:HD3	1.70	0.40
1:B:189:GLU:C	1:B:190:ILE:HG13	2.42	0.40
1:B:112:GLU:O	1:B:113:LYS:C	2.64	0.40

All (2) 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:A:267:GLU:O	1:A:291:ARG:NH1[2_555]	2.06	0.14
1:A:177:ARG:NH1	1:B:34:GLU:OE2[2_544]	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	A	333/339 (98%)	303 (91%)	19 (6%)	11 (3%)	3	2
1	B	315/339 (93%)	283 (90%)	18 (6%)	14 (4%)	2	1
All	All	648/678 (96%)	586 (90%)	37 (6%)	25 (4%)	2	1

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	GLU
1	A	186	ASP
1	A	188	PHE
1	A	189	GLU
1	A	190	ILE
1	A	243	ILE
1	A	282	GLU
1	A	308	TRP
1	A	309	ARG
1	B	90	ARG
1	B	190	ILE
1	B	206	HIS
1	B	287	LYS
1	B	288	ALA
1	A	91	GLY
1	A	206	HIS
1	B	153	ALA
1	B	156	GLU
1	B	285	ILE
1	B	89	GLN
1	B	113	LYS
1	B	286	ARG
1	B	39	GLU
1	B	307	GLY
1	B	310	LYS

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	293/297 (99%)	250 (85%)	43 (15%)	3	3
1	B	282/297 (95%)	230 (82%)	52 (18%)	1	1
All	All	575/594 (97%)	480 (84%)	95 (16%)	2	2

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	75	SER
1	A	89	GLN
1	A	90	ARG
1	A	109	MET
1	A	111	LYS
1	A	112	GLU
1	A	114	VAL
1	A	132	LYS
1	A	148	SER
1	A	152	GLU
1	A	155	LYS
1	A	156	GLU
1	A	157	ILE
1	A	161	LEU
1	A	174	GLN
1	A	176	VAL
1	A	187	TYR
1	A	188	PHE
1	A	190	ILE
1	A	210	ARG
1	A	235	GLU
1	A	236	VAL
1	A	237	ARG
1	A	239	GLU
1	A	244	LYS
1	A	246	LYS

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Mol	Chain	Res	Type
1	A	247	GLU
1	A	259	GLU
1	A	268	ILE
1	A	270	VAL
1	A	286	ARG
1	A	298	LYS
1	A	306	ILE
1	A	308	TRP
1	A	309	ARG
1	A	310	LYS
1	A	315	THR
1	A	318	LYS
1	A	319	GLU
1	A	327	LYS
1	A	330	THR
1	A	332	ARG
1	B	18	LYS
1	B	20[A]	GLN
1	B	20[B]	GLN
1	B	27	GLU
1	B	38	GLN
1	B	63	LYS
1	B	88	THR
1	B	89	GLN
1	B	90	ARG
1	B	111	LYS
1	B	112	GLU
1	B	113	LYS
1	B	143	MET
1	B	146	MET
1	B	152	GLU
1	B	155	LYS
1	B	157	ILE
1	B	160	ARG
1	B	161	LEU
1	B	163	ARG
1	B	174	GLN
1	B	176	VAL
1	B	177	ARG
1	B	190	ILE
1	B	236	VAL
1	B	237	ARG

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Mol	Chain	Res	Type
1	B	240	TRP
1	B	243	ILE
1	B	246	LYS
1	B	248	ARG
1	B	257	ILE
1	B	259	GLU
1	B	262	LYS
1	B	267	GLU
1	B	269	LYS
1	B	270	VAL
1	B	285	ILE
1	B	286	ARG
1	B	287	LYS
1	B	289	ILE
1	B	292	LEU
1	B	296	ILE
1	B	298	LYS
1	B	305	ASN
1	B	306	ILE
1	B	308	TRP
1	B	309	ARG
1	B	316	GLU
1	B	320	LEU
1	B	327	LYS
1	B	331	TRP
1	B	332	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	74	HIS
1	A	174	GLN
1	B	31	ASN
1	B	38	GLN
1	B	141	HIS
1	B	167	ASN
1	B	299	ASN
1	B	305	ASN
1	B	322	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](#)

Of 4 ligands modelled in this entry, 4 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	332/339 (97%)	0.23	17 (5%)	33 35	18, 35, 55, 76	15 (4%)
1	B	318/339 (93%)	0.41	34 (10%)	11 12	15, 34, 65, 87	21 (6%)
All	All	650/678 (95%)	0.32	51 (7%)	19 21	15, 35, 59, 87	36 (5%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	LYS	6.0
1	B	288	ALA	5.1
1	A	186	ASP	4.6
1	A	187	TYR	4.5
1	B	286	ARG	4.5
1	B	285	ILE	4.5
1	B	110	ARG	4.1
1	B	189	GLU	4.1
1	A	188	PHE	3.8
1	B	289	ILE	3.7
1	A	329	ASP	3.6
1	A	190	ILE	3.5
1	B	284	GLU	3.5
1	B	188	PHE	3.3
1	B	122	GLU	3.0
1	A	90	ARG	3.0
1	A	332	ARG	3.0
1	B	290	LYS	2.9
1	B	307	GLY	2.9
1	B	240	TRP	2.9
1	B	331	TRP	2.9
1	B	243	ILE	2.9
1	B	31	ASN	2.8
1	A	184	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	242	GLY	2.7
1	A	189	GLU	2.7
1	A	330	THR	2.7
1	B	89	GLN	2.6
1	A	308	TRP	2.5
1	B	320	LEU	2.5
1	A	331	TRP	2.5
1	B	317	ILE	2.5
1	A	309	ARG	2.4
1	B	278	ILE	2.4
1	B	237	ARG	2.4
1	B	306	ILE	2.4
1	B	146	MET	2.4
1	B	292	LEU	2.4
1	B	249	TYR	2.4
1	B	310	LYS	2.3
1	A	89	GLN	2.3
1	B	90	ARG	2.3
1	B	38	GLN	2.3
1	B	153	ALA	2.2
1	B	20[A]	GLN	2.2
1	B	291	ARG	2.2
1	B	190	ILE	2.1
1	B	279	LYS	2.1
1	A	152	GLU	2.1
1	B	242	GLY	2.1
1	A	185	GLU	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(Å ²)	Q<0.9
2	MN	A	401	1/1	0.94	0.10	52,52,52,52	0
2	MN	A	402	1/1	0.97	0.06	41,41,41,41	0
2	MN	B	401	1/1	0.98	0.05	41,41,41,41	0
2	MN	B	402	1/1	0.98	0.09	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.