



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:13 PM UTC

PDB ID : 3CSQ / pdb_00003csq
Title : Crystal and cryoEM structural studies of a cell wall degrading enzyme in the bacteriophage phi29 tail
Authors : Xiang, Y.; Rossmann, M.G.
Deposited on : 2008-04-10
Resolution : 1.80 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

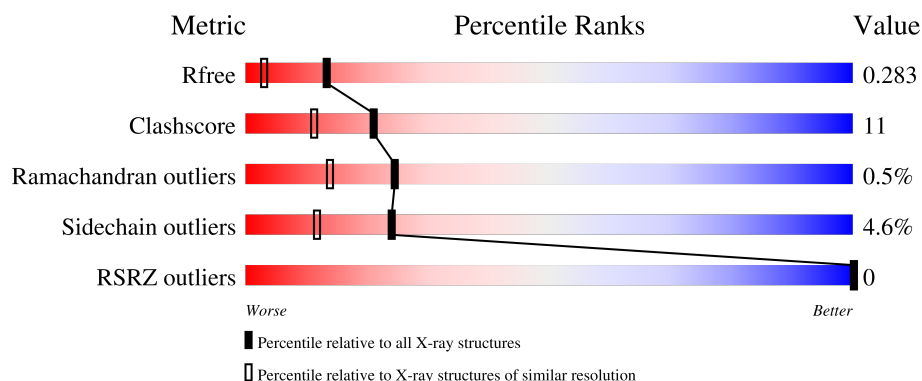
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	334	
1	B	334	
1	C	334	
1	D	334	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10684 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 Morphogenesis protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	3	0
			2614	1664	435	497	18			
1	B	324	Total	C	N	O	S	0	0	0
			2597	1652	433	494	18			
1	C	324	Total	C	N	O	S	0	4	0
			2616	1665	436	497	18			
1	D	326	Total	C	N	O	S	0	4	0
			2633	1676	443	496	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	ASN	ASP	SEE REMARK 999	UNP P15132
B	89	ASN	ASP	SEE REMARK 999	UNP P15132
C	89	ASN	ASP	SEE REMARK 999	UNP P15132
D	89	ASN	ASP	SEE REMARK 999	UNP P15132

- 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		

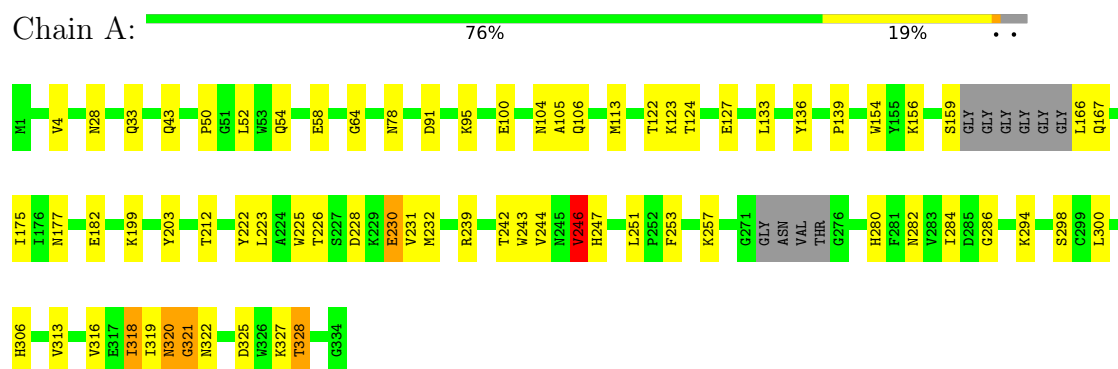
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	49	Total 49	O 49	0	0
3	B	54	Total 54	O 54	0	0
3	C	58	Total 62	O 62	0	4
3	D	55	Total 55	O 55	0	0

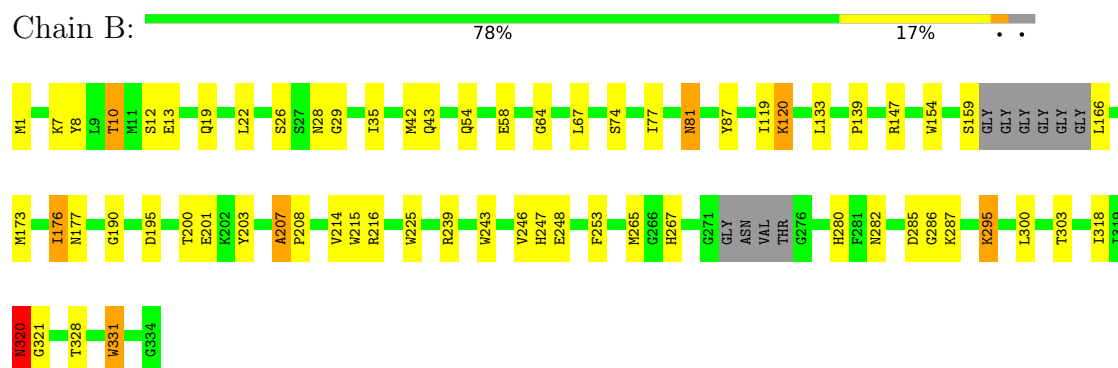
3 Residue-property plots

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: Morphogenesis protein 1



• Molecule 1: Morphogenesis protein 1

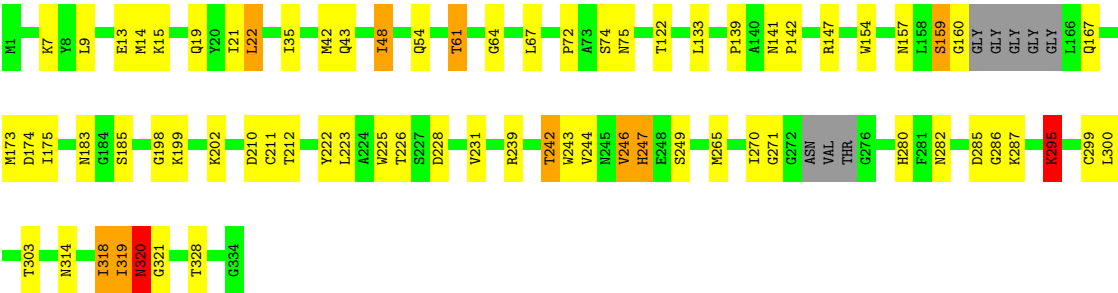


• Molecule 1: Morphogenesis protein 1





● Molecule 1: Morphogenesis protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.84Å 133.96Å 85.72Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	19.90 – 1.80 19.90 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.90-1.80) 97.5 (19.90-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.84 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.238 , 0.282 0.239 , 0.283	Depositor DCC
R_{free} test set	5487 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 16.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.450 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10684	wwPDB-VP
Average B, all atoms (Å ²)	18.0	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 48.74 % 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 8.2421e-05.*

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	0.82	0/2694	0.98	7/3656 (0.2%)
1	B	0.87	0/2668	1.04	8/3622 (0.2%)
1	C	0.82	0/2699	0.94	1/3663 (0.0%)
1	D	0.86	1/2716 (0.0%)	0.98	6/3682 (0.2%)
All	All	0.84	1/10777 (0.0%)	0.99	22/14623 (0.2%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	270	ILE	CA-CB	5.21	1.60	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	GLY	N-CA-C	-10.07	89.31	113.18
1	A	320	ASN	O-C-N	-7.05	116.43	123.62
1	B	173	MET	CA-C-N	6.83	130.35	120.38
1	B	173	MET	C-N-CA	6.83	130.35	120.38
1	B	320	ASN	CA-C-N	6.56	134.26	121.41
1	B	320	ASN	C-N-CA	6.56	134.26	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	320	ASN	O-C-N	-6.54	115.15	123.26
1	A	320	ASN	CA-C-N	5.70	131.97	121.70
1	A	320	ASN	C-N-CA	5.70	131.97	121.70
1	C	172	PRO	N-CA-C	5.40	120.94	113.65
1	B	207	ALA	N-CA-C	5.40	117.37	109.71
1	A	321	GLY	N-CA-C	-5.37	97.74	113.30
1	D	286	GLY	N-CA-C	5.33	121.90	112.83
1	A	328	THR	N-CA-CB	-5.32	101.95	110.46
1	D	183	ASN	CA-C-N	5.19	124.91	119.92
1	D	183	ASN	C-N-CA	5.19	124.91	119.92
1	A	246	VAL	CB-CA-C	5.19	118.82	110.82
1	A	320	ASN	CB-CA-C	-5.15	105.04	111.43
1	B	286	GLY	N-CA-C	5.14	118.55	112.33
1	D	295	LYS	CA-C-N	5.05	139.12	127.00
1	D	295	LYS	C-N-CA	5.05	139.12	127.00
1	D	320	ASN	CB-CA-C	-5.02	104.59	111.51

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	320	ASN	Peptide
1	D	320	ASN	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	2614	0	2492	48	0
1	B	2597	0	2467	58	0
1	C	2616	0	2497	57	0
1	D	2633	0	2525	67	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	49	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	54	0	0	2	0
3	C	62	0	0	6	0
3	D	55	0	0	5	0
All	All	10684	0	9981	224	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 11.

All (224) 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:174:ASP:OD2	1:D:175:ILE:HD12	1.46	1.15
1:C:246:VAL:HG22	1:C:280:HIS:HB3	1.35	1.07
1:B:42:MET:HE3	1:B:67:LEU:HB3	1.09	1.04
1:B:42:MET:CE	1:B:67:LEU:HB3	1.87	1.03
1:B:246:VAL:CG1	1:B:280:HIS:HB3	1.94	0.97
1:B:28:ASN:OD1	1:D:122:THR:HG23	1.64	0.96
3:A:343:HOH:O	1:C:303:THR:HG22	1.65	0.95
1:C:246:VAL:CG2	1:C:280:HIS:HB3	1.97	0.94
1:C:246:VAL:HG23	1:C:247:HIS:CD2	2.04	0.93
1:A:313:VAL:HG13	1:A:316:VAL:HB	1.50	0.93
1:B:54:GLN:HE21	1:B:64:GLY:H	1.15	0.93
1:D:19:GLN:HE22	1:D:159:SER:H	1.10	0.93
1:B:42:MET:HE3	1:B:67:LEU:CB	1.99	0.92
1:A:54:GLN:HE21	1:A:64:GLY:H	1.21	0.85
1:A:167:GLN:O	1:A:231:VAL:HG13	1.76	0.85
1:B:176:ILE:CG2	1:B:318:ILE:HG12	2.07	0.84
1:D:318:ILE:HD11	1:D:321:GLY:HA2	1.60	0.83
1:D:174:ASP:OD2	1:D:175:ILE:CD1	2.27	0.83
1:D:167:GLN:O	1:D:231:VAL:HG13	1.80	0.82
1:D:42:MET:HE2	1:D:48:ILE:HG23	1.61	0.82
1:D:42:MET:CE	1:D:48:ILE:HG23	2.09	0.81
1:B:19:GLN:HE22	1:B:159:SER:H	1.27	0.81
1:C:54:GLN:HE21	1:C:64:GLY:H	1.27	0.81
1:C:122:THR:HG21	3:C:344:HOH:O	1.81	0.80
1:C:133:LEU:HD11	1:C:139:PRO:HG3	1.63	0.79
1:A:212:THR:HG23	1:A:228:ASP:OD1	1.82	0.78
1:D:61:THR:HG23	1:D:74:SER:HB3	1.67	0.77
1:C:19:GLN:HE22	1:C:159:SER:H	1.34	0.75
1:D:54:GLN:HE21	1:D:64:GLY:H	1.35	0.74
1:A:223:LEU:CD2	1:A:251:LEU:HD22	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:LEU:C	1:C:22:LEU:HD23	2.12	0.74
1:D:212:THR:HG23	1:D:228:ASP:OD1	1.89	0.73
1:A:133:LEU:HD11	1:A:139:PRO:HG3	1.71	0.72
1:A:320:ASN:HB3	3:A:372:HOH:O	1.89	0.72
1:D:42:MET:HE3	1:D:67:LEU:HD22	1.70	0.72
1:D:19:GLN:NE2	1:D:159:SER:H	1.87	0.72
1:B:42:MET:CE	1:B:67:LEU:HD22	2.20	0.71
1:D:226:THR:HG23	3:D:379:HOH:O	1.91	0.71
1:D:19:GLN:HE22	1:D:159:SER:N	1.88	0.71
1:C:246:VAL:HG22	1:C:280:HIS:CB	2.16	0.70
1:C:239:ARG:HD3	1:C:285:ASP:OD2	1.92	0.70
1:D:22:LEU:C	1:D:22:LEU:HD23	2.17	0.70
1:A:43:GLN:NE2	1:A:154:TRP:HE1	1.91	0.69
1:B:176:ILE:HG21	1:B:318:ILE:HG12	1.75	0.69
1:C:327:LYS:CE	3:C:378:HOH:O	2.41	0.69
1:C:216:ARG:HH12	1:C:218:ASP:HB3	1.58	0.69
1:A:242:THR:OG1	1:A:284:ILE:HG13	1.92	0.68
1:B:246:VAL:HG12	1:B:280:HIS:HB3	1.75	0.68
1:A:91:ASP:HB3	1:A:95:LYS:HE3	1.75	0.68
1:C:173:MET:HE1	1:C:196:PHE:HB3	1.76	0.67
1:A:182:GLU:OE2	1:A:306:HIS:HD2	1.78	0.67
1:A:43:GLN:HE21	1:A:154:TRP:HE1	1.42	0.67
1:A:4:VAL:HG22	1:A:50:PRO:HG2	1.76	0.66
1:B:74:SER:CB	1:D:303:THR:HG21	2.26	0.66
1:B:214:VAL:HG13	3:B:358:HOH:O	1.97	0.65
1:A:78:ASN:HD21	1:C:303:THR:HG21	1.62	0.64
1:B:214:VAL:CG1	3:B:358:HOH:O	2.45	0.64
1:B:282:ASN:ND2	1:B:300:LEU:H	1.96	0.64
1:D:167:GLN:HE22	1:D:210:ASP:H	1.46	0.64
1:D:175:ILE:HD11	1:D:199:LYS:NZ	2.13	0.63
1:A:226:THR:OG1	1:A:242:THR:HG22	1.98	0.63
1:B:246:VAL:HG13	1:B:247:HIS:CD2	2.34	0.63
1:B:22:LEU:O	1:B:26:SER:HB2	1.99	0.62
1:C:327:LYS:HE2	3:C:378:HOH:O	1.97	0.62
1:A:321:GLY:CA	3:A:369:HOH:O	2.48	0.62
1:C:327:LYS:NZ	3:C:378:HOH:O	2.32	0.62
1:B:176:ILE:HG23	1:B:318:ILE:HA	1.82	0.62
1:C:173:MET:HE2	1:C:279:TRP:CE3	2.35	0.62
1:B:74:SER:HB3	1:D:303:THR:HG21	1.81	0.61
1:C:22:LEU:HD23	1:C:22:LEU:O	2.00	0.61
1:D:175:ILE:HD11	1:D:199:LYS:HZ1	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLN:NE2	1:A:122:THR:OG1	2.35	0.60
1:D:222:TYR:HB3	1:D:246:VAL:HB	1.83	0.59
1:B:29:GLY:O	1:B:120:LYS:HE2	2.01	0.59
1:D:173:MET:HE1	1:D:198:GLY:HA2	1.84	0.59
1:D:22:LEU:HD22	3:D:349:HOH:O	2.01	0.59
1:B:7:LYS:HD2	1:B:8:TYR:H	1.68	0.59
1:B:246:VAL:HG13	1:B:280:HIS:HB3	1.81	0.58
1:B:166:LEU:HB2	1:B:331:TRP:CZ3	2.38	0.58
1:B:42:MET:HE2	1:B:67:LEU:HD22	1.84	0.58
1:B:207:ALA:HA	1:B:265:MET:HE3	1.84	0.58
1:A:124:THR:OG1	1:A:127:GLU:HG3	2.03	0.58
1:B:133:LEU:HD13	1:B:147:ARG:HD2	1.86	0.57
1:A:54:GLN:NE2	1:A:64:GLY:H	1.98	0.57
1:B:246:VAL:CG1	1:B:280:HIS:CB	2.77	0.57
1:A:313:VAL:HG12	1:A:313:VAL:O	2.04	0.57
1:C:216:ARG:NH1	1:C:218:ASP:HB3	2.19	0.57
1:D:42:MET:CE	1:D:67:LEU:HD22	2.35	0.57
1:B:243:TRP:HZ2	1:B:265:MET:HE1	1.69	0.57
1:D:22:LEU:HD23	1:D:22:LEU:O	2.04	0.57
1:D:72:PRO:HD2	1:D:75:ASN:HD21	1.70	0.57
1:D:320:ASN:HB3	3:D:361:HOH:O	2.03	0.57
1:B:177:ASN:ND2	1:B:320:ASN:HD22	2.03	0.56
1:A:177:ASN:ND2	1:A:320:ASN:HD22	2.04	0.56
1:A:113:MET:HE1	1:A:123:LYS:HD2	1.87	0.56
1:B:119:ILE:HG13	1:B:120:LYS:HE3	1.86	0.56
1:D:282:ASN:ND2	1:D:300:LEU:H	2.03	0.56
1:D:243:TRP:HZ2	1:D:265:MET:HE1	1.71	0.56
1:A:294:LYS:HE2	1:A:298:SER:OG	2.04	0.56
1:C:226:THR:HG22	1:C:242:THR:OG1	2.06	0.56
1:C:175:ILE:HD12	1:C:199:LYS:HG3	1.88	0.56
1:B:282:ASN:HD21	1:B:300:LEU:H	1.52	0.55
1:C:4:VAL:HG22	1:C:50:PRO:HG2	1.88	0.55
1:D:42:MET:HE1	1:D:48:ILE:HG23	1.88	0.55
1:B:176:ILE:HG23	1:B:318:ILE:HG12	1.88	0.55
1:D:246:VAL:O	1:D:247:HIS:HB2	2.06	0.55
1:A:242:THR:OG1	1:A:284:ILE:CG1	2.54	0.55
1:D:173:MET:CE	1:D:198:GLY:HA2	2.37	0.55
1:D:319:ILE:O	1:D:320:ASN:OD1	2.25	0.55
1:A:282:ASN:ND2	1:A:300:LEU:H	2.05	0.55
1:A:313:VAL:CG1	1:A:316:VAL:HB	2.31	0.55
1:B:10:THR:HG22	1:B:13:GLU:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:LYS:NZ	1:D:157:ASN:O	2.40	0.54
1:C:100:GLU:CD	1:C:106:GLN:HG3	2.33	0.54
1:C:218:ASP:OD1	1:C:218:ASP:N	2.41	0.54
1:D:246:VAL:HG13	1:D:280:HIS:HB3	1.90	0.54
1:D:21:ILE:CD1	1:D:42:MET:HE1	2.38	0.54
1:D:22:LEU:C	1:D:22:LEU:CD2	2.80	0.54
1:A:175:ILE:HG21	1:A:199:LYS:HE3	1.89	0.53
1:A:313:VAL:HG13	1:A:316:VAL:CB	2.32	0.53
1:C:22:LEU:C	1:C:22:LEU:CD2	2.81	0.53
1:C:270:ILE:HD13	3:C:362:HOH:O	2.08	0.53
1:A:223:LEU:HD22	1:A:251:LEU:HD22	1.91	0.53
1:D:173:MET:HE2	1:D:175:ILE:O	2.09	0.53
1:A:253:PHE:CE2	1:A:257:LYS:HE2	2.44	0.53
1:B:246:VAL:HG12	1:B:280:HIS:CB	2.38	0.52
1:B:42:MET:CE	1:B:67:LEU:CB	2.75	0.52
1:B:225:TRP:HB2	1:B:243:TRP:CE2	2.45	0.52
1:A:177:ASN:HD21	1:A:320:ASN:HD22	1.57	0.52
1:B:303:THR:HG21	1:C:78:ASN:OD1	2.11	0.51
1:B:239:ARG:NH1	1:B:285:ASP:OD1	2.44	0.51
1:C:246:VAL:CG2	1:C:247:HIS:CD2	2.88	0.51
1:C:77:ILE:HG12	1:C:87:TYR:CD1	2.46	0.50
1:C:122:THR:HG22	3:C:361:HOH:O	2.10	0.50
1:B:208:PRO:HD2	1:B:265:MET:HE1	1.93	0.50
1:A:242:THR:HG23	1:A:286:GLY:O	2.11	0.50
1:B:42:MET:HE1	1:B:67:LEU:HD13	1.92	0.50
1:D:239:ARG:HD3	1:D:285:ASP:OD2	2.12	0.50
1:B:54:GLN:HE21	1:B:64:GLY:N	1.97	0.50
1:C:173:MET:HE2	1:C:279:TRP:CZ3	2.47	0.50
1:B:43:GLN:HE21	1:B:154:TRP:HE1	1.58	0.50
1:D:295:LYS:HD3	1:D:299:CYS:SG	2.53	0.49
1:B:133:LEU:HD13	1:B:147:ARG:CD	2.44	0.48
1:D:226:THR:CG2	3:D:379:HOH:O	2.55	0.47
1:B:77:ILE:HG12	1:B:87:TYR:CD1	2.49	0.47
1:B:200:THR:HG22	1:B:203:TYR:HD1	1.79	0.47
1:C:11:MET:HE2	1:C:14:MET:CE	2.44	0.47
1:C:177:ASN:ND2	1:C:320:ASN:HD22	2.12	0.47
1:C:246:VAL:HG23	1:C:247:HIS:CG	2.49	0.47
1:B:248:GLU:CD	1:B:267:HIS:H	2.23	0.47
1:B:166:LEU:O	1:B:331:TRP:HZ3	1.97	0.46
1:B:81:ASN:HD22	1:B:81:ASN:C	2.23	0.46
1:A:43:GLN:NE2	1:A:154:TRP:NE1	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:ARG:HH11	1:C:285:ASP:CG	2.23	0.46
1:C:177:ASN:HD21	1:C:320:ASN:HD22	1.63	0.46
1:C:207:ALA:HA	1:C:265:MET:HE3	1.98	0.46
1:D:133:LEU:HD13	1:D:147:ARG:HD2	1.97	0.46
1:A:222:TYR:HB3	1:A:246:VAL:HB	1.97	0.46
1:B:42:MET:HE1	1:B:67:LEU:HD22	1.97	0.46
1:C:243:TRP:HZ2	1:C:265:MET:HE1	1.79	0.46
1:B:243:TRP:CZ2	1:B:265:MET:HE1	2.50	0.46
1:C:11:MET:HE2	1:C:14:MET:HE3	1.98	0.46
1:C:175:ILE:CD1	1:C:199:LYS:HG3	2.45	0.46
1:A:246:VAL:HG13	1:A:280:HIS:CD2	2.51	0.45
1:B:22:LEU:HD12	1:B:35:ILE:HD13	1.98	0.45
1:B:190:GLY:HA3	1:B:295:LYS:O	2.17	0.45
1:D:249:SER:OG	1:D:271:GLY:CA	2.65	0.45
1:C:313:VAL:HG21	1:C:326:TRP:HB3	1.97	0.45
1:D:14:MET:SD	1:D:43:GLN:HG3	2.57	0.45
1:A:177:ASN:HD22	1:A:320:ASN:HB2	1.82	0.45
1:C:22:LEU:HA	1:C:35:ILE:HG21	1.99	0.45
1:A:313:VAL:O	1:A:313:VAL:CG1	2.64	0.45
1:B:215:TRP:HH2	1:D:139:PRO:O	2.00	0.45
1:D:225:TRP:HB2	1:D:243:TRP:CE2	2.51	0.45
1:A:222:TYR:HB2	1:A:244:VAL:CG2	2.46	0.45
1:D:226:THR:HG23	1:D:226:THR:O	2.17	0.45
1:D:246:VAL:CG1	1:D:280:HIS:CD2	3.00	0.45
1:A:106:GLN:HG2	1:A:136:TYR:CZ	2.52	0.44
1:A:318:ILE:HD11	3:A:369:HOH:O	2.18	0.44
1:B:195:ASP:OD1	1:B:280:HIS:HB2	2.17	0.44
1:C:280:HIS:C	1:C:280:HIS:CD2	2.96	0.44
1:D:9:LEU:HB3	1:D:13:GLU:HB2	1.98	0.44
1:C:173:MET:HE2	1:C:279:TRP:HE3	1.81	0.44
1:D:43:GLN:HE21	1:D:154:TRP:HE1	1.65	0.44
1:A:230:GLU:H	1:A:230:GLU:HG2	1.41	0.44
1:C:141:ASN:HA	1:C:142:PRO:HD3	1.87	0.44
1:D:133:LEU:HD13	1:D:147:ARG:CD	2.48	0.43
1:C:134:ALA:O	1:C:138:ARG:HG2	2.18	0.43
1:B:216:ARG:NH1	1:B:253:PHE:O	2.52	0.43
1:A:225:TRP:HB2	1:A:243:TRP:CE2	2.52	0.43
1:D:42:MET:HE2	1:D:42:MET:HB3	1.58	0.43
1:C:54:GLN:NE2	1:C:64:GLY:H	2.06	0.43
1:D:225:TRP:O	1:D:242:THR:HB	2.18	0.43
1:D:22:LEU:HA	1:D:35:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:159:SER:O	1:D:160:GLY:C	2.63	0.42
1:A:199:LYS:HB2	1:A:203:TYR:CE1	2.54	0.42
1:C:189:LYS:HD2	1:C:297:ASP:OD2	2.19	0.42
1:D:314:ASN:CG	1:D:328:THR:HG1	2.26	0.42
1:A:231:VAL:HG12	1:A:232:MET:N	2.34	0.42
1:B:177:ASN:HD21	1:B:320:ASN:HD22	1.66	0.42
1:D:61:THR:CG2	1:D:74:SER:HB3	2.45	0.42
1:C:208:PRO:HD2	1:C:265:MET:HE1	2.02	0.42
1:B:133:LEU:HD11	1:B:139:PRO:HG3	2.02	0.42
1:C:248:GLU:HB2	1:C:267:HIS:O	2.19	0.42
1:D:211:CYS:SG	1:D:265:MET:HE1	2.60	0.42
1:A:321:GLY:HA2	3:A:369:HOH:O	2.18	0.41
1:C:72:PRO:HD2	1:C:75:ASN:OD1	2.20	0.41
1:D:141:ASN:HA	1:D:142:PRO:HD3	1.87	0.41
1:C:201:GLU:HG2	1:C:202:LYS:HG2	2.03	0.41
1:C:11:MET:CE	1:C:14:MET:HE3	2.51	0.41
1:D:173:MET:CE	1:D:175:ILE:HB	2.51	0.41
1:A:325:ASP:OD2	1:A:327:LYS:NZ	2.48	0.41
1:D:246:VAL:CG1	1:D:280:HIS:HD2	2.34	0.41
1:B:177:ASN:C	1:B:177:ASN:HD22	2.28	0.41
1:C:133:LEU:HD22	1:C:147:ARG:HD2	2.03	0.41
1:C:246:VAL:O	1:C:247:HIS:HB2	2.21	0.41
1:D:54:GLN:NE2	1:D:64:GLY:H	2.11	0.41
1:A:100:GLU:HA	1:A:105:ALA:HB3	2.03	0.41
1:D:320:ASN:CA	3:D:361:HOH:O	2.69	0.41
1:D:246:VAL:HG13	1:D:280:HIS:CD2	2.56	0.40
1:D:222:TYR:HB2	1:D:244:VAL:HG22	2.04	0.40
1:C:223:LEU:HD11	1:C:251:LEU:HB3	2.03	0.40
1:D:246:VAL:O	1:D:247:HIS:CB	2.70	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	321/334 (96%)	305 (95%)	15 (5%)	1 (0%)	36	25
1	B	318/334 (95%)	303 (95%)	13 (4%)	2 (1%)	21	11
1	C	322/334 (96%)	311 (97%)	9 (3%)	2 (1%)	21	11
1	D	324/334 (97%)	305 (94%)	17 (5%)	2 (1%)	21	11
All	All	1285/1336 (96%)	1224 (95%)	54 (4%)	7 (0%)	24	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	295	LYS
1	D	247	HIS
1	A	247	HIS
1	B	58	GLU
1	C	247	HIS
1	B	295	LYS
1	C	295	LYS

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	283/283 (100%)	270 (95%)	13 (5%)	24	12
1	B	280/283 (99%)	270 (96%)	10 (4%)	31	18
1	C	284/283 (100%)	267 (94%)	17 (6%)	17	7
1	D	284/283 (100%)	271 (95%)	13 (5%)	24	12
All	All	1131/1132 (100%)	1078 (95%)	53 (5%)	24	11

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	52	LEU
1	A	58	GLU
1	A	156	LYS

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Mol	Chain	Res	Type
1	A	159	SER
1	A	166	LEU
1	A	230	GLU
1	A	239	ARG
1	A	246	VAL
1	A	318	ILE
1	A	319	ILE
1	A	322	ASN
1	A	328	THR
1	B	1	MET
1	B	10	THR
1	B	12	SER
1	B	81	ASN
1	B	120	LYS
1	B	176	ILE
1	B	201	GLU
1	B	287	LYS
1	B	328	THR
1	B	331	TRP
1	C	22	LEU
1	C	48	ILE
1	C	106	GLN
1	C	135	SER
1	C	156	LYS
1	C	173	MET
1	C	175	ILE
1	C	189	LYS
1	C	218	ASP
1	C	231	VAL
1	C	237[A]	SER
1	C	237[B]	SER
1	C	246	VAL
1	C	270	ILE
1	C	280	HIS
1	C	287	LYS
1	C	330	ASP
1	D	7	LYS
1	D	22	LEU
1	D	48	ILE
1	D	61	THR
1	D	159	SER
1	D	185	SER

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Mol	Chain	Res	Type
1	D	202	LYS
1	D	223	LEU
1	D	242	THR
1	D	246	VAL
1	D	287	LYS
1	D	318	ILE
1	D	319	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	33	GLN
1	A	43	GLN
1	A	54	GLN
1	A	81	ASN
1	A	103	ASN
1	A	143	ASN
1	A	150	GLN
1	A	170	GLN
1	A	177	ASN
1	A	282	ASN
1	A	290	GLN
1	A	306	HIS
1	A	320	ASN
1	A	322	ASN
1	B	19	GLN
1	B	23	ASN
1	B	43	GLN
1	B	54	GLN
1	B	55	ASN
1	B	69	GLN
1	B	75	ASN
1	B	78	ASN
1	B	81	ASN
1	B	143	ASN
1	B	150	GLN
1	B	177	ASN
1	B	247	HIS
1	B	282	ASN
1	B	290	GLN
1	C	19	GLN

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Mol	Chain	Res	Type
1	C	23	ASN
1	C	43	GLN
1	C	54	GLN
1	C	150	GLN
1	C	177	ASN
1	C	332	GLN
1	D	19	GLN
1	D	23	ASN
1	D	43	GLN
1	D	54	GLN
1	D	75	ASN
1	D	78	ASN
1	D	103	ASN
1	D	143	ASN
1	D	150	GLN
1	D	167	GLN
1	D	282	ASN
1	D	290	GLN
1	D	320	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 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

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 [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	324/334 (97%)	-1.25	0 100 100	9, 18, 27, 34	3 (0%)
1	B	324/334 (97%)	-1.27	0 100 100	8, 17, 26, 37	0
1	C	324/334 (97%)	-1.25	0 100 100	7, 17, 26, 34	4 (1%)
1	D	326/334 (97%)	-1.25	0 100 100	8, 17, 28, 32	4 (1%)
All	All	1298/1336 (97%)	-1.26	0 100 100	7, 17, 28, 37	11 (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	335	1/1	1.00	0.03	28,28,28,28	0
2	ZN	B	335	1/1	1.00	0.06	23,23,23,23	0
2	ZN	C	335	1/1	1.00	0.05	25,25,25,25	0
2	ZN	D	335	1/1	1.00	0.05	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.