



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:00 PM UTC

PDB ID : 9I1U / pdb_00009i1u
Title : Lytic polysaccharide monooxygenase from Cellvibrio japonicus - CjAA10B
Authors : Branch, J.; Hemsworth, G.R.
Deposited on : 2025-01-17
Resolution : 1.90 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
Mogul : 2022.3.0, CSD as543be (2022)
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

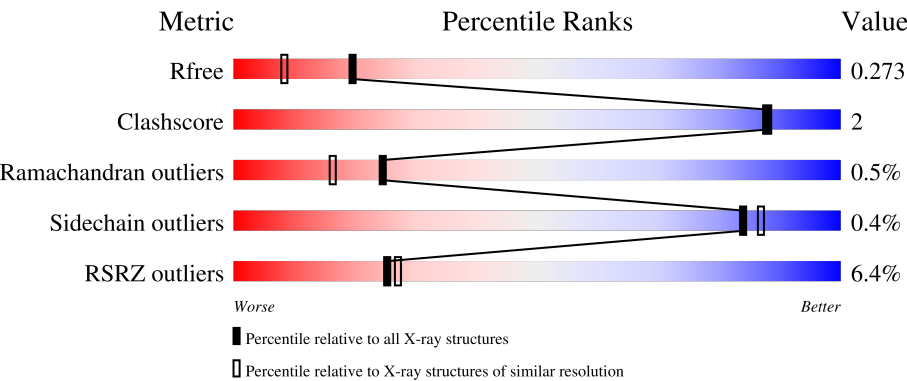
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	211	<div><div>4%</div><div>91%</div><div>6%</div><div>.</div></div>
1	B	211	<div><div>6%</div><div>95%</div><div>.</div><div>.</div></div>
1	C	211	<div><div>13%</div><div>91%</div><div>6%</div><div>.</div></div>
1	D	211	<div><div>%</div><div>95%</div><div>.</div><div>.</div></div>
1	E	211	<div><div>8%</div><div>93%</div><div>.</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
1	F	211	<div> <div></div> <div>3%</div> <div>94%</div> <div>8%</div> <div>3%</div> <div>• •</div> </div>
1	G	211	<div> <div></div> <div>11%</div> <div>90%</div> <div>8%</div> <div>1%</div> <div>•</div> </div>
1	H	211	<div> <div></div> <div>3%</div> <div>87%</div> <div>11%</div> <div>0%</div> <div>•</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 25819 atoms, of which 11821 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 Chitin binding protein, putative, cbp33/10B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	206	Total	C	H	N	O	S	57	0	0
			3110	1034	1477	287	304	8			
1	B	206	Total	C	H	N	O	S	59	1	0
			3102	1034	1472	282	305	9			
1	C	206	Total	C	H	N	O	S	61	0	0
			3076	1026	1454	284	304	8			
1	D	207	Total	C	H	N	O	S	61	0	0
			3117	1037	1481	287	304	8			
1	E	205	Total	C	H	N	O	S	59	1	0
			3112	1034	1482	287	301	8			
1	F	206	Total	C	H	N	O	S	61	1	0
			3104	1034	1475	283	303	9			
1	G	206	Total	C	H	N	O	S	61	1	0
			3114	1036	1482	285	302	9			
1	H	208	Total	C	H	N	O	S	60	1	0
			3153	1047	1498	292	308	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	HIS	-	expression tag	UNP B3PDT6
A	207	HIS	-	expression tag	UNP B3PDT6
A	208	HIS	-	expression tag	UNP B3PDT6
A	209	HIS	-	expression tag	UNP B3PDT6
A	210	HIS	-	expression tag	UNP B3PDT6
A	211	HIS	-	expression tag	UNP B3PDT6
B	206	HIS	-	expression tag	UNP B3PDT6
B	207	HIS	-	expression tag	UNP B3PDT6
B	208	HIS	-	expression tag	UNP B3PDT6
B	209	HIS	-	expression tag	UNP B3PDT6
B	210	HIS	-	expression tag	UNP B3PDT6
B	211	HIS	-	expression tag	UNP B3PDT6
C	206	HIS	-	expression tag	UNP B3PDT6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	207	HIS	-	expression tag	UNP B3PDT6
C	208	HIS	-	expression tag	UNP B3PDT6
C	209	HIS	-	expression tag	UNP B3PDT6
C	210	HIS	-	expression tag	UNP B3PDT6
C	211	HIS	-	expression tag	UNP B3PDT6
D	206	HIS	-	expression tag	UNP B3PDT6
D	207	HIS	-	expression tag	UNP B3PDT6
D	208	HIS	-	expression tag	UNP B3PDT6
D	209	HIS	-	expression tag	UNP B3PDT6
D	210	HIS	-	expression tag	UNP B3PDT6
D	211	HIS	-	expression tag	UNP B3PDT6
E	206	HIS	-	expression tag	UNP B3PDT6
E	207	HIS	-	expression tag	UNP B3PDT6
E	208	HIS	-	expression tag	UNP B3PDT6
E	209	HIS	-	expression tag	UNP B3PDT6
E	210	HIS	-	expression tag	UNP B3PDT6
E	211	HIS	-	expression tag	UNP B3PDT6
F	206	HIS	-	expression tag	UNP B3PDT6
F	207	HIS	-	expression tag	UNP B3PDT6
F	208	HIS	-	expression tag	UNP B3PDT6
F	209	HIS	-	expression tag	UNP B3PDT6
F	210	HIS	-	expression tag	UNP B3PDT6
F	211	HIS	-	expression tag	UNP B3PDT6
G	206	HIS	-	expression tag	UNP B3PDT6
G	207	HIS	-	expression tag	UNP B3PDT6
G	208	HIS	-	expression tag	UNP B3PDT6
G	209	HIS	-	expression tag	UNP B3PDT6
G	210	HIS	-	expression tag	UNP B3PDT6
G	211	HIS	-	expression tag	UNP B3PDT6
H	206	HIS	-	expression tag	UNP B3PDT6
H	207	HIS	-	expression tag	UNP B3PDT6
H	208	HIS	-	expression tag	UNP B3PDT6
H	209	HIS	-	expression tag	UNP B3PDT6
H	210	HIS	-	expression tag	UNP B3PDT6
H	211	HIS	-	expression tag	UNP B3PDT6

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

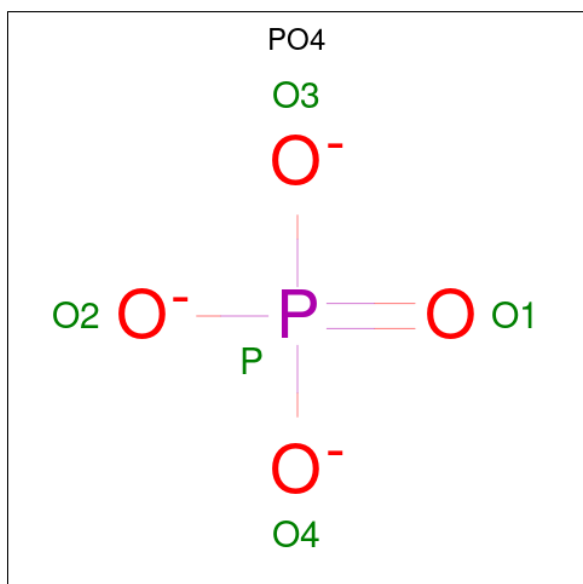
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Cu	0	0
			1	1		
2	D	1	Total	Cu	0	0
			1	1		
2	E	1	Total	Cu	0	0
			1	1		
2	F	1	Total	Cu	0	0
			1	1		
2	G	1	Total	Cu	0	0
			1	1		
2	H	1	Total	Cu	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		
3	G	1	Total	O	P	0	0
			5	4	1		
3	H	1	Total	O	P	0	0
			5	4	1		

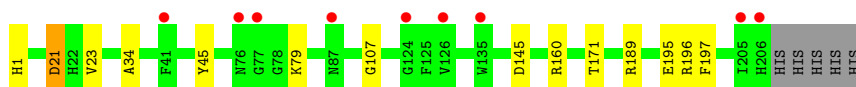
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	104	Total	O	0	0
			104	104		
4	B	124	Total	O	0	0
			124	124		
4	C	94	Total	O	0	0
			94	94		
4	D	129	Total	O	0	0
			129	129		
4	E	93	Total	O	0	0
			93	93		
4	F	122	Total	O	0	0
			122	122		
4	G	104	Total	O	0	0
			104	104		
4	H	108	Total	O	0	0
			108	108		

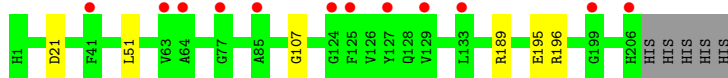
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

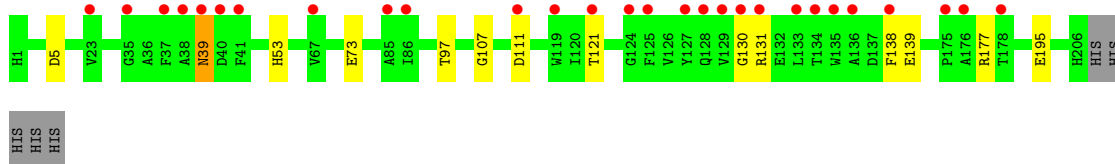
- Molecule 1: Chitin binding protein, putative, cbp33/10B



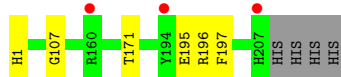
- Molecule 1: Chitin binding protein, putative, cbp33/10B



- Molecule 1: Chitin binding protein, putative, cbp33/10B

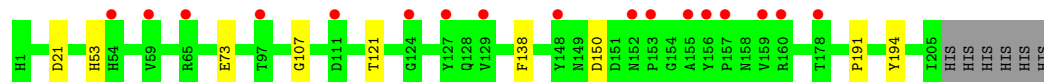


- Molecule 1: Chitin binding protein, putative, cbp33/10B

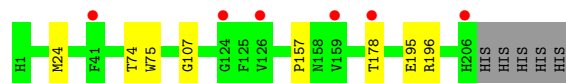


- Molecule 1: Chitin binding protein, putative, cbp33/10B

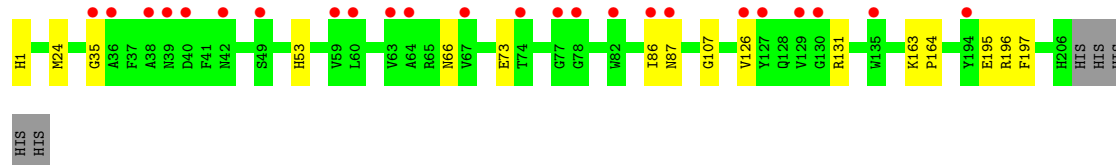
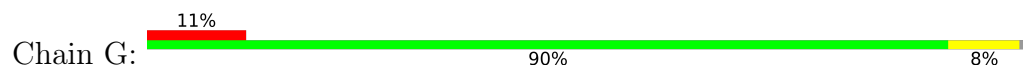




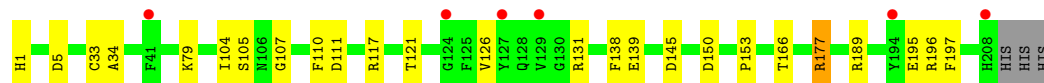
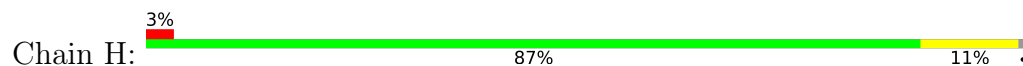
- Molecule 1: Chitin binding protein, putative, cbp33/10B



- Molecule 1: Chitin binding protein, putative, cbp33/10B



- Molecule 1: Chitin binding protein, putative, cbp33/10B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.82Å 74.92Å 137.46Å 90.00° 102.09° 90.00°	Depositor
Resolution (Å)	75.12 – 1.90 75.12 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (75.12-1.90) 97.3 (75.12-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.230 , 0.276 0.226 , 0.273	Depositor DCC
R_{free} test set	5903 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	20.5	Xtrriage
Anisotropy	0.528	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 25.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	25819	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.78 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3423e-05. 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: CU, PO4

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	0.50	0/1694	0.91	2/2319 (0.1%)
1	B	0.50	0/1694	0.91	0/2320
1	C	0.50	0/1683	0.93	2/2305 (0.1%)
1	D	0.53	0/1697	0.93	0/2323
1	E	0.50	0/1694	0.90	0/2318
1	F	0.51	0/1693	0.95	0/2318
1	G	0.51	0/1696	0.92	0/2321
1	H	0.51	0/1720	0.92	3/2354 (0.1%)
All	All	0.51	0/13571	0.92	7/18578 (0.0%)

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	0	1
1	D	0	1
1	F	0	1
1	G	0	1
1	H	0	2
All	All	0	6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	111	ASP	CA-CB-CG	5.51	118.11	112.60
1	C	5	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	79	LYS	N-CA-CB	-5.30	102.05	110.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	5	ASP	CA-CB-CG	5.14	117.75	112.60
1	A	145	ASP	CA-CB-CG	5.09	117.69	112.60
1	C	97	THR	CA-CB-OG1	-5.05	102.03	109.60
1	H	79	LYS	N-CA-CB	-5.04	102.15	109.95

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	ARG	Sidechain
1	D	196	ARG	Sidechain
1	F	196	ARG	Sidechain
1	G	196	ARG	Sidechain
1	H	177	ARG	Sidechain
1	H	196	ARG	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	1633	1477	1463	6	0
1	B	1630	1472	1456	3	0
1	C	1622	1454	1436	7	0
1	D	1636	1481	1463	3	0
1	E	1630	1482	1466	4	0
1	F	1629	1475	1457	4	0
1	G	1632	1482	1464	11	0
1	H	1655	1498	1483	11	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	1	0
3	C	5	0	0	1	0
3	D	10	0	0	1	0
3	E	5	0	0	0	0
3	F	5	0	0	1	0
3	G	5	0	0	1	0
3	H	5	0	0	1	0
4	A	104	0	0	0	0
4	B	124	0	0	0	0
4	C	94	0	0	1	0
4	D	129	0	0	1	0
4	E	93	0	0	1	0
4	F	122	0	0	1	0
4	G	104	0	0	1	0
4	H	108	0	0	0	0
All	All	13998	11821	11688	49	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 2.

All (49) 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:G:24[A]:MET:SD	4:G:436:HOH:O	2.48	0.72
1:C:111:ASP:OD1	4:C:401:HOH:O	2.14	0.65
1:B:195:GLU:OE1	3:B:302:PO4:O2	2.23	0.57
1:G:86:ILE:HG22	1:G:87:ASN:N	2.20	0.56
1:A:160:ARG:NH2	1:A:171:THR:OG1	2.40	0.55
1:G:86:ILE:HG22	1:G:87:ASN:H	1.71	0.55
1:H:1:HIS:HA	1:H:197:PHE:CE1	2.41	0.55
1:H:117:ARG:HD3	1:H:145:ASP:OD1	2.08	0.54
1:F:24[B]:MET:HA	1:F:24[B]:MET:HE2	1.90	0.53
1:C:195:GLU:OE1	3:C:302:PO4:O4	2.28	0.52
1:H:195:GLU:OE1	3:H:302:PO4:O1	2.28	0.51
1:C:139:GLU:OE2	1:C:177:ARG:NH2	2.38	0.51
1:G:126:VAL:O	1:G:131:ARG:NH2	2.44	0.50
1:C:121:THR:HA	1:C:138:PHE:HA	1.93	0.50
1:H:126:VAL:HG23	1:H:131:ARG:NH2	2.25	0.50
1:A:195:GLU:OE1	3:A:302:PO4:O3	2.29	0.49
1:C:53:HIS:HD1	1:C:73:GLU:CD	2.19	0.49
1:D:171:THR:HG23	4:D:489:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:GLY:HA3	1:G:86:ILE:HG21	1.94	0.48
1:G:195:GLU:OE1	3:G:302:PO4:O3	2.32	0.48
1:G:1:HIS:HA	1:G:197:PHE:CE2	2.48	0.47
1:G:86:ILE:CG2	1:G:87:ASN:H	2.27	0.47
1:B:51:LEU:HA	1:B:196:ARG:O	2.16	0.46
1:F:195:GLU:OE1	3:F:302:PO4:O2	2.34	0.45
1:E:191:PRO:HD3	1:E:194:TYR:CE1	2.52	0.45
1:G:163:LYS:HB2	1:G:164:PRO:HD3	1.99	0.44
1:E:53:HIS:ND1	1:E:73:GLU:OE1	2.50	0.44
1:E:121:THR:HA	1:E:138:PHE:HA	1.99	0.44
1:G:86:ILE:CG2	1:G:87:ASN:N	2.81	0.44
1:A:1:HIS:HA	1:A:197:PHE:CE2	2.54	0.43
1:H:104:ILE:HD11	1:H:110:PHE:CZ	2.53	0.43
1:E:150:ASP:OD2	4:E:401:HOH:O	2.21	0.43
1:A:21:ASP:HB2	1:A:45:TYR:OH	2.18	0.42
1:F:74:THR:HB	1:F:75:TRP:CE3	2.54	0.42
1:H:121:THR:HA	1:H:138:PHE:HA	2.01	0.42
1:H:139:GLU:OE2	1:H:177:ARG:NH2	2.51	0.42
1:H:150:ASP:O	1:H:153:PRO:HD3	2.19	0.42
1:C:130:GLY:O	1:C:131:ARG:C	2.62	0.42
1:B:189:ARG:HD3	1:B:195:GLU:HB3	2.02	0.42
1:D:195:GLU:OE1	3:D:303:PO4:O2	2.38	0.42
1:F:157:PRO:O	4:F:401:HOH:O	2.22	0.41
1:H:105[A]:SER:HB3	1:H:166:THR:HG1	1.85	0.41
1:H:189:ARG:HD3	1:H:195:GLU:HB3	2.03	0.41
1:D:1:HIS:HA	1:D:197:PHE:CE1	2.55	0.41
1:A:189:ARG:HD3	1:A:195:GLU:HB3	2.03	0.41
1:H:33:CYS:O	1:H:34:ALA:C	2.64	0.40
1:A:23:VAL:HG11	1:A:34:ALA:HA	2.04	0.40
1:G:53:HIS:ND1	1:G:73:GLU:OE2	2.47	0.40
1:C:39:ASN:O	1:C:39:ASN:CG	2.64	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	204/211 (97%)	195 (96%)	8 (4%)	1 (0%)	24	16
1	B	205/211 (97%)	197 (96%)	7 (3%)	1 (0%)	24	16
1	C	204/211 (97%)	188 (92%)	15 (7%)	1 (0%)	24	16
1	D	205/211 (97%)	198 (97%)	6 (3%)	1 (0%)	24	16
1	E	204/211 (97%)	191 (94%)	12 (6%)	1 (0%)	24	16
1	F	205/211 (97%)	194 (95%)	10 (5%)	1 (0%)	24	16
1	G	205/211 (97%)	194 (95%)	10 (5%)	1 (0%)	24	16
1	H	207/211 (98%)	196 (95%)	10 (5%)	1 (0%)	24	16
All	All	1639/1688 (97%)	1553 (95%)	78 (5%)	8 (0%)	24	16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	GLY
1	D	107	GLY
1	H	107	GLY
1	E	107	GLY
1	G	107	GLY
1	C	107	GLY
1	B	107	GLY
1	F	107	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	170/177 (96%)	169 (99%)	1 (1%)	78	81
1	B	170/177 (96%)	169 (99%)	1 (1%)	78	81
1	C	167/177 (94%)	166 (99%)	1 (1%)	78	81
1	D	169/177 (96%)	169 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	169/177 (96%)	168 (99%)	1 (1%)	78	81
1	F	169/177 (96%)	168 (99%)	1 (1%)	78	81
1	G	169/177 (96%)	168 (99%)	1 (1%)	78	81
1	H	173/177 (98%)	173 (100%)	0	100	100
All	All	1356/1416 (96%)	1350 (100%)	6 (0%)	84	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASP
1	B	21	ASP
1	C	39	ASN
1	E	21	ASP
1	F	178	THR
1	G	66	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	HIS
1	A	92	ASN
1	A	204	GLN
1	B	55	GLN
1	C	39	ASN
1	C	84	ASN
1	D	42	ASN
1	D	84	ASN
1	D	141	GLN
1	D	158	ASN
1	E	165	ASN
1	E	204	GLN
1	F	25	ASN
1	F	54	HIS
1	F	87	ASN
1	F	204	GLN
1	G	141	GLN
1	H	92	ASN
1	H	141	GLN
1	H	204	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](#)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PO4	F	302	2	4,4,4	0.82	0	6,6,6	0.55	0
3	PO4	D	302	-	4,4,4	0.89	0	6,6,6	0.65	0
3	PO4	G	302	2	4,4,4	0.80	0	6,6,6	0.58	0
3	PO4	D	303	2	4,4,4	0.52	0	6,6,6	0.44	0
3	PO4	C	302	2	4,4,4	0.91	0	6,6,6	0.45	0
3	PO4	E	302	2	4,4,4	0.89	0	6,6,6	0.48	0
3	PO4	A	302	2	4,4,4	0.56	0	6,6,6	0.39	0
3	PO4	H	302	2	4,4,4	0.98	0	6,6,6	0.55	0
3	PO4	B	302	2	4,4,4	0.66	0	6,6,6	0.56	0

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.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	302	PO4	1	0
3	G	302	PO4	1	0
3	D	303	PO4	1	0
3	C	302	PO4	1	0
3	A	302	PO4	1	0
3	H	302	PO4	1	0
3	B	302	PO4	1	0

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	206/211 (97%)	0.63	9 (4%) 39 41	16, 27, 42, 55	0
1	B	206/211 (97%)	0.57	12 (5%) 29 30	16, 25, 38, 46	1 (0%)
1	C	206/211 (97%)	1.01	28 (13%) 7 7	16, 29, 50, 62	0
1	D	207/211 (98%)	0.37	3 (1%) 73 76	15, 24, 35, 44	0
1	E	205/211 (97%)	0.62	17 (8%) 17 18	13, 26, 45, 52	1 (0%)
1	F	206/211 (97%)	0.35	6 (2%) 53 57	14, 22, 33, 43	1 (0%)
1	G	206/211 (97%)	0.81	24 (11%) 9 10	16, 26, 41, 53	1 (0%)
1	H	208/211 (98%)	0.42	6 (2%) 53 57	9, 26, 38, 44	1 (0%)
All	All	1650/1688 (97%)	0.60	105 (6%) 25 27	9, 26, 41, 62	5 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	129	VAL	6.4
1	G	39	ASN	4.9
1	D	207	HIS	4.4
1	G	36	ALA	4.3
1	C	131	ARG	3.7
1	C	133	LEU	3.7
1	C	86	ILE	3.7
1	G	35	GLY	3.6
1	G	38	ALA	3.5
1	C	124	GLY	3.5
1	E	111	ASP	3.5
1	C	41	PHE	3.5
1	E	155	ALA	3.4
1	G	64	ALA	3.4
1	E	152	ASN	3.3
1	C	39	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	124	GLY	3.2
1	A	206	HIS	3.2
1	A	126	VAL	3.1
1	G	67	VAL	3.1
1	C	130	GLY	3.1
1	G	60	LEU	3.0
1	B	129	VAL	3.0
1	B	41	PHE	3.0
1	C	37	PHE	3.0
1	C	135	TRP	2.9
1	G	40	ASP	2.9
1	C	138	PHE	2.8
1	C	128	GLN	2.8
1	C	125	PHE	2.8
1	E	156	TYR	2.7
1	B	85	ALA	2.7
1	G	86	ILE	2.7
1	B	127	TYR	2.7
1	H	208	HIS	2.7
1	E	129	VAL	2.7
1	G	63	VAL	2.7
1	C	178	THR	2.7
1	G	129	VAL	2.7
1	A	77	GLY	2.6
1	B	124	GLY	2.6
1	C	40	ASP	2.6
1	C	67	VAL	2.6
1	G	127	TYR	2.5
1	B	125	PHE	2.5
1	C	35	GLY	2.5
1	D	194	TYR	2.5
1	H	194	TYR	2.5
1	A	41	PHE	2.5
1	F	124	GLY	2.5
1	A	76	ASN	2.4
1	E	127	TYR	2.4
1	F	206	HIS	2.4
1	E	159	VAL	2.4
1	G	135	TRP	2.4
1	C	136	ALA	2.4
1	A	135	TRP	2.4
1	E	65	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	127	TYR	2.3
1	C	127	TYR	2.3
1	E	178	THR	2.3
1	G	194	TYR	2.3
1	C	175	PRO	2.3
1	E	153	PRO	2.3
1	H	124	GLY	2.3
1	B	206	HIS	2.3
1	C	38	ALA	2.3
1	E	124	GLY	2.3
1	F	159	VAL	2.3
1	C	134	THR	2.3
1	B	77	GLY	2.2
1	H	41	PHE	2.2
1	C	111	ASP	2.2
1	G	59	VAL	2.2
1	E	97	THR	2.2
1	G	49	SER	2.2
1	A	205	ILE	2.2
1	H	129	VAL	2.2
1	B	64	ALA	2.2
1	A	87	ASN	2.2
1	E	59	VAL	2.2
1	B	133	LEU	2.2
1	G	42	ASN	2.1
1	C	23	VAL	2.1
1	C	121	THR	2.1
1	F	126	VAL	2.1
1	G	130	GLY	2.1
1	D	160	ARG	2.1
1	G	74	THR	2.1
1	G	82	TRP	2.1
1	B	63	VAL	2.1
1	G	126	VAL	2.1
1	E	157	PRO	2.1
1	C	85	ALA	2.1
1	G	77	GLY	2.1
1	G	78	GLY	2.1
1	C	176	ALA	2.1
1	E	148	TYR	2.0
1	B	199	GLY	2.0
1	G	87	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	119	TRP	2.0
1	E	54[A]	HIS	2.0
1	F	41	PHE	2.0
1	F	178	THR	2.0
1	E	160	ARG	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](#)

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
3	PO4	C	302	5/5	0.84	0.17	34,39,41,43	0
3	PO4	D	302	5/5	0.84	0.18	31,32,38,39	0
3	PO4	E	302	5/5	0.86	0.16	43,46,49,50	0
3	PO4	F	302	5/5	0.88	0.16	36,36,39,42	0
3	PO4	D	303	5/5	0.91	0.13	29,34,37,40	0
3	PO4	A	302	5/5	0.92	0.12	29,30,34,40	0
3	PO4	G	302	5/5	0.93	0.09	32,35,37,40	0
3	PO4	B	302	5/5	0.94	0.10	34,36,37,43	0
3	PO4	H	302	5/5	0.94	0.12	31,31,32,33	0
2	CU	C	301	1/1	0.97	0.04	26,26,26,26	0
2	CU	B	301	1/1	0.98	0.03	25,25,25,25	0
2	CU	H	301	1/1	0.99	0.03	22,22,22,22	0
2	CU	A	301	1/1	0.99	0.02	22,22,22,22	0
2	CU	D	301	1/1	0.99	0.02	21,21,21,21	0
2	CU	F	301	1/1	0.99	0.02	21,21,21,21	0
2	CU	G	301	1/1	0.99	0.03	23,23,23,23	0
2	CU	E	301	1/1	1.00	0.02	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.