



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:07 PM UTC

PDB ID : 2J8A / pdb_00002j8a
Title : X-ray structure of the N-terminus RRM domain of Set1
Authors : Tresaugues, L.; Dehe, P.M.; Guerois, R.; Rodriguez-Gil, A.; Varlet, I.; Salah, P.; Pamblanco, M.; Luciano, P.; Quevillon-Cheruel, S.; Sollier, J.; Leulliot, N.; Couprie, J.; Tordera, V.; Zinn-Justin, S.; Chavez, S.; Van Tilbeurgh, H.; Geli, V.
Deposited on : 2006-10-24
Resolution : 3.00 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

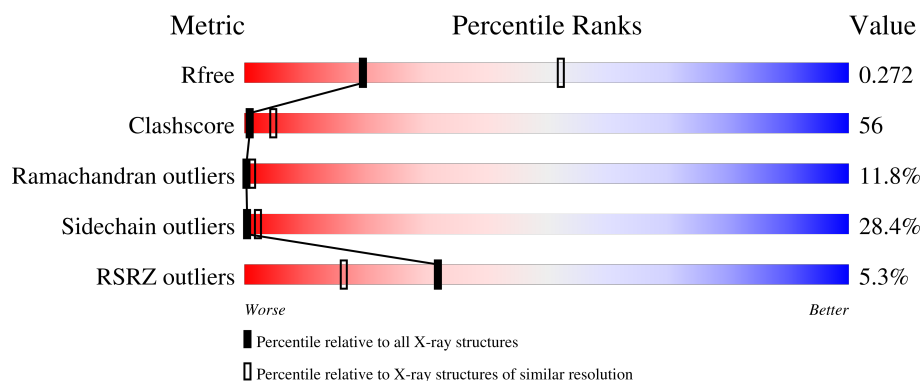
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	136	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 915 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.

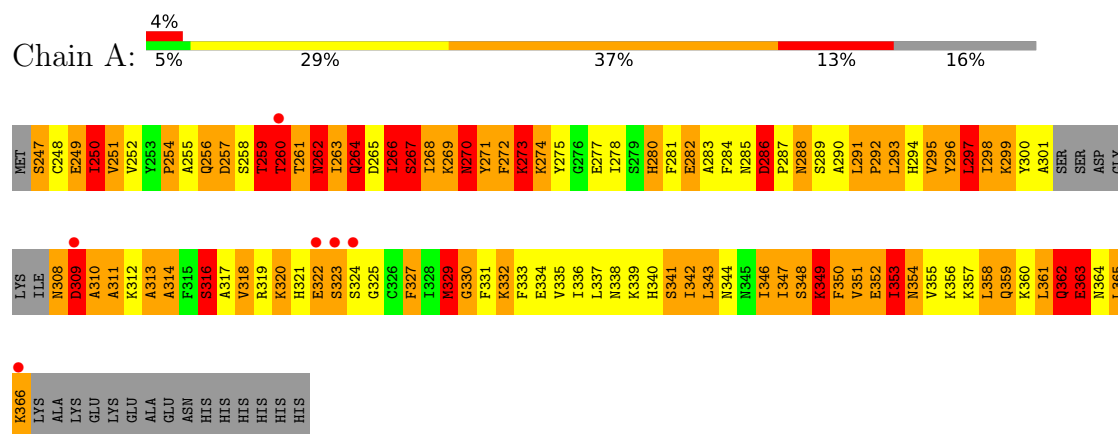
- Molecule 1 is a protein called HISTONE-LYSINE N-METHYLTRANSFERASE, H3 LYSINE-4 SPECIFIC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	S	0	0	0
			915	592	152	168	3			

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: HISTONE-LYSINE N-METHYLTRANSFERASE, H3 LYSINE-4 SPECIFIC



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 3 2	Depositor
Cell constants a, b, c, α , β , γ	123.79Å 123.79Å 123.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 10.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (10.00-3.00) 96.5 (10.00-3.00)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.86 (at 2.99Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.246 , 0.277 0.244 , 0.272	Depositor DCC
R_{free} test set	321 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	79.2	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	915	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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

5.1 Standard geometry

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	2.85	75/933 (8.0%)	2.46	59/1255 (4.7%)

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	A	1	5

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	260	THR	CA-CB	13.98	1.70	1.52
1	A	353	ILE	CA-CB	-10.90	1.38	1.54
1	A	351	VAL	CA-CB	-10.84	1.41	1.54
1	A	349	LYS	CA-C	-10.11	1.39	1.52
1	A	266	ILE	CG1-CD1	10.09	1.91	1.51
1	A	348	SER	C-O	9.90	1.36	1.24
1	A	347	ILE	CA-CB	-9.51	1.41	1.54
1	A	354	ASN	N-CA	-9.50	1.34	1.46
1	A	295	VAL	C-O	9.34	1.35	1.24
1	A	343	LEU	C-O	9.28	1.35	1.24
1	A	340	HIS	CA-C	-8.84	1.41	1.53
1	A	346	ILE	CA-CB	-8.15	1.44	1.54
1	A	346	ILE	C-O	8.08	1.33	1.24
1	A	355	VAL	C-O	-7.98	1.14	1.24
1	A	366	LYS	CG-CD	7.83	1.75	1.52
1	A	356	LYS	C-O	-7.75	1.14	1.24
1	A	327	PHE	CA-CB	-7.67	1.40	1.53
1	A	323	SER	CA-C	7.56	1.62	1.52
1	A	349	LYS	CE-NZ	7.49	1.71	1.49
1	A	293	LEU	CA-C	-7.19	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	LEU	N-CA	7.09	1.54	1.45
1	A	311	ALA	CA-CB	-6.76	1.42	1.53
1	A	338	ASN	CA-C	-6.67	1.46	1.53
1	A	283	ALA	CA-CB	-6.62	1.42	1.53
1	A	349	LYS	CD-CE	6.59	1.72	1.52
1	A	351	VAL	C-O	6.42	1.31	1.24
1	A	268	ILE	CA-C	-6.41	1.44	1.52
1	A	323	SER	CA-CB	6.37	1.64	1.53
1	A	298	ILE	CA-CB	-6.29	1.46	1.54
1	A	301	ALA	N-CA	6.17	1.57	1.46
1	A	325	GLY	C-O	-6.05	1.15	1.23
1	A	356	LYS	CE-NZ	6.02	1.67	1.49
1	A	366	LYS	CD-CE	5.95	1.70	1.52
1	A	249	GLU	CB-CG	-5.94	1.34	1.52
1	A	362	GLN	N-CA	-5.91	1.39	1.46
1	A	351	VAL	N-CA	-5.91	1.39	1.46
1	A	320	LYS	CG-CD	5.91	1.70	1.52
1	A	286	ASP	CA-C	5.85	1.59	1.52
1	A	254	PRO	C-O	-5.84	1.16	1.23
1	A	249	GLU	CA-CB	-5.84	1.44	1.53
1	A	266	ILE	CB-CG1	5.82	1.65	1.53
1	A	344	ASN	CA-CB	-5.76	1.43	1.53
1	A	355	VAL	CA-C	-5.67	1.44	1.52
1	A	273	LYS	N-CA	5.64	1.53	1.46
1	A	366	LYS	CE-NZ	5.62	1.66	1.49
1	A	266	ILE	CA-C	5.57	1.59	1.52
1	A	349	LYS	C-O	5.52	1.30	1.24
1	A	263	ILE	CA-CB	-5.47	1.48	1.54
1	A	324	SER	CA-CB	5.46	1.63	1.53
1	A	277	GLU	C-O	5.42	1.30	1.23
1	A	260	THR	CA-C	5.38	1.59	1.52
1	A	251	VAL	C-O	5.36	1.29	1.24
1	A	283	ALA	N-CA	5.36	1.52	1.45
1	A	336	ILE	C-O	5.35	1.30	1.23
1	A	284	PHE	C-O	5.34	1.30	1.24
1	A	356	LYS	CA-C	-5.31	1.45	1.52
1	A	295	VAL	N-CA	-5.31	1.39	1.46
1	A	287	PRO	C-O	-5.30	1.17	1.24
1	A	365	LEU	CA-C	5.30	1.59	1.52
1	A	342	ILE	N-CA	-5.28	1.38	1.46
1	A	352	GLU	CG-CD	5.24	1.65	1.52
1	A	282	GLU	CB-CG	-5.23	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	320	LYS	CB-CG	5.21	1.68	1.52
1	A	260	THR	CB-CG2	5.19	1.69	1.52
1	A	270	ASN	CA-C	-5.19	1.45	1.52
1	A	296	TYR	N-CA	5.19	1.52	1.46
1	A	354	ASN	CA-CB	-5.16	1.45	1.53
1	A	280	HIS	N-CA	5.15	1.52	1.46
1	A	292	PRO	N-CA	-5.14	1.41	1.47
1	A	297	LEU	C-O	5.03	1.29	1.24
1	A	248	CYS	CA-C	5.03	1.58	1.52
1	A	329	MET	SD-CE	5.03	1.92	1.79
1	A	249	GLU	CA-C	-5.02	1.46	1.52
1	A	354	ASN	CA-C	-5.02	1.46	1.52
1	A	271	TYR	CB-CG	-5.00	1.40	1.51

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	HIS	N-CA-C	12.86	129.10	113.16
1	A	259	THR	N-CA-C	12.82	130.66	109.24
1	A	268	ILE	N-CA-C	-11.98	100.29	111.67
1	A	262	ASN	N-CA-C	-11.07	97.35	110.41
1	A	277	GLU	N-CA-C	-10.21	94.64	109.96
1	A	316	SER	N-CA-C	-9.20	100.38	111.69
1	A	287	PRO	CB-CA-C	-8.93	99.17	111.85
1	A	257	ASP	CA-C-N	-8.45	109.12	120.95
1	A	257	ASP	C-N-CA	-8.45	109.12	120.95
1	A	362	GLN	CA-C-N	-8.01	107.57	121.66
1	A	362	GLN	C-N-CA	-8.01	107.57	121.66
1	A	320	LYS	CA-C-N	-7.71	108.43	122.38
1	A	320	LYS	C-N-CA	-7.71	108.43	122.38
1	A	251	VAL	N-CA-CB	7.26	122.11	111.52
1	A	352	GLU	N-CA-CB	-6.88	99.19	110.40
1	A	266	ILE	CB-CG1-CD1	6.74	127.96	113.80
1	A	286	ASP	CB-CA-C	6.71	120.89	109.82
1	A	297	LEU	CB-CA-C	-6.55	100.30	110.78
1	A	250	ILE	CB-CG1-CD1	-6.55	100.05	113.80
1	A	349	LYS	CA-C-O	6.52	127.88	120.90
1	A	269	LYS	CD-CE-NZ	-6.47	91.21	111.90
1	A	335	VAL	CB-CA-C	-6.47	99.27	110.65
1	A	290	ALA	CA-C-N	-6.33	111.60	120.39
1	A	290	ALA	C-N-CA	-6.33	111.60	120.39
1	A	268	ILE	CB-CA-C	-6.27	104.40	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	SER	N-CA-C	6.24	120.84	113.23
1	A	338	ASN	N-CA-C	-6.18	101.12	110.70
1	A	350	PHE	CA-C-O	-6.05	112.65	119.79
1	A	314	ALA	CA-C-N	-6.03	110.66	120.72
1	A	314	ALA	C-N-CA	-6.03	110.66	120.72
1	A	348	SER	CA-CB-OG	-6.00	99.10	111.10
1	A	322	GLU	N-CA-C	5.97	120.42	113.20
1	A	250	ILE	CA-C-N	-5.97	114.69	122.99
1	A	250	ILE	C-N-CA	-5.97	114.69	122.99
1	A	354	ASN	N-CA-C	-5.94	104.39	111.69
1	A	353	ILE	CA-CB-CG2	-5.90	100.47	110.50
1	A	291	LEU	N-CA-C	5.89	117.12	109.64
1	A	263	ILE	N-CA-C	-5.87	102.00	109.80
1	A	341	SER	CA-CB-OG	-5.64	99.81	111.10
1	A	332	LYS	N-CA-C	5.63	117.86	109.25
1	A	272	PHE	N-CA-C	5.58	117.45	111.36
1	A	263	ILE	CA-C-N	-5.56	113.47	122.81
1	A	263	ILE	C-N-CA	-5.56	113.47	122.81
1	A	346	ILE	CA-C-N	-5.55	111.98	121.97
1	A	346	ILE	C-N-CA	-5.55	111.98	121.97
1	A	285	ASN	N-CA-C	5.47	118.62	110.14
1	A	288	ASN	CA-C-N	-5.43	113.58	122.54
1	A	288	ASN	C-N-CA	-5.43	113.58	122.54
1	A	259	THR	CA-C-O	5.40	126.87	120.66
1	A	292	PRO	CB-CA-C	-5.37	104.74	111.56
1	A	318	VAL	N-CA-C	-5.37	106.02	113.00
1	A	256	GLN	CA-CB-CG	-5.31	103.47	114.10
1	A	343	LEU	CB-CG-CD1	-5.27	94.90	110.70
1	A	348	SER	N-CA-CB	-5.20	101.70	110.49
1	A	320	LYS	CB-CG-CD	5.16	123.16	111.30
1	A	262	ASN	N-CA-CB	-5.12	105.65	111.79
1	A	264	GLN	N-CA-CB	5.07	119.41	111.20
1	A	365	LEU	CA-CB-CG	5.04	133.96	116.30
1	A	351	VAL	CB-CA-C	5.03	118.63	112.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	259	THR	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	SER	Peptide
1	A	260	THR	Peptide
1	A	300	TYR	Peptide
1	A	309	ASP	Peptide
1	A	363	GLU	Peptide

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	915	0	923	102	0
All	All	915	0	923	102	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 56.

All (102) 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:366:LYS:CD	1:A:366:LYS:CG	1.75	1.54
1:A:349:LYS:CE	1:A:349:LYS:NZ	1.71	1.48
1:A:266:ILE:CD1	1:A:266:ILE:CG1	1.91	1.46
1:A:363:GLU:CB	1:A:366:LYS:HE3	1.60	1.31
1:A:363:GLU:HB2	1:A:366:LYS:HE3	1.12	1.07
1:A:363:GLU:CB	1:A:366:LYS:CE	2.37	1.03
1:A:363:GLU:HB3	1:A:366:LYS:CE	1.89	1.02
1:A:262:ASN:HD22	1:A:262:ASN:H	0.94	0.93
1:A:256:GLN:HE21	1:A:259:THR:HG21	1.32	0.93
1:A:264:GLN:HE21	1:A:264:GLN:H	1.15	0.92
1:A:254:PRO:HD3	1:A:294:HIS:O	1.71	0.90
1:A:258:SER:O	1:A:259:THR:HG23	1.73	0.88
1:A:363:GLU:HB3	1:A:366:LYS:HE3	1.52	0.87
1:A:262:ASN:HD22	1:A:262:ASN:N	1.65	0.86
1:A:250:ILE:CG2	1:A:298:ILE:HB	2.06	0.85
1:A:250:ILE:HG22	1:A:298:ILE:HB	1.64	0.80
1:A:264:GLN:HE21	1:A:264:GLN:N	1.79	0.79
1:A:250:ILE:HG22	1:A:298:ILE:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:THR:CB	1:A:331:PHE:HZ	1.97	0.77
1:A:363:GLU:HB3	1:A:366:LYS:HE2	1.66	0.74
1:A:366:LYS:CD	1:A:366:LYS:CB	2.66	0.74
1:A:259:THR:HB	1:A:331:PHE:CZ	2.23	0.73
1:A:308:ASN:HD22	1:A:308:ASN:C	2.00	0.70
1:A:289:SER:OG	1:A:291:LEU:HD12	1.90	0.70
1:A:270:ASN:O	1:A:271:TYR:C	2.31	0.69
1:A:347:ILE:O	1:A:348:SER:C	2.34	0.69
1:A:262:ASN:H	1:A:262:ASN:ND2	1.78	0.68
1:A:348:SER:O	1:A:352:GLU:HG3	1.93	0.68
1:A:247:SER:HA	1:A:339:LYS:HZ2	1.59	0.68
1:A:342:ILE:O	1:A:346:ILE:HG12	1.94	0.67
1:A:249:GLU:HG2	1:A:299:LYS:HB2	1.76	0.67
1:A:297:LEU:HG	1:A:343:LEU:HD22	1.76	0.66
1:A:309:ASP:HB2	1:A:312:LYS:HB3	1.77	0.66
1:A:316:SER:O	1:A:319:ARG:N	2.25	0.65
1:A:259:THR:OG1	1:A:331:PHE:HZ	1.78	0.65
1:A:329:MET:O	1:A:331:PHE:N	2.31	0.64
1:A:259:THR:HB	1:A:331:PHE:HZ	1.58	0.63
1:A:259:THR:CB	1:A:331:PHE:CZ	2.81	0.62
1:A:309:ASP:CG	1:A:309:ASP:O	2.41	0.62
1:A:256:GLN:NE2	1:A:259:THR:HG21	2.09	0.61
1:A:292:PRO:HB2	1:A:294:HIS:CE1	2.37	0.59
1:A:266:ILE:O	1:A:267:SER:C	2.43	0.59
1:A:264:GLN:O	1:A:265:ASP:C	2.46	0.59
1:A:262:ASN:ND2	1:A:262:ASN:C	2.58	0.59
1:A:366:LYS:CG	1:A:366:LYS:CE	2.81	0.57
1:A:262:ASN:N	1:A:262:ASN:ND2	2.36	0.56
1:A:329:MET:O	1:A:330:GLY:C	2.47	0.56
1:A:309:ASP:HB2	1:A:312:LYS:CB	2.36	0.55
1:A:359:GLN:HA	1:A:362:GLN:NE2	2.22	0.55
1:A:252:VAL:HG12	1:A:333:PHE:CD1	2.44	0.53
1:A:261:THR:HB	1:A:263:ILE:H	1.74	0.52
1:A:247:SER:HA	1:A:339:LYS:NZ	2.23	0.52
1:A:266:ILE:O	1:A:268:ILE:N	2.43	0.51
1:A:309:ASP:O	1:A:309:ASP:OD1	2.27	0.51
1:A:258:SER:OG	1:A:357:LYS:NZ	2.45	0.49
1:A:308:ASN:C	1:A:308:ASN:ND2	2.69	0.49
1:A:265:ASP:O	1:A:268:ILE:N	2.34	0.49
1:A:258:SER:O	1:A:259:THR:CG2	2.54	0.48
1:A:352:GLU:O	1:A:353:ILE:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLU:O	1:A:296:TYR:HA	2.13	0.48
1:A:272:PHE:O	1:A:275:TYR:HD1	1.95	0.48
1:A:265:ASP:HB2	1:A:266:ILE:HD12	1.94	0.47
1:A:256:GLN:CG	1:A:256:GLN:O	2.62	0.47
1:A:264:GLN:O	1:A:267:SER:HB2	2.13	0.47
1:A:252:VAL:HA	1:A:334:GLU:O	2.15	0.47
1:A:273:LYS:O	1:A:275:TYR:N	2.45	0.47
1:A:266:ILE:CD1	1:A:266:ILE:H	2.29	0.46
1:A:310:ALA:O	1:A:313:ALA:HB3	2.16	0.46
1:A:327:PHE:CE2	1:A:332:LYS:HB2	2.51	0.46
1:A:273:LYS:N	1:A:278:ILE:CD1	2.79	0.46
1:A:318:VAL:HG12	1:A:318:VAL:O	2.16	0.45
1:A:329:MET:C	1:A:331:PHE:N	2.75	0.45
1:A:293:LEU:O	1:A:294:HIS:HB2	2.16	0.45
1:A:337:LEU:O	1:A:339:LYS:N	2.48	0.44
1:A:347:ILE:C	1:A:349:LYS:N	2.74	0.44
1:A:255:ALA:HB2	1:A:332:LYS:HG2	2.00	0.44
1:A:358:LEU:HA	1:A:358:LEU:HD23	1.40	0.44
1:A:361:LEU:HA	1:A:361:LEU:HD12	1.66	0.44
1:A:286:ASP:C	1:A:286:ASP:OD2	2.60	0.44
1:A:316:SER:O	1:A:317:ALA:C	2.60	0.44
1:A:266:ILE:HD12	1:A:266:ILE:H	1.83	0.43
1:A:270:ASN:O	1:A:272:PHE:N	2.52	0.43
1:A:347:ILE:O	1:A:349:LYS:N	2.51	0.43
1:A:337:LEU:C	1:A:339:LYS:N	2.76	0.43
1:A:363:GLU:HB2	1:A:366:LYS:CE	2.07	0.43
1:A:250:ILE:HG23	1:A:250:ILE:HD13	1.56	0.43
1:A:271:TYR:C	1:A:271:TYR:CD2	2.97	0.42
1:A:286:ASP:OD2	1:A:288:ASN:N	2.43	0.42
1:A:273:LYS:N	1:A:278:ILE:HD11	2.34	0.42
1:A:256:GLN:HE21	1:A:259:THR:CG2	2.16	0.42
1:A:348:SER:O	1:A:349:LYS:C	2.61	0.42
1:A:329:MET:C	1:A:331:PHE:H	2.28	0.42
1:A:313:ALA:O	1:A:314:ALA:C	2.62	0.42
1:A:337:LEU:C	1:A:339:LYS:H	2.28	0.42
1:A:281:PHE:CD2	1:A:281:PHE:C	2.98	0.41
1:A:349:LYS:NZ	1:A:349:LYS:CD	2.76	0.41
1:A:343:LEU:HA	1:A:343:LEU:HD12	1.38	0.41
1:A:351:VAL:O	1:A:354:ASN:HB2	2.20	0.41
1:A:252:VAL:O	1:A:295:VAL:HA	2.20	0.41
1:A:281:PHE:CD1	1:A:298:ILE:HG12	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LYS:O	1:A:270:ASN:C	2.64	0.41
1:A:293:LEU:HD22	1:A:350:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

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	110/136 (81%)	81 (74%)	16 (14%)	13 (12%)	0 1

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	266	ILE
1	A	267	SER
1	A	323	SER
1	A	270	ASN
1	A	273	LYS
1	A	274	LYS
1	A	330	GLY
1	A	280	HIS
1	A	311	ALA
1	A	313	ALA
1	A	364	ASN
1	A	257	ASP
1	A	310	ALA

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	102/121 (84%)	73 (72%)	29 (28%)	0 2

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	250	ILE
1	A	251	VAL
1	A	259	THR
1	A	260	THR
1	A	261	THR
1	A	262	ASN
1	A	264	GLN
1	A	266	ILE
1	A	267	SER
1	A	274	LYS
1	A	286	ASP
1	A	297	LEU
1	A	299	LYS
1	A	308	ASN
1	A	309	ASP
1	A	316	SER
1	A	320	LYS
1	A	322	GLU
1	A	329	MET
1	A	341	SER
1	A	349	LYS
1	A	353	ILE
1	A	358	LEU
1	A	359	GLN
1	A	360	LYS
1	A	361	LEU
1	A	362	GLN
1	A	363	GLU
1	A	365	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	262	ASN
1	A	264	GLN
1	A	294	HIS
1	A	308	ASN
1	A	359	GLN
1	A	362	GLN

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](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	114/136 (83%)	-0.19	6 (5%) 32 16	39, 65, 96, 102	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	SER	2.8
1	A	309	ASP	2.4
1	A	323	SER	2.4
1	A	260	THR	2.2
1	A	366	LYS	2.1
1	A	322	GLU	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.