Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2024 – 03:04 pm BST

PDB ID	:	9GP1
Title	:	Jumonji domain-containing protein 2A with crystallization epitope mutatios 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:

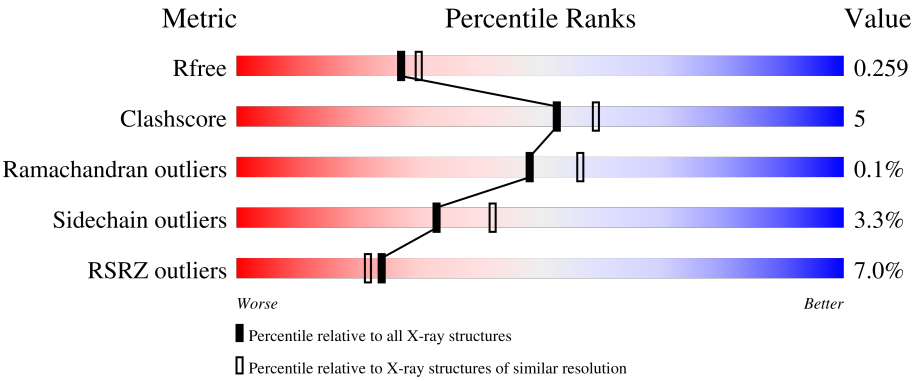
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 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}	164625	7167 (2.24-2.20)
Clashscore	180529	8096 (2.24-2.20)
Ramachandran outliers	177936	8010 (2.24-2.20)
Sidechain outliers	177891	8011 (2.24-2.20)
RSRZ outliers	164620	7166 (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 <=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	14% 85% 11%
1	B	360	4% 86% 11%
1	C	360	7% 87% 9%
1	D	360	2% 85% 11%

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 (three-letter code: 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 Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

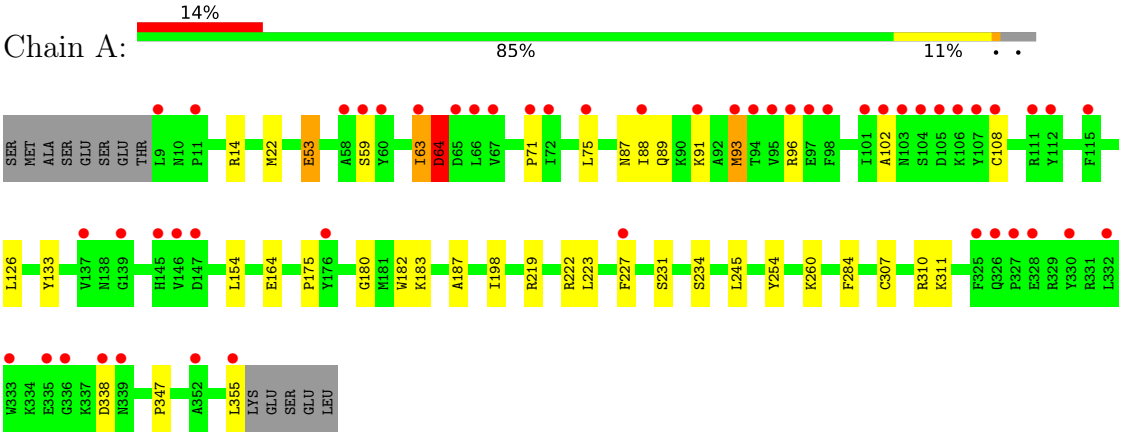
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	50	Total O 50 50	0	0
4	B	157	Total O 157 157	0	0
4	C	115	Total O 115 115	0	0
4	D	215	Total O 215 215	0	0

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.

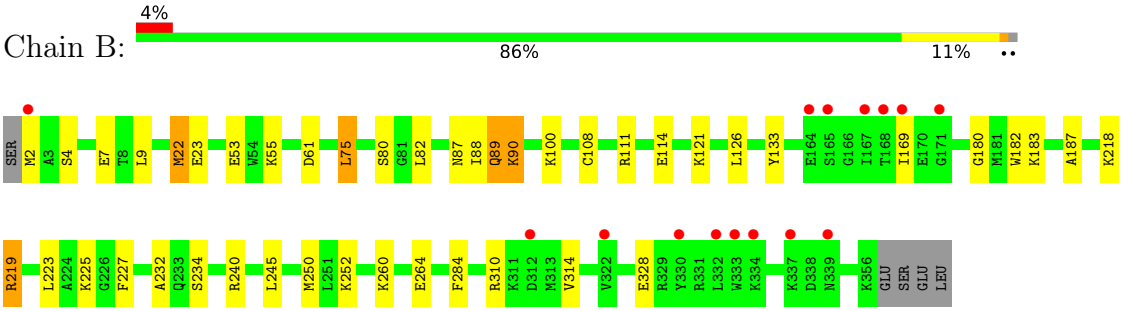
• Molecule 1: Lysine-specific demethylase 4A

Chain A:



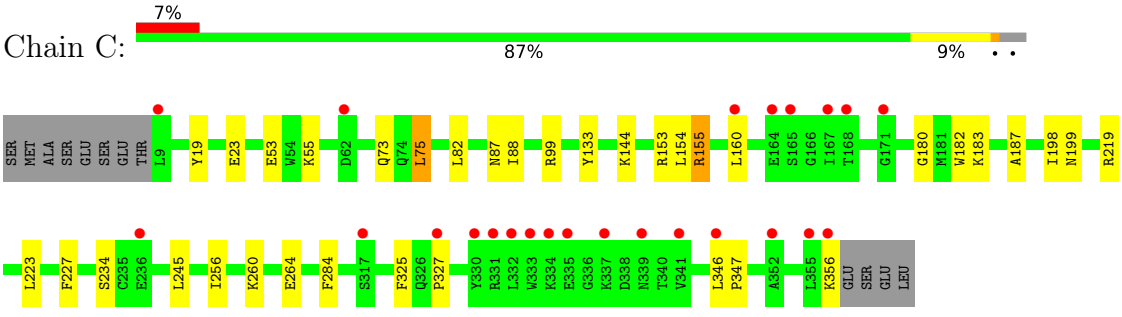
• Molecule 1: Lysine-specific demethylase 4A

Chain B:



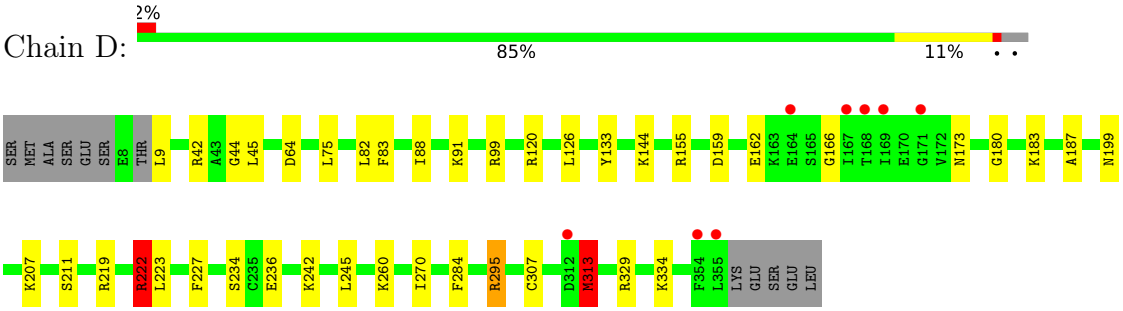
• Molecule 1: Lysine-specific demethylase 4A

Chain C:



• Molecule 1: Lysine-specific demethylase 4A

Chain D:


2%
85%
11%
SER MET ALA SER GLU SER E8 THR L9 R42 A43 G44 L45 D64 L75 L82 F83 I88 K91 R99 R120 L126 Y133 K144 R155 D159 E162 K163 E164 S165 G166 I167 T168 I169 E170 G171 V172 N173 G180 K183 A187 N199
K207 S211 R219 R222 L223 F227 S234 C235 E236 K242 L245 K260 I270 F284 R295 C307 D312 M313 R329 K334 F354 L355 LYS GLU SER GLU LEU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.41	0/2749	0.85	3/3752 (0.1%)
1	B	0.48	0/2936	0.95	8/3989 (0.2%)
1	C	0.44	0/2870	0.90	3/3904 (0.1%)
1	D	0.51	0/2911	0.95	6/3952 (0.2%)
All	All	0.46	0/11466	0.91	20/15597 (0.1%)

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 (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	121	LYS	CD-CE-NZ	-6.62	96.47	111.70
1	B	82	LEU	CB-CG-CD2	-6.42	100.08	111.00
1	D	222	ARG	CG-CD-NE	6.38	125.20	111.80
1	B	75	LEU	CB-CG-CD2	-6.12	100.59	111.00
1	B	260	LYS	CB-CA-C	-6.12	98.17	110.40
1	A	93	MET	CG-SD-CE	5.85	109.56	100.20
1	B	219	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	338	ASP	CB-CA-C	5.71	121.82	110.40
1	C	264	GLU	CB-CG-CD	5.69	129.57	114.20
1	C	155	ARG	CA-CB-CG	5.67	125.87	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	260	LYS	CB-CA-C	-5.50	99.41	110.40
1	D	42	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	250	MET	CG-SD-CE	-5.43	91.52	100.20
1	D	313	MET	CB-CG-SD	5.41	128.64	112.40
1	B	310	ARG	CA-CB-CG	5.38	125.24	113.40
1	B	22	MET	CG-SD-CE	-5.29	91.74	100.20
1	D	260	LYS	CB-CA-C	-5.26	99.88	110.40
1	D	120	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	D	295	ARG	CG-CD-NE	-5.18	100.92	111.80
1	A	260	LYS	CB-CA-C	-5.09	100.23	110.40

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 (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	A	2667	0	2433	29	0
1	B	2849	0	2690	24	0
1	C	2783	0	2620	22	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	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	215	0	0	9	1
All	All	11668	0	10433	105	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 (105) 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:C:87:ASN:C	1:C:88:ILE:HD13	2.11	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:B:87:ASN:C	1:B:88:ILE:HD13	2.11	0.69
1:A:87:ASN:C	1:A:88:ILE:HD13	2.15	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:87:ASN:O	1:A:88:ILE:HD13	2.10	0.52
1:A:254:TYR:CE2	1:C:19:TYR:CD1	2.98	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:A:88:ILE:HD13	1:A:88:ILE:N	2.25	0.51
1:B:225:LYS:HG3	1:B:232:ALA:CB	2.40	0.51
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: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:D:242:LYS:NZ	4:D:516:HOH:O	2.44	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: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: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:D:75[B]:LEU:C	1:D:75[B]:LEU:HD23	2.38	0.45
1:C:99:ARG:NH1	4:C:519:HOH:O	2.50	0.45
1:D:64:ASP:CG	1:D:99:ARG:HH22	2.21	0.45
1:B:183:LYS:HE3	4:B:568:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:89:GLN:O	1:B:90:LYS:NZ	2.50	0.43
1:A:154:LEU:HD11	1:A:198:ILE:HG21	2.00	0.43
1:C:325:PHE:C	1:C:327:PRO:HD3	2.39	0.43
1:D:207:LYS:HE3	4:D:653:HOH:O	2.19	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
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%)	37	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
1	D	347/360 (96%)	340 (98%)	6 (2%)	1 (0%)	37	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 (i)

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%)	27	35
1	B	295/317 (93%)	281 (95%)	14 (5%)	22	27
1	C	286/317 (90%)	280 (98%)	6 (2%)	48	61
1	D	294/317 (93%)	287 (98%)	7 (2%)	44	56
All	All	1133/1268 (89%)	1096 (97%)	37 (3%)	33	42

All (37) 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	133	TYR
1	A	164	GLU
1	A	231	SER
1	A	234	SER
1	B	2	MET
1	B	9	LEU
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	133	TYR
1	B	234	SER
1	B	252	LYS
1	B	264	GLU
1	B	328	GLU
1	C	23	GLU
1	C	53	GLU
1	C	75	LEU
1	C	82	LEU
1	C	133	TYR
1	C	234	SER
1	D	82	LEU
1	D	91	LYS
1	D	133	TYR
1	D	222	ARG
1	D	234	SER
1	D	313	MET
1	D	334	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	138	ASN

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Mol	Chain	Res	Type
1	B	87	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.79	51 (14%) 7 6	24, 51, 89, 113	0
1	B	355/360 (98%)	0.11	15 (4%) 41 38	16, 34, 76, 103	0
1	C	348/360 (96%)	0.46	24 (6%) 24 22	24, 42, 80, 129	0
1	D	348/360 (96%)	-0.16	8 (2%) 61 58	10, 29, 63, 114	1 (0%)
All	All	1398/1440 (97%)	0.30	98 (7%) 24 21	10, 39, 83, 129	1 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	ASN	4.9
1	D	167	ILE	4.3
1	A	9	LEU	3.8
1	B	167	ILE	3.6
1	D	169	ILE	3.6
1	C	332	LEU	3.5
1	A	102	ALA	3.5
1	D	168	THR	3.5
1	C	335	GLU	3.5
1	B	332	LEU	3.5
1	B	2	MET	3.4
1	A	325	PHE	3.4
1	A	98	PHE	3.4
1	C	330	TYR	3.3
1	A	355	LEU	3.2
1	C	167	ILE	3.2
1	A	71	PRO	3.2
1	A	339	ASN	3.1
1	A	106	LYS	3.1
1	A	91	LYS	3.1
1	A	105	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	171	GLY	3.1
1	B	164	GLU	3.1
1	A	227	PHE	3.0
1	D	312	ASP	3.0
1	B	169	ILE	3.0
1	A	330	TYR	3.0
1	B	339	ASN	3.0
1	A	63	ILE	2.9
1	C	333	TRP	2.9
1	A	115	PHE	2.9
1	B	312	ASP	2.9
1	B	168	THR	2.9
1	A	66	LEU	2.8
1	A	104	SER	2.8
1	A	94	THR	2.8
1	A	147	ASP	2.8
1	C	331	ARG	2.8
1	C	171	GLY	2.8
1	C	9	LEU	2.8
1	A	65	ASP	2.8
1	A	88	ILE	2.7
1	C	160	LEU	2.7
1	A	328	GLU	2.7
1	A	146	VAL	2.7
1	A	335	GLU	2.7
1	A	107	TYR	2.7
1	C	168	THR	2.7
1	A	96	ARG	2.6
1	A	332	LEU	2.6
1	B	337	LYS	2.6
1	C	334	LYS	2.6
1	D	355	LEU	2.6
1	B	334	LYS	2.6
1	A	93	MET	2.5
1	C	165	SER	2.5
1	A	327	PRO	2.5
1	A	67	VAL	2.5
1	A	72	ILE	2.5
1	A	59	SER	2.4
1	A	108	CYS	2.4
1	C	352	ALA	2.4
1	A	137	VAL	2.4

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

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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, 95^{th} 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	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	0.03	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.