



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:59 AM UTC

PDB ID : 5AF0 / pdb_00005af0
Title : MAEL domain from Bombyx mori Maelstrom
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Deposited on : 2015-01-13
Resolution : 2.40 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

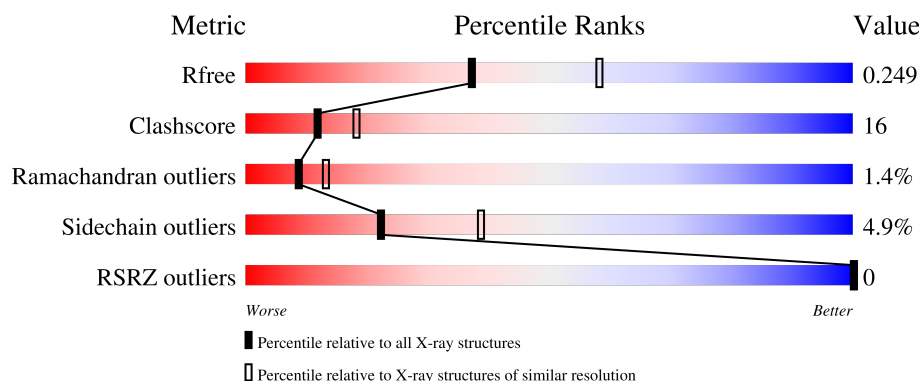
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	261	56% 32% • 9%
1	B	261	61% 25% • 10%
1	C	261	56% 31% • 8%
1	D	261	57% 32% • 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7297 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 MAELSTROM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1829	1170	297	350	12			
1	B	236	Total	C	N	O	S	0	0	0
			1797	1147	292	345	13			
1	C	239	Total	C	N	O	S	0	0	0
			1809	1163	291	342	13			
1	D	238	Total	C	N	O	S	0	0	0
			1823	1170	295	345	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	298	LYS	ARG	conflict	UNP H9JFX7
B	298	LYS	ARG	conflict	UNP H9JFX7
C	298	LYS	ARG	conflict	UNP H9JFX7
D	298	LYS	ARG	conflict	UNP H9JFX7

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

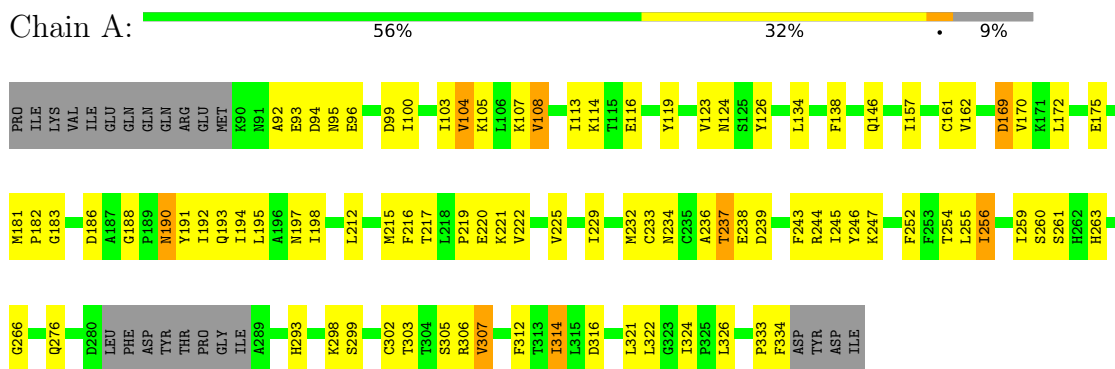
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total 14	O 14	0	0
3	B	9	Total 9	O 9	0	0
3	C	7	Total 7	O 7	0	0
3	D	5	Total 5	O 5	0	0

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.

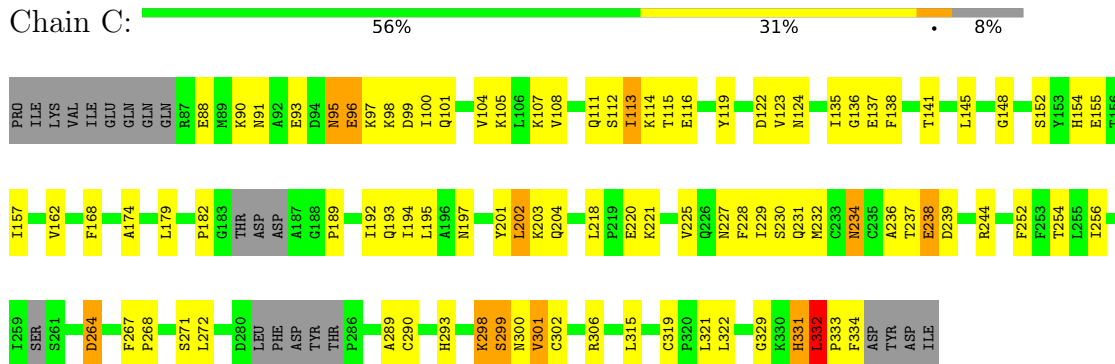
• Molecule 1: MAELSTROM



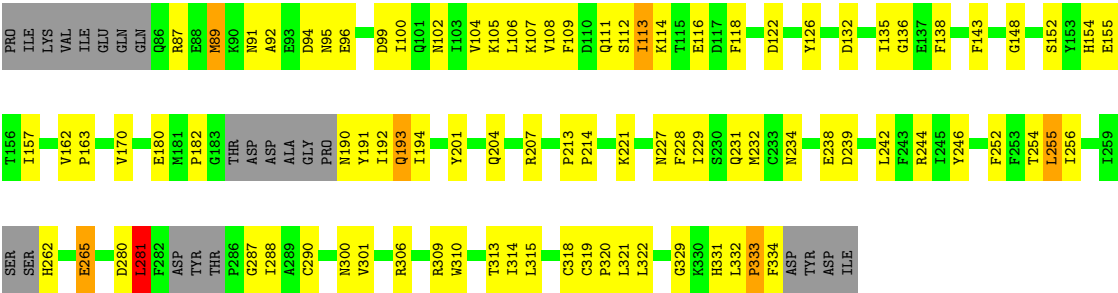
• Molecule 1: MAELSTROM



• Molecule 1: MAELSTROM



● Molecule 1: MAELSTROM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.37Å 101.21Å 101.64Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	45.42 – 2.40 45.42 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.2 (45.42-2.40) 81.1 (45.42-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.39Å)	Xtriage
Refinement program	PHENIX dev_1839	Depositor
R, R_{free}	0.227 , 0.263 (Not available) , 0.249	Depositor DCC
R_{free} test set	2870 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.951	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.426 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7297	wwPDB-VP
Average B, all atoms (Å ²)	59.0	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 29.39 % 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 1.5621e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.67	0/1869	1.09	10/2544 (0.4%)
1	B	0.66	0/1833	1.10	10/2495 (0.4%)
1	C	0.71	1/1846 (0.1%)	1.15	14/2509 (0.6%)
1	D	0.64	0/1862	1.11	14/2528 (0.6%)
All	All	0.67	1/7410 (0.0%)	1.11	48/10076 (0.5%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	95	ASN	CA-C	-5.40	1.45	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	319	CYS	CA-C-N	-8.36	111.12	119.56
1	C	319	CYS	C-N-CA	-8.36	111.12	119.56
1	C	96	GLU	N-CA-C	-8.25	102.28	111.28
1	A	93	GLU	N-CA-C	-7.86	103.50	113.72
1	B	236	ALA	N-CA-C	-7.61	99.74	108.49
1	D	319	CYS	CA-C-N	-6.97	112.52	119.56
1	D	319	CYS	C-N-CA	-6.97	112.52	119.56
1	C	301	VAL	N-CA-C	-6.68	106.01	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	293	HIS	N-CA-C	6.48	118.00	111.07
1	D	301	VAL	N-CA-C	-6.39	106.28	112.29
1	C	234	ASN	N-CA-C	-6.30	104.65	112.90
1	B	108	VAL	N-CA-C	-6.28	103.50	112.35
1	A	94	ASP	N-CA-C	-6.22	104.61	111.82
1	D	256	ILE	N-CA-C	6.05	116.79	110.62
1	C	332	LEU	CA-C-N	6.02	127.36	119.84
1	C	332	LEU	C-N-CA	6.02	127.36	119.84
1	D	288	ILE	N-CA-C	5.91	116.04	108.12
1	B	319	CYS	CA-C-N	-5.88	113.62	119.56
1	B	319	CYS	C-N-CA	-5.88	113.62	119.56
1	C	298	LYS	CA-C-N	5.85	132.23	121.70
1	C	298	LYS	C-N-CA	5.85	132.23	121.70
1	B	218	LEU	CA-C-N	5.76	127.04	119.84
1	B	218	LEU	C-N-CA	5.76	127.04	119.84
1	A	157	ILE	N-CA-C	5.60	115.66	107.37
1	C	331	HIS	N-CA-C	-5.58	106.60	113.41
1	D	213	PRO	CA-C-N	-5.57	114.85	120.31
1	D	213	PRO	C-N-CA	-5.57	114.85	120.31
1	C	111	GLN	N-CA-C	5.55	118.90	111.24
1	B	298	LYS	CA-C-N	5.54	132.12	121.54
1	B	298	LYS	C-N-CA	5.54	132.12	121.54
1	D	193	GLN	N-CA-C	5.54	117.12	111.14
1	C	218	LEU	CA-C-N	5.52	125.61	119.32
1	C	218	LEU	C-N-CA	5.52	125.61	119.32
1	D	287	GLY	N-CA-C	5.50	121.48	114.66
1	A	191	TYR	N-CA-C	5.48	117.25	111.28
1	D	265	GLU	N-CA-C	5.29	118.85	109.96
1	D	234	ASN	N-CA-C	-5.29	105.97	112.90
1	A	192	ILE	N-CA-C	-5.20	105.43	110.42
1	A	108	VAL	N-CA-C	-5.15	105.09	112.35
1	A	266	GLY	N-CA-C	5.13	120.41	112.45
1	D	281	LEU	N-CA-C	-5.11	105.36	111.03
1	D	255	LEU	N-CA-C	5.04	116.47	110.97
1	B	109	PHE	CA-C-N	-5.02	114.65	122.73
1	B	109	PHE	C-N-CA	-5.02	114.65	122.73
1	A	161	CYS	N-CA-C	5.01	116.61	109.14
1	D	300	ASN	N-CA-C	-5.01	107.02	114.64
1	A	298	LYS	CA-C-N	5.00	130.71	121.70
1	A	298	LYS	C-N-CA	5.00	130.71	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	298	LYS	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	1829	0	1731	61	0
1	B	1797	0	1693	50	0
1	C	1809	0	1698	59	0
1	D	1823	0	1698	55	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	14	0	0	1	0
3	B	9	0	0	1	0
3	C	7	0	0	0	0
3	D	5	0	0	0	0
All	All	7297	0	6820	223	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 16.

All (223) 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:D:262:HIS:HB2	1:D:265:GLU:HG3	1.58	0.85
1:A:260:SER:HA	1:A:321:LEU:HD13	1.59	0.83
1:D:91:ASN:O	1:D:95:ASN:ND2	2.15	0.80
1:C:99:ASP:OD2	1:C:244:ARG:NH1	2.15	0.80
1:A:124:ASN:OD1	1:A:306:ARG:NH2	2.14	0.80
1:B:124:ASN:OD1	1:B:306:ARG:NH2	2.15	0.79
1:B:259:ILE:HB	1:B:322:LEU:HD11	1.63	0.79
1:D:227:ASN:OD1	1:D:231:GLN:NE2	2.16	0.78
1:C:95:ASN:O	1:C:99:ASP:N	2.11	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ILE:HB	1:A:322:LEU:HD11	1.65	0.76
1:D:122:ASP:OD2	1:D:306:ARG:NH1	2.19	0.76
1:B:132:ASP:HB3	1:B:231:GLN:HE21	1.53	0.72
1:B:276:GLN:HE22	1:B:317:ARG:HH11	1.38	0.72
1:B:146:GLN:HA	1:B:324:ILE:HD13	1.70	0.72
1:C:152:SER:HA	1:C:201:TYR:OH	1.91	0.70
1:A:306:ARG:NH1	3:A:2006:HOH:O	2.21	0.70
1:A:212:LEU:O	1:A:244:ARG:NH2	2.25	0.69
1:B:190:ASN:HB2	1:B:193:GLN:HB3	1.73	0.69
1:D:94:ASP:OD1	1:D:95:ASN:ND2	2.26	0.69
1:B:145:LEU:HD11	1:B:255:LEU:HD11	1.75	0.69
1:A:252:PHE:CZ	1:A:314:ILE:HA	2.27	0.68
1:C:96:GLU:O	1:C:100:ILE:HG13	1.93	0.68
1:C:104:VAL:HG21	1:C:254:THR:HG22	1.76	0.68
1:B:146:GLN:O	1:B:331:HIS:NE2	2.25	0.67
1:A:194:ILE:HA	1:A:197:ASN:HD22	1.58	0.67
1:B:293:HIS:HB3	1:B:299:SER:HA	1.76	0.67
1:D:104:VAL:HG11	1:D:254:THR:HG22	1.78	0.66
1:B:111:GLN:OE1	3:B:2001:HOH:O	2.13	0.66
1:B:181:MET:HE3	1:B:182:PRO:HD2	1.78	0.66
1:A:302:CYS:HB3	1:A:305:SER:HB2	1.79	0.65
1:C:193:GLN:HG3	1:C:197:ASN:HD21	1.62	0.64
1:C:268:PRO:HD2	1:C:272:LEU:HD22	1.80	0.63
1:D:138:PHE:O	1:D:154:HIS:HD2	1.82	0.63
1:A:221:LYS:O	1:A:225:VAL:HG22	1.99	0.63
1:C:227:ASN:OD1	1:C:231:GLN:NE2	2.31	0.63
1:C:194:ILE:HA	1:C:197:ASN:HD22	1.63	0.62
1:D:239:ASP:HB3	1:D:242:LEU:HD13	1.80	0.62
1:A:312:PHE:O	1:A:316:ASP:HB2	2.00	0.62
1:B:96:GLU:O	1:B:100:ILE:HG13	2.00	0.61
1:B:270:GLU:CD	1:B:270:GLU:H	2.04	0.61
1:A:126:TYR:HB2	1:A:134:LEU:HD23	1.83	0.59
1:A:162:VAL:HG22	1:A:182:PRO:HG2	1.85	0.59
1:B:274:LEU:O	1:B:278:THR:N	2.34	0.59
1:A:198:ILE:HD12	1:A:232:MET:HE1	1.83	0.59
1:B:119:TYR:OH	1:B:142:GLN:NE2	2.33	0.59
1:D:126:TYR:OH	1:D:180:GLU:O	2.07	0.59
1:A:169:ASP:OD1	1:A:169:ASP:N	2.36	0.58
1:D:105:LYS:HG2	1:D:106:LEU:HD12	1.86	0.58
1:A:225:VAL:HG23	1:A:245:ILE:HG21	1.86	0.58
1:D:329:GLY:N	1:D:332:LEU:O	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ILE:HG13	1:C:228:PHE:CD1	2.39	0.57
1:A:162:VAL:HG13	1:A:170:VAL:HG21	1.85	0.56
1:B:274:LEU:H	1:B:274:LEU:HD12	1.68	0.56
1:D:281:LEU:HG	1:D:310:TRP:HE1	1.69	0.56
1:B:190:ASN:O	1:B:194:ILE:HG23	2.06	0.56
1:C:95:ASN:HA	1:C:98:LYS:HB2	1.88	0.55
1:A:220:GLU:HG3	1:A:221:LYS:N	2.22	0.55
1:B:169:ASP:OD1	1:B:169:ASP:N	2.39	0.55
1:D:107:LYS:HE3	1:D:116:GLU:HG3	1.87	0.55
1:D:99:ASP:OD2	1:D:244:ARG:NH1	2.40	0.55
1:A:303:THR:O	1:A:307:VAL:HB	2.07	0.54
1:B:220:GLU:HG3	1:B:221:LYS:HG2	1.90	0.54
1:C:138:PHE:O	1:C:154:HIS:HD2	1.90	0.54
1:B:107:LYS:HZ3	1:B:116:GLU:CD	2.15	0.54
1:C:112:SER:O	1:C:116:GLU:HG2	2.06	0.54
1:C:100:ILE:O	1:C:104:VAL:HG22	2.08	0.54
1:C:124:ASN:HB2	1:C:137:GLU:HB3	1.90	0.54
1:C:193:GLN:O	1:C:197:ASN:ND2	2.41	0.54
1:D:104:VAL:HG21	1:D:255:LEU:HA	1.89	0.53
1:A:236:ALA:C	1:A:238:GLU:H	2.16	0.53
1:D:163:PRO:HD2	1:D:170:VAL:HG21	1.89	0.53
1:C:91:ASN:O	1:C:95:ASN:N	2.23	0.53
1:A:162:VAL:CG2	1:A:182:PRO:HG2	2.39	0.53
1:D:136:GLY:HA2	1:D:157:ILE:O	2.08	0.52
1:A:96:GLU:O	1:A:100:ILE:HG13	2.10	0.52
1:C:202:LEU:O	1:C:204:GLN:NE2	2.39	0.52
1:C:333:PRO:O	1:C:334:PHE:HB2	2.09	0.52
1:D:194:ILE:HD11	1:D:232:MET:SD	2.49	0.52
1:D:108:VAL:HG12	1:D:113:ILE:HG21	1.92	0.52
1:D:152:SER:HA	1:D:201:TYR:OH	2.09	0.52
1:C:195:LEU:HD22	1:C:232:MET:O	2.10	0.52
1:A:186:ASP:O	1:A:188:GLY:N	2.44	0.51
1:C:264:ASP:OD1	1:C:264:ASP:N	2.33	0.51
1:D:100:ILE:O	1:D:104:VAL:HG12	2.10	0.51
1:C:289:ALA:HB1	1:C:302:CYS:SG	2.51	0.51
1:B:90:LYS:NZ	1:B:93:GLU:OE2	2.44	0.51
1:B:162:VAL:HG13	1:B:170:VAL:HG21	1.93	0.51
1:A:193:GLN:O	1:A:197:ASN:ND2	2.44	0.50
1:C:230:SER:O	1:C:234:ASN:N	2.43	0.50
1:B:122:ASP:OD2	1:B:306:ARG:NH1	2.43	0.50
1:A:172:LEU:O	1:A:175:GLU:HB3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:LYS:HA	1:B:93:GLU:HB3	1.92	0.50
1:B:145:LEU:HD21	1:B:255:LEU:HD21	1.94	0.50
1:A:188:GLY:O	1:A:190:ASN:ND2	2.45	0.50
1:D:112:SER:O	1:D:116:GLU:HG2	2.10	0.50
1:C:148:GLY:HA2	1:C:315:LEU:HD11	1.93	0.50
1:D:122:ASP:OD1	1:D:221:LYS:HE3	2.12	0.50
1:C:108:VAL:HB	1:C:113:ILE:HD13	1.93	0.49
1:D:190:ASN:HA	1:D:193:GLN:HB3	1.95	0.49
1:D:333:PRO:O	1:D:334:PHE:HB2	2.13	0.49
1:A:236:ALA:O	1:A:238:GLU:N	2.45	0.49
1:D:111:GLN:O	1:D:114:LYS:NZ	2.45	0.49
1:A:219:PRO:HG3	1:A:247:LYS:HE3	1.93	0.49
1:D:315:LEU:HD13	1:D:331:HIS:CD2	2.48	0.48
1:A:233:CYS:O	1:A:238:GLU:N	2.46	0.48
1:C:225:VAL:O	1:C:229:ILE:HG12	2.13	0.48
1:B:296:LEU:O	1:B:298:LYS:N	2.42	0.48
1:C:95:ASN:O	1:C:96:GLU:C	2.56	0.48
1:B:290:CYS:HB2	1:B:302:CYS:SG	2.54	0.48
1:B:255:LEU:O	1:B:259:ILE:HG12	2.13	0.48
1:C:107:LYS:HD3	1:C:116:GLU:HG3	1.94	0.48
1:A:123:VAL:HG12	1:A:138:PHE:HB3	1.95	0.48
1:A:193:GLN:HG2	1:A:197:ASN:HD21	1.79	0.47
1:B:162:VAL:HG23	1:B:182:PRO:HG2	1.96	0.47
1:A:99:ASP:OD2	1:A:246:TYR:OH	2.28	0.47
1:A:236:ALA:C	1:A:238:GLU:N	2.72	0.47
1:A:234:ASN:C	1:A:236:ALA:H	2.23	0.47
1:D:280:ASP:HB3	1:D:313:THR:HG21	1.97	0.47
1:A:146:GLN:HA	1:A:324:ILE:HD13	1.97	0.47
1:B:239:ASP:O	1:B:242:LEU:HD13	2.15	0.47
1:C:124:ASN:ND2	1:C:301:VAL:O	2.39	0.47
1:B:227:ASN:O	1:B:231:GLN:HB2	2.15	0.47
1:A:92:ALA:HA	1:A:95:ASN:ND2	2.30	0.47
1:C:136:GLY:HA2	1:C:157:ILE:O	2.14	0.47
1:C:220:GLU:HG2	1:C:221:LYS:N	2.29	0.47
1:A:195:LEU:HD11	1:A:243:PHE:CZ	2.50	0.46
1:A:104:VAL:HG11	1:A:254:THR:HG22	1.98	0.46
1:B:177:PHE:HB2	1:B:179:LEU:HG	1.96	0.46
1:B:276:GLN:NE2	1:B:317:ARG:HH11	2.10	0.46
1:C:138:PHE:CE2	1:C:155:GLU:HB2	2.50	0.46
1:A:107:LYS:HD3	1:A:116:GLU:HG2	1.97	0.46
1:C:315:LEU:HD13	1:C:331:HIS:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:318:CYS:O	1:D:321:LEU:HB2	2.16	0.46
1:C:93:GLU:O	1:C:97:LYS:HG2	2.16	0.46
1:A:181:MET:HE3	1:A:182:PRO:HD2	1.98	0.46
1:B:269:LYS:O	1:B:272:LEU:HB2	2.16	0.45
1:C:154:HIS:CE1	1:C:290:CYS:HB2	2.51	0.45
1:D:118:PHE:HB2	1:D:143:PHE:CE1	2.51	0.45
1:D:252:PHE:CZ	1:D:314:ILE:HA	2.51	0.45
1:D:136:GLY:O	1:D:157:ILE:N	2.46	0.45
1:B:234:ASN:C	1:B:236:ALA:H	2.23	0.45
1:D:320:PRO:C	1:D:322:LEU:H	2.25	0.45
1:C:124:ASN:OD1	1:C:306:ARG:NH1	2.49	0.45
1:D:162:VAL:HG22	1:D:182:PRO:HG2	1.99	0.45
1:C:114:LYS:HA	1:C:145:LEU:HB2	1.98	0.45
1:C:138:PHE:O	1:C:154:HIS:CD2	2.69	0.45
1:A:107:LYS:HE3	1:C:168:PHE:CD2	2.52	0.45
1:C:195:LEU:HD13	1:C:232:MET:HB3	1.99	0.44
1:A:252:PHE:O	1:A:256:ILE:HG22	2.18	0.44
1:D:281:LEU:O	1:D:309:ARG:NE	2.51	0.43
1:D:320:PRO:C	1:D:322:LEU:N	2.76	0.43
1:B:233:CYS:HB3	1:B:238:GLU:O	2.17	0.43
1:B:252:PHE:O	1:B:256:ILE:HG22	2.17	0.43
1:D:227:ASN:O	1:D:231:GLN:HG3	2.18	0.43
1:A:186:ASP:C	1:A:188:GLY:N	2.75	0.43
1:A:263:HIS:CE1	1:D:191:TYR:CE2	3.06	0.43
1:B:107:LYS:NZ	1:B:116:GLU:CD	2.77	0.43
1:B:138:PHE:CE2	1:B:155:GLU:HB2	2.54	0.43
1:B:190:ASN:ND2	1:B:190:ASN:H	2.15	0.43
1:B:218:LEU:HD23	1:B:218:LEU:HA	1.74	0.43
1:C:154:HIS:CE1	1:C:290:CYS:CB	3.01	0.43
1:C:193:GLN:HG3	1:C:197:ASN:ND2	2.31	0.43
1:C:145:LEU:HD13	1:C:322:LEU:CD1	2.48	0.43
1:C:329:GLY:N	1:C:332:LEU:O	2.52	0.43
1:A:225:VAL:O	1:A:229:ILE:HG12	2.19	0.43
1:A:293:HIS:HB3	1:A:299:SER:HA	2.00	0.43
1:A:123:VAL:HG12	1:A:138:PHE:CB	2.48	0.43
1:A:293:HIS:HB3	1:A:299:SER:N	2.34	0.43
1:A:255:LEU:O	1:A:259:ILE:HG12	2.19	0.43
1:C:98:LYS:HA	1:C:101:GLN:OE1	2.19	0.43
1:C:123:VAL:HG12	1:C:138:PHE:HB3	2.01	0.43
1:D:102:ASN:O	1:D:106:LEU:HD13	2.18	0.43
1:A:293:HIS:HB3	1:A:299:SER:H	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ASP:OD1	1:C:221:LYS:HE3	2.19	0.42
1:C:138:PHE:CD1	1:C:138:PHE:C	2.97	0.42
1:D:94:ASP:OD1	1:D:95:ASN:N	2.52	0.42
1:B:122:ASP:OD2	1:B:306:ARG:HD2	2.19	0.42
1:C:157:ILE:HG23	1:C:189:PRO:CB	2.48	0.42
1:A:216:PHE:HA	1:A:246:TYR:O	2.19	0.42
1:A:238:GLU:HG3	1:A:239:ASP:N	2.34	0.42
1:A:293:HIS:HB3	1:A:299:SER:CA	2.49	0.42
1:D:96:GLU:O	1:D:100:ILE:HG13	2.19	0.42
1:D:109:PHE:HD1	1:D:109:PHE:HA	1.71	0.42
1:D:214:PRO:HG3	1:D:244:ARG:CZ	2.49	0.42
1:A:333:PRO:O	1:A:334:PHE:HB2	2.20	0.42
1:A:114:LYS:HG2	1:A:322:LEU:HD23	2.01	0.42
1:C:119:TYR:HA	1:C:141:THR:O	2.20	0.42
1:C:267:PHE:HA	1:C:268:PRO:HD3	1.87	0.42
1:A:103:ILE:O	1:A:107:LYS:HG3	2.20	0.42
1:A:316:ASP:HA	1:A:326:LEU:HD21	2.01	0.42
1:B:194:ILE:HG13	1:B:195:LEU:N	2.34	0.42
1:D:154:HIS:CE1	1:D:290:CYS:CB	3.03	0.42
1:D:190:ASN:O	1:D:194:ILE:N	2.38	0.42
1:B:120:VAL:HG23	1:B:216:PHE:O	2.20	0.41
1:C:298:LYS:HA	1:C:299:SER:CB	2.49	0.41
1:D:138:PHE:CE2	1:D:155:GLU:HB2	2.55	0.41
1:A:119:TYR:O	1:A:215:MET:HA	2.20	0.41
1:C:162:VAL:HG22	1:C:182:PRO:HG2	2.02	0.41
1:D:89:MET:O	1:D:89:MET:HG3	2.12	0.41
1:D:96:GLU:HG3	1:D:246:TYR:CE1	2.55	0.41
1:C:321:LEU:HD23	1:C:321:LEU:HA	1.85	0.41
1:D:204:GLN:HB2	1:D:207:ARG:HB2	2.01	0.41
1:C:174:ALA:HA	1:C:179:LEU:HB2	2.03	0.41
1:D:229:ILE:HD13	1:D:229:ILE:HA	1.88	0.41
1:A:105:LYS:O	1:A:108:VAL:HG12	2.20	0.41
1:C:236:ALA:C	1:C:238:GLU:H	2.28	0.41
1:C:252:PHE:O	1:C:256:ILE:HG22	2.21	0.41
1:D:92:ALA:HA	1:D:95:ASN:HB2	2.02	0.41
1:A:260:SER:HA	1:A:321:LEU:CD1	2.40	0.41
1:B:162:VAL:CG2	1:B:182:PRO:HG2	2.51	0.41
1:B:213:PRO:HA	1:B:214:PRO:HD3	1.95	0.41
1:B:218:LEU:HG	1:B:310:TRP:CZ2	2.56	0.41
1:C:227:ASN:O	1:C:231:GLN:HG3	2.21	0.41
1:D:148:GLY:HA2	1:D:315:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:LYS:NZ	1:B:116:GLU:OE2	2.54	0.40
1:C:104:VAL:HG23	1:C:105:LYS:N	2.36	0.40
1:A:217:THR:HG21	1:A:225:VAL:HG21	2.04	0.40
1:D:132:ASP:HA	1:D:227:ASN:OD1	2.22	0.40
1:D:135:ILE:HG13	1:D:228:PHE:CD1	2.57	0.40
1:B:247:LYS:HB3	1:B:247:LYS:HE2	1.85	0.40
1:A:220:GLU:HG3	1:A:221:LYS:CG	2.52	0.40
1:B:327:GLN:HA	1:B:328:PRO:HD3	1.79	0.40
1:D:107:LYS:HB2	1:D:113:ILE:HD12	2.03	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	233/261 (89%)	220 (94%)	10 (4%)	3 (1%)	9	14
1	B	230/261 (88%)	216 (94%)	10 (4%)	4 (2%)	7	10
1	C	231/261 (88%)	218 (94%)	9 (4%)	4 (2%)	7	10
1	D	230/261 (88%)	215 (94%)	13 (6%)	2 (1%)	14	22
All	All	924/1044 (88%)	869 (94%)	42 (4%)	13 (1%)	9	13

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	205	LYS
1	B	299	SER
1	B	184	THR
1	C	88	GLU
1	C	300	ASN
1	A	237	THR

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Mol	Chain	Res	Type
1	C	90	LYS
1	D	87	ARG
1	A	261	SER
1	D	333	PRO
1	C	299	SER
1	A	183	GLY
1	B	182	PRO

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	198/239 (83%)	188 (95%)	10 (5%)	21	37
1	B	192/239 (80%)	180 (94%)	12 (6%)	16	29
1	C	189/239 (79%)	178 (94%)	11 (6%)	18	32
1	D	191/239 (80%)	186 (97%)	5 (3%)	40	63
All	All	770/956 (80%)	732 (95%)	38 (5%)	22	39

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	VAL
1	A	113	ILE
1	A	169	ASP
1	A	190	ASN
1	A	222	VAL
1	A	237	THR
1	A	256	ILE
1	A	276	GLN
1	A	307	VAL
1	A	314	ILE
1	B	113	ILE
1	B	134	LEU
1	B	169	ASP
1	B	176	GLU

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Mol	Chain	Res	Type
1	B	190	ASN
1	B	192	ILE
1	B	194	ILE
1	B	202	LEU
1	B	205	LYS
1	B	238	GLU
1	B	270	GLU
1	B	272	LEU
1	C	113	ILE
1	C	115	THR
1	C	192	ILE
1	C	202	LEU
1	C	203	LYS
1	C	237	THR
1	C	238	GLU
1	C	239	ASP
1	C	264	ASP
1	C	271	SER
1	C	332	LEU
1	D	89	MET
1	D	113	ILE
1	D	192	ILE
1	D	238	GLU
1	D	281	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	GLN
1	A	190	ASN
1	A	197	ASN
1	A	204	GLN
1	A	300	ASN
1	B	102	ASN
1	B	142	GLN
1	B	190	ASN
1	B	204	GLN
1	B	231	GLN
1	C	151	ASN
1	C	154	HIS
1	C	197	ASN
1	C	331	HIS

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Mol	Chain	Res	Type
1	D	154	HIS
1	D	193	GLN
1	D	210	GLN
1	D	331	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	237/261 (90%)	-1.17	0 100 100	32, 53, 98, 120	0
1	B	236/261 (90%)	-1.00	0 100 100	33, 60, 109, 134	0
1	C	239/261 (91%)	-1.04	0 100 100	32, 57, 91, 135	0
1	D	238/261 (91%)	-1.07	0 100 100	32, 58, 92, 136	0
All	All	950/1044 (90%)	-1.07	0 100 100	32, 57, 98, 136	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	ZN	A	501	1/1	1.00	0.01	85,85,85,85	0
2	ZN	B	501	1/1	1.00	0.01	86,86,86,86	0
2	ZN	C	501	1/1	1.00	0.02	73,73,73,73	0
2	ZN	D	501	1/1	1.00	0.02	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.