



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:39 AM UTC

PDB ID : 9GP1 / pdb_00009gp1
Title : Jumonji domain-containing protein 2A with crystallization epitope mutations K330R:A334E
Authors : Fairhead, M.; Strain-Damerell, C.; Ye, M.; Mackinnon, S.R.; Pinkas, D.; MacLean, E.M.; Koekemoer, L.; Damerell, D.; Krojer, T.; Arrowsmith, C.H.; Edwards, A.; Bountra, C.; Yue, W.; Burgess-Brown, N.; Marsden, B.; von Delft, F.; Structural Genomics Consortium (SGC)
Deposited on : 2024-09-06
Resolution : 2.21 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)	:	Engl & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

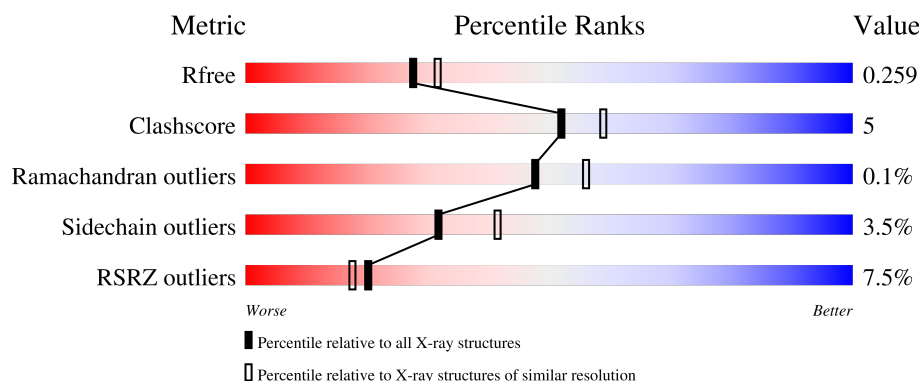
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	360	15% 84% 11% ..
1	B	360	4% 85% 13% ..
1	C	360	7% 85% 11% ..
1	D	360	2% 83% 12% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11668 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 Lysine-specific demethylase 4A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2667	1727	442	484	14			
1	B	355	Total	C	N	O	S	0	0	0
			2849	1839	473	522	15			
1	C	348	Total	C	N	O	S	0	0	0
			2783	1805	457	507	14			
1	D	348	Total	C	N	O	S	0	1	0
			2824	1827	471	511	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP O75164
A	331	ARG	LYS	engineered mutation	UNP O75164
A	335	GLU	ALA	engineered mutation	UNP O75164
B	1	SER	-	expression tag	UNP O75164
B	331	ARG	LYS	engineered mutation	UNP O75164
B	335	GLU	ALA	engineered mutation	UNP O75164
C	1	SER	-	expression tag	UNP O75164
C	331	ARG	LYS	engineered mutation	UNP O75164
C	335	GLU	ALA	engineered mutation	UNP O75164
D	2	SER	-	expression tag	UNP O75164
D	331	ARG	LYS	engineered mutation	UNP O75164
D	335	GLU	ALA	engineered mutation	UNP O75164

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ni	0	0
			1	1		
2	B	1	Total	Ni	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Ni 1	0	0
2	D	1	Total 1	Ni 1	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0

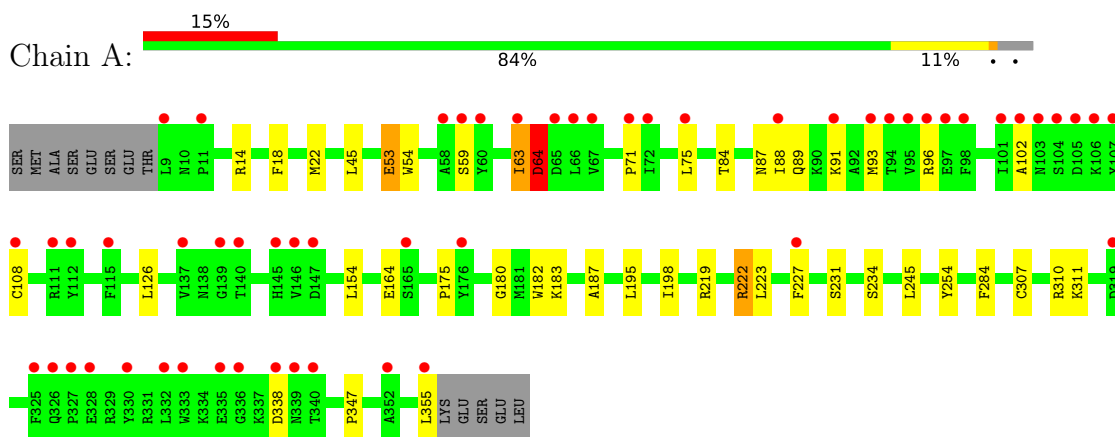
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total 50	O 50	0	0
4	B	157	Total 157	O 157	0	0
4	C	115	Total 115	O 115	0	0
4	D	215	Total 215	O 215	0	0

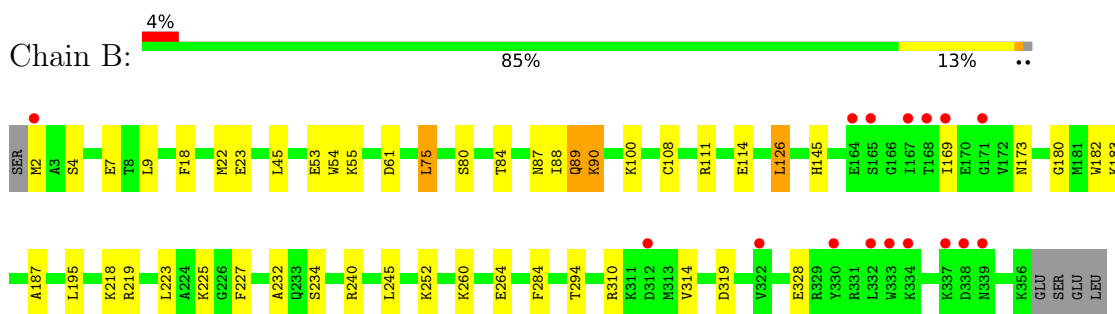
3 Residue-property plots [i](#)

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

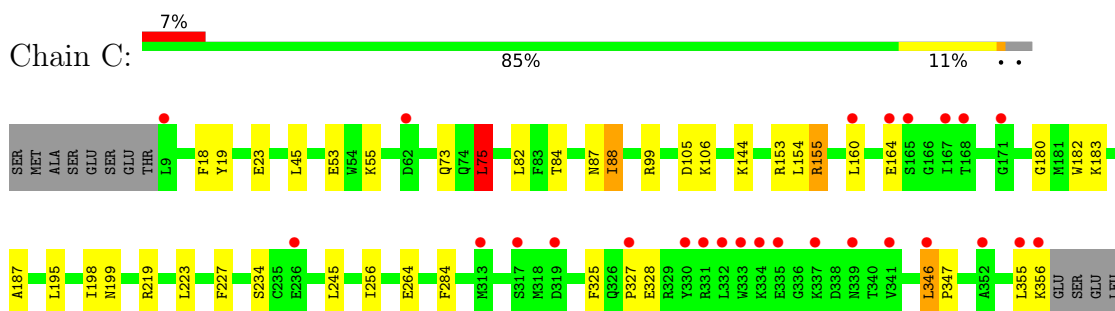
- Molecule 1: Lysine-specific demethylase 4A



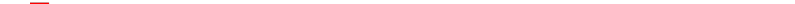
- Molecule 1: Lysine-specific demethylase 4A

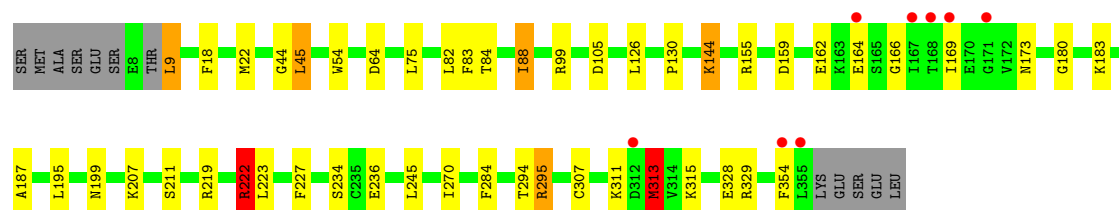


- Molecule 1: Lysine-specific demethylase 4A



- Molecule 1: Lysine-specific demethylase 4A

Chain D:  2% 83% 12% ...



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.03Å 101.60Å 141.43Å 90.00° 99.38° 90.00°	Depositor
Resolution (Å)	82.14 – 2.21 82.14 – 2.21	Depositor EDS
% Data completeness (in resolution range)	97.6 (82.14-2.21) 97.6 (82.14-2.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.82)	Depositor
R, R_{free}	0.215 , 0.259 0.215 , 0.259	Depositor DCC
R_{free} test set	3949 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.064 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11668	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.94 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1500e-03.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	0/2749	1.13	5/3752 (0.1%)
1	B	0.64	0/2936	1.23	11/3989 (0.3%)
1	C	0.58	0/2870	1.19	11/3904 (0.3%)
1	D	0.68	0/2911	1.21	15/3952 (0.4%)
All	All	0.62	0/11466	1.19	42/15597 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	264	GLU	CB-CG-CD	9.98	129.57	112.60
1	B	84	THR	CA-CB-OG1	-7.29	98.67	109.60
1	B	18	PHE	CA-CB-CG	-7.29	106.52	113.80
1	D	105	ASP	CA-CB-CG	7.05	119.65	112.60
1	C	84	THR	CA-CB-OG1	-6.76	99.46	109.60
1	C	328	GLU	CB-CG-CD	6.60	123.82	112.60
1	D	328	GLU	CB-CG-CD	6.49	123.64	112.60
1	C	164	GLU	CB-CG-CD	6.41	123.50	112.60
1	D	84	THR	CA-CB-OG1	-6.24	100.24	109.60
1	B	145	HIS	CA-CB-CG	-6.12	107.69	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	130	PRO	CB-CA-C	6.08	118.34	110.92
1	A	18	PHE	CA-CB-CG	-6.06	107.74	113.80
1	D	222	ARG	CG-CD-NE	6.00	125.20	112.00
1	D	18	PHE	CA-CB-CG	-5.99	107.81	113.80
1	D	45	LEU	N-CA-CB	-5.92	100.42	111.13
1	D	354	PHE	CA-CB-CG	5.90	119.70	113.80
1	C	155	ARG	CA-CB-CG	5.88	125.87	114.10
1	C	105	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	338	ASP	CB-CA-C	5.73	121.82	110.42
1	C	45	LEU	N-CA-CB	-5.70	100.82	111.13
1	B	294	THR	CA-CB-OG1	-5.69	101.06	109.60
1	C	164	GLU	N-CA-CB	5.64	118.94	110.19
1	D	294	THR	CA-CB-OG1	-5.64	101.14	109.60
1	B	310	ARG	CA-CB-CG	5.57	125.24	114.10
1	A	195	LEU	N-CA-CB	-5.53	102.81	110.38
1	B	75	LEU	N-CA-CB	-5.48	101.12	110.16
1	B	45	LEU	N-CA-CB	-5.47	101.33	111.13
1	D	311	LYS	CB-CA-C	5.44	118.72	109.53
1	D	315	LYS	CG-CD-CE	5.37	123.66	111.30
1	A	84	THR	CA-CB-OG1	-5.35	101.57	109.60
1	D	313	MET	CB-CG-SD	5.31	128.64	112.70
1	C	195	LEU	N-CA-CB	-5.29	103.06	110.25
1	A	45	LEU	N-CA-CB	-5.21	101.69	111.13
1	C	18	PHE	CA-CB-CG	-5.20	108.60	113.80
1	B	195	LEU	N-CA-CB	-5.17	103.30	110.38
1	D	195	LEU	N-CA-CB	-5.15	103.25	110.25
1	B	260	LYS	CB-CA-C	-5.13	98.17	109.56
1	B	173	ASN	CB-CA-C	5.06	119.11	110.56
1	C	75	LEU	N-CA-CB	-5.04	101.84	110.16
1	D	295	ARG	CG-CD-NE	-5.04	100.92	112.00
1	D	164	GLU	CB-CG-CD	5.03	121.15	112.60
1	B	126	LEU	N-CA-CB	5.00	118.70	110.39

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	219	ARG	Sidechain
1	D	219	ARG	Sidechain

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	2667	0	2433	32	0
1	B	2849	0	2690	25	0
1	C	2783	0	2620	23	0
1	D	2824	0	2690	34	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	50	0	0	2	0
4	B	157	0	0	8	1
4	C	115	0	0	8	0
4	D	215	0	0	8	1
All	All	11668	0	10433	110	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:CB	1:D:166:GLY:O	2.04	1.04
1:D:75[A]:LEU:CD1	1:D:88:ILE:HD11	1.88	1.03
1:D:199:ASN:HB2	4:D:677:HOH:O	1.62	0.98
1:D:295:ARG:NH1	1:D:295:ARG:HG3	1.83	0.93
1:D:75[A]:LEU:HD12	1:D:88:ILE:HD11	1.49	0.91
1:A:75:LEU:HD12	1:A:88:ILE:HG12	1.54	0.86
1:D:211:SER:OG	4:D:501:HOH:O	1.95	0.84
1:D:75[A]:LEU:HD11	1:D:88:ILE:HD11	1.61	0.81
1:D:295:ARG:HG3	1:D:295:ARG:HH11	1.44	0.78
1:D:22:MET:HE1	1:D:54:TRP:HB2	1.65	0.77
1:C:87:ASN:C	1:C:88:ILE:HD13	2.11	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ASN:C	1:B:88:ILE:HD13	2.11	0.74
1:A:87:ASN:C	1:A:88:ILE:HD13	2.15	0.72
1:A:22:MET:HE1	1:A:54:TRP:HB2	1.72	0.71
1:C:144:LYS:O	1:C:153:ARG:NH1	2.25	0.70
1:C:73:GLN:OE1	4:C:501:HOH:O	2.09	0.70
1:D:155:ARG:HH11	1:D:155:ARG:HG3	1.56	0.70
1:A:64:ASP:OD1	1:A:96:ARG:N	2.23	0.69
1:C:356:LYS:O	4:C:502:HOH:O	2.12	0.67
1:D:44:GLY:HA3	4:D:501:HOH:O	1.96	0.66
1:D:64:ASP:OD1	1:D:99:ARG:NH2	2.29	0.66
1:A:222:ARG:HG3	1:A:222:ARG:HH11	1.61	0.65
1:C:88:ILE:HD13	1:C:88:ILE:N	2.11	0.63
1:B:223:LEU:HD11	1:B:227:PHE:CE2	2.33	0.63
1:D:183:LYS:HG2	4:D:616:HOH:O	1.99	0.62
1:A:223:LEU:HD11	1:A:227:PHE:CE2	2.35	0.61
1:A:311:LYS:CA	1:D:166:GLY:O	2.48	0.60
1:C:223:LEU:HD11	1:C:227:PHE:CE2	2.37	0.60
1:A:59:SER:HB2	4:A:501:HOH:O	2.02	0.60
1:A:102:ALA:O	1:A:108:CYS:HA	2.02	0.58
1:A:63:ILE:O	1:A:64:ASP:HB2	2.04	0.58
1:A:75:LEU:HD12	1:A:88:ILE:CG1	2.33	0.57
1:D:222:ARG:HG2	1:D:222:ARG:HH11	1.69	0.57
1:D:329:ARG:NE	4:D:510:HOH:O	2.36	0.57
1:C:153:ARG:HG3	4:C:560:HOH:O	2.05	0.57
1:B:88:ILE:HD13	1:B:88:ILE:N	2.19	0.57
1:B:183:LYS:HG2	4:B:572:HOH:O	2.03	0.56
1:C:55:LYS:HG2	4:C:614:HOH:O	2.06	0.56
1:B:218:LYS:NZ	4:B:504:HOH:O	2.38	0.56
1:A:59:SER:CB	4:A:501:HOH:O	2.54	0.55
1:B:80:SER:HB2	4:B:612:HOH:O	2.05	0.55
1:D:223:LEU:HD11	1:D:227:PHE:CE2	2.42	0.55
1:D:75[A]:LEU:HD12	1:D:88:ILE:CD1	2.31	0.54
1:B:22:MET:HE1	1:B:54:TRP:HB2	1.89	0.54
1:D:159:ASP:HA	4:D:505:HOH:O	2.07	0.54
1:B:22:MET:CE	1:B:53:GLU:HG2	2.39	0.53
1:C:199:ASN:HB2	4:C:517:HOH:O	2.09	0.52
1:A:254:TYR:CE2	1:C:19:TYR:CD1	2.98	0.52
1:A:87:ASN:O	1:A:88:ILE:HD13	2.10	0.52
1:A:75:LEU:CD1	1:A:88:ILE:HG12	2.34	0.52
1:D:236:GLU:O	4:D:502:HOH:O	2.19	0.51
1:B:225:LYS:HG3	1:B:232:ALA:CB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:162:GLU:HB2	1:D:173:ASN:ND2	2.25	0.51
1:A:63:ILE:O	1:A:64:ASP:CB	2.60	0.49
1:D:75[B]:LEU:C	1:D:75[B]:LEU:HD23	2.38	0.49
1:D:64:ASP:CG	1:D:99:ARG:HH22	2.21	0.49
1:A:88:ILE:HD13	1:A:88:ILE:N	2.25	0.49
1:D:295:ARG:HH11	1:D:295:ARG:CG	2.21	0.49
1:B:4:SER:OG	1:B:7:GLU:HG3	2.13	0.49
1:B:111:ARG:HA	4:B:534:HOH:O	2.12	0.48
1:B:187:ALA:HA	1:B:245:LEU:HD23	1.96	0.48
1:C:73:GLN:HB3	4:C:501:HOH:O	2.13	0.47
1:D:187:ALA:HA	1:D:245:LEU:HD23	1.95	0.47
1:A:22:MET:HE3	1:A:53:GLU:HG2	1.96	0.47
1:A:64:ASP:OD1	1:A:96:ARG:HB2	2.15	0.47
1:D:222:ARG:HH11	1:D:222:ARG:CG	2.27	0.47
1:C:325:PHE:C	1:C:327:PRO:HD3	2.39	0.47
1:A:175:PRO:HD2	1:D:144:LYS:NZ	2.30	0.47
1:A:71:PRO:HG3	1:A:93:MET:HG2	1.97	0.46
1:B:225:LYS:HE3	1:B:225:LYS:HB2	1.49	0.46
1:C:187:ALA:HA	1:C:245:LEU:HD23	1.98	0.45
1:B:126:LEU:H	1:B:126:LEU:HD23	1.81	0.45
1:C:182:TRP:O	1:C:183:LYS:HB3	2.17	0.45
1:C:154:LEU:HD11	1:C:198:ILE:HG21	1.98	0.45
1:B:75:LEU:HD12	1:B:88:ILE:HG12	1.98	0.45
1:B:89:GLN:O	1:B:90:LYS:NZ	2.50	0.45
1:C:99:ARG:NH1	4:C:519:HOH:O	2.50	0.45
1:B:183:LYS:HE3	4:B:568:HOH:O	2.16	0.44
1:B:225:LYS:HG3	1:B:232:ALA:HB1	1.98	0.44
1:A:22:MET:CE	1:A:53:GLU:HG2	2.47	0.44
1:B:87:ASN:O	1:B:88:ILE:HD13	2.17	0.44
1:B:182:TRP:O	1:B:183:LYS:HB3	2.18	0.44
1:B:87:ASN:ND2	4:B:519:HOH:O	2.50	0.44
1:D:155:ARG:HH11	1:D:155:ARG:CG	2.29	0.44
1:A:154:LEU:HD11	1:A:198:ILE:HG21	2.00	0.43
1:C:106:LYS:NZ	4:C:518:HOH:O	2.50	0.43
1:D:207:LYS:HE3	4:D:653:HOH:O	2.19	0.42
1:A:64:ASP:CG	1:A:96:ARG:HB2	2.44	0.42
1:D:307:CYS:HB3	1:D:313:MET:HG3	2.01	0.42
1:D:83:PHE:CZ	1:D:126:LEU:HD21	2.54	0.42
1:D:75[A]:LEU:CD1	1:D:88:ILE:CD1	2.79	0.42
1:A:307:CYS:SG	1:A:310:ARG:HG2	2.60	0.41
1:C:219:ARG:HD2	1:C:256:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:TRP:O	1:A:183:LYS:HB3	2.20	0.41
1:A:219:ARG:HE	1:A:219:ARG:HB2	1.54	0.41
1:C:160:LEU:CD1	1:C:325:PHE:HE2	2.32	0.41
1:A:187:ALA:HA	1:A:245:LEU:HD23	2.02	0.41
1:C:154:LEU:O	1:C:155:ARG:HG2	2.20	0.41
1:C:180:GLY:O	1:C:284:PHE:HA	2.21	0.41
1:A:347:PRO:HG3	1:A:355:LEU:HD11	2.02	0.41
1:C:75:LEU:HD12	1:C:88:ILE:HG12	2.02	0.41
1:C:346:LEU:HD22	1:C:347:PRO:HD2	2.02	0.41
1:D:180:GLY:O	1:D:284:PHE:HA	2.20	0.41
1:B:169:ILE:HG21	1:B:314:VAL:HG13	2.02	0.41
1:A:126:LEU:HD23	1:A:126:LEU:H	1.86	0.40
1:A:180:GLY:O	1:A:284:PHE:HA	2.21	0.40
1:B:180:GLY:O	1:B:284:PHE:HA	2.21	0.40
1:B:108:CYS:HB2	4:B:622:HOH:O	2.22	0.40
1:D:45:LEU:HA	1:D:270:ILE:O	2.22	0.40
1:B:240:ARG:HG2	4:B:514:HOH:O	2.21	0.40

All (1) 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)
4:B:639:HOH:O	4:D:634:HOH:O[2_545]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	345/360 (96%)	336 (97%)	8 (2%)	1 (0%)	36	41
1	B	353/360 (98%)	345 (98%)	8 (2%)	0	100	100
1	C	346/360 (96%)	340 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	347/360 (96%)	340 (98%)	6 (2%)	1 (0%)	36	41
All	All	1391/1440 (97%)	1361 (98%)	28 (2%)	2 (0%)	48	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ASP
1	D	9	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	258/317 (81%)	248 (96%)	10 (4%)	28	37
1	B	295/317 (93%)	281 (95%)	14 (5%)	23	29
1	C	286/317 (90%)	278 (97%)	8 (3%)	38	50
1	D	294/317 (93%)	286 (97%)	8 (3%)	39	52
All	All	1133/1268 (89%)	1093 (96%)	40 (4%)	32	41

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ARG
1	A	53	GLU
1	A	63	ILE
1	A	64	ASP
1	A	89	GLN
1	A	91	LYS
1	A	164	GLU
1	A	222	ARG
1	A	231	SER
1	A	234	SER
1	B	2	MET
1	B	9	LEU

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Mol	Chain	Res	Type
1	B	23	GLU
1	B	55	LYS
1	B	61	ASP
1	B	89	GLN
1	B	90	LYS
1	B	100	LYS
1	B	114	GLU
1	B	234	SER
1	B	252	LYS
1	B	264	GLU
1	B	319	ASP
1	B	328	GLU
1	C	23	GLU
1	C	53	GLU
1	C	75	LEU
1	C	82	LEU
1	C	88	ILE
1	C	234	SER
1	C	346	LEU
1	C	355	LEU
1	D	9	LEU
1	D	82	LEU
1	D	88	ILE
1	D	144	LYS
1	D	169	ILE
1	D	222	ARG
1	D	234	SER
1	D	313	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	B	87	ASN
1	C	216	HIS
1	D	216	HIS

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 oligosaccharides 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	A	347/360 (96%)	0.89	55 (15%) 5 4	24, 51, 89, 113	0
1	B	355/360 (98%)	0.21	16 (4%) 38 35	16, 34, 76, 103	0
1	C	348/360 (96%)	0.56	26 (7%) 20 17	24, 42, 80, 129	0
1	D	348/360 (96%)	-0.06	8 (2%) 61 59	10, 29, 63, 114	1 (0%)
All	All	1398/1440 (97%)	0.40	105 (7%) 20 17	10, 39, 83, 129	1 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ASN	5.0
1	D	167	ILE	4.4
1	A	9	LEU	3.9
1	B	167	ILE	3.7
1	D	169	ILE	3.7
1	A	102	ALA	3.7
1	C	332	LEU	3.6
1	D	168	THR	3.6
1	B	332	LEU	3.6
1	A	325	PHE	3.6
1	B	2	MET	3.5
1	A	98	PHE	3.5
1	C	335	GLU	3.5
1	C	330	TYR	3.4
1	A	355	LEU	3.3
1	C	167	ILE	3.3
1	A	71	PRO	3.3
1	A	339	ASN	3.2
1	D	171	GLY	3.2
1	A	227	PHE	3.2
1	A	105	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	330	TYR	3.1
1	B	169	ILE	3.1
1	A	106	LYS	3.1
1	A	91	LYS	3.1
1	D	312	ASP	3.1
1	B	164	GLU	3.1
1	C	333	TRP	3.1
1	B	339	ASN	3.1
1	A	115	PHE	3.0
1	A	63	ILE	3.0
1	B	168	THR	3.0
1	A	66	LEU	2.9
1	B	312	ASP	2.9
1	A	94	THR	2.9
1	A	104	SER	2.9
1	C	171	GLY	2.9
1	C	9	LEU	2.9
1	A	88	ILE	2.9
1	A	147	ASP	2.9
1	C	160	LEU	2.8
1	A	146	VAL	2.8
1	A	65	ASP	2.8
1	C	331	ARG	2.8
1	A	107	TYR	2.8
1	C	168	THR	2.8
1	A	332	LEU	2.8
1	A	328	GLU	2.7
1	D	355	LEU	2.7
1	A	335	GLU	2.7
1	A	96	ARG	2.7
1	B	337	LYS	2.6
1	C	334	LYS	2.6
1	A	93	MET	2.6
1	B	334	LYS	2.6
1	A	67	VAL	2.6
1	A	327	PRO	2.6
1	C	165	SER	2.6
1	A	72	ILE	2.6
1	C	352	ALA	2.5
1	A	59	SER	2.5
1	A	108	CYS	2.5
1	A	137	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	176	TYR	2.5
1	B	330	TYR	2.5
1	A	95	VAL	2.4
1	A	139	GLY	2.4
1	B	171	GLY	2.4
1	D	354	PHE	2.4
1	A	97	GLU	2.4
1	A	145	HIS	2.4
1	B	333	TRP	2.4
1	C	327	PRO	2.3
1	C	317	SER	2.3
1	A	111	ARG	2.3
1	B	322	VAL	2.3
1	B	165	SER	2.3
1	A	60	TYR	2.3
1	A	112	TYR	2.3
1	A	58	ALA	2.3
1	A	333	TRP	2.2
1	C	355	LEU	2.2
1	A	338	ASP	2.2
1	A	75	LEU	2.2
1	C	341	VAL	2.2
1	C	62	ASP	2.2
1	C	164	GLU	2.2
1	A	326	GLN	2.2
1	A	336	GLY	2.2
1	A	352	ALA	2.2
1	A	101	ILE	2.1
1	A	11	PRO	2.1
1	C	346	LEU	2.1
1	C	236	GLU	2.1
1	D	164	GLU	2.1
1	A	140	THR	2.1
1	C	339	ASN	2.1
1	A	165	SER	2.1
1	C	337	LYS	2.1
1	C	313	MET	2.1
1	C	319	ASP	2.1
1	C	356	LYS	2.0
1	A	340	THR	2.0
1	B	338	ASP	2.0
1	A	319	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NI	A	401	1/1	0.99	0.02	48,48,48,48	0
2	NI	B	401	1/1	0.99	0.05	40,40,40,40	0
2	NI	C	401	1/1	0.99	0.03	49,49,49,49	0
2	NI	D	401	1/1	0.99	0.02	34,34,34,34	0
3	ZN	A	402	1/1	0.99	0.04	47,47,47,47	0
3	ZN	B	402	1/1	0.99	0.04	40,40,40,40	0
3	ZN	C	402	1/1	0.99	0.04	51,51,51,51	0
3	ZN	D	402	1/1	1.00	0.01	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.