



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:03 PM UTC

PDB ID : 4FBW / pdb_00004fbw
Title : Crystal structure of an unfused Mre11-Nbs1 complex with two manganese ions per active site
Authors : Schiller, C.B.; Lammens, K.; Hopfner, K.P.
Deposited on : 2012-05-23
Resolution : 2.20 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

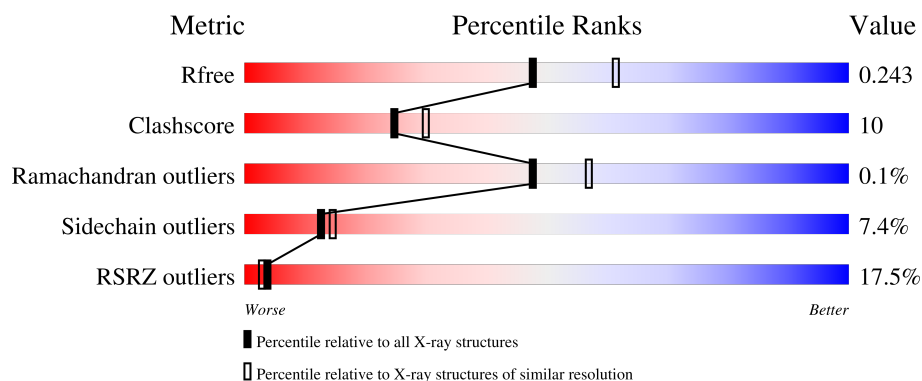
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	417	16% 71% 17% • 9%
1	B	417	11% 74% 16% • 7%
2	C	59	31% 20% 7% 7% • 64%
2	D	59	19% 20% • • 73%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6703 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 repair protein rad32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	83	0	0
			3056	1953	527	569	7			
1	B	386	Total	C	N	O	S	70	0	0
			3107	1981	535	583	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	GLY	-	expression tag	UNP Q09683
A	6	PRO	-	expression tag	UNP Q09683
A	414	VAL	-	cloning artifact	UNP Q09683
A	415	ASP	-	cloning artifact	UNP Q09683
A	416	GLU	-	cloning artifact	UNP Q09683
A	417	ASN	-	cloning artifact	UNP Q09683
A	418	LEU	-	cloning artifact	UNP Q09683
A	419	TYR	-	cloning artifact	UNP Q09683
A	420	PHE	-	cloning artifact	UNP Q09683
A	421	GLN	-	cloning artifact	UNP Q09683
B	5	GLY	-	expression tag	UNP Q09683
B	6	PRO	-	expression tag	UNP Q09683
B	414	VAL	-	cloning artifact	UNP Q09683
B	415	ASP	-	cloning artifact	UNP Q09683
B	416	GLU	-	cloning artifact	UNP Q09683
B	417	ASN	-	cloning artifact	UNP Q09683
B	418	LEU	-	cloning artifact	UNP Q09683
B	419	TYR	-	cloning artifact	UNP Q09683
B	420	PHE	-	cloning artifact	UNP Q09683
B	421	GLN	-	cloning artifact	UNP Q09683

- Molecule 2 is a protein called DNA repair and telomere maintenance protein nbs1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	35	0	0
			188	119	40	29			
2	D	16	Total	C	N	O	29	0	0
			140	84	30	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	473	GLY	-	cloning artifact	UNP O43070
D	473	GLY	-	cloning artifact	UNP O43070

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

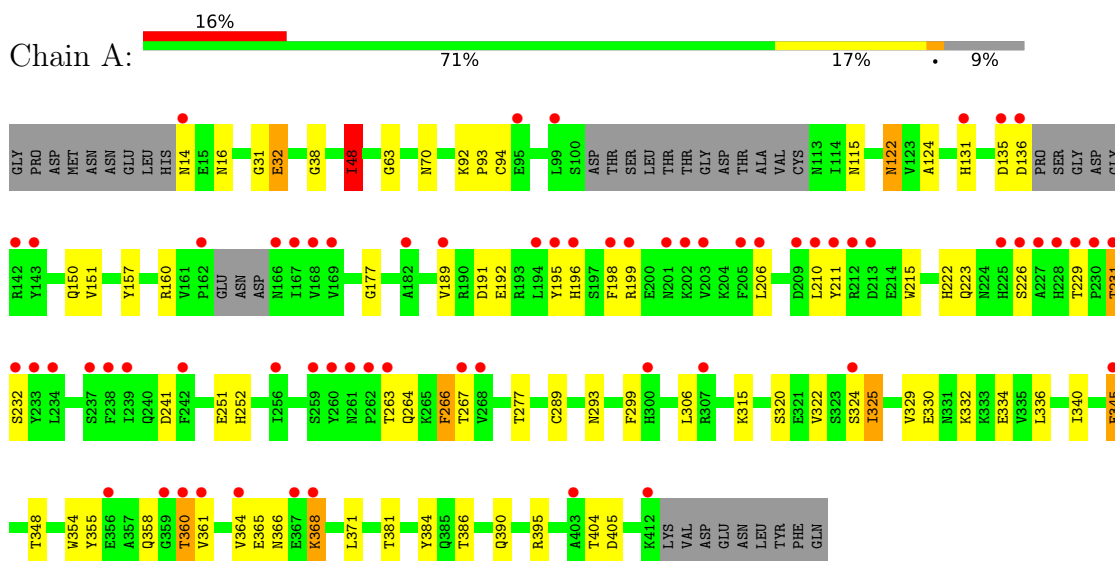
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	92	Total	O	0	0
			92	92		
4	B	115	Total	O	0	0
			115	115		
4	C	1	Total	O	0	0
			1	1		

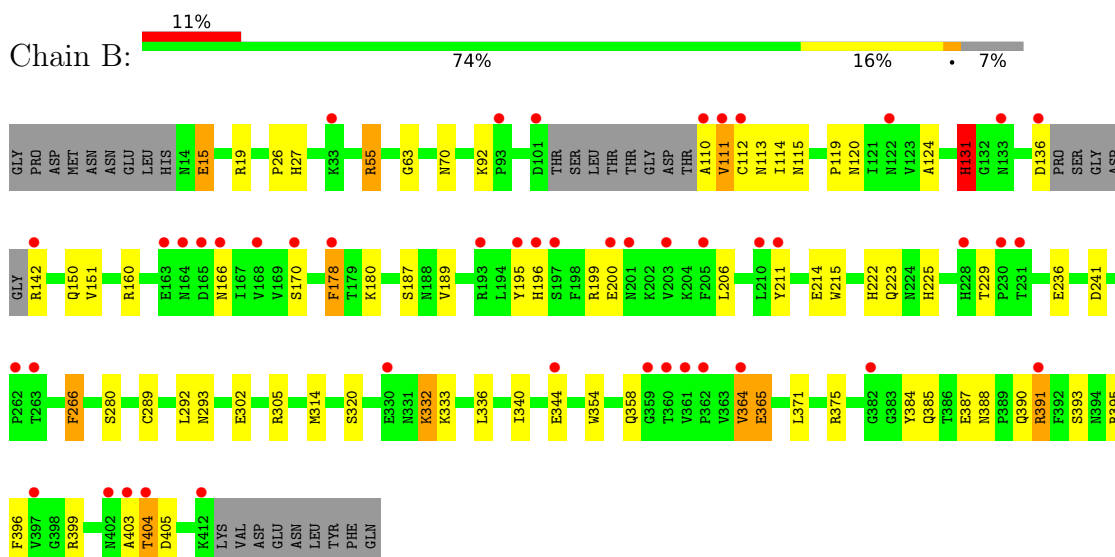
3 Residue-property plots [i](#)

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.

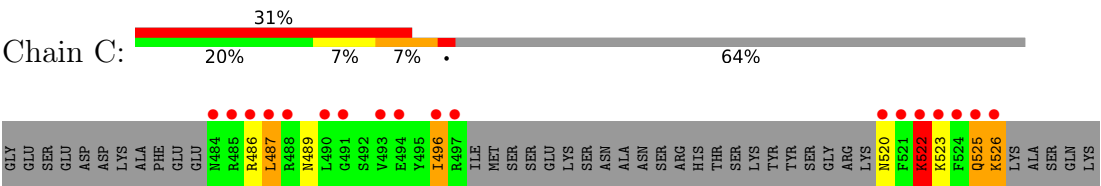
- Molecule 1: DNA repair protein rad32



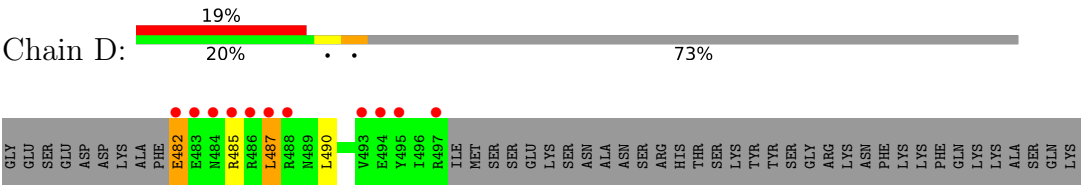
- Molecule 1: DNA repair protein rad32



- Molecule 2: DNA repair and telomere maintenance protein nbs1



● Molecule 2: DNA repair and telomere maintenance protein nbs1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.12Å 79.95Å 220.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.54 – 2.20 47.54 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.54-2.20) 99.4 (47.54-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.233 , 0.244 0.230 , 0.243	Depositor DCC
R_{free} test set	2000 reflections (3.71%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6703	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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	0.83	2/3127 (0.1%)	1.25	13/4247 (0.3%)
1	B	0.84	1/3179 (0.0%)	1.26	12/4320 (0.3%)
2	C	0.70	0/189	1.27	4/246 (1.6%)
2	D	0.80	0/140	1.12	0/185
All	All	0.83	3/6635 (0.0%)	1.25	29/8998 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	PRO	C-N	-5.98	1.25	1.33
1	A	198	PHE	C-N	5.58	1.41	1.33
1	A	48	ILE	CG1-CD1	-5.53	1.30	1.51

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	PRO	CA-C-N	-16.88	99.91	123.20
1	B	26	PRO	C-N-CA	-16.88	99.91	123.20
1	A	122	ASN	CA-CB-CG	8.09	120.69	112.60
1	B	113	ASN	CB-CA-C	8.05	125.72	110.51
1	B	266	PHE	CA-CB-CG	7.95	121.75	113.80
1	A	266	PHE	CA-CB-CG	7.63	121.43	113.80
1	B	114	ILE	N-CA-C	-6.95	100.62	109.30
2	C	522	LYS	CB-CA-C	-6.90	97.75	109.83
1	A	14	ASN	CA-CB-CG	6.64	119.24	112.60
1	B	26	PRO	N-CA-C	-6.46	101.11	111.38
2	C	523	LYS	N-CA-CB	-6.44	100.89	110.61
2	C	486	ARG	N-CA-C	6.36	119.16	111.40
1	A	31	GLY	CA-C-N	6.22	128.91	120.38
1	A	31	GLY	C-N-CA	6.22	128.91	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	487	LEU	N-CA-C	-6.12	102.45	110.53
1	B	115	ASN	N-CA-C	5.87	118.43	111.33
1	A	241	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	131	HIS	CB-CA-C	5.64	119.16	109.51
1	A	381	THR	CB-CA-C	5.55	119.75	109.54
1	B	241	ASP	CA-CB-CG	5.48	118.08	112.60
1	B	195	TYR	CA-C-N	5.45	127.58	120.28
1	B	195	TYR	C-N-CA	5.45	127.58	120.28
1	B	289	CYS	N-CA-C	-5.33	102.01	109.69
1	A	405	ASP	N-CA-C	5.21	116.69	109.54
1	A	325	ILE	N-CA-C	5.20	112.70	107.55
1	A	115	ASN	N-CA-C	5.12	117.52	111.33
1	A	38	GLY	N-CA-C	5.09	120.04	113.27
1	A	289	CYS	N-CA-C	-5.09	102.36	109.69
1	A	32	GLU	CB-CA-C	-5.05	102.10	110.68

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	3056	0	3026	61	0
1	B	3107	0	3066	49	0
2	C	188	0	198	15	0
2	D	140	0	140	4	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	92	0	0	1	0
4	B	115	0	0	0	0
4	C	1	0	0	0	0
All	All	6703	0	6430	122	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 10.

All (122) 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:ALA:O	1:B:111:VAL:HG22	1.29	1.24
1:A:195:TYR:CD2	1:A:231:THR:CG2	2.26	1.19
1:A:195:TYR:CD2	1:A:231:THR:HG22	1.78	1.17
2:C:525:GLN:O	2:C:526:LYS:HB2	1.46	1.13
1:A:195:TYR:CE2	1:A:231:THR:HG23	1.83	1.13
2:D:482:GLU:HA	2:D:482:GLU:OE1	1.31	1.13
1:B:110:ALA:O	1:B:111:VAL:CG2	1.96	1.11
1:B:391:ARG:HH11	1:B:391:ARG:CG	1.64	1.10
2:C:520:ASN:OD1	2:C:522:LYS:HG2	1.58	1.03
1:B:178:PHE:O	1:B:178:PHE:HD2	1.45	0.99
1:B:391:ARG:HH11	1:B:391:ARG:HG3	1.28	0.99
1:A:358:GLN:HB2	1:A:360:THR:HG22	1.45	0.98
1:A:229:THR:HG22	1:A:231:THR:H	1.27	0.97
1:A:229:THR:HB	1:A:232:SER:OG	1.67	0.94
1:B:110:ALA:C	1:B:111:VAL:HG22	1.92	0.94
2:D:482:GLU:OE1	2:D:482:GLU:CA	2.19	0.87
1:A:195:TYR:CD2	1:A:231:THR:HG23	1.99	0.86
1:A:195:TYR:HD2	1:A:231:THR:HG22	1.42	0.85
1:A:315:LYS:HZ1	1:A:345:GLU:HG2	1.42	0.84
1:A:70:ASN:ND2	1:A:136:ASP:HB2	1.91	0.84
1:B:178:PHE:O	1:B:178:PHE:CD2	2.30	0.84
1:B:391:ARG:HH11	1:B:391:ARG:HG2	1.45	0.81
1:A:355:TYR:HD1	1:A:360:THR:HG23	1.45	0.80
2:C:520:ASN:OD1	2:C:522:LYS:CG	2.30	0.79
1:A:229:THR:CB	1:A:232:SER:OG	2.32	0.78
1:A:315:LYS:NZ	1:A:345:GLU:HG2	1.97	0.77
1:B:178:PHE:CD2	1:B:178:PHE:C	2.69	0.71
1:A:315:LYS:HZ3	1:A:345:GLU:CD	1.99	0.70
1:B:320:SER:HA	1:B:384:TYR:OH	1.92	0.69
1:B:131:HIS:CD2	1:B:187:SER:HB3	2.29	0.68
1:A:16:ASN:HD22	1:A:177:GLY:HA3	1.59	0.68
1:B:119:PRO:HA	2:C:526:LYS:HE2	1.75	0.67
1:B:391:ARG:HG3	1:B:391:ARG:NH1	2.00	0.67
1:B:55:ARG:NH2	1:B:302:GLU:OE2	2.29	0.66
1:A:150:GLN:OE1	1:A:160:ARG:NH2	2.28	0.66
1:A:315:LYS:NZ	1:A:345:GLU:OE1	2.20	0.66
1:B:388:ASN:HD22	1:B:391:ARG:H	1.44	0.66
2:C:525:GLN:O	2:C:526:LYS:CB	2.33	0.65
1:A:211:TYR:O	1:A:215:TRP:CD1	2.50	0.65
1:B:387:GLU:OE2	1:B:395:ARG:NH2	2.27	0.64
1:B:391:ARG:CG	1:B:391:ARG:NH1	2.37	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:HD22	1:B:120:ASN:HD22	1.46	0.63
1:B:189:VAL:H	1:B:223:GLN:HE22	1.47	0.63
1:B:150:GLN:OE1	1:B:160:ARG:NH2	2.31	0.63
1:B:170:SER:OG	1:B:206:LEU:HD12	1.99	0.63
1:B:63:GLY:O	1:B:222:HIS:HD2	1.83	0.62
1:B:344:GLU:OE2	1:B:399:ARG:NH1	2.33	0.62
1:A:191:ASP:HB3	1:A:232:SER:O	2.00	0.62
1:A:189:VAL:H	1:A:223:GLN:HE22	1.47	0.61
1:B:211:TYR:HD1	1:B:214:GLU:OE1	1.83	0.61
1:B:180:LYS:HB3	1:B:215:TRP:CE3	2.36	0.60
1:A:63:GLY:O	1:A:222:HIS:HD2	1.84	0.60
1:A:191:ASP:CB	1:A:232:SER:O	2.50	0.60
1:A:70:ASN:HD21	1:A:136:ASP:HB2	1.65	0.59
1:A:195:TYR:HD2	1:A:231:THR:CG2	1.98	0.59
1:B:391:ARG:HG2	1:B:391:ARG:NH1	2.14	0.58
1:A:206:LEU:HD21	2:C:496:ILE:CG2	2.34	0.58
1:B:390:GLN:HE22	1:B:404:THR:HA	1.69	0.58
1:A:229:THR:CG2	1:A:232:SER:OG	2.53	0.57
1:A:340:ILE:HD11	1:A:395:ARG:HE	1.69	0.57
1:A:315:LYS:NZ	1:A:345:GLU:CG	2.68	0.56
1:A:135:ASP:O	1:A:136:ASP:C	2.49	0.56
1:B:364:VAL:HG23	1:B:365:GLU:OE2	2.06	0.56
1:A:366:ASN:O	1:A:368:LYS:HE2	2.06	0.55
1:A:191:ASP:HB3	1:A:232:SER:C	2.31	0.55
1:A:195:TYR:CE2	1:A:231:THR:CG2	2.61	0.55
1:B:110:ALA:O	1:B:111:VAL:HG23	1.99	0.54
2:C:520:ASN:CG	2:C:522:LYS:HG2	2.32	0.54
1:A:355:TYR:CD1	1:A:360:THR:HG23	2.35	0.53
1:B:19:ARG:HE	1:B:293:ASN:HD21	1.56	0.53
1:A:320:SER:HA	1:A:384:TYR:OH	2.08	0.53
1:A:360:THR:HG21	4:A:663:HOH:O	2.09	0.53
1:A:264:GLN:NE2	2:C:489:ASN:OD1	2.42	0.52
1:B:387:GLU:CD	1:B:395:ARG:HH21	2.16	0.52
2:D:487:LEU:HD23	2:D:487:LEU:N	2.23	0.52
1:B:196:HIS:O	1:B:200:GLU:HG2	2.11	0.51
2:C:520:ASN:OD1	2:C:522:LYS:CD	2.59	0.50
1:A:48:ILE:HD11	1:A:306:LEU:HD21	1.94	0.50
1:A:93:PRO:HA	2:C:522:LYS:HD3	1.94	0.50
1:B:70:ASN:ND2	1:B:136:ASP:HB3	2.28	0.49
1:A:329:VAL:HG12	1:A:330:GLU:H	1.77	0.48
1:A:192:GLU:HA	1:A:231:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:GLN:NE2	1:A:404:THR:HG23	2.30	0.47
1:A:70:ASN:HD22	1:A:136:ASP:HB2	1.73	0.47
1:A:92:LYS:HB3	1:A:124:ALA:HB1	1.97	0.46
1:A:252:HIS:CE1	1:A:277:THR:OG1	2.69	0.46
1:B:55:ARG:HH22	1:B:302:GLU:CD	2.23	0.46
1:A:206:LEU:HD21	2:C:496:ILE:HG21	1.97	0.46
2:C:526:LYS:O	2:C:526:LYS:HD3	2.16	0.46
1:A:229:THR:HG21	1:A:232:SER:OG	2.16	0.46
1:B:92:LYS:HB3	1:B:124:ALA:HB1	1.96	0.46
1:B:390:GLN:NE2	1:B:404:THR:HA	2.30	0.46
2:C:522:LYS:HG2	2:C:522:LYS:H	1.51	0.45
2:C:520:ASN:CG	2:C:522:LYS:CG	2.89	0.45
1:A:368:LYS:HD3	1:A:368:LYS:HA	1.41	0.45
1:B:388:ASN:ND2	1:B:391:ARG:H	2.12	0.45
2:D:487:LEU:HB3	2:D:490:LEU:HD21	1.99	0.44
1:B:15:GLU:CD	1:B:15:GLU:H	2.23	0.44
1:B:393:SER:HB3	1:B:403:ALA:C	2.43	0.44
1:B:314:MET:HE2	1:B:375:ARG:HD3	2.00	0.44
1:A:354:TRP:O	1:A:358:GLN:HG2	2.18	0.44
1:B:340:ILE:O	1:B:344:GLU:HG2	2.18	0.44
1:A:315:LYS:NZ	1:A:345:GLU:CD	2.70	0.44
1:A:322:VAL:HB	1:A:325:ILE:HD12	1.99	0.44
1:A:390:GLN:HE22	1:A:404:THR:HG23	1.84	0.43
1:B:354:TRP:O	1:B:358:GLN:HG2	2.18	0.43
1:B:19:ARG:HE	1:B:293:ASN:ND2	2.17	0.43
1:B:332:LYS:H	1:B:385:GLN:HE21	1.68	0.42
1:A:131:HIS:HD2	1:A:157:TYR:OH	2.02	0.42
1:B:225:HIS:HE1	1:B:236:GLU:OE1	2.03	0.42
1:A:94:CYS:H	2:C:522:LYS:HD2	1.85	0.42
1:A:358:GLN:HB2	1:A:360:THR:CG2	2.31	0.42
1:B:178:PHE:HD2	1:B:178:PHE:C	2.08	0.42
1:B:211:TYR:HD1	1:B:214:GLU:CD	2.28	0.41
1:A:229:THR:HG22	1:A:231:THR:N	2.11	0.41
1:A:322:VAL:CG1	1:A:325:ILE:HD12	2.51	0.41
1:A:360:THR:OG1	1:A:361:VAL:N	2.53	0.41
1:B:396:PHE:O	1:B:399:ARG:HB2	2.20	0.41
1:A:332:LYS:HD2	1:A:386:THR:O	2.21	0.41
1:A:192:GLU:HG2	1:A:231:THR:HB	2.03	0.40
1:A:293:ASN:O	1:A:299:PHE:HA	2.22	0.40
1:B:131:HIS:CD2	1:B:187:SER:CB	3.02	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	371/417 (89%)	358 (96%)	13 (4%)	0	100	100
1	B	380/417 (91%)	362 (95%)	17 (4%)	1 (0%)	36	42
2	C	17/59 (29%)	15 (88%)	2 (12%)	0	100	100
2	D	14/59 (24%)	13 (93%)	1 (7%)	0	100	100
All	All	782/952 (82%)	748 (96%)	33 (4%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	VAL

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	343/376 (91%)	321 (94%)	22 (6%)	16	19
1	B	349/376 (93%)	325 (93%)	24 (7%)	14	16
2	C	20/53 (38%)	15 (75%)	5 (25%)	0	0
2	D	15/53 (28%)	12 (80%)	3 (20%)	1	1
All	All	727/858 (85%)	673 (93%)	54 (7%)	13	14

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	48	ILE
1	A	151	VAL
1	A	196	HIS
1	A	199	ARG
1	A	210	LEU
1	A	226	SER
1	A	231	THR
1	A	251	GLU
1	A	263	THR
1	A	266	PHE
1	A	267	THR
1	A	324	SER
1	A	334	GLU
1	A	336	LEU
1	A	345	GLU
1	A	348	THR
1	A	360	THR
1	A	364	VAL
1	A	365	GLU
1	A	368	LYS
1	A	371	LEU
1	B	15	GLU
1	B	27	HIS
1	B	55	ARG
1	B	112	CYS
1	B	131	HIS
1	B	142	ARG
1	B	151	VAL
1	B	166	ASN
1	B	178	PHE
1	B	199	ARG
1	B	229	THR
1	B	266	PHE
1	B	280	SER
1	B	292	LEU
1	B	305	ARG
1	B	332	LYS
1	B	333	LYS
1	B	336	LEU
1	B	364	VAL
1	B	365	GLU
1	B	371	LEU

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Mol	Chain	Res	Type
1	B	391	ARG
1	B	404	THR
1	B	405	ASP
2	C	487	LEU
2	C	496	ILE
2	C	522	LYS
2	C	525	GLN
2	C	526	LYS
2	D	482	GLU
2	D	485	ARG
2	D	487	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	70	ASN
1	A	222	HIS
1	A	223	GLN
1	A	240	GLN
1	A	353	GLN
1	A	366	ASN
1	A	390	GLN
1	A	394	ASN
1	B	70	ASN
1	B	120	ASN
1	B	188	ASN
1	B	222	HIS
1	B	223	GLN
1	B	224	ASN
1	B	225	HIS
1	B	264	GLN
1	B	293	ASN
1	B	385	GLN
1	B	388	ASN
1	B	390	GLN
2	C	484	ASN
2	D	484	ASN
2	D	489	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	379/417 (90%)	0.91	65 (17%) 4 3	19, 44, 80, 116	21 (5%)
1	B	386/417 (92%)	0.61	46 (11%) 9 7	25, 40, 71, 116	19 (4%)
2	C	21/59 (35%)	3.33	18 (85%) 0 0	18, 72, 94, 105	7 (33%)
2	D	16/59 (27%)	2.36	11 (68%) 0 0	41, 73, 107, 140	6 (37%)
All	All	802/952 (84%)	0.86	140 (17%) 4 3	18, 43, 82, 140	53 (6%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	110	ALA	7.9
2	C	490	LEU	5.9
1	B	403	ALA	5.8
1	B	165	ASP	5.6
1	A	360	THR	5.6
2	C	497	ARG	5.3
2	C	521	PHE	4.9
2	C	487	LEU	4.8
1	A	230	PRO	4.7
1	A	166	ASN	4.7
1	A	239	ILE	4.6
1	B	404	THR	4.6
1	B	163	GLU	4.5
1	A	228	HIS	4.5
1	A	232	SER	4.4
1	B	136	ASP	4.4
2	C	488	ARG	4.3
1	B	228	HIS	4.2
1	A	226	SER	4.1
1	A	142	ARG	4.1
1	A	263	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	230	PRO	4.0
2	C	486	ARG	4.0
1	B	361	VAL	4.0
2	D	497	ARG	4.0
1	A	267	THR	4.0
2	C	526	LYS	3.9
1	B	360	THR	3.9
1	B	101	ASP	3.9
1	B	211	TYR	3.9
1	A	227	ALA	3.9
1	A	199	ARG	3.9
1	B	112	CYS	3.8
1	A	135	ASP	3.7
1	A	361	VAL	3.7
2	D	493	VAL	3.7
1	B	142	ARG	3.7
2	C	524	PHE	3.6
2	D	487	LEU	3.6
1	A	268	VAL	3.6
2	D	482	GLU	3.6
1	A	206	LEU	3.6
2	C	523	LYS	3.5
1	A	262	PRO	3.5
1	A	14	ASN	3.4
1	A	136	ASP	3.4
1	A	211	TYR	3.4
1	B	359	GLY	3.4
1	A	234	LEU	3.3
1	B	170	SER	3.3
1	B	166	ASN	3.3
1	A	238	PHE	3.3
1	A	198	PHE	3.3
1	A	229	THR	3.3
2	C	491	GLY	3.3
1	A	195	TYR	3.2
1	A	162	PRO	3.2
2	D	484	ASN	3.2
1	A	231	THR	3.2
1	B	178	PHE	3.1
1	A	182	ALA	3.1
1	A	237	SER	3.0
2	C	520	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	412	LYS	3.0
1	A	364	VAL	3.0
1	B	330	GLU	3.0
2	C	493	VAL	3.0
1	A	209	ASP	3.0
1	B	210	LEU	2.9
2	C	525	GLN	2.9
2	C	496	ILE	2.9
1	B	197	SER	2.9
1	B	412	LYS	2.9
1	A	300	HIS	2.9
1	A	205	PHE	2.9
1	A	210	LEU	2.9
1	A	203	VAL	2.8
2	D	483	GLU	2.8
2	C	522	LYS	2.8
1	B	111	VAL	2.8
1	B	402	ASN	2.7
1	B	196	HIS	2.7
1	B	203	VAL	2.7
1	A	345	GLU	2.7
1	B	344	GLU	2.7
1	B	397	VAL	2.7
1	A	99	LEU	2.7
1	A	168	VAL	2.6
1	B	391	ARG	2.6
1	B	231	THR	2.6
1	A	403	ALA	2.6
2	C	485	ARG	2.6
1	B	164	ASN	2.6
1	A	169	VAL	2.6
1	A	194	LEU	2.5
1	B	201	ASN	2.5
1	A	368	LYS	2.5
1	A	242	PHE	2.5
1	A	261	ASN	2.5
1	B	364	VAL	2.5
2	D	485	ARG	2.5
1	A	201	ASN	2.5
1	A	233	TYR	2.4
1	A	260	TYR	2.4
1	A	189	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	256	ILE	2.4
2	C	484	ASN	2.3
1	B	263	THR	2.3
1	B	168	VAL	2.3
1	A	131	HIS	2.3
1	A	212	ARG	2.3
2	D	486	ARG	2.3
2	D	494	GLU	2.3
1	B	93	PRO	2.3
1	A	259	SER	2.3
1	B	133	ASN	2.3
1	A	356	GLU	2.3
1	B	33	LYS	2.3
1	B	205	PHE	2.2
2	D	488	ARG	2.2
1	A	202	LYS	2.2
1	B	362	PRO	2.2
1	A	95	GLU	2.2
1	A	225	HIS	2.2
1	B	122	ASN	2.2
1	A	367	GLU	2.2
1	A	359	GLY	2.2
1	A	324	SER	2.2
1	A	213	ASP	2.1
1	A	196	HIS	2.1
1	B	195	TYR	2.1
1	A	167	ILE	2.1
1	B	382	GLY	2.1
2	C	494	GLU	2.1
1	B	262	PRO	2.1
1	A	307	ARG	2.1
1	A	143	TYR	2.0
2	D	495	TYR	2.0
1	B	200	GLU	2.0
1	B	193	ARG	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 [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
3	MN	A	501	1/1	0.96	0.05	45,45,45,45	0
3	MN	B	502	1/1	0.96	0.06	34,34,34,34	0
3	MN	B	501	1/1	0.97	0.07	40,40,40,40	0
3	MN	A	502	1/1	0.98	0.06	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.