



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:37 PM UTC

PDB ID : 5GZT / pdb_00005gzt
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 : 2.10 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

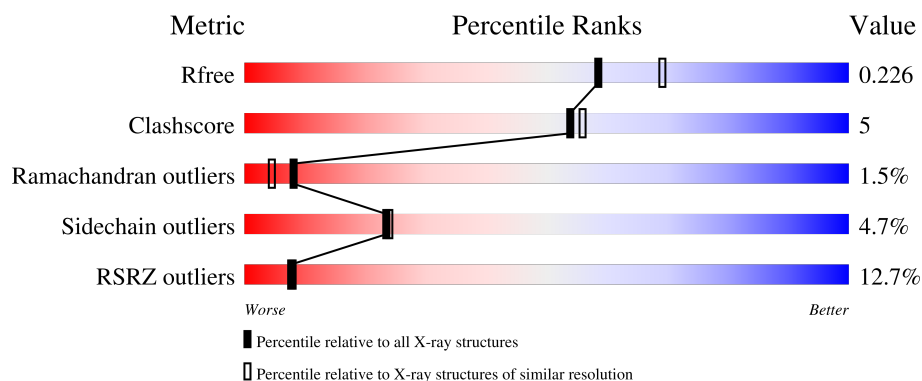
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	108	
2	B	1136	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PO4	B	4002	-	X	-	-
5	FMT	B	4006	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10611 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	69	Total	C	N	O	0	0	0
			481	297	81	103			

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	175	MET	-	initiating methionine	UNP K7ZLW6
A	176	ASN	-	expression tag	UNP K7ZLW6
A	177	HIS	-	expression tag	UNP K7ZLW6
A	178	LYS	-	expression tag	UNP K7ZLW6
A	179	VAL	-	expression tag	UNP K7ZLW6
A	180	HIS	-	expression tag	UNP K7ZLW6
A	181	HIS	-	expression tag	UNP K7ZLW6
A	182	HIS	-	expression tag	UNP K7ZLW6
A	183	HIS	-	expression tag	UNP K7ZLW6
A	184	HIS	-	expression tag	UNP K7ZLW6
A	185	HIS	-	expression tag	UNP K7ZLW6
A	186	ILE	-	expression tag	UNP K7ZLW6
A	187	GLU	-	expression tag	UNP K7ZLW6
A	188	GLY	-	expression tag	UNP K7ZLW6
A	189	ARG	-	expression tag	UNP K7ZLW6
A	190	HIS	-	expression tag	UNP K7ZLW6
A	191	MET	-	expression tag	UNP K7ZLW6
A	192	GLU	-	expression tag	UNP K7ZLW6
A	193	LEU	-	expression tag	UNP K7ZLW6
A	194	GLY	-	expression tag	UNP K7ZLW6
A	195	THR	-	expression tag	UNP K7ZLW6
A	196	LEU	-	expression tag	UNP K7ZLW6
A	197	GLU	-	expression tag	UNP K7ZLW6

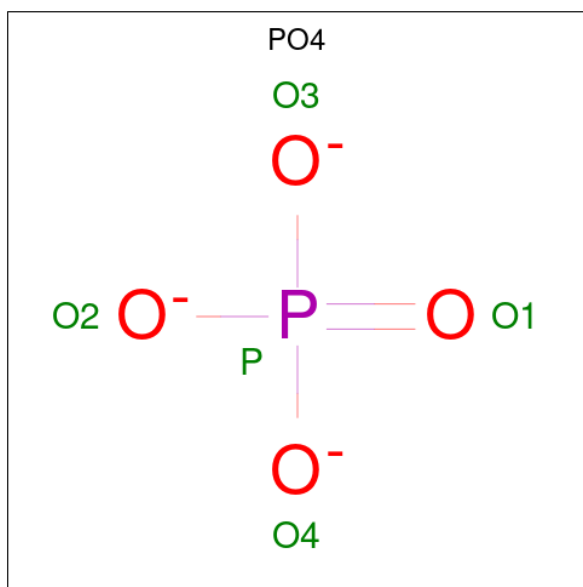
- Molecule 2 is a protein called Chitinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1134	Total	C	N	O	S	0	6	0
			8736	5560	1443	1721	12			

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

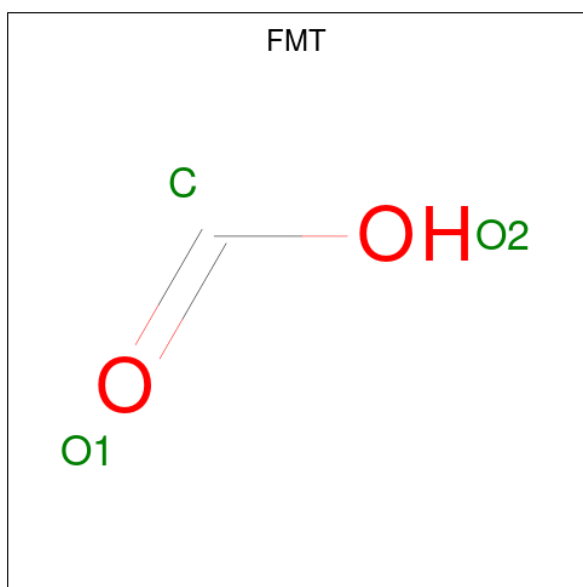
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		
5	B	1	Total	C	O	0	0
			3	1	2		

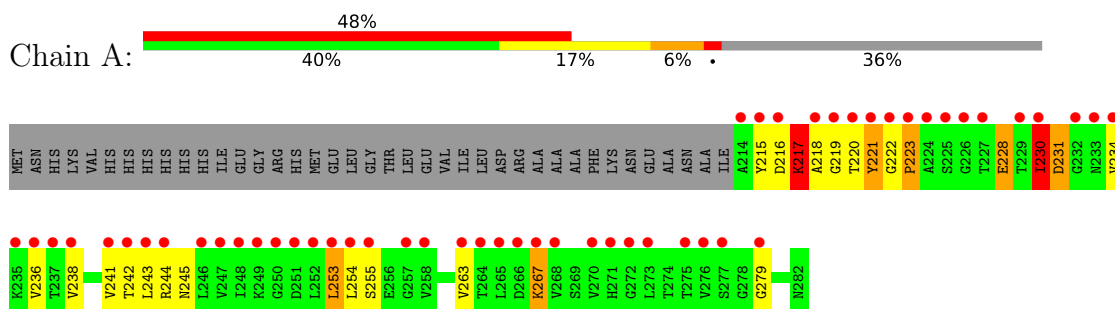
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	18	Total	O	0	0
			18	18		
6	B	1340	Total	O	0	0
			1340	1340		

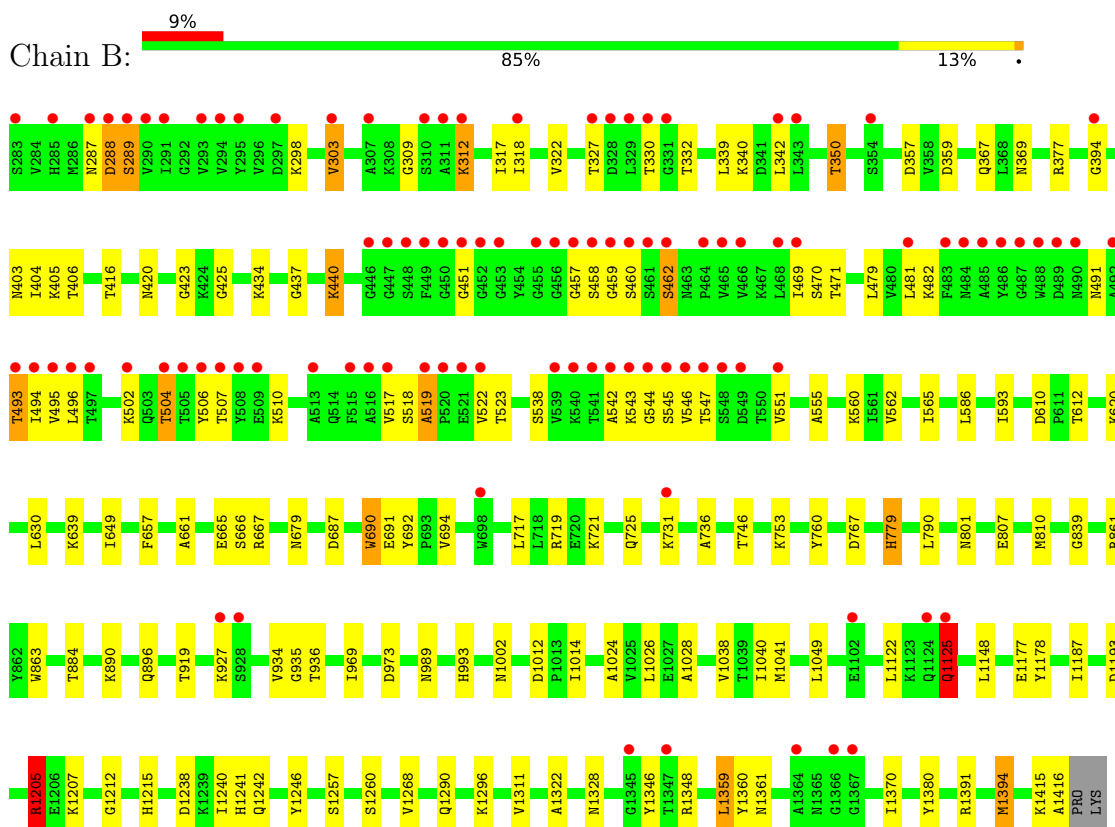
3 Residue-property plots

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: Chitinase



• Molecule 2: Chitinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.34Å 123.49Å 130.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.10 50.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.01-2.10) 99.7 (50.01-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.175 , 0.221 0.185 , 0.226	Depositor DCC
R_{free} test set	5370 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10611	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

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, NA, FMT

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	1.34	4/485 (0.8%)	1.37	4/659 (0.6%)
2	B	1.35	22/8954 (0.2%)	1.16	16/12192 (0.1%)
All	All	1.35	26/9439 (0.3%)	1.17	20/12851 (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	A	0	2

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1012	ASP	C-O	-8.23	1.17	1.24
2	B	1205	ARG	CD-NE	-8.23	1.34	1.46
1	A	215	TYR	CA-C	7.73	1.61	1.53
2	B	649	ILE	CA-C	-7.62	1.43	1.52
2	B	884	THR	N-CA	-6.79	1.38	1.46
2	B	394	GLY	N-CA	6.57	1.54	1.45
1	A	216	ASP	N-CA	6.37	1.53	1.46
1	A	217	LYS	N-CA	6.17	1.53	1.46
2	B	666	SER	N-CA	5.93	1.53	1.46
2	B	1148	LEU	C-O	-5.90	1.17	1.24
2	B	1241	HIS	CA-C	-5.79	1.44	1.52
2	B	1242	GLN	C-O	-5.76	1.16	1.24
2	B	1394	MET	N-CA	-5.59	1.38	1.45
2	B	919	THR	C-O	5.53	1.30	1.24
2	B	423	GLY	C-O	5.44	1.30	1.23
2	B	746	THR	CA-C	5.31	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1193	ASP	N-CA	5.31	1.53	1.46
2	B	1212	GLY	N-CA	-5.26	1.39	1.45
2	B	1380	TYR	CA-C	5.25	1.59	1.52
2	B	935	GLY	CA-C	5.24	1.56	1.52
2	B	1240	ILE	CA-CB	-5.20	1.48	1.54
2	B	1207	LYS	C-O	-5.16	1.18	1.24
2	B	1246	TYR	C-O	5.14	1.29	1.23
1	A	221	TYR	CA-C	5.06	1.59	1.52
2	B	1187	ILE	CA-C	-5.06	1.46	1.52
2	B	1038	VAL	CA-C	5.03	1.58	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1205	ARG	NE-CZ-NH1	12.67	134.17	121.50
2	B	1205	ARG	NE-CZ-NH2	-11.28	109.05	119.20
2	B	519	ALA	CA-C-N	-8.34	111.21	119.64
2	B	519	ALA	C-N-CA	-8.34	111.21	119.64
2	B	1205	ARG	CD-NE-CZ	7.36	134.70	124.40
1	A	216	ASP	N-CA-C	6.80	119.60	110.35
2	B	440	LYS	CB-CA-C	-6.79	99.46	110.74
2	B	934	VAL	CA-C-N	6.76	127.26	122.33
2	B	934	VAL	C-N-CA	6.76	127.26	122.33
1	A	222	GLY	CA-C-N	6.50	127.97	119.84
1	A	222	GLY	C-N-CA	6.50	127.97	119.84
1	A	215	TYR	N-CA-C	6.00	118.17	109.71
2	B	690	TRP	CA-CB-CG	5.34	123.74	113.60
2	B	936	THR	N-CA-C	5.33	118.26	109.85
2	B	1296	LYS	CA-CB-CG	-5.28	103.55	114.10
2	B	303	VAL	CB-CA-C	-5.24	104.34	111.15
2	B	1125	GLN	N-CA-C	5.23	119.38	113.15
2	B	1028	ALA	CA-C-N	-5.23	113.25	123.13
2	B	1028	ALA	C-N-CA	-5.23	113.25	123.13
2	B	753	LYS	N-CA-C	5.07	116.89	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	218	ALA	Peptide
1	A	230	ILE	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	481	0	483	9	0
2	B	8736	0	8553	81	0
3	B	1	0	0	0	0
4	B	5	0	0	0	0
5	B	30	0	14	4	0
6	A	18	0	0	1	0
6	B	1340	0	0	14	1
All	All	10611	0	9050	90	1

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 (90) 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)
2:B:767:ASP:H	2:B:779:HIS:HD2	1.23	0.86
2:B:495:VAL:HG12	2:B:538:SER:OG	1.76	0.86
2:B:312:LYS:NZ	2:B:332:THR:OG1	2.09	0.85
2:B:993:HIS:HD2	6:B:5115:HOH:O	1.62	0.82
2:B:679:ASN:HD21	2:B:725:GLN:HE22	1.26	0.81
2:B:458:SER:HB3	2:B:459:GLY:HA2	1.63	0.80
2:B:1205:ARG:O	2:B:1205:ARG:HD3	1.89	0.73
2:B:969:ILE:H	2:B:989:ASN:HD21	1.35	0.71
2:B:367:GLN:HE21	2:B:369:ASN:HD21	1.40	0.69
2:B:403:ASN:HD21	2:B:420:ASN:HD22	1.39	0.68
2:B:593:ILE:O	6:B:4101:HOH:O	2.12	0.67
2:B:839:GLY:HA3	6:B:4362:HOH:O	1.95	0.67
2:B:801:ASN:HB3	6:B:4814:HOH:O	1.97	0.65
2:B:458:SER:CB	2:B:459:GLY:HA2	2.27	0.64
2:B:1041:MET:HE1	2:B:1391:ARG:NH1	2.13	0.64
2:B:479:LEU:HD11	2:B:555:ALA:CB	2.29	0.63
2:B:317:ILE:HG23	2:B:340:LYS:HG3	1.81	0.61
2:B:404:ILE:O	2:B:406[A]:THR:HG23	1.99	0.61
2:B:482:LYS:HG2	2:B:523:THR:HG22	1.83	0.60
2:B:350:THR:HB	2:B:369:ASN:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:THR:HG22	1:A:220:THR:O	2.01	0.59
2:B:437:GLY:O	2:B:440:LYS:HG3	2.02	0.59
2:B:679:ASN:ND2	2:B:725:GLN:HE22	1.97	0.59
2:B:458:SER:CB	2:B:459:GLY:CA	2.83	0.57
2:B:1359:LEU:HB2	2:B:1370:ILE:HB	1.87	0.57
2:B:479:LEU:HD11	2:B:555:ALA:HB1	1.88	0.56
2:B:403:ASN:ND2	2:B:420:ASN:HD22	2.03	0.56
2:B:493:THR:HB	2:B:507:THR:HG22	1.90	0.54
2:B:350:THR:HG23	6:B:4949:HOH:O	2.07	0.54
2:B:1415:LYS:HG2	6:B:4780:HOH:O	2.06	0.54
2:B:309:GLY:C	2:B:330:THR:HG22	2.34	0.52
2:B:767:ASP:N	2:B:779:HIS:HD2	2.00	0.52
2:B:717:LEU:HD11	2:B:721:LYS:HE2	1.91	0.52
2:B:767:ASP:H	2:B:779:HIS:CD2	2.14	0.52
1:A:230:ILE:HG13	1:A:231:ASP:N	2.26	0.51
2:B:1215:HIS:HE1	6:B:4302:HOH:O	1.94	0.51
2:B:1311:VAL:O	2:B:1360:TYR:OH	2.26	0.50
2:B:1177:GLU:HA	2:B:1178:TYR:CD1	2.46	0.50
2:B:969:ILE:H	2:B:989:ASN:ND2	2.07	0.50
2:B:1416:ALA:C	6:B:4799:HOH:O	2.55	0.50
2:B:861:ARG:HH11	5:B:4006:FMT:C	2.25	0.48
2:B:562:VAL:HG23	2:B:810:MET:HE2	1.95	0.48
2:B:896:GLN:HG2	6:B:5190:HOH:O	2.12	0.48
2:B:318:ILE:HD13	2:B:322:VAL:HG11	1.95	0.47
1:A:223:PRO:HG2	1:A:228:GLU:HB3	1.96	0.47
2:B:350:THR:HB	2:B:369:ASN:CB	2.44	0.47
2:B:1205:ARG:HD3	2:B:1205:ARG:C	2.40	0.47
1:A:279:GLY:O	2:B:298:LYS:HE3	2.15	0.47
2:B:350:THR:CG2	6:B:4949:HOH:O	2.63	0.47
2:B:471:THR:HG22	2:B:481:LEU:HD23	1.97	0.47
2:B:339:LEU:N	2:B:339:LEU:HD12	2.30	0.46
2:B:457:GLY:HA3	2:B:458:SER:OG	2.15	0.46
2:B:610:ASP:OD1	2:B:612:THR:HB	2.14	0.46
2:B:691:GLU:HA	2:B:692:TYR:CD1	2.50	0.46
1:A:230:ILE:CG1	1:A:231:ASP:N	2.79	0.46
2:B:969:ILE:N	2:B:989:ASN:HD21	2.08	0.46
2:B:1260:SER:O	2:B:1322:ALA:HB3	2.15	0.46
2:B:863:TRP:CE3	5:B:4006:FMT:H	2.50	0.46
2:B:287:ASN:O	2:B:289:SER:N	2.49	0.45
2:B:405:LYS:HE3	2:B:425:GLY:O	2.16	0.45
2:B:1049:LEU:O	2:B:1394:MET:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:560:LYS:HE3	2:B:760:TYR:CD1	2.52	0.45
1:A:241:VAL:HG12	1:A:243:LEU:CD1	2.47	0.44
2:B:973:ASP:HB3	2:B:1024:ALA:HB2	1.98	0.44
2:B:657:PHE:HB3	2:B:690:TRP:CD2	2.52	0.44
2:B:807[B]:GLU:CD	2:B:807[B]:GLU:H	2.26	0.44
5:B:4007:FMT:O1	6:B:4102:HOH:O	2.21	0.43
2:B:298:LYS:HG2	2:B:303:VAL:HG23	1.99	0.43
2:B:687:ASP:HA	2:B:736:ALA:O	2.18	0.43
2:B:1346:TYR:CD1	2:B:1361:ASN:HB2	2.54	0.43
2:B:993:HIS:HE1	6:B:5140:HOH:O	2.01	0.43
2:B:1348:ARG:HA	2:B:1359:LEU:HD12	2.01	0.43
2:B:496:LEU:HD12	6:B:4752:HOH:O	2.19	0.42
1:A:253:LEU:O	1:A:254:LEU:HD12	2.20	0.42
2:B:1257:SER:HB3	2:B:1328:ASN:ND2	2.34	0.42
2:B:491:ASN:HD21	2:B:542:ALA:HB3	1.84	0.42
2:B:1014:ILE:HB	2:B:1040:ILE:HB	2.02	0.42
2:B:357:ASP:CG	2:B:377[A]:ARG:HH21	2.27	0.42
1:A:217:LYS:HB3	6:A:309:HOH:O	2.19	0.41
2:B:661:ALA:HA	2:B:667:ARG:HG2	2.00	0.41
2:B:494:ILE:HA	2:B:538:SER:O	2.20	0.41
2:B:1125:GLN:HE21	2:B:1125:GLN:HB3	1.66	0.41
1:A:242:THR:O	1:A:243:LEU:HD12	2.21	0.41
2:B:1026:LEU:CD1	5:B:4006:FMT:H	2.51	0.41
2:B:1238[A]:ASP:HB2	2:B:1290:GLN:O	2.20	0.41
2:B:691:GLU:HA	2:B:692:TYR:CG	2.55	0.41
2:B:504:THR:CG2	2:B:506:TYR:CE2	3.04	0.41
2:B:377[B]:ARG:HD3	6:B:4876:HOH:O	2.20	0.40
2:B:1049:LEU:HD23	2:B:1049:LEU:C	2.46	0.40
2:B:416:THR:HA	2:B:434:LYS:O	2.22	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
6:B:4775:HOH:O	6:B:4968:HOH:O[4_555]	1.57	0.63

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	67/108 (62%)	51 (76%)	8 (12%)	8 (12%)	0	0
2	B	1138/1136 (100%)	1087 (96%)	41 (4%)	10 (1%)	14	10
All	All	1205/1244 (97%)	1138 (94%)	49 (4%)	18 (2%)	8	4

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	255	SER
2	B	288	ASP
2	B	460	SER
2	B	462	SER
2	B	519	ALA
2	B	451	GLY
2	B	544	GLY
2	B	545	SER
1	A	221	TYR
1	A	223	PRO
1	A	245	ASN
2	B	546	VAL
1	A	236	VAL
1	A	267	LYS
2	B	470	SER
1	A	219	GLY
1	A	263	VAL
2	B	694	VAL

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	53/85 (62%)	44 (83%)	9 (17%)	2	1
2	B	928/924 (100%)	891 (96%)	37 (4%)	28	29
All	All	981/1009 (97%)	935 (95%)	46 (5%)	23	24

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	LYS
1	A	228	GLU
1	A	230	ILE
1	A	231	ASP
1	A	234	VAL
1	A	238	VAL
1	A	244	ARG
1	A	253	LEU
1	A	267	LYS
2	B	288	ASP
2	B	289	SER
2	B	312	LYS
2	B	327	THR
2	B	342	LEU
2	B	350	THR
2	B	359	ASP
2	B	462	SER
2	B	469	ILE
2	B	493	THR
2	B	502	LYS
2	B	504	THR
2	B	510	LYS
2	B	517	VAL
2	B	518	SER
2	B	522	VAL
2	B	543	LYS
2	B	547	THR
2	B	551	VAL
2	B	565	ILE
2	B	586	LEU
2	B	620	LYS
2	B	630	LEU
2	B	639	LYS

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Mol	Chain	Res	Type
2	B	665	GLU
2	B	719	ARG
2	B	731	LYS
2	B	779	HIS
2	B	790	LEU
2	B	890	LYS
2	B	927	LYS
2	B	1002	ASN
2	B	1122	LEU
2	B	1125	GLN
2	B	1205	ARG
2	B	1268	VAL
2	B	1359	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	287	ASN
2	B	365	ASN
2	B	369	ASN
2	B	420	ASN
2	B	484	ASN
2	B	595	ASN
2	B	679	ASN
2	B	779	HIS
2	B	821	GLN
2	B	822	ASN
2	B	989	ASN
2	B	993	HIS
2	B	1093	ASN
2	B	1125	GLN
2	B	1215	HIS
2	B	1242	GLN
2	B	1315	ASN

5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	$\# Z > 2$
5	FMT	B	4003	-	2,2,2	1.43	0	1,1,1	0.14	0
5	FMT	B	4004	-	2,2,2	1.09	0	1,1,1	0.52	0
5	FMT	B	4009	-	2,2,2	1.04	0	1,1,1	0.34	0
4	PO4	B	4002	-	4,4,4	2.03	2 (50%)	6,6,6	1.76	2 (33%)
5	FMT	B	4006	-	2,2,2	1.73	1 (50%)	1,1,1	0.67	0
5	FMT	B	4011	-	2,2,2	0.35	0	1,1,1	0.97	0
5	FMT	B	4005	-	2,2,2	1.02	0	1,1,1	0.23	0
5	FMT	B	4008	-	2,2,2	1.41	0	1,1,1	0.13	0
5	FMT	B	4007	-	2,2,2	1.59	0	1,1,1	0.07	0
5	FMT	B	4012	-	2,2,2	0.83	0	1,1,1	0.42	0
5	FMT	B	4010	-	2,2,2	0.72	0	1,1,1	0.22	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	4002	PO4	P-O3	-3.07	1.45	1.54
4	B	4002	PO4	P-O2	-2.18	1.48	1.54
5	B	4006	FMT	O2-C	2.16	1.39	1.28

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	4002	PO4	O2-P-O1	-2.91	100.65	110.95
4	B	4002	PO4	O3-P-O2	2.44	115.50	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	4006	FMT	3	0
5	B	4007	FMT	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	69/108 (63%)	2.96	52 (75%) 0 0	59, 83, 113, 119	0
2	B	1134/1136 (99%)	0.25	101 (8%) 15 16	12, 29, 76, 123	6 (0%)
All	All	1203/1244 (96%)	0.41	153 (12%) 8 8	12, 30, 86, 123	6 (0%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	485	ALA	6.9
1	A	234	VAL	6.1
2	B	457	GLY	6.0
1	A	221	TYR	5.7
2	B	542	ALA	5.5
2	B	447	GLY	5.4
1	A	224	ALA	5.3
1	A	248	ILE	4.9
1	A	214	ALA	4.9
2	B	451	GLY	4.7
1	A	247	VAL	4.7
2	B	450	GLY	4.7
2	B	465	VAL	4.7
2	B	449	PHE	4.6
2	B	486	TYR	4.6
1	A	233	ASN	4.6
1	A	252	LEU	4.5
2	B	448	SER	4.5
2	B	493	THR	4.5
2	B	446	GLY	4.4
1	A	241	VAL	4.4
1	A	276	VAL	4.4
1	A	267	LYS	4.3
1	A	253	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	218	ALA	4.2
1	A	215	TYR	4.2
2	B	492	ALA	4.1
2	B	546	VAL	4.1
1	A	270	VAL	4.1
1	A	238	VAL	4.0
1	A	219	GLY	4.0
1	A	232	GLY	4.0
2	B	513	ALA	3.9
1	A	226	GLY	3.9
2	B	515	PHE	3.9
2	B	461	SER	3.9
1	A	264	THR	3.9
2	B	458	SER	3.8
1	A	236	VAL	3.8
2	B	456	GLY	3.8
2	B	508	TYR	3.8
2	B	551	VAL	3.7
2	B	310	SER	3.7
1	A	265	LEU	3.6
2	B	342	LEU	3.6
1	A	230	ILE	3.6
1	A	272	GLY	3.6
2	B	927	LYS	3.5
1	A	220	THR	3.5
2	B	520	PRO	3.5
2	B	1124	GLN	3.4
2	B	459	GLY	3.3
1	A	243	LEU	3.3
2	B	312	LYS	3.3
1	A	227	THR	3.3
2	B	544	GLY	3.2
2	B	466	VAL	3.2
1	A	250	GLY	3.2
2	B	460	SER	3.2
2	B	509	GLU	3.2
1	A	244	ARG	3.1
2	B	541	THR	3.1
2	B	290	VAL	3.1
2	B	468	LEU	3.1
1	A	246	LEU	3.1
2	B	488	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	295	TYR	3.1
2	B	452	GLY	3.1
2	B	330	THR	3.1
2	B	507	THR	3.1
1	A	225	SER	3.1
2	B	329	LEU	3.0
2	B	283	SER	3.0
2	B	455	GLY	3.0
2	B	543	LYS	3.0
2	B	311	ALA	3.0
2	B	547	THR	3.0
1	A	258	VAL	3.0
2	B	469	ILE	3.0
2	B	328	ASP	3.0
1	A	242	THR	2.9
2	B	327	THR	2.9
2	B	464	PRO	2.9
1	A	249	LYS	2.9
2	B	548	SER	2.8
1	A	254	LEU	2.8
2	B	517	VAL	2.8
2	B	539	VAL	2.8
2	B	291	ILE	2.7
1	A	266	ASP	2.7
2	B	516	ALA	2.7
2	B	519	ALA	2.7
2	B	1345	GLY	2.7
2	B	1364	ALA	2.7
2	B	303	VAL	2.7
1	A	237	THR	2.6
2	B	484	ASN	2.6
2	B	505	THR	2.6
1	A	223	PRO	2.6
1	A	263	VAL	2.6
1	A	222	GLY	2.6
2	B	522	VAL	2.5
2	B	285	HIS	2.5
2	B	497	THR	2.5
2	B	453	GLY	2.5
1	A	216	ASP	2.5
2	B	506	TYR	2.4
2	B	502	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	698	TRP	2.4
2	B	288	ASP	2.4
2	B	928	SER	2.4
2	B	521	GLU	2.3
1	A	273	LEU	2.3
2	B	489	ASP	2.3
1	A	268	VAL	2.3
1	A	275	THR	2.3
2	B	394	GLY	2.3
2	B	1366	GLY	2.3
2	B	462	SER	2.3
2	B	331	GLY	2.3
2	B	487	GLY	2.3
2	B	481	LEU	2.3
2	B	496	LEU	2.3
1	A	251	ASP	2.2
1	A	277	SER	2.2
2	B	294	VAL	2.2
2	B	289	SER	2.2
2	B	354	SER	2.2
2	B	549	ASP	2.2
2	B	495	VAL	2.2
2	B	1125	GLN	2.2
2	B	504	THR	2.2
2	B	1347	THR	2.2
2	B	318	ILE	2.1
2	B	483	PHE	2.1
1	A	235	LYS	2.1
2	B	545	SER	2.1
1	A	271	HIS	2.1
2	B	1367	GLY	2.1
2	B	307	ALA	2.1
1	A	255	SER	2.1
2	B	343	LEU	2.1
2	B	297	ASP	2.1
2	B	494	ILE	2.1
2	B	293	VAL	2.1
2	B	1102	GLU	2.0
2	B	287	ASN	2.0
2	B	490	ASN	2.0
1	A	229	THR	2.0
2	B	540	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	731	LYS	2.0
1	A	257	GLY	2.0
1	A	279	GLY	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($\text{\AA}^2$)	Q<0.9
5	FMT	B	4004	3/3	0.82	0.20	57,57,58,69	0
3	NA	B	4001	1/1	0.84	0.12	50,50,50,50	0
5	FMT	B	4009	3/3	0.87	0.15	51,51,56,67	0
5	FMT	B	4005	3/3	0.88	0.26	49,49,56,61	0
5	FMT	B	4012	3/3	0.88	0.15	47,47,52,57	0
5	FMT	B	4003	3/3	0.91	0.18	41,41,45,50	0
5	FMT	B	4007	3/3	0.93	0.15	25,25,37,39	0
5	FMT	B	4006	3/3	0.94	0.19	25,25,26,39	0
5	FMT	B	4008	3/3	0.94	0.13	33,33,37,44	0
5	FMT	B	4010	3/3	0.95	0.09	37,37,38,41	0
5	FMT	B	4011	3/3	0.96	0.08	28,28,29,30	0
4	PO4	B	4002	5/5	0.99	0.04	16,17,18,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.