



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 10:42 PM GMT

PDB ID : 4DM1  
Title : Contribution of disulfide bond toward thermostability in hyperthermostable endocellulase  
Authors : Kim, H.-W.; Ishikawa, K.  
Deposited on : 2012-02-06  
Resolution : 1.75 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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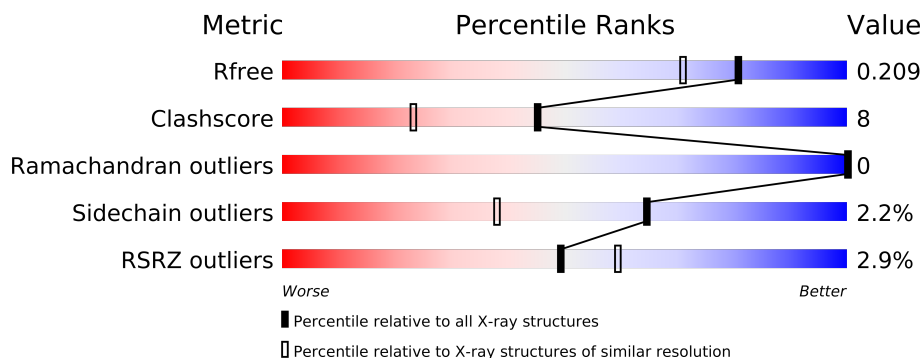
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.75 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))
$R_{free}$	66092	1134 (1.76-1.76)
Clashscore	79885	1304 (1.76-1.76)
Ramachandran outliers	78287	1288 (1.76-1.76)
Sidechain outliers	78261	1288 (1.76-1.76)
RSRZ outliers	66119	1135 (1.76-1.76)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	377	
1	B	377	
1	C	377	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	PO4	A	501	-	X
2	PO4	A	503	-	X
2	PO4	B	507	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10364 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

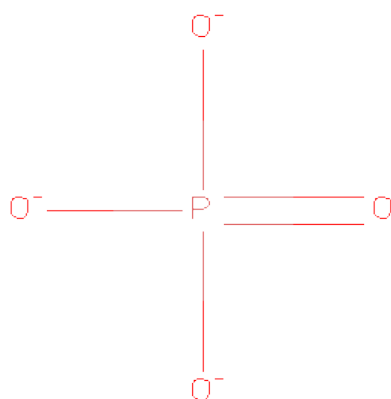
- Molecule 1 is a protein called 458aa long hypothetical endo-1,4-beta-glucanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	377	Total	C	N	O	S	0	0	0
			3069	2002	500	557	10			
1	B	377	Total	C	N	O	S	0	0	0
			3069	2002	500	557	10			
1	C	377	Total	C	N	O	S	0	0	0
			3069	2002	500	557	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	289	LYS	ARG	CONFLICT	UNP O58925
B	289	LYS	ARG	CONFLICT	UNP O58925
C	289	LYS	ARG	CONFLICT	UNP O58925

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is water.

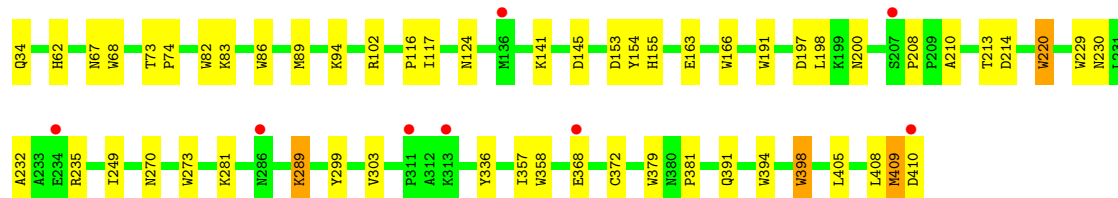
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	369	Total O 369 369	0	0
3	B	359	Total O 359 359	0	0
3	C	354	Total O 354 354	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

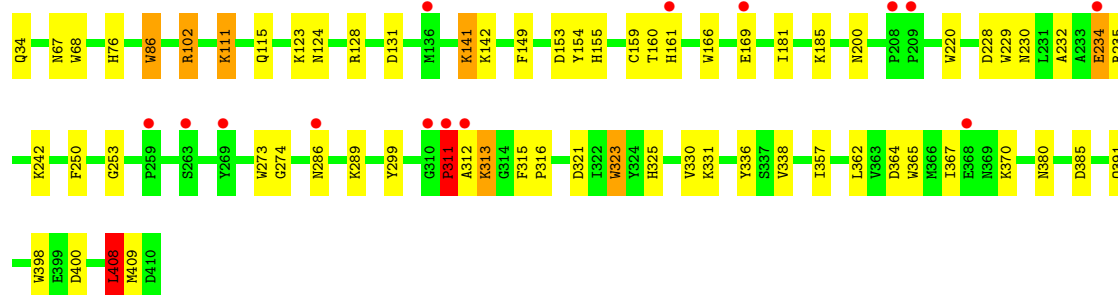
- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase

Chain A: 



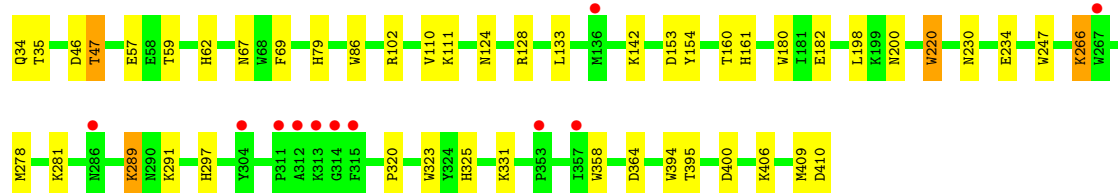
- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase

Chain B: 



- Molecule 1: 458aa long hypothetical endo-1,4-beta-glucanase

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	163.10Å 58.34Å 137.91Å 90.00° 109.65° 90.00°	Depositor
Resolution (Å)	44.69 – 1.75 44.46 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.69-1.75) 98.3 (44.46-1.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.74 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.160 , 0.209 0.160 , 0.209	Depositor DCC
$R_{free}$ test set	6097 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.8	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 52.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 121183 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	10364	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.32	11/3180 (0.3%)	1.14	11/4341 (0.3%)
1	B	1.27	8/3180 (0.3%)	1.13	15/4341 (0.3%)
1	C	1.14	5/3180 (0.2%)	0.96	3/4341 (0.1%)
All	All	1.25	24/9540 (0.3%)	1.08	29/13023 (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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	229	TRP	CD2-CE2	7.89	1.50	1.41
1	A	220	TRP	CD2-CE2	6.85	1.49	1.41
1	B	323	TRP	CD2-CE2	6.77	1.49	1.41
1	A	398	TRP	CD2-CE2	6.54	1.49	1.41
1	A	191	TRP	CD2-CE2	6.25	1.48	1.41
1	B	273	TRP	CD2-CE2	6.17	1.48	1.41
1	B	365	TRP	CD2-CE2	6.11	1.48	1.41
1	A	409	MET	N-CA	-5.99	1.34	1.46
1	B	229	TRP	CD2-CE2	5.97	1.48	1.41
1	C	220	TRP	CD2-CE2	5.96	1.48	1.41
1	C	394	TRP	CD2-CE2	5.91	1.48	1.41
1	C	247	TRP	CD2-CE2	5.86	1.48	1.41
1	B	68	TRP	CD2-CE2	5.80	1.48	1.41
1	A	358	TRP	CD2-CE2	5.61	1.48	1.41
1	A	273	TRP	CD2-CE2	5.58	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	TRP	CD2-CE2	5.51	1.48	1.41
1	B	86	TRP	CD2-CE2	5.43	1.47	1.41
1	A	82	TRP	CD2-CE2	5.39	1.47	1.41
1	A	379	TRP	CD2-CE2	5.27	1.47	1.41
1	A	163	GLU	CD-OE1	5.18	1.31	1.25
1	B	234	GLU	CD-OE1	5.16	1.31	1.25
1	B	273	TRP	CG-CD1	5.13	1.44	1.36
1	C	180	TRP	CD2-CE2	5.11	1.47	1.41
1	C	358	TRP	CD2-CE2	5.04	1.47	1.41

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	364	ASP	CB-CG-OD1	9.81	127.13	118.30
1	A	289	LYS	CD-CE-NZ	-9.77	89.22	111.70
1	A	409	MET	CG-SD-CE	-9.57	84.88	100.20
1	A	235	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	B	400	ASP	CB-CG-OD1	7.50	125.05	118.30
1	A	235	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	408	LEU	CB-CG-CD1	6.73	122.44	111.00
1	B	250	PHE	CB-CG-CD1	-6.53	116.23	120.80
1	A	89	MET	CG-SD-CE	-6.22	90.24	100.20
1	B	153	ASP	CB-CG-OD1	6.14	123.82	118.30
1	B	131	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	235	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	299	TYR	CB-CG-CD1	-5.84	117.50	121.00
1	B	102	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	C	198	LEU	CB-CG-CD1	-5.80	101.13	111.00
1	A	405	LEU	CB-CG-CD2	-5.77	101.20	111.00
1	B	311	PRO	N-CA-C	-5.75	97.16	112.10
1	B	228	ASP	CB-CG-OD1	5.74	123.47	118.30
1	B	409	MET	CG-SD-CE	-5.71	91.06	100.20
1	C	364	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	197	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	380	ASN	CB-CA-C	-5.47	99.46	110.40
1	B	250	PHE	CZ-CE2-CD2	-5.39	113.64	120.10
1	B	299	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	A	336	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	C	400	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	385	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	153	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	145	ASP	CB-CG-OD2	-5.10	113.71	118.30



There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	311	PRO	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3069	0	2908	56	0
1	B	3069	0	2908	51	2
1	C	3069	0	2908	44	1
2	A	20	0	0	0	0
2	B	40	0	0	1	0
2	C	15	0	0	2	0
3	A	369	0	0	29	2
3	B	359	0	0	22	4
3	C	354	0	0	21	0
All	All	10364	0	8724	152	6

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (152) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:372:CYS:HB3	3:A:641:HOH:O	1.20	1.28
1:A:270:ASN:OD1	3:A:911:HOH:O	1.60	1.19
1:B:330:VAL:HG12	3:B:802:HOH:O	0.98	1.16
1:A:214:ASP:CG	3:A:961:HOH:O	1.85	1.15
1:B:312:ALA:HA	3:B:919:HOH:O	0.95	1.12
1:B:311:PRO:HA	3:B:919:HOH:O	1.51	1.08
1:A:410:ASP:HA	3:A:864:HOH:O	1.51	1.08
1:B:313:LYS:HA	3:B:921:HOH:O	1.56	1.05
1:C:182:GLU:OE2	3:C:953:HOH:O	1.76	1.03
1:C:320:PRO:HG3	3:C:944:HOH:O	1.60	1.00
1:B:115:GLN:HB3	3:B:799:HOH:O	1.60	0.98

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:69:PHE:O	3:C:830:HOH:O	1.82	0.97
1:C:266:LYS:HD3	1:C:266:LYS:H	1.30	0.96
1:B:286:ASN:HB3	3:B:751:HOH:O	1.67	0.95
1:C:323:TRP:CZ3	3:C:944:HOH:O	2.22	0.91
1:B:128:ARG:HD3	3:C:655:HOH:O	1.71	0.90
1:C:289:LYS:HE3	3:C:942:HOH:O	1.72	0.90
1:A:210:ALA:O	3:A:961:HOH:O	1.90	0.90
1:C:79:HIS:N	3:C:830:HOH:O	1.68	0.88
1:C:406:LYS:HD3	3:C:867:HOH:O	1.72	0.88
1:A:62:HIS:ND1	1:A:372:CYS:SG	2.47	0.88
1:B:311:PRO:O	3:B:886:HOH:O	1.91	0.86
1:C:395:THR:HB	3:C:795:HOH:O	0.68	0.85
1:B:312:ALA:O	3:B:921:HOH:O	1.93	0.85
1:B:242:LYS:HD2	3:B:908:HOH:O	1.75	0.84
1:B:315:PHE:CE2	1:B:357:ILE:HD11	2.13	0.84
1:A:303:VAL:HG23	3:A:817:HOH:O	1.82	0.79
1:C:323:TRP:HZ3	3:C:944:HOH:O	1.59	0.78
1:A:67:ASN:HD21	1:A:102:ARG:HH11	1.31	0.77
1:C:67:ASN:HD21	1:C:102:ARG:HH11	1.33	0.76
1:A:410:ASP:CA	3:A:864:HOH:O	2.21	0.75
1:A:213:THR:C	3:A:965:HOH:O	2.25	0.74
1:C:142:LYS:NZ	3:C:761:HOH:O	2.16	0.73
1:A:409:MET:O	1:A:410:ASP:CG	2.28	0.72
1:B:123:LYS:HE3	3:C:913:HOH:O	1.91	0.71
1:A:67:ASN:HD21	1:A:102:ARG:HD3	1.55	0.71
1:A:34:GLN:HG3	3:A:673:HOH:O	1.90	0.71
1:B:67:ASN:HD21	1:B:102:ARG:HH11	1.38	0.70
1:A:213:THR:OG1	3:A:965:HOH:O	2.08	0.70
1:A:86:TRP:H	1:A:124:ASN:HD21	1.40	0.70
1:C:406:LYS:NZ	3:C:853:HOH:O	2.25	0.70
1:A:410:ASP:HA	3:A:794:HOH:O	1.93	0.67
1:C:102:ARG:HH22	1:C:200:ASN:HD22	1.40	0.67
1:A:102:ARG:HH22	1:A:200:ASN:HD22	1.42	0.66
1:A:67:ASN:ND2	1:A:102:ARG:HH11	1.92	0.66
1:C:62:HIS:HE1	2:C:502:PO4:O4	1.77	0.66
1:A:372:CYS:CB	3:A:641:HOH:O	1.98	0.65
1:A:281:LYS:NZ	3:A:963:HOH:O	2.26	0.65
1:A:214:ASP:CB	3:A:961:HOH:O	2.37	0.64
1:C:266:LYS:HD3	1:C:266:LYS:N	2.09	0.64
1:A:62:HIS:CE1	1:A:372:CYS:SG	2.91	0.64
1:B:149:PHE:HE2	3:B:810:HOH:O	1.81	0.64
1:B:336:TYR:HB2	3:B:802:HOH:O	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:34:GLN:N	3:A:914:HOH:O	2.31	0.63
1:A:213:THR:CB	3:A:965:HOH:O	2.46	0.63
1:C:67:ASN:HD21	1:C:102:ARG:HD3	1.63	0.63
1:A:86:TRP:H	1:A:124:ASN:ND2	1.97	0.62
1:A:372:CYS:SG	3:A:641:HOH:O	2.52	0.62
1:A:213:THR:CA	3:A:965:HOH:O	2.48	0.61
1:A:214:ASP:N	3:A:965:HOH:O	2.33	0.61
1:C:47:THR:HG23	3:C:840:HOH:O	1.99	0.61
1:A:62:HIS:CG	1:A:372:CYS:HG	2.18	0.60
1:C:281:LYS:NZ	3:C:806:HOH:O	2.35	0.60
1:B:316:PRO:HG3	1:B:357:ILE:HD13	1.84	0.60
1:A:409:MET:O	1:A:410:ASP:CB	2.51	0.59
1:C:406:LYS:HA	1:C:409:MET:CE	2.33	0.59
1:B:338:VAL:CG2	3:B:802:HOH:O	2.50	0.58
1:B:67:ASN:ND2	1:B:102:ARG:HH11	2.00	0.58
1:B:86:TRP:HD1	1:B:124:ASN:HD22	1.52	0.58
1:A:214:ASP:OD2	3:A:961:HOH:O	2.09	0.58
1:B:67:ASN:HD21	1:B:102:ARG:HD3	1.69	0.57
1:C:62:HIS:HD2	3:C:846:HOH:O	1.87	0.57
1:B:86:TRP:H	1:B:124:ASN:HD21	1.53	0.57
1:B:253:GLY:O	1:B:274:GLY:HA2	2.04	0.56
1:B:242:LYS:HB2	3:B:908:HOH:O	2.04	0.56
1:C:67:ASN:ND2	1:C:102:ARG:HH11	2.02	0.56
1:C:230:ASN:O	1:C:234:GLU:HG3	2.06	0.55
1:C:161:HIS:HE1	3:C:927:HOH:O	1.88	0.55
1:C:102:ARG:HH22	1:C:200:ASN:ND2	2.05	0.55
1:B:316:PRO:HG3	1:B:357:ILE:CD1	2.38	0.54
1:C:62:HIS:CE1	2:C:502:PO4:O4	2.60	0.54
1:C:86:TRP:H	1:C:124:ASN:HD21	1.55	0.53
1:A:62:HIS:CG	1:A:372:CYS:SG	3.02	0.52
1:A:86:TRP:HD1	1:A:124:ASN:HD22	1.56	0.52
1:B:102:ARG:HH22	1:B:200:ASN:HD22	1.55	0.52
1:B:160:THR:OG1	1:B:161:HIS:HD2	1.92	0.52
1:A:208:PRO:C	3:A:964:HOH:O	2.47	0.52
1:C:406:LYS:HA	1:C:409:MET:HE2	1.91	0.51
1:B:367:ILE:HG13	1:B:408:LEU:CD1	2.41	0.51
1:A:166:TRP:CZ2	1:A:232:ALA:HB2	2.46	0.50
1:C:291:LYS:HE2	1:C:291:LYS:HA	1.93	0.50
1:A:270:ASN:HB2	3:A:911:HOH:O	2.11	0.50
1:A:86:TRP:N	1:A:124:ASN:HD21	2.07	0.50
1:A:270:ASN:CB	3:A:911:HOH:O	2.57	0.50
1:B:338:VAL:HG23	3:B:802:HOH:O	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:331:LYS:HE3	1:B:370:LYS:O	2.12	0.49
1:B:391:GLN:HG2	1:B:398:TRP:CE2	2.47	0.49
1:B:321:ASP:OD1	1:B:325:HIS:HE1	1.95	0.49
1:C:409:MET:O	1:C:410:ASP:HB2	2.13	0.49
1:B:86:TRP:H	1:B:124:ASN:ND2	2.10	0.49
1:B:367:ILE:HG13	1:B:408:LEU:HD13	1.95	0.49
1:A:391:GLN:HG2	1:A:398:TRP:CE2	2.48	0.48
1:C:34:GLN:NE2	3:C:936:HOH:O	2.44	0.48
1:C:46:ASP:OD2	1:C:331:LYS:HE2	2.14	0.48
1:B:102:ARG:HH22	1:B:200:ASN:ND2	2.12	0.48
1:A:73:THR:HB	1:A:74:PRO:CD	2.42	0.48
1:B:242:LYS:CD	3:B:908:HOH:O	2.46	0.48
1:A:73:THR:HB	1:A:74:PRO:HD2	1.96	0.48
2:B:503:PO4:O3	3:B:697:HOH:O	2.20	0.48
1:C:110:VAL:HA	1:C:133:LEU:HD13	1.96	0.47
1:C:86:TRP:H	1:C:124:ASN:ND2	2.11	0.47
1:B:111:LYS:NZ	3:B:860:HOH:O	2.48	0.47
1:B:220:TRP:CE2	1:B:230:ASN:HB3	2.50	0.47
1:B:242:LYS:CB	3:B:908:HOH:O	2.63	0.46
1:A:270:ASN:CG	3:A:911:HOH:O	2.25	0.46
1:C:160:THR:OG1	1:C:161:HIS:HD2	1.99	0.46
1:C:79:HIS:HB2	3:C:830:HOH:O	2.15	0.46
1:A:102:ARG:HH22	1:A:200:ASN:ND2	2.11	0.46
1:B:315:PHE:CZ	1:B:357:ILE:HD11	2.51	0.46
1:A:116:PRO:C	1:A:117:ILE:HD13	2.36	0.46
1:C:406:LYS:HA	1:C:409:MET:HE3	1.97	0.45
1:A:141:LYS:HD2	3:A:671:HOH:O	2.16	0.45
1:A:381:PRO:HD2	1:A:394:TRP:CH2	2.51	0.45
1:B:321:ASP:OD1	1:B:325:HIS:CE1	2.69	0.45
1:C:200:ASN:ND2	1:C:297:HIS:HE1	2.15	0.45
1:B:76:HIS:HE1	1:B:159:CYS:SG	2.40	0.45
1:B:311:PRO:CA	3:B:919:HOH:O	2.32	0.44
1:B:181:ILE:HG22	1:B:185:LYS:HE2	1.97	0.44
1:B:313:LYS:CA	3:B:921:HOH:O	2.36	0.44
1:B:286:ASN:ND2	3:B:736:HOH:O	2.50	0.44
1:B:76:HIS:HD2	3:B:773:HOH:O	1.99	0.44
1:C:86:TRP:HD1	1:C:124:ASN:HD22	1.64	0.44
1:A:381:PRO:HD2	1:A:394:TRP:CZ2	2.53	0.44
1:A:368:GLU:OE2	3:A:804:HOH:O	2.21	0.44
1:B:234:GLU:CD	1:B:286:ASN:HB2	2.38	0.44
1:B:155:HIS:HA	1:B:200:ASN:CB	2.48	0.44
1:B:166:TRP:CZ2	1:B:232:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:116:PRO:O	1:A:117:ILE:HD13	2.18	0.43
1:A:220:TRP:CE2	1:A:230:ASN:HB3	2.53	0.43
1:A:198:LEU:HD21	1:A:249:ILE:HG23	2.01	0.42
1:C:79:HIS:CB	3:C:830:HOH:O	2.67	0.42
1:A:62:HIS:CD2	3:A:895:HOH:O	2.73	0.42
1:A:410:ASP:CB	3:A:864:HOH:O	2.62	0.42
1:A:368:GLU:HG3	3:A:871:HOH:O	2.19	0.42
1:C:57:GLU:HG2	3:C:796:HOH:O	2.19	0.42
1:C:220:TRP:CE2	1:C:230:ASN:HB3	2.55	0.41
1:A:155:HIS:HA	1:A:200:ASN:HB3	2.02	0.41
1:B:86:TRP:N	1:B:124:ASN:HD21	2.17	0.41
1:A:155:HIS:HA	1:A:200:ASN:CB	2.50	0.41
1:C:111:LYS:HD3	1:C:111:LYS:HA	1.88	0.41
1:C:278:MET:HG2	1:C:325:HIS:O	2.21	0.41
1:B:323:TRP:CH2	1:B:362:LEU:HA	2.56	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:A:836:HOH:O	3:A:954:HOH:O[4_546]	1.84	0.36
1:C:128:ARG:NH1	3:B:714:HOH:O[1_565]	1.95	0.25
3:A:835:HOH:O	3:A:946:HOH:O[4_556]	2.04	0.16
1:B:142:LYS:NZ	3:B:859:HOH:O[4_555]	2.13	0.07
3:B:896:HOH:O	3:B:897:HOH:O[2_555]	2.16	0.04
1:B:141:LYS:NZ	3:B:932:HOH:O[4_555]	2.19	0.01

## 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	375/377 (100%)	362 (96%)	13 (4%)	0	100	100
1	B	375/377 (100%)	365 (97%)	10 (3%)	0	100	100
1	C	375/377 (100%)	365 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1125/1131 (100%)	1092 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	324/324 (100%)	318 (98%)	6 (2%)	69	47
1	B	324/324 (100%)	316 (98%)	8 (2%)	60	33
1	C	324/324 (100%)	317 (98%)	7 (2%)	64	38
All	All	972/972 (100%)	951 (98%)	21 (2%)	64	38

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	94	LYS
1	A	154	TYR
1	A	289	LYS
1	A	357	ILE
1	A	408	LEU
1	B	34	GLN
1	B	111	LYS
1	B	141	LYS
1	B	154	TYR
1	B	169	GLU
1	B	289	LYS
1	B	313	LYS
1	B	408	LEU
1	C	35	THR
1	C	47	THR
1	C	59	THR
1	C	153	ASP
1	C	154	TYR
1	C	266	LYS

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Mol	Chain	Res	Type
1	C	289	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	67	ASN
1	A	124	ASN
1	A	200	ASN
1	A	270	ASN
1	A	359	GLN
1	B	67	ASN
1	B	76	HIS
1	B	124	ASN
1	B	161	HIS
1	B	200	ASN
1	B	286	ASN
1	B	359	GLN
1	C	34	GLN
1	C	62	HIS
1	C	67	ASN
1	C	76	HIS
1	C	124	ASN
1	C	161	HIS
1	C	200	ASN
1	C	359	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

15 ligands are modelled in this entry.

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
2	PO4	A	501	-	4,4,4	0.47	0	6,6,6	0.31	0
2	PO4	A	502	-	4,4,4	0.44	0	6,6,6	0.33	0
2	PO4	A	503	-	4,4,4	0.38	0	6,6,6	0.33	0
2	PO4	A	504	-	4,4,4	0.19	0	6,6,6	0.30	0
2	PO4	B	501	-	4,4,4	0.31	0	6,6,6	0.29	0
2	PO4	B	502	-	4,4,4	0.96	0	6,6,6	0.31	0
2	PO4	B	503	-	4,4,4	0.42	0	6,6,6	0.35	0
2	PO4	B	504	-	4,4,4	1.37	1 (25%)	6,6,6	0.37	0
2	PO4	B	505	-	4,4,4	0.19	0	6,6,6	0.36	0
2	PO4	B	506	-	4,4,4	0.17	0	6,6,6	0.32	0
2	PO4	B	507	-	4,4,4	0.48	0	6,6,6	0.30	0
2	PO4	B	508	-	4,4,4	0.72	0	6,6,6	0.37	0
2	PO4	C	501	-	4,4,4	0.52	0	6,6,6	0.32	0
2	PO4	C	502	-	4,4,4	0.57	0	6,6,6	0.36	0
2	PO4	C	503	-	4,4,4	0.30	0	6,6,6	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	501	-	-	0/0/0/0	0/0/0/0
2	PO4	A	502	-	-	0/0/0/0	0/0/0/0
2	PO4	A	503	-	-	0/0/0/0	0/0/0/0
2	PO4	A	504	-	-	0/0/0/0	0/0/0/0
2	PO4	B	501	-	-	0/0/0/0	0/0/0/0
2	PO4	B	502	-	-	0/0/0/0	0/0/0/0
2	PO4	B	503	-	-	0/0/0/0	0/0/0/0
2	PO4	B	504	-	-	0/0/0/0	0/0/0/0
2	PO4	B	505	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	B	506	-	-	0/0/0/0	0/0/0/0
2	PO4	B	507	-	-	0/0/0/0	0/0/0/0
2	PO4	B	508	-	-	0/0/0/0	0/0/0/0
2	PO4	C	501	-	-	0/0/0/0	0/0/0/0
2	PO4	C	502	-	-	0/0/0/0	0/0/0/0
2	PO4	C	503	-	-	0/0/0/0	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	504	PO4	P-O3	2.69	1.63	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	377/377 (100%)	-0.23	8 (2%) 60 72	8, 20, 36, 54	8 (2%)
1	B	377/377 (100%)	-0.21	14 (3%) 39 48	11, 21, 38, 63	10 (2%)
1	C	377/377 (100%)	-0.14	11 (2%) 49 59	11, 25, 40, 59	9 (2%)
All	All	1131/1131 (100%)	-0.19	33 (2%) 49 59	8, 22, 38, 63	27 (2%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	ASN	4.5
1	C	136	MET	4.4
1	B	311	PRO	4.4
1	B	286	ASN	4.0
1	B	310	GLY	3.8
1	A	136	MET	3.6
1	B	234	GLU	3.4
1	A	234	GLU	3.4
1	B	136	MET	3.4
1	C	311	PRO	3.3
1	B	208	PRO	3.1
1	B	312	ALA	3.0
1	C	315	PHE	2.9
1	A	207	SER	2.9
1	B	161	HIS	2.8
1	C	267	TRP	2.8
1	C	353	PRO	2.8
1	B	209	PRO	2.8
1	B	259	PRO	2.4
1	C	313	LYS	2.4
1	C	314	GLY	2.4
1	C	286	ASN	2.4
1	A	313	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	304	TYR	2.3
1	A	368	GLU	2.3
1	B	269	TYR	2.3
1	C	312	ALA	2.3
1	A	311	PRO	2.2
1	C	357	ILE	2.1
1	B	169	GLU	2.1
1	B	368	GLU	2.1
1	B	263	SER	2.0
1	A	410	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	PO4	A	503	5/5	0.17	6.73	26,34,38,40	0
2	PO4	B	507	5/5	0.25	5.66	40,44,56,60	0
2	PO4	A	501	5/5	0.16	3.07	55,58,67,73	0
2	PO4	A	504	5/5	0.14	1.85	81,82,89,92	0
2	PO4	B	505	5/5	0.21	1.62	62,74,79,84	0
2	PO4	C	502	5/5	0.12	1.46	29,32,36,37	0
2	PO4	B	504	5/5	0.11	1.01	28,28,34,35	0
2	PO4	C	503	5/5	0.15	0.93	55,63,69,77	0
2	PO4	A	502	5/5	0.17	0.92	37,45,50,58	0
2	PO4	B	506	5/5	0.15	0.66	53,60,68,75	0
2	PO4	B	508	5/5	0.08	-0.65	33,36,43,46	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PO4	B	502	5/5	0.05	-1.15	23,24,28,28	0
2	PO4	B	503	5/5	0.07	-1.50	34,38,42,44	0
2	PO4	B	501	5/5	0.04	-2.36	23,25,27,28	0
2	PO4	C	501	5/5	0.06	-3.34	21,23,33,39	0

## 6.5 Other polymers

There are no such residues in this entry.