



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:02 am BST

PDB ID : 5GZU
Title : Crystal Structure of Chitinase ChiW from *Paenibacillus* sp. str. FPU-7 Reveals a Novel Type of Bacterial Cell-Surface-Expressed Multi-Modular Enzyme Machinery
Authors : Itoh, T.; Hibi, T.; Suzuki, F.; Sugimoto, I.; Fujiwara, A.; Inaka, K.; Tanaka, H.; Ohta, K.; Fujii, Y.; Taketo, A.; Kimoto, H.
Deposited on : 2016-10-01
Resolution : 2.03 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

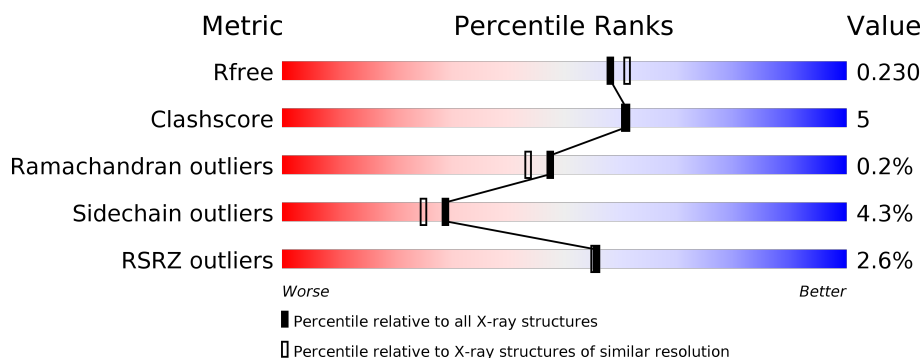
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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 ≥ 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	885	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>14%</div> <div>••</div> </div> </div>
1	B	885	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>••</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14861 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 Chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	858	Total	C	N	O	S	0	5	0
			6753	4318	1109	1315	11			
1	B	859	Total	C	N	O	S	0	7	0
			6776	4337	1111	1314	14			

There are 46 discrepancies between the modelled and reference sequences:

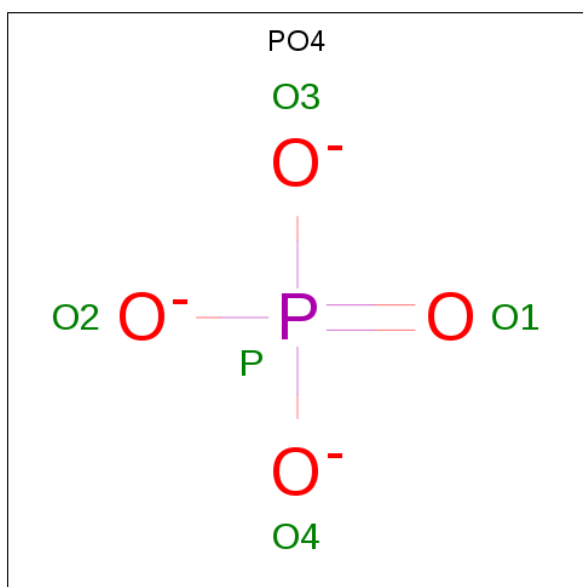
Chain	Residue	Modelled	Actual	Comment	Reference
A	534	MET	-	initiating methionine	UNP K7ZLW6
A	535	ASN	-	expression tag	UNP K7ZLW6
A	536	HIS	-	expression tag	UNP K7ZLW6
A	537	LYS	-	expression tag	UNP K7ZLW6
A	538	VAL	-	expression tag	UNP K7ZLW6
A	539	HIS	-	expression tag	UNP K7ZLW6
A	540	HIS	-	expression tag	UNP K7ZLW6
A	541	HIS	-	expression tag	UNP K7ZLW6
A	542	HIS	-	expression tag	UNP K7ZLW6
A	543	HIS	-	expression tag	UNP K7ZLW6
A	544	HIS	-	expression tag	UNP K7ZLW6
A	545	ILE	-	expression tag	UNP K7ZLW6
A	546	GLU	-	expression tag	UNP K7ZLW6
A	547	GLY	-	expression tag	UNP K7ZLW6
A	548	ARG	-	expression tag	UNP K7ZLW6
A	549	HIS	-	expression tag	UNP K7ZLW6
A	550	MET	-	expression tag	UNP K7ZLW6
A	551	GLU	-	expression tag	UNP K7ZLW6
A	552	LEU	-	expression tag	UNP K7ZLW6
A	553	GLY	-	expression tag	UNP K7ZLW6
A	554	THR	-	expression tag	UNP K7ZLW6
A	555	LEU	-	expression tag	UNP K7ZLW6
A	556	GLU	-	expression tag	UNP K7ZLW6
B	534	MET	-	initiating methionine	UNP K7ZLW6
B	535	ASN	-	expression tag	UNP K7ZLW6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	536	HIS	-	expression tag	UNP K7ZLW6
B	537	LYS	-	expression tag	UNP K7ZLW6
B	538	VAL	-	expression tag	UNP K7ZLW6
B	539	HIS	-	expression tag	UNP K7ZLW6
B	540	HIS	-	expression tag	UNP K7ZLW6
B	541	HIS	-	expression tag	UNP K7ZLW6
B	542	HIS	-	expression tag	UNP K7ZLW6
B	543	HIS	-	expression tag	UNP K7ZLW6
B	544	HIS	-	expression tag	UNP K7ZLW6
B	545	ILE	-	expression tag	UNP K7ZLW6
B	546	GLU	-	expression tag	UNP K7ZLW6
B	547	GLY	-	expression tag	UNP K7ZLW6
B	548	ARG	-	expression tag	UNP K7ZLW6
B	549	HIS	-	expression tag	UNP K7ZLW6
B	550	MET	-	expression tag	UNP K7ZLW6
B	551	GLU	-	expression tag	UNP K7ZLW6
B	552	LEU	-	expression tag	UNP K7ZLW6
B	553	GLY	-	expression tag	UNP K7ZLW6
B	554	THR	-	expression tag	UNP K7ZLW6
B	555	LEU	-	expression tag	UNP K7ZLW6
B	556	GLU	-	expression tag	UNP K7ZLW6

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

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

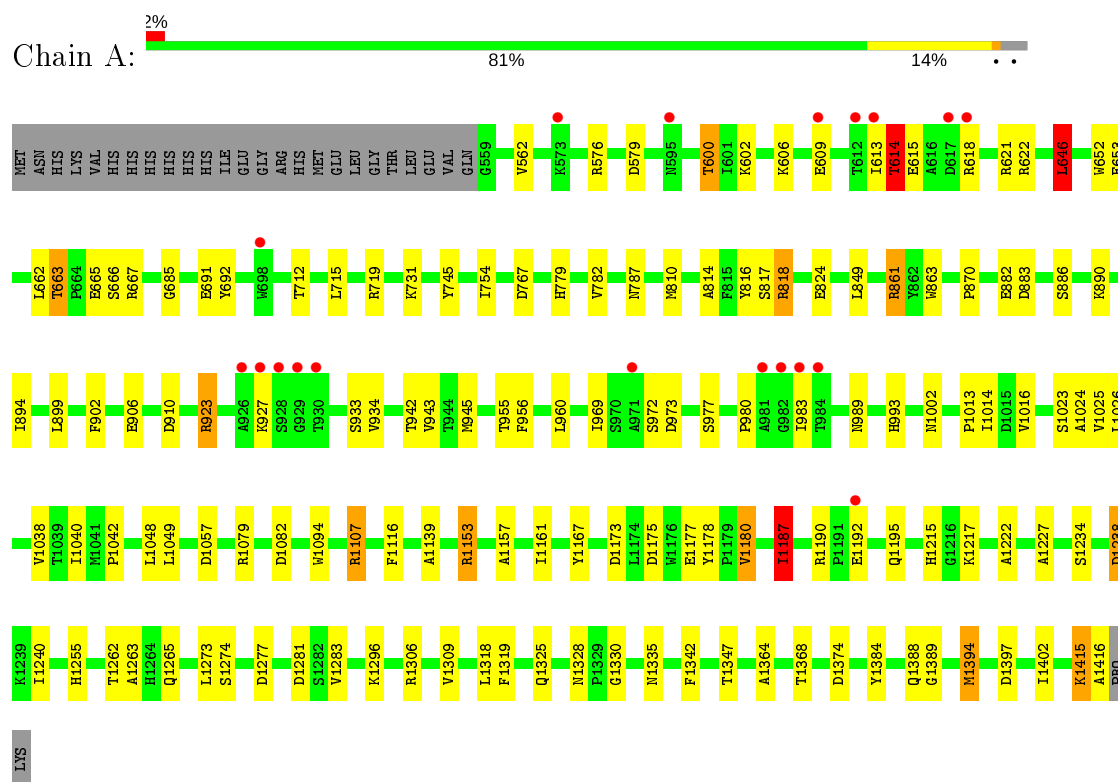
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	652	Total	O	0	0
			652	652		
3	B	670	Total	O	0	0
			670	670		

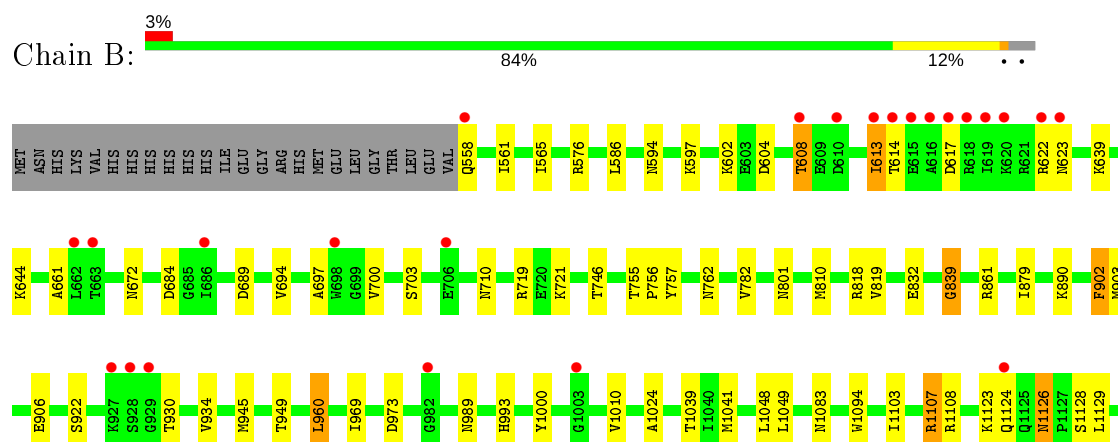
3 Residue-property plots [i](#)

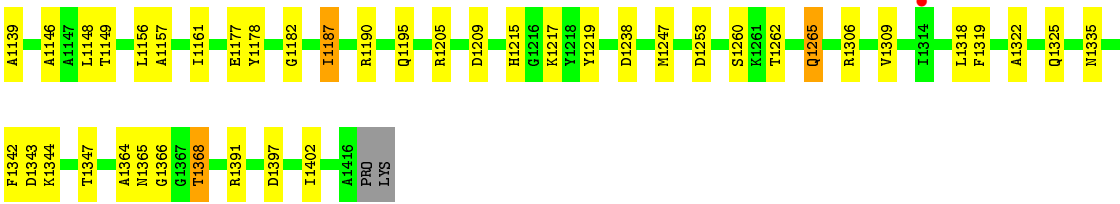
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Chitinase



• Molecule 1: Chitinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.98Å 127.99Å 162.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.03 41.28 – 2.03	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.01-2.03) 98.8 (41.28-2.03)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.27 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.182 , 0.226 0.190 , 0.230	Depositor DCC
R_{free} test set	7476 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14861	wwPDB-VP
Average B, all atoms (Å ²)	31.0	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 22.42 % 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 5.7242e-03.*

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: 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	1.02	3/6942 (0.0%)	1.09	36/9460 (0.4%)
1	B	1.01	6/6969 (0.1%)	1.06	27/9494 (0.3%)
All	All	1.01	9/13911 (0.1%)	1.07	63/18954 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	839	GLY	N-CA	6.54	1.55	1.46
1	A	745	TYR	CE1-CZ	-6.49	1.30	1.38
1	A	1306	ARG	CD-NE	-6.17	1.35	1.46
1	B	839	GLY	CA-C	5.84	1.61	1.51
1	B	1306	ARG	CD-NE	-5.78	1.36	1.46
1	A	824	GLU	CD-OE2	5.45	1.31	1.25
1	B	832	GLU	CD-OE2	5.40	1.31	1.25
1	B	922	SER	CB-OG	-5.28	1.35	1.42
1	B	757	TYR	CG-CD1	5.13	1.45	1.39

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1306	ARG	NE-CZ-NH2	-19.03	110.78	120.30
1	B	1306	ARG	NE-CZ-NH2	-18.56	111.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1306	ARG	NE-CZ-NH1	16.26	128.43	120.30
1	A	1306	ARG	NE-CZ-NH1	14.16	127.38	120.30
1	A	818	ARG	NE-CZ-NH1	12.81	126.70	120.30
1	A	923	ARG	NE-CZ-NH1	10.95	125.78	120.30
1	B	1107	ARG	NE-CZ-NH1	10.38	125.49	120.30
1	A	1107	ARG	NE-CZ-NH1	10.16	125.38	120.30
1	A	818	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	A	1153	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	B	1190	ARG	NE-CZ-NH1	9.43	125.02	120.30
1	B	1190	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	A	1107	ARG	NE-CZ-NH2	-8.40	116.10	120.30
1	A	861[A]	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	A	861[B]	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	B	861	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	A	1306	ARG	CG-CD-NE	-7.28	96.51	111.80
1	B	1366	GLY	N-CA-C	7.26	131.26	113.10
1	B	1108	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	719	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	B	719	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	1107	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	A	923	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	A	1397	ASP	CB-CG-OD1	6.42	124.08	118.30
1	B	1342	PHE	C-N-CA	-6.28	105.99	121.70
1	A	579	ASP	CB-CG-OD2	6.23	123.91	118.30
1	B	1343	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	1374	ASP	CB-CG-OD1	6.14	123.82	118.30
1	A	646	LEU	CA-CB-CG	6.09	129.31	115.30
1	A	646	LEU	CB-CG-CD2	6.02	121.24	111.00
1	A	1306	ARG	CD-NE-CZ	5.96	131.94	123.60
1	A	910	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	1394	MET	CG-SD-CE	5.86	109.58	100.20
1	A	1281	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	B	1205	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	667	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	1306	ARG	CG-CD-NE	-5.74	99.75	111.80
1	B	1391	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	B	1306	ARG	CD-NE-CZ	5.68	131.55	123.60
1	A	1079	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	1190	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	1108	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	1397	ASP	CB-CG-OD1	5.56	123.30	118.30
1	A	1296	LYS	CD-CE-NZ	-5.53	98.97	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1394	MET	CA-CB-CG	5.53	122.70	113.30
1	A	1057	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	1209	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	B	1247	MET	CG-SD-CE	-5.41	91.55	100.20
1	B	818	ARG	CB-CG-CD	5.29	125.37	111.60
1	A	818	ARG	CB-CG-CD	5.29	125.36	111.60
1	B	604	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	1205	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	A	1153	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	818	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	579	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	A	1238[A]	ASP	CB-CG-OD1	5.19	122.97	118.30
1	A	1238[B]	ASP	CB-CG-OD1	5.19	122.97	118.30
1	B	960	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	1187	ILE	CA-CB-CG2	5.07	121.04	110.90
1	A	1342	PHE	C-N-CA	-5.07	109.04	121.70
1	B	684	ASP	CB-CG-OD2	5.06	122.85	118.30
1	A	621	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	861	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	839	GLY	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	6753	0	6529	73	0
1	B	6776	0	6561	48	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	652	0	0	7	0
3	B	670	0	0	10	0
All	All	14861	0	13090	121	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 5.

All (121) 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:A:1335:ASN:HD21	1:A:1402:ILE:H	1.21	0.86
1:B:694:VAL:O	1:B:703:SER:OG	1.94	0.85
1:A:614:THR:HG22	1:A:618:ARG:HE	1.47	0.79
1:B:1335:ASN:HD21	1:B:1402:ILE:H	1.29	0.78
1:A:1002:ASN:HB2	3:A:3552:HOH:O	1.84	0.76
1:B:993:HIS:HD2	3:B:2151:HOH:O	1.69	0.74
1:A:614:THR:HG22	1:A:618:ARG:NE	2.06	0.71
1:B:1364:ALA:O	1:B:1368:THR:HG22	1.90	0.70
1:B:1238:ASP:OD1	3:B:1601:HOH:O	2.08	0.70
1:A:1328:ASN:HD22	1:A:1330:GLY:H	1.38	0.69
1:B:672:ASN:OD1	1:B:721:LYS:HE2	1.92	0.69
1:A:1309:VAL:HG12	1:A:1368[A]:THR:HG22	1.75	0.68
1:B:1124:GLN:N	3:B:1604:HOH:O	2.28	0.66
1:A:1180:VAL:HG13	1:A:1234:SER:HB3	1.81	0.63
1:A:1368[A]:THR:HG21	3:A:3313:HOH:O	1.99	0.63
1:A:712:THR:HA	1:A:754:ILE:CD1	2.29	0.63
1:B:993:HIS:HE1	3:B:2129:HOH:O	1.82	0.61
1:B:782:VAL:HG22	1:B:890:LYS:HG2	1.83	0.59
1:A:1328:ASN:ND2	1:A:1330:GLY:H	2.01	0.59
1:A:1364:ALA:O	1:A:1368[A]:THR:HG23	2.04	0.58
1:B:934:VAL:HG13	1:B:960:LEU:HD13	1.86	0.57
1:B:565:ILE:HG13	1:B:586:LEU:HD21	1.85	0.57
1:A:1094:TRP:CH2	1:A:1107:ARG:HG2	2.39	0.57
1:A:712:THR:HA	1:A:754:ILE:HD11	1.87	0.57
1:B:1217:LYS:HE3	1:B:1219:TYR:CE1	2.41	0.56
1:A:1215:HIS:HE1	3:A:3133:HOH:O	1.90	0.54
1:A:973:ASP:OD1	1:A:1023:SER:OG	2.22	0.54
1:B:1368:THR:HG21	3:B:2117:HOH:O	2.07	0.54
1:A:1415:LYS:O	1:A:1416:ALA:HB2	2.07	0.54
1:A:1153:ARG:HD2	3:A:3502:HOH:O	2.06	0.53
1:A:814:ALA:HB1	1:A:816:TYR:CE1	2.43	0.53
1:A:767:ASP:OD1	1:A:818:ARG:HD3	2.08	0.53
1:A:652:TRP:CD1	1:A:653:GLU:HG3	2.44	0.52
1:A:943:VAL:HG23	1:A:956:PHE:CE1	2.45	0.52
1:A:973:ASP:HB3	1:A:1024:ALA:HB2	1.90	0.52
1:A:782:VAL:HG22	1:A:890:LYS:HG2	1.92	0.51
1:B:746:THR:O	3:B:1602:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:ALA:O	1:B:710:ASN:HB3	2.11	0.51
1:B:1083:ASN:HD21	1:B:1146:ALA:HA	1.75	0.51
1:A:993:HIS:HD2	3:A:3632:HOH:O	1.94	0.50
1:B:969:ILE:H	1:B:989:ASN:HD21	1.59	0.50
1:B:1148:LEU:HB3	1:B:1149:THR:HG23	1.93	0.50
1:A:1335:ASN:HD21	1:A:1402:ILE:N	2.01	0.50
1:A:576:ARG:HB2	3:A:3185:HOH:O	2.11	0.50
1:B:1182:GLY:HA2	1:B:1187:ILE:HG22	1.93	0.50
1:B:945[A]:MET:HE3	1:B:1010:VAL:HG21	1.93	0.50
1:B:973:ASP:HB3	1:B:1024:ALA:HB2	1.93	0.50
1:A:1384:TYR:CE2	1:A:1388:GLN:HG3	2.48	0.49
1:B:1309:VAL:H	1:B:1325:GLN:HE22	1.59	0.49
1:B:819:VAL:HG22	1:B:879:ILE:HG12	1.94	0.49
1:A:1016:VAL:HB	1:A:1038:VAL:HG23	1.94	0.49
1:B:755:THR:N	1:B:756:PRO:CD	2.76	0.49
1:A:1139:ALA:C	1:A:1187:ILE:HD11	2.33	0.48
1:A:715:LEU:HD12	1:A:754:ILE:CG1	2.42	0.48
1:A:1157:ALA:O	1:A:1161:ILE:HG12	2.14	0.48
1:A:1139:ALA:HA	1:A:1187:ILE:CD1	2.44	0.48
1:B:1039:THR:HG21	1:B:1041:MET:CE	2.43	0.48
1:B:565:ILE:HG13	1:B:586:LEU:CD2	2.44	0.48
1:A:609:GLU:HA	1:A:618:ARG:HD2	1.96	0.47
1:A:1227:ALA:HB1	1:A:1283:VAL:HG21	1.97	0.47
1:A:663:THR:HG23	1:A:666:SER:H	1.79	0.47
1:B:1049:LEU:HD23	1:B:1049:LEU:C	2.35	0.47
1:A:1415:LYS:O	1:A:1416:ALA:CB	2.63	0.47
1:A:969:ILE:H	1:A:989:ASN:HD21	1.61	0.47
1:A:861[B]:ARG:NH1	1:A:883:ASP:OD2	2.47	0.47
1:A:1014:ILE:HB	1:A:1040:ILE:HB	1.97	0.47
1:B:1157:ALA:O	1:B:1161:ILE:HG12	2.16	0.47
1:A:945:MET:HE2	1:A:1040:ILE:HG22	1.96	0.46
1:A:779:HIS:CG	1:A:818:ARG:HG2	2.50	0.46
1:A:562:VAL:HG23	1:A:810:MET:CE	2.45	0.46
1:A:1384:TYR:CZ	1:A:1388:GLN:HG3	2.52	0.46
1:B:1000:TYR:OH	3:B:1603:HOH:O	2.19	0.45
1:A:934:VAL:HG13	1:A:960:LEU:HD13	1.97	0.45
1:A:782:VAL:HG22	1:A:890:LYS:CG	2.46	0.45
1:A:715:LEU:HD12	1:A:754:ILE:HD11	1.99	0.45
1:B:1094:TRP:CH2	1:B:1107:ARG:HG2	2.52	0.45
1:B:762:ASN:HA	1:B:810:MET:HB2	1.98	0.45
1:B:1039:THR:HG21	1:B:1041:MET:HE1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1325:GLN:O	1:A:1328:ASN:HB2	2.18	0.44
1:A:861[B]:ARG:HH22	1:A:863:TRP:HB2	1.83	0.44
1:A:609:GLU:OE2	1:A:622:ARG:NH1	2.50	0.44
1:B:1177:GLU:HA	1:B:1178:TYR:CD1	2.53	0.44
1:A:1173:ASP:OD2	1:A:1175:ASP:OD1	2.35	0.44
1:A:1274:SER:O	1:A:1277:ASP:HB2	2.17	0.44
1:A:993:HIS:HE1	3:A:3625:HOH:O	2.01	0.44
1:A:863:TRP:CD1	1:A:1026:LEU:HD22	2.53	0.43
1:A:980:PRO:HG2	1:A:983:ILE:HG13	2.00	0.43
1:A:942:THR:OG1	1:A:1389:GLY:HA2	2.19	0.43
1:A:646:LEU:HD13	1:A:685:GLY:HA3	2.00	0.43
1:B:1124:GLN:HA	3:B:1604:HOH:O	2.16	0.43
1:A:1173:ASP:HA	1:A:1222:ALA:O	2.18	0.43
1:B:1103:ILE:HG22	1:B:1107:ARG:HD3	2.00	0.43
1:A:1116:PHE:CD2	1:A:1167:TYR:CD1	3.06	0.43
1:B:697:ALA:O	1:B:700:VAL:HG23	2.19	0.43
1:A:817:SER:HB3	1:A:849:LEU:HD11	2.01	0.42
1:A:1240:ILE:HG21	1:A:1240:ILE:HD13	1.77	0.42
1:A:600:THR:CG2	1:A:602:LYS:HG2	2.48	0.42
1:B:1126:ASN:HB3	1:B:1129:LEU:HB2	2.01	0.42
1:B:561:ILE:HA	1:B:902:PHE:O	2.19	0.42
1:A:894:ILE:HA	1:A:899:LEU:HD12	2.02	0.42
1:B:1335:ASN:HD21	1:B:1402:ILE:N	2.08	0.42
1:A:1177:GLU:HA	1:A:1178:TYR:CD1	2.55	0.42
1:A:691:GLU:HA	1:A:692:TYR:CD2	2.54	0.42
1:B:1124:GLN:CA	3:B:1604:HOH:O	2.68	0.42
1:A:870:PRO:HD3	1:A:886:SER:HB3	2.00	0.42
1:B:1146:ALA:HB1	1:B:1156:LEU:HD22	2.02	0.42
1:B:602:LYS:O	1:B:608:THR:HG21	2.19	0.41
1:A:1049:LEU:O	1:A:1394:MET:HA	2.21	0.41
1:A:1013:PRO:HA	1:A:1042:PRO:HD3	2.03	0.41
1:B:1260:SER:O	1:B:1322:ALA:N	2.47	0.41
1:A:1139:ALA:HA	1:A:1187:ILE:HD13	2.03	0.41
1:A:1049:LEU:HD23	1:A:1049:LEU:C	2.41	0.41
1:A:1262:THR:OG1	1:A:1319:PHE:N	2.53	0.40
1:B:1126:ASN:ND2	1:B:1128:SER:OG	2.52	0.40
1:A:1335:ASN:ND2	1:A:1402:ILE:HG12	2.36	0.40
1:A:1255:HIS:CD2	1:A:1263:ALA:HB3	2.56	0.40
1:B:1262:THR:O	1:B:1319:PHE:HA	2.21	0.40
1:B:1253:ASP:H	1:B:1265:GLN:NE2	2.19	0.40
1:B:1139:ALA:C	1:B:1187:ILE:HD11	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1215:HIS:HE1	3:B:1719:HOH:O	2.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	861/885 (97%)	828 (96%)	31 (4%)	2 (0%)	47	43
1	B	864/885 (98%)	835 (97%)	27 (3%)	2 (0%)	47	43
All	All	1725/1770 (98%)	1663 (96%)	58 (3%)	4 (0%)	47	43

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	614	THR
1	A	615	GLU
1	B	613	ILE
1	B	1365	ASN

5.3.2 Protein sidechains [i](#)

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	710/730 (97%)	678 (96%)	32 (4%)	27	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	712/730 (98%)	681 (96%)	31 (4%)	28	24
All	All	1422/1460 (97%)	1359 (96%)	63 (4%)	29	24

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	600	THR
1	A	606	LYS
1	A	613	ILE
1	A	614	THR
1	A	646	LEU
1	A	662	LEU
1	A	663	THR
1	A	665	GLU
1	A	731	LYS
1	A	787	ASN
1	A	882	GLU
1	A	902	PHE
1	A	906	GLU
1	A	923	ARG
1	A	927	LYS
1	A	933	SER
1	A	955	THR
1	A	972	SER
1	A	977	SER
1	A	1025	VAL
1	A	1048	LEU
1	A	1082	ASP
1	A	1180	VAL
1	A	1187	ILE
1	A	1192	GLU
1	A	1195	GLN
1	A	1217	LYS
1	A	1265	GLN
1	A	1273	LEU
1	A	1318	LEU
1	A	1347	THR
1	A	1415	LYS
1	B	558	GLN
1	B	576	ARG
1	B	594	ASN
1	B	597	LYS

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Mol	Chain	Res	Type
1	B	608	THR
1	B	613	ILE
1	B	614	THR
1	B	617	ASP
1	B	622	ARG
1	B	623	ASN
1	B	639	LYS
1	B	644	LYS
1	B	689	ASP
1	B	801	ASN
1	B	902	PHE
1	B	903[A]	MET
1	B	903[B]	MET
1	B	906	GLU
1	B	930	THR
1	B	949	THR
1	B	1048	LEU
1	B	1123[A]	LYS
1	B	1123[B]	LYS
1	B	1126	ASN
1	B	1187	ILE
1	B	1195	GLN
1	B	1265	GLN
1	B	1318	LEU
1	B	1344	LYS
1	B	1347	THR
1	B	1368	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	821	GLN
1	A	822	ASN
1	A	857	ASN
1	A	989	ASN
1	A	993	HIS
1	A	1009	ASN
1	A	1060	ASN
1	A	1083	ASN
1	A	1215	HIS
1	A	1265	GLN
1	A	1328	ASN

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Mol	Chain	Res	Type
1	A	1335	ASN
1	B	558	GLN
1	B	642	ASN
1	B	762	ASN
1	B	821	GLN
1	B	822	ASN
1	B	857	ASN
1	B	989	ASN
1	B	993	HIS
1	B	1009	ASN
1	B	1060	ASN
1	B	1083	ASN
1	B	1106	GLN
1	B	1126	ASN
1	B	1215	HIS
1	B	1265	GLN
1	B	1320	GLN
1	B	1321	GLN
1	B	1325	GLN
1	B	1328	ASN
1	B	1335	ASN
1	B	1365	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	3001	-	4,4,4	1.39	0	6,6,6	1.53	1 (16%)
2	PO4	B	1501	-	4,4,4	1.26	0	6,6,6	1.34	1 (16%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	PO4	O2-P-O1	-2.91	100.23	110.89
2	B	1501	PO4	O4-P-O3	-2.90	98.68	107.97

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 ⓘ

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	858/885 (96%)	-0.04	19 (2%) 62 61	14, 29, 54, 106	0
1	B	859/885 (97%)	-0.06	25 (2%) 51 51	12, 26, 52, 131	0
All	All	1717/1770 (97%)	-0.05	44 (2%) 56 55	12, 28, 53, 131	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	614	THR	9.4
1	A	929	GLY	8.4
1	B	619	ILE	6.6
1	B	929	GLY	6.1
1	A	928	SER	5.6
1	A	927	LYS	5.2
1	B	927	LYS	4.8
1	B	616	ALA	4.5
1	B	617	ASP	3.7
1	B	928	SER	3.6
1	B	615	GLU	3.5
1	B	618	ARG	3.4
1	A	930	THR	3.3
1	B	613	ILE	3.3
1	A	613	ILE	3.2
1	A	981	ALA	3.2
1	B	1314	ILE	2.9
1	B	608	THR	2.8
1	A	618	ARG	2.8
1	A	982	GLY	2.8
1	B	1003	GLY	2.7
1	B	982	GLY	2.6
1	B	558	GLN	2.5
1	B	623	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	573	LYS	2.5
1	B	610	ASP	2.5
1	A	983	ILE	2.5
1	B	620	LYS	2.4
1	A	984	THR	2.4
1	A	609	GLU	2.4
1	A	1192	GLU	2.4
1	B	1124	GLN	2.3
1	B	622	ARG	2.3
1	A	698	TRP	2.2
1	B	698	TRP	2.2
1	B	663	THR	2.2
1	B	706	GLU	2.2
1	A	595	ASN	2.2
1	A	617	ASP	2.1
1	B	662	LEU	2.1
1	A	926	ALA	2.1
1	B	686	ILE	2.1
1	A	612	THR	2.0
1	A	971	ALA	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 carbohydrates 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(\AA^2)	Q<0.9
2	PO4	A	3001	5/5	0.99	0.10	25,26,28,29	0
2	PO4	B	1501	5/5	0.99	0.07	23,24,26,29	0

6.5 Other polymers

There are no such residues in this entry.