



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 08:29 AM EDT

PDB ID : 5B02 / pdb_00005b02
Title : Structure of the prenyltransferase MoeN5 with a fusion protein tag of Sso7d
Authors : Ko, T.-P.; Zhang, L.; Chen, C.-C.; Guo, R.-T.; Oldfield, E.O.
Deposited on : 2015-10-27
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)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

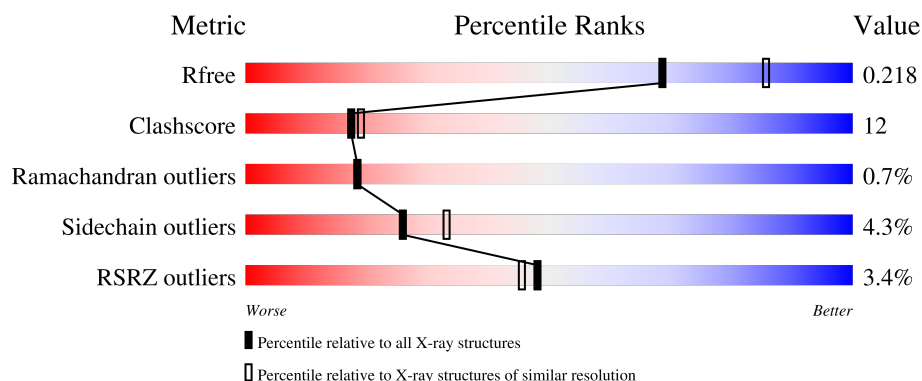
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	343	0% 62% 13% • 23%
1	B	343	2% 75% 20% • •
1	C	343	57% 17% • 24%
1	D	343	9% 73% 21% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9942 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 MoeN5,DNA-binding protein 7d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2013	1243	374	385	11			
1	B	332	Total	C	N	O	S	0	0	0
			2533	1571	463	485	14			
1	C	262	Total	C	N	O	S	0	0	0
			1998	1234	372	381	11			
1	D	333	Total	C	N	O	S	0	0	0
			2544	1579	466	485	14			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP A0A010
A	-12	ALA	-	expression tag	UNP A0A010
A	-11	HIS	-	expression tag	UNP A0A010
A	-10	HIS	-	expression tag	UNP A0A010
A	-9	HIS	-	expression tag	UNP A0A010
A	-8	HIS	-	expression tag	UNP A0A010
A	-7	HIS	-	expression tag	UNP A0A010
A	-6	HIS	-	expression tag	UNP A0A010
A	-5	VAL	-	expression tag	UNP A0A010
A	-4	ASP	-	expression tag	UNP A0A010
A	-3	ASP	-	expression tag	UNP A0A010
A	-2	ASP	-	expression tag	UNP A0A010
A	-1	ASP	-	expression tag	UNP A0A010
A	0	LYS	-	expression tag	UNP A0A010
A	261	ALA	-	linker	UNP A0A010
A	262	GLY	-	linker	UNP A0A010
A	263	ALA	-	linker	UNP A0A010
A	264	GLY	-	linker	UNP A0A010
A	265	ALA	-	linker	UNP A0A010
B	-13	MET	-	expression tag	UNP A0A010
B	-12	ALA	-	expression tag	UNP A0A010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP A0A010
B	-10	HIS	-	expression tag	UNP A0A010
B	-9	HIS	-	expression tag	UNP A0A010
B	-8	HIS	-	expression tag	UNP A0A010
B	-7	HIS	-	expression tag	UNP A0A010
B	-6	HIS	-	expression tag	UNP A0A010
B	-5	VAL	-	expression tag	UNP A0A010
B	-4	ASP	-	expression tag	UNP A0A010
B	-3	ASP	-	expression tag	UNP A0A010
B	-2	ASP	-	expression tag	UNP A0A010
B	-1	ASP	-	expression tag	UNP A0A010
B	0	LYS	-	expression tag	UNP A0A010
B	261	ALA	-	linker	UNP A0A010
B	262	GLY	-	linker	UNP A0A010
B	263	ALA	-	linker	UNP A0A010
B	264	GLY	-	linker	UNP A0A010
B	265	ALA	-	linker	UNP A0A010
C	-13	MET	-	expression tag	UNP A0A010
C	-12	ALA	-	expression tag	UNP A0A010
C	-11	HIS	-	expression tag	UNP A0A010
C	-10	HIS	-	expression tag	UNP A0A010
C	-9	HIS	-	expression tag	UNP A0A010
C	-8	HIS	-	expression tag	UNP A0A010
C	-7	HIS	-	expression tag	UNP A0A010
C	-6	HIS	-	expression tag	UNP A0A010
C	-5	VAL	-	expression tag	UNP A0A010
C	-4	ASP	-	expression tag	UNP A0A010
C	-3	ASP	-	expression tag	UNP A0A010
C	-2	ASP	-	expression tag	UNP A0A010
C	-1	ASP	-	expression tag	UNP A0A010
C	0	LYS	-	expression tag	UNP A0A010
C	261	ALA	-	linker	UNP A0A010
C	262	GLY	-	linker	UNP A0A010
C	263	ALA	-	linker	UNP A0A010
C	264	GLY	-	linker	UNP A0A010
C	265	ALA	-	linker	UNP A0A010
D	-13	MET	-	expression tag	UNP A0A010
D	-12	ALA	-	expression tag	UNP A0A010
D	-11	HIS	-	expression tag	UNP A0A010
D	-10	HIS	-	expression tag	UNP A0A010
D	-9	HIS	-	expression tag	UNP A0A010
D	-8	HIS	-	expression tag	UNP A0A010

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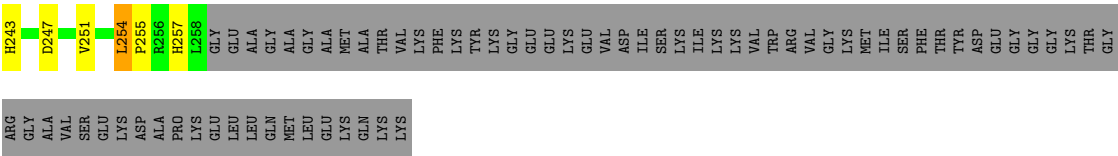
Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	HIS	-	expression tag	UNP A0A010
D	-6	HIS	-	expression tag	UNP A0A010
D	-5	VAL	-	expression tag	UNP A0A010
D	-4	ASP	-	expression tag	UNP A0A010
D	-3	ASP	-	expression tag	UNP A0A010
D	-2	ASP	-	expression tag	UNP A0A010
D	-1	ASP	-	expression tag	UNP A0A010
D	0	LYS	-	expression tag	UNP A0A010
D	261	ALA	-	linker	UNP A0A010
D	262	GLY	-	linker	UNP A0A010
D	263	ALA	-	linker	UNP A0A010
D	264	GLY	-	linker	UNP A0A010
D	265	ALA	-	linker	UNP A0A010

- Molecule 2 is water.

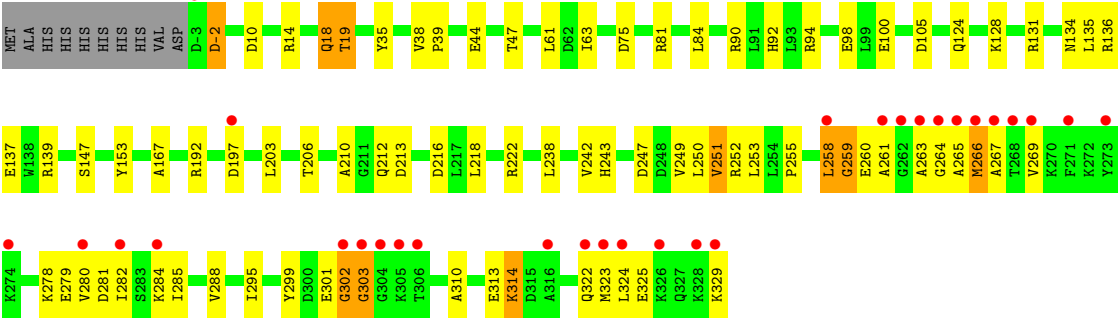
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	229	Total O 229 229	0	0
2	B	235	Total O 235 235	0	0
2	C	176	Total O 176 176	0	0
2	D	214	Total O 214 214	0	0

- Molecule 1: MoeN5,DNA-binding protein 7d





● Molecule 1: MoeN5,DNA-binding protein 7d



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.88Å 217.44Å 104.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.21 25.00 – 2.21	Depositor EDS
% Data completeness (in resolution range)	96.1 (25.00-2.21) 96.0 (25.00-2.21)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.22Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.176 , 0.218 0.176 , 0.218	Depositor DCC
R_{free} test set	3842 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9942	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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	1.02	3/2045 (0.1%)	1.12	6/2780 (0.2%)
1	B	0.99	4/2572 (0.2%)	1.08	8/3478 (0.2%)
1	C	1.09	2/2030 (0.1%)	1.16	9/2759 (0.3%)
1	D	0.93	0/2583	1.12	10/3489 (0.3%)
All	All	1.01	9/9230 (0.1%)	1.12	33/12506 (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	D	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	183	MET	SD-CE	11.85	2.09	1.79
1	B	1	MET	SD-CE	8.80	2.01	1.79
1	B	239	VAL	CA-CB	7.40	1.58	1.54
1	A	204	MET	SD-CE	-6.98	1.62	1.79
1	B	179	MET	SD-CE	-6.79	1.62	1.79
1	B	140	ALA	CA-CB	5.73	1.62	1.53
1	C	1	MET	SD-CE	5.44	1.93	1.79
1	A	165	GLN	C-O	-5.29	1.20	1.25
1	A	239	VAL	CA-CB	5.16	1.56	1.54

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	-2	ASP	N-CA-C	-12.57	96.43	112.90
1	D	258	LEU	N-CA-C	-8.72	95.03	109.24
1	D	253	LEU	N-CA-C	8.35	120.39	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	ALA	N-CA-C	-7.99	102.57	111.28
1	C	165	GLN	N-CA-C	-7.78	99.28	110.40
1	A	147	SER	N-CA-C	7.52	119.12	111.07
1	B	285	ILE	N-CA-C	7.10	118.22	108.84
1	D	167	ALA	N-CA-C	6.93	119.43	111.11
1	A	253	LEU	N-CA-C	6.50	119.69	111.69
1	B	190	TYR	N-CA-C	-6.47	104.15	111.07
1	B	253	LEU	N-CA-C	6.42	119.59	111.69
1	B	147	SER	N-CA-C	6.36	117.88	111.07
1	D	147	SER	N-CA-C	6.34	117.86	111.07
1	A	188	THR	N-CA-C	-6.20	104.68	112.93
1	C	104	ARG	N-CA-C	-6.19	104.44	111.07
1	A	33	ARG	N-CA-C	6.03	118.38	111.02
1	D	265	ALA	N-CA-C	-5.97	104.74	112.68
1	D	47	THR	N-CA-C	5.89	117.78	111.36
1	C	257	HIS	N-CA-C	5.74	120.44	113.38
1	D	250	LEU	N-CA-C	5.67	117.14	111.07
1	C	33	ARG	N-CA-C	5.56	117.78	111.11
1	B	180	THR	N-CA-C	-5.46	105.23	111.07
1	D	259	GLY	N-CA-C	-5.44	107.50	115.72
1	A	154	GLY	N-CA-C	-5.33	106.04	112.49
1	A	104	ARG	N-CA-C	-5.33	105.47	111.28
1	B	306	THR	N-CA-C	5.14	116.79	108.41
1	C	82	VAL	CA-C-N	5.11	127.08	120.44
1	C	82	VAL	C-N-CA	5.11	127.08	120.44
1	C	115	GLN	N-CA-C	5.08	117.47	111.33
1	C	94	ARG	CG-CD-NE	-5.04	100.91	112.00
1	D	278	LYS	N-CA-C	5.01	117.51	110.14
1	B	-3	ASP	N-CA-C	-5.01	106.01	111.82
1	C	94	ARG	CB-CG-CD	5.00	122.80	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	153	TYR	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	2013	0	1996	42	0
1	B	2533	0	2532	57	0
1	C	1998	0	1983	66	0
1	D	2544	0	2554	69	0
2	A	229	0	0	4	0
2	B	235	0	0	3	0
2	C	176	0	0	6	0
2	D	214	0	0	1	0
All	All	9942	0	9065	226	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 12.

All (226) 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:1:MET:SD	1:B:1:MET:CE	2.01	1.48
1:C:183:MET:CE	1:C:183:MET:SD	2.09	1.40
1:D:131:ARG:HG2	1:D:131:ARG:HH11	1.36	0.86
1:A:139:ARG:HD3	1:A:179:MET:HE1	1.59	0.84
1:D:222:ARG:HH11	1:D:243:HIS:HD2	1.27	0.83
1:D:267:ALA:HB1	1:D:282:ILE:HB	1.61	0.83
1:B:273:TYR:CE2	1:B:274:LYS:HD2	2.16	0.81
1:D:325:GLU:HA	1:D:329:LYS:HB3	1.65	0.79
1:D:10:ASP:HB2	2:D:521:HOH:O	1.85	0.77
1:B:222:ARG:HH11	1:B:243:HIS:HD2	1.33	0.76
1:C:183:MET:HE1	1:C:218:LEU:HG	1.67	0.75
1:C:201:ALA:HA	1:C:204:MET:HE3	1.67	0.74
1:B:284:LYS:HE3	1:B:284:LYS:HA	1.71	0.73
1:C:22:SER:N	1:C:83:GLU:OE1	2.21	0.73
1:A:61:LEU:HD13	1:A:94:ARG:HG3	1.71	0.72
1:C:145:TYR:HD1	1:C:146:GLY:H	1.37	0.72
1:C:131:ARG:HH11	1:C:131:ARG:HG2	1.55	0.71
1:D:10:ASP:O	1:D:14:ARG:HG3	1.89	0.71
1:D:94:ARG:HD2	1:D:98:GLU:OE2	1.90	0.71
1:A:192:ARG:HD2	1:C:80:ASP:HB2	1.72	0.71
1:C:145:TYR:CD1	1:C:146:GLY:N	2.58	0.70
1:D:325:GLU:HB2	1:D:329:LYS:HD3	1.73	0.70
1:D:247:ASP:O	1:D:251:VAL:HG13	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:THR:HG21	1:D:90:ARG:HG3	1.73	0.69
1:D:251:VAL:O	1:D:255:PRO:HG2	1.93	0.69
1:B:179:MET:CE	1:B:217:LEU:HD21	2.22	0.69
1:A:189:ASP:HB3	1:A:195:GLU:OE1	1.92	0.68
1:D:131:ARG:HG2	1:D:131:ARG:NH1	2.09	0.68
1:D:75:ASP:HB2	1:D:81:ARG:NH1	2.09	0.67
1:C:94:ARG:HD2	1:C:98:GLU:OE2	1.95	0.66
1:B:187:LEU:HD21	1:B:204:MET:CE	2.25	0.66
1:D:61:LEU:HD13	1:D:94:ARG:HG3	1.77	0.66
1:D:19:THR:CG2	1:D:90:ARG:HG3	2.26	0.66
1:A:195:GLU:O	1:A:196:ARG:HD2	1.97	0.65
1:B:295:ILE:HD12	1:B:324:LEU:HD11	1.79	0.65
1:A:94:ARG:HD2	1:A:98:GLU:OE2	1.97	0.65
1:C:183:MET:CE	1:C:183:MET:HB3	2.28	0.64
1:C:136:ARG:HB3	1:C:136:ARG:HH11	1.64	0.63
1:B:111:ASP:O	1:B:115:GLN:HG2	1.98	0.62
1:C:222:ARG:NH1	1:C:243:HIS:HD2	1.98	0.61
1:D:218:LEU:HD11	1:D:249:VAL:CG1	2.30	0.61
1:C:145:TYR:HB2	2:C:532:HOH:O	1.99	0.61
1:C:179:MET:CE	1:C:217:LEU:HD11	2.29	0.61
1:C:1:MET:HE2	2:C:504:HOH:O	2.00	0.61
1:C:247:ASP:O	1:C:251:VAL:HG12	2.00	0.61
1:D:134:ASN:HD21	1:D:136:ARG:NH2	1.99	0.61
1:C:81:ARG:HD3	1:D:81:ARG:NH2	2.16	0.60
1:D:75:ASP:HB2	1:D:81:ARG:HH12	1.64	0.60
1:C:145:TYR:HD1	1:C:146:GLY:N	1.98	0.59
1:A:187:LEU:HD21	1:A:204:MET:CE	2.32	0.59
1:B:301:GLU:CD	1:B:305:LYS:HE3	2.28	0.59
1:A:38:VAL:HG12	1:A:39:PRO:HD3	1.84	0.59
1:D:222:ARG:NH1	1:D:243:HIS:HD2	1.96	0.59
1:B:200:LEU:HG	1:B:204:MET:HE2	1.85	0.59
1:C:1:MET:SD	1:C:1:MET:C	2.86	0.58
1:C:219:GLU:CD	1:C:222:ARG:HE	2.09	0.58
1:A:187:LEU:HD21	1:A:204:MET:HE1	1.86	0.58
1:B:187:LEU:HD21	1:B:204:MET:HE1	1.85	0.58
1:D:218:LEU:HD11	1:D:249:VAL:HG12	1.84	0.58
1:D:281:ASP:HB3	1:D:284:LYS:HG3	1.86	0.58
1:D:255:PRO:O	1:D:258:LEU:O	2.22	0.58
1:D:285:ILE:HG22	1:D:323:MET:HE1	1.85	0.58
1:B:319:GLU:CD	1:B:319:GLU:H	2.13	0.57
1:C:5:GLU:OE2	1:C:33:ARG:HG2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLU:OE1	1:C:222:ARG:NE	2.38	0.57
1:C:183:MET:HB3	1:C:183:MET:HE2	1.87	0.57
1:C:107:LYS:O	1:C:107:LYS:HD3	2.05	0.57
1:D:192:ARG:HG2	1:D:192:ARG:HH11	1.70	0.57
1:A:90:ARG:C	1:A:90:ARG:HD3	2.30	0.57
1:B:200:LEU:HG	1:B:204:MET:CE	2.35	0.57
1:A:107:LYS:O	1:A:107:LYS:HD3	2.05	0.56
1:B:301:GLU:HB3	1:B:305:LYS:HD3	1.86	0.56
1:D:124:GLN:HE21	1:D:128:LYS:HE2	1.71	0.56
1:A:200:LEU:HG	1:A:204:MET:HE2	1.88	0.55
1:B:35:TYR:CE2	1:B:67:LYS:HG3	2.41	0.55
1:B:301:GLU:OE2	1:B:305:LYS:HE3	2.05	0.55
1:B:303:GLY:C	1:B:305:LYS:H	2.14	0.54
1:A:201:ALA:HB1	1:A:257:HIS:CE1	2.42	0.54
1:C:111:ASP:O	1:C:115:GLN:HG2	2.08	0.54
1:C:222:ARG:HH11	1:C:243:HIS:CD2	2.26	0.54
1:A:187:LEU:CD2	1:A:204:MET:HE1	2.38	0.53
1:B:65:SER:HB2	1:B:91:LEU:HB2	1.91	0.53
1:B:243:HIS:HE1	2:B:559:HOH:O	1.92	0.53
1:D:222:ARG:HH11	1:D:243:HIS:CD2	2.17	0.53
1:D:269:VAL:O	1:D:279:GLU:HA	2.08	0.53
1:A:94:ARG:HD3	1:A:98:GLU:HG3	1.91	0.53
1:C:44:GLU:HG2	1:C:238:LEU:HG	1.91	0.53
1:D:18:GLN:HG2	1:D:18:GLN:O	2.08	0.53
1:C:38:VAL:HG12	1:C:39:PRO:HD3	1.90	0.52
1:D:238:LEU:O	1:D:242:VAL:HG23	2.10	0.52
1:D:280:VAL:HG21	1:D:299:TYR:CZ	2.45	0.52
1:D:288:VAL:HG12	1:D:324:LEU:HD13	1.92	0.52
1:A:179:MET:HE2	1:A:221:LEU:HD21	1.90	0.52
1:C:183:MET:CE	1:C:183:MET:CB	2.88	0.52
1:C:201:ALA:HA	1:C:204:MET:CE	2.38	0.52
1:A:9:ARG:HD2	2:A:468:HOH:O	2.10	0.52
1:B:187:LEU:HD21	1:B:204:MET:HE3	1.90	0.52
1:B:295:ILE:CD1	1:B:324:LEU:HD11	2.39	0.52
1:D:313:GLU:HG3	1:D:314:LYS:N	2.25	0.51
1:D:90:ARG:HD3	1:D:90:ARG:C	2.36	0.51
1:C:187:LEU:HD21	1:C:204:MET:HE1	1.92	0.51
1:C:210:ALA:HB3	1:C:213:ASP:OD2	2.10	0.51
1:D:281:ASP:HB3	1:D:284:LYS:CG	2.40	0.51
1:D:61:LEU:CD1	1:D:94:ARG:HG3	2.41	0.51
1:D:251:VAL:CG2	1:D:252:ARG:N	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ARG:HD3	1:B:90:ARG:C	2.35	0.51
1:D:267:ALA:HB1	1:D:282:ILE:CB	2.38	0.50
1:B:98:GLU:OE1	2:B:401:HOH:O	2.19	0.50
1:A:192:ARG:HD2	1:C:80:ASP:CB	2.41	0.50
1:C:10:ASP:OD2	1:C:14:ARG:NH1	2.44	0.50
1:A:38:VAL:CG1	1:A:39:PRO:HD3	2.42	0.50
1:D:75:ASP:CB	1:D:81:ARG:NH1	2.75	0.50
1:C:11:HIS:CE1	1:C:57:ARG:HD2	2.47	0.49
1:D:267:ALA:C	1:D:282:ILE:HG12	2.37	0.49
1:D:325:GLU:CB	1:D:329:LYS:HD3	2.41	0.49
1:B:273:TYR:HB3	1:B:278:LYS:HD2	1.94	0.49
1:B:322:GLN:O	1:B:325:GLU:HG3	2.12	0.49
1:B:269:VAL:HG21	1:B:320:LEU:HD22	1.95	0.49
1:D:203:LEU:O	1:D:206:THR:HG22	2.12	0.48
1:A:183:MET:HE1	1:A:218:LEU:HG	1.95	0.48
1:B:19:THR:HG22	1:B:19:THR:O	2.14	0.48
1:C:187:LEU:CD2	1:C:204:MET:HE1	2.43	0.48
1:B:201:ALA:HB1	1:B:257:HIS:CE1	2.49	0.48
1:A:131:ARG:HG3	1:A:197:ASP:HB3	1.96	0.47
1:C:14:ARG:HG3	2:C:486:HOH:O	2.13	0.47
1:A:222:ARG:NH1	1:A:243:HIS:ND1	2.61	0.47
1:B:285:ILE:CD1	1:B:320:LEU:HD13	2.44	0.47
1:A:10:ASP:CG	1:C:192:ARG:HD2	2.39	0.47
1:C:126:ARG:NH2	2:C:402:HOH:O	2.31	0.47
1:D:252:ARG:O	1:D:255:PRO:HD2	2.14	0.47
1:B:295:ILE:O	1:B:310:ALA:HA	2.15	0.47
1:B:266:MET:HE3	1:B:266:MET:HA	1.96	0.47
1:D:259:GLY:O	1:D:260:GLU:HG2	2.15	0.47
1:B:202:HIS:O	1:B:206:THR:HB	2.15	0.47
1:C:100:GLU:OE1	1:D:100:GLU:OE1	2.33	0.47
1:D:210:ALA:O	1:D:213:ASP:HB2	2.14	0.47
1:B:303:GLY:C	1:B:305:LYS:N	2.74	0.46
1:A:195:GLU:C	1:A:196:ARG:HD2	2.41	0.46
1:C:131:ARG:HH11	1:C:131:ARG:CG	2.25	0.46
1:C:136:ARG:HH11	1:C:136:ARG:CG	2.29	0.46
1:C:119:HIS:CD2	2:C:402:HOH:O	2.69	0.45
1:C:46:THR:HG21	1:C:51:ARG:HG2	1.99	0.45
1:C:138:TRP:CH2	1:C:183:MET:HG2	2.51	0.45
1:A:147:SER:O	1:A:175:GLU:HG2	2.17	0.45
1:B:139:ARG:HG3	1:B:179:MET:HE1	1.99	0.45
1:C:222:ARG:NH1	1:C:243:HIS:CD2	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ASN:OD1	1:A:137:GLU:HG3	2.17	0.45
1:B:187:LEU:HD23	1:B:201:ALA:HB2	1.98	0.45
1:B:266:MET:HE2	1:B:267:ALA:N	2.31	0.45
1:D:38:VAL:HG12	1:D:39:PRO:HD3	1.97	0.45
1:C:73:MET:HE1	1:C:124:GLN:NE2	2.32	0.45
1:D:259:GLY:HA2	1:D:322:GLN:HG3	1.99	0.45
1:D:325:GLU:CA	1:D:329:LYS:HB3	2.42	0.45
1:D:44:GLU:HG3	1:D:44:GLU:O	2.17	0.44
1:D:295:ILE:O	1:D:310:ALA:HA	2.17	0.44
1:B:321:LEU:O	1:B:324:LEU:HB2	2.17	0.44
1:A:61:LEU:CD1	1:A:94:ARG:HG3	2.44	0.44
1:A:192:ARG:HA	2:A:494:HOH:O	2.18	0.44
1:C:136:ARG:HB2	2:C:448:HOH:O	2.17	0.44
1:D:218:LEU:HD11	1:D:249:VAL:HG11	1.99	0.44
1:B:105:ASP:CG	1:B:106:PRO:HD2	2.43	0.44
1:C:136:ARG:HH11	1:C:136:ARG:CB	2.29	0.44
1:C:179:MET:HE2	1:C:217:LEU:HD11	1.98	0.44
1:A:10:ASP:OD2	1:C:192:ARG:HD2	2.18	0.44
1:B:267:ALA:O	1:B:282:ILE:HG12	2.18	0.44
1:A:44:GLU:HG2	1:A:238:LEU:HG	1.99	0.43
1:B:302:GLY:H	1:B:305:LYS:HB3	1.82	0.43
1:A:14:ARG:HD2	2:A:543:HOH:O	2.17	0.43
1:C:81:ARG:HD3	1:D:81:ARG:HH22	1.82	0.43
1:D:280:VAL:HG11	1:D:299:TYR:CD2	2.53	0.43
1:C:19:THR:O	1:C:19:THR:HG22	2.18	0.43
1:B:87:VAL:O	1:B:91:LEU:HG	2.18	0.43
1:B:90:ARG:NH1	1:B:94:ARG:HB2	2.34	0.43
1:B:269:VAL:O	1:B:279:GLU:HA	2.18	0.43
1:D:258:LEU:HA	1:D:258:LEU:HD12	1.81	0.43
1:D:301:GLU:O	1:D:303:GLY:N	2.51	0.43
1:B:206:THR:HG22	1:B:208:ALA:H	1.83	0.43
1:B:266:MET:CE	1:B:267:ALA:N	2.82	0.43
1:B:115:GLN:HG3	2:B:581:HOH:O	2.18	0.43
1:D:301:GLU:O	1:D:302:GLY:C	2.62	0.43
1:A:165:GLN:HE21	1:A:165:GLN:HB2	1.60	0.43
1:C:254:LEU:N	1:C:255:PRO:CD	2.82	0.43
1:B:271:PHE:HB3	1:B:311:VAL:CG1	2.49	0.43
1:A:187:LEU:CD2	1:A:204:MET:CE	2.95	0.42
1:A:80:ASP:OD1	1:A:82:VAL:HB	2.19	0.42
1:B:131:ARG:HA	1:B:131:ARG:HD2	1.83	0.42
1:C:70:ASP:OD2	1:C:128:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:NH1	1:A:33:ARG:HG2	2.34	0.42
1:A:81:ARG:HG2	1:A:81:ARG:HH11	1.85	0.42
1:D:134:ASN:OD1	1:D:137:GLU:HG3	2.19	0.42
1:D:266:MET:H	1:D:266:MET:HG3	1.64	0.42
1:D:285:ILE:HG22	1:D:323:MET:CE	2.49	0.42
1:C:231:ALA:HA	1:C:232:PRO:HD3	1.85	0.42
1:B:271:PHE:HB3	1:B:311:VAL:HG12	2.01	0.42
1:C:183:MET:CE	1:C:183:MET:CG	2.94	0.42
1:C:189:ASP:O	1:C:190:TYR:C	2.63	0.42
1:D:131:ARG:NH1	1:D:131:ARG:CG	2.76	0.42
1:A:158:ALA:CB	1:A:165:GLN:HG2	2.49	0.42
1:B:317:PRO:O	1:B:318:LYS:C	2.62	0.42
1:C:70:ASP:HA	1:C:73:MET:HE3	2.02	0.42
1:B:131:ARG:HG3	1:B:197:ASP:HB3	2.02	0.41
1:B:285:ILE:HG22	1:B:323:MET:HE1	2.02	0.41
1:C:131:ARG:HG2	1:C:131:ARG:NH1	2.31	0.41
1:C:134:ASN:C	1:C:134:ASN:OD1	2.63	0.41
1:D:35:TYR:HB3	1:D:63:ILE:HG22	2.02	0.41
1:A:107:LYS:HD3	1:A:107:LYS:C	2.46	0.41
1:B:285:ILE:HG22	1:B:285:ILE:O	2.19	0.41
1:C:92:HIS:NE2	1:D:92:HIS:NE2	2.63	0.41
1:A:131:ARG:CG	1:A:131:ARG:HH11	2.33	0.41
1:B:1:MET:HB2	1:B:1:MET:HE3	2.02	0.41
1:B:281:ASP:C	1:B:283:SER:N	2.78	0.41
1:C:38:VAL:N	1:C:39:PRO:CD	2.84	0.41
1:D:124:GLN:NE2	1:D:128:LYS:HE2	2.34	0.41
1:A:9:ARG:HG2	2:A:443:HOH:O	2.20	0.41
1:C:179:MET:HE2	1:C:221:LEU:HD11	2.02	0.41
1:D:135:LEU:CD2	1:D:213:ASP:HB3	2.51	0.41
1:D:288:VAL:HG12	1:D:324:LEU:CD1	2.50	0.41
1:A:163:GLU:H	1:A:163:GLU:HG2	1.79	0.40
1:C:139:ARG:HG3	1:C:179:MET:HE1	2.03	0.40
1:B:1:MET:CE	1:B:1:MET:HB2	2.52	0.40
1:B:301:GLU:HB3	1:B:305:LYS:CD	2.50	0.40
1:C:131:ARG:CG	1:C:131:ARG:NH1	2.84	0.40
1:A:254:LEU:HB2	1:A:255:PRO:HD3	2.02	0.40
1:D:212:GLN:NE2	1:D:216:ASP:OD1	2.48	0.40
1:D:251:VAL:HG22	1:D:252:ARG:N	2.36	0.40
1:D:84:LEU:HD23	1:D:84:LEU:HA	1.94	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	262/343 (76%)	256 (98%)	6 (2%)	0	100	100
1	B	330/343 (96%)	311 (94%)	17 (5%)	2 (1%)	21	22
1	C	260/343 (76%)	252 (97%)	7 (3%)	1 (0%)	30	33
1	D	331/343 (96%)	310 (94%)	16 (5%)	5 (2%)	8	6
All	All	1183/1372 (86%)	1129 (95%)	46 (4%)	8 (1%)	18	18

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	261	ALA
1	C	164	GLY
1	D	302	GLY
1	B	261	ALA
1	D	263	ALA
1	D	303	GLY
1	B	302	GLY
1	D	264	GLY

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	208/270 (77%)	197 (95%)	11 (5%)	20	24
1	B	260/270 (96%)	247 (95%)	13 (5%)	22	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	206/270 (76%)	199 (97%)	7 (3%)	32	42
1	D	261/270 (97%)	252 (97%)	9 (3%)	32	42
All	All	935/1080 (87%)	895 (96%)	40 (4%)	26	33

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

Mol	Chain	Res	Type
1	A	18	GLN
1	A	29	THR
1	A	107	LYS
1	A	130	SER
1	A	131	ARG
1	A	139	ARG
1	A	163	GLU
1	A	165	GLN
1	A	186	ASP
1	A	191	ASP
1	A	197	ASP
1	B	18	GLN
1	B	38	VAL
1	B	131	ARG
1	B	186	ASP
1	B	206	THR
1	B	229	VAL
1	B	254	LEU
1	B	266	MET
1	B	277	GLU
1	B	284	LYS
1	B	288	VAL
1	B	293	LYS
1	B	325	GLU
1	C	29	THR
1	C	83	GLU
1	C	94	ARG
1	C	107	LYS
1	C	136	ARG
1	C	212	GLN
1	C	254	LEU
1	D	-2	ASP
1	D	18	GLN
1	D	19	THR

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Mol	Chain	Res	Type
1	D	105	ASP
1	D	139	ARG
1	D	197	ASP
1	D	251	VAL
1	D	266	MET
1	D	314	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	18	GLN
1	B	243	HIS
1	C	119	HIS
1	C	124	GLN
1	C	165	GLN
1	C	243	HIS
1	D	124	GLN
1	D	165	GLN
1	D	193	ASN
1	D	243	HIS
1	D	322	GLN

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 ⓘ

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

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	264/343 (76%)	-0.49	4 (1%) 72 70	17, 26, 52, 81	0
1	B	332/343 (96%)	-0.35	6 (1%) 67 65	16, 28, 66, 84	0
1	C	262/343 (76%)	-0.46	1 (0%) 88 87	15, 29, 45, 73	0
1	D	333/343 (97%)	-0.07	30 (9%) 15 13	15, 30, 100, 120	0
All	All	1191/1372 (86%)	-0.32	41 (3%) 48 45	15, 28, 78, 120	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	265	ALA	4.6
1	D	269	VAL	4.2
1	B	264	GLY	3.7
1	D	328	LYS	3.7
1	B	263	ALA	3.5
1	D	266	MET	3.5
1	D	263	ALA	3.5
1	B	261	ALA	3.3
1	D	304	GLY	3.3
1	D	267	ALA	3.2
1	D	262	GLY	3.0
1	D	268	THR	3.0
1	D	326	LYS	3.0
1	A	164	GLY	3.0
1	B	262	GLY	2.9
1	D	303	GLY	2.9
1	D	264	GLY	2.8
1	D	-3	ASP	2.8
1	D	258	LEU	2.8
1	D	305	LYS	2.7
1	C	145	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	192	ARG	2.6
1	A	-5	VAL	2.5
1	D	261	ALA	2.5
1	D	282	ILE	2.5
1	B	265	ALA	2.4
1	D	280	VAL	2.4
1	D	284	LYS	2.4
1	B	304	GLY	2.4
1	D	316	ALA	2.4
1	D	273	TYR	2.3
1	D	322	GLN	2.3
1	D	274	LYS	2.3
1	D	324	LEU	2.3
1	D	271	PHE	2.2
1	D	302	GLY	2.2
1	A	190	TYR	2.2
1	D	306	THR	2.2
1	D	197	ASP	2.1
1	D	329	LYS	2.1
1	D	323	MET	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.