



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:53 am GMT

PDB ID : 5GZV  
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 : 2.61 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

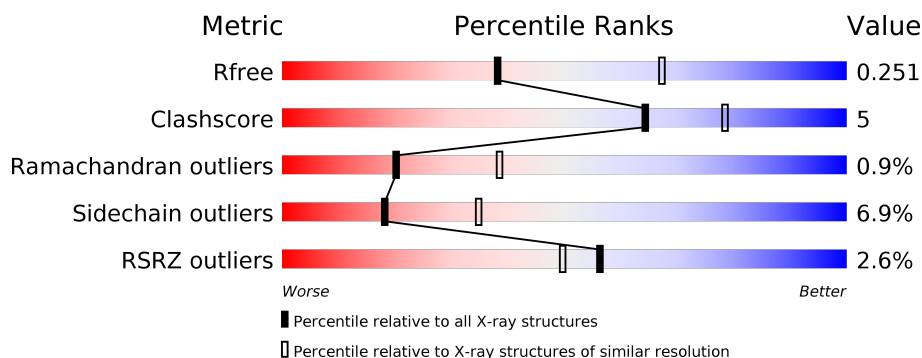
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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))
$R_{free}$	100719	2983 (2.64-2.60)
Clashscore	112137	3351 (2.64-2.60)
Ramachandran outliers	110173	3298 (2.64-2.60)
Sidechain outliers	110143	3298 (2.64-2.60)
RSRZ outliers	101464	2992 (2.64-2.60)

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. 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>82%</div> <div>14%</div> <div>••</div> </div> </div>
1	B	885	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>••</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13773 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	860	Total	C	N	O	S	0	3	0
			6762	4324	1112	1314	12			
1	B	859	Total	C	N	O	S	0	1	0
			6741	4310	1108	1311	12			

There are 46 discrepancies between the modelled and reference sequences:

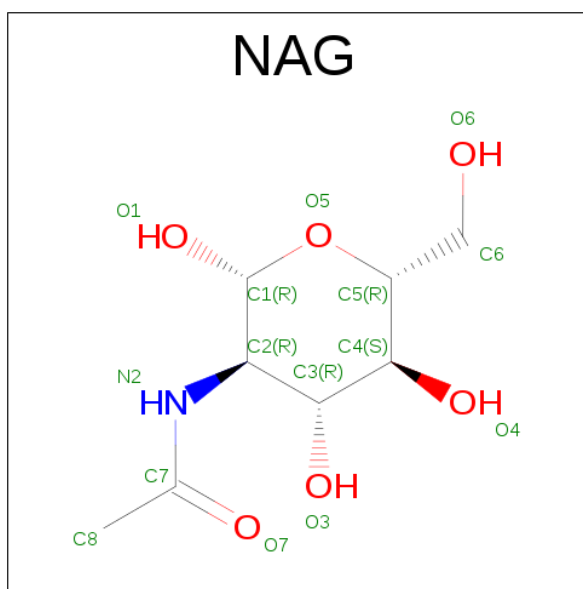
Chain	Residue	Modelled	Actual	Comment	Reference
A	534	MET	-	initiating methionine	UNP K7ZLW6
A	535	ASN	-	expression tag	UNP K7ZLW6
A	536	HIS	-	expression tag	UNP K7ZLW6
A	537	LYS	-	expression tag	UNP K7ZLW6
A	538	VAL	-	expression tag	UNP K7ZLW6
A	539	HIS	-	expression tag	UNP K7ZLW6
A	540	HIS	-	expression 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 N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



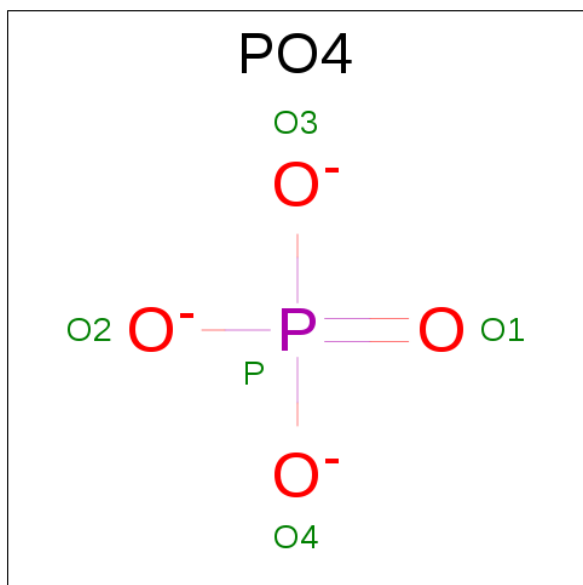
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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		

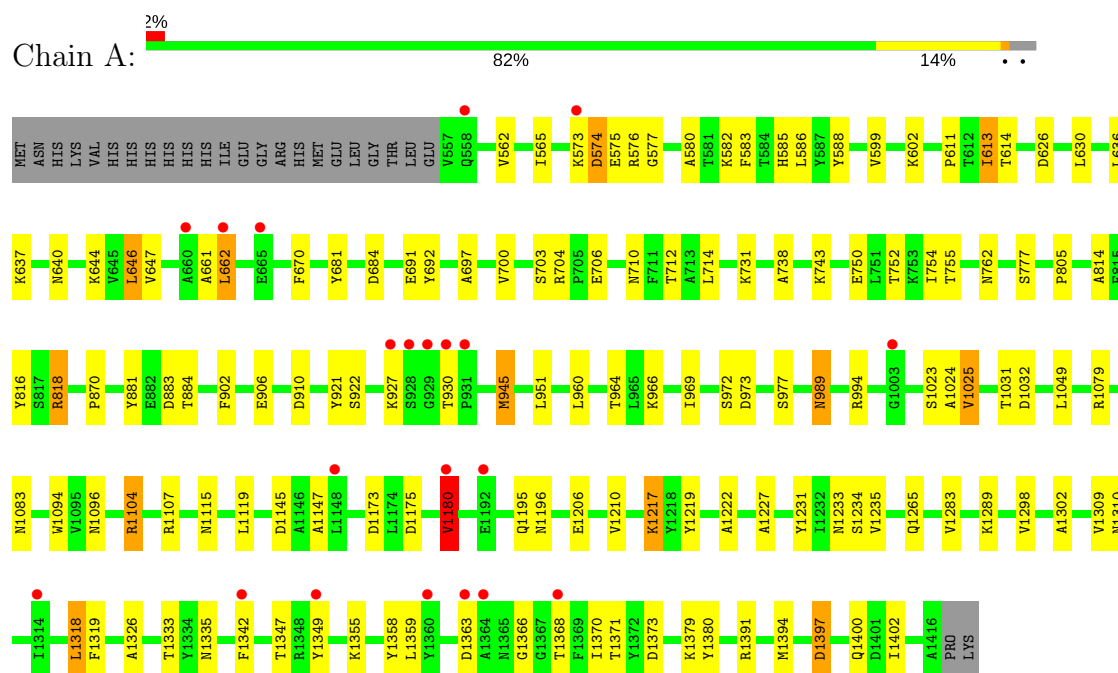
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	117	Total	O	0	0
			117	117		
4	B	85	Total	O	0	0
			85	85		

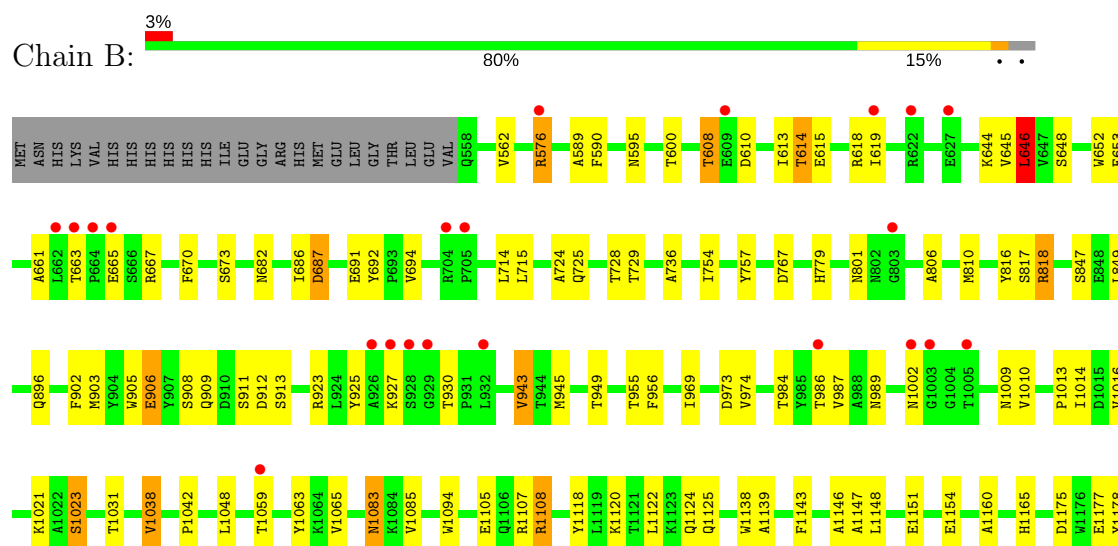
### 3 Residue-property plots

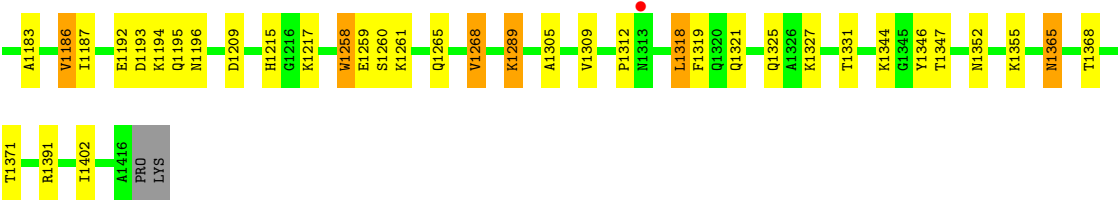
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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, $\alpha$ , $\beta$ , $\gamma$	112.99Å 127.23Å 161.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 2.61 41.08 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.01-2.61) 99.1 (41.08-2.61)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.20 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, $R_{free}$	0.203 , 0.253 0.206 , 0.251	Depositor DCC
$R_{free}$ test set	3459 reflections (5.16%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13773	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	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 28.55 % 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 1.8065e-03.*

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

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NAG

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	0.77	0/6945	0.89	5/9463 (0.1%)
1	B	0.79	0/6918	0.92	6/9427 (0.1%)
All	All	0.78	0/13863	0.90	11/18890 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	818	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	818	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	994	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	B	646	LEU	CA-CB-CG	6.97	131.34	115.30
1	A	1391	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	1391	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	B	1108	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	687	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	818	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	910	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	1209	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	6762	0	6539	63	0
1	B	6741	0	6511	67	0
2	A	29	0	27	0	0
2	B	29	0	27	6	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	117	0	0	0	0
4	B	85	0	0	1	0
All	All	13773	0	13104	129	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 (129) 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:B:906:GLU:OE2	1:B:908:SER:OG	2.07	0.70
1:A:1094:TRP:CZ3	1:A:1107:ARG:HG3	2.26	0.70
1:B:1010:VAL:HG11	1:B:1014:ILE:HD11	1.75	0.69
1:B:909:GLN:HE22	2:B:1501:NAG:H81	1.57	0.68
1:A:1310:ASN:HA	1:A:1366:GLY:HA3	1.74	0.68
1:B:1094:TRP:CH2	1:B:1107:ARG:HG2	2.29	0.67
1:A:973:ASP:HB3	1:A:1024:ALA:HB2	1.76	0.66
1:B:909:GLN:NE2	2:B:1501:NAG:H81	2.11	0.64
1:B:562:VAL:HG23	1:B:810:MET:CE	2.29	0.63
1:A:1206:GLU:O	1:A:1210:VAL:HG23	1.99	0.62
1:A:969:ILE:H	1:A:989:ASN:HD21	1.50	0.60
1:B:905:TRP:HE1	2:B:1501:NAG:H83	1.67	0.59
1:B:1186:VAL:HG23	1:B:1187:ILE:HD13	1.85	0.58
1:A:884:THR:HG1	1:A:964:THR:HG1	1.37	0.58
1:A:1326:ALA:HB1	1:B:682:ASN:HB3	1.86	0.58
1:A:588:TYR:OH	1:A:626:ASP:OD2	2.16	0.58
1:A:945:MET:CE	1:A:951:LEU:HD13	2.34	0.57
1:A:574:ASP:OD1	1:A:577:GLY:N	2.38	0.56
1:A:712:THR:HA	1:A:754:ILE:CD1	2.36	0.56
1:B:1059:THR:HG22	1:B:1118:TYR:HB2	1.86	0.56
1:A:1309:VAL:HA	1:A:1368:THR:HG22	1.88	0.55
1:A:644:LYS:HA	1:A:684:ASP:OD2	2.08	0.54
1:A:712:THR:HA	1:A:754:ILE:HD11	1.89	0.54
1:B:645:VAL:O	1:B:645:VAL:HG12	2.07	0.54
1:B:1083:ASN:HD21	1:B:1146:ALA:HA	1.73	0.54
2:B:1502:NAG:H1	2:B:1502:NAG:H82	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:ASP:HA	1:B:736:ALA:O	2.08	0.53
1:B:1289:LYS:HE3	1:B:1289:LYS:HA	1.90	0.53
1:B:613:ILE:HG23	1:B:613:ILE:O	2.08	0.53
1:A:1335:ASN:HD21	1:A:1402:ILE:H	1.57	0.53
1:A:637:LYS:HA	1:A:640:ASN:O	2.08	0.53
1:B:1318:LEU:HD22	1:B:1319:PHE:CE2	2.43	0.53
1:A:1355:LYS:HE3	1:A:1380:TYR:CE1	2.45	0.52
1:B:905:TRP:CD2	2:B:1502:NAG:H83	2.44	0.52
1:A:750:GLU:O	1:A:754:ILE:HB	2.09	0.52
1:B:974:VAL:HG12	1:B:987:VAL:HG21	1.92	0.52
1:B:1260:SER:OG	1:B:1321:GLN:NE2	2.41	0.52
1:B:576:ARG:HD3	1:B:912:ASP:HA	1.92	0.51
1:B:969:ILE:H	1:B:989:ASN:HD21	1.57	0.51
1:B:1177:GLU:HA	1:B:1178:TYR:CD1	2.46	0.51
1:A:1180:VAL:HG22	1:A:1234:SER:HB3	1.92	0.51
1:B:1177:GLU:HG2	1:B:1178:TYR:CE1	2.46	0.51
1:B:1183:ALA:HB3	1:B:1186:VAL:HG22	1.92	0.51
1:B:1085:VAL:HG21	1:B:1160:ALA:HB2	1.91	0.51
1:B:661:ALA:HB2	1:B:714:LEU:HD22	1.92	0.51
1:B:608:THR:O	1:B:618:ARG:HD2	2.11	0.50
1:B:610:ASP:HB3	1:B:613:ILE:HG22	1.94	0.50
1:A:1318:LEU:HD22	1:A:1319:PHE:CD2	2.47	0.50
1:B:562:VAL:HG23	1:B:810:MET:HE2	1.92	0.50
1:A:945:MET:HE2	1:A:951:LEU:HD13	1.93	0.50
1:A:755:THR:HG21	1:A:805:PRO:HD2	1.94	0.50
1:B:1151:GLU:O	1:B:1154:GLU:HB3	2.12	0.50
1:A:1173:ASP:HA	1:A:1222:ALA:O	2.12	0.49
1:A:646:LEU:HD23	1:A:646:LEU:N	2.27	0.49
1:B:1138:TRP:O	1:B:1139:ALA:HB3	2.11	0.49
1:A:1309:VAL:HG12	1:A:1368:THR:CG2	2.43	0.49
1:B:1258:TRP:CD1	1:B:1259:GLU:HG3	2.47	0.49
1:A:814:ALA:HB1	1:A:816:TYR:CE1	2.47	0.49
1:B:715:LEU:HD13	1:B:754:ILE:HG23	1.94	0.49
1:A:1096:ASN:HA	1:A:1104:ARG:HD2	1.95	0.49
1:A:1049:LEU:HD23	1:A:1049:LEU:C	2.34	0.48
1:B:943:VAL:HG23	1:B:956:PHE:CZ	2.48	0.48
1:B:1346:TYR:HE2	1:B:1368:THR:HG23	1.77	0.48
1:A:964:THR:H	1:A:1025:VAL:HG22	1.78	0.47
1:B:663:THR:O	1:B:667:ARG:HG3	2.14	0.47
1:B:1309:VAL:HG11	1:B:1327:LYS:O	2.15	0.47
1:B:1013:PRO:HA	1:B:1042:PRO:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1217:LYS:HE2	1:A:1219:TYR:CE1	2.50	0.47
1:A:580:ALA:HB2	1:A:636:LEU:HD13	1.97	0.47
1:B:973:ASP:O	1:B:1021:LYS:HG3	2.16	0.46
1:B:1346:TYR:CE2	1:B:1368:THR:HG23	2.51	0.46
1:B:1165:HIS:CE1	1:B:1215:HIS:CE1	3.04	0.46
1:B:1105:GLU:OE1	1:B:1108:ARG:NH2	2.49	0.46
1:A:670:PHE:CD2	1:A:714:LEU:HD11	2.51	0.45
1:B:1309:VAL:HG12	1:B:1368:THR:HB	1.98	0.45
1:B:925:TYR:HB3	4:B:1644:HOH:O	2.16	0.45
1:A:630:LEU:HD13	1:A:681:TYR:CG	2.52	0.45
1:A:945:MET:HE1	1:A:951:LEU:HD13	1.97	0.45
1:B:1365:ASN:OD1	1:B:1365:ASN:N	2.50	0.45
1:A:989:ASN:HD22	1:A:989:ASN:H	1.64	0.44
1:A:1227:ALA:HB1	1:A:1283:VAL:HG21	1.99	0.44
1:A:611:PRO:HA	1:A:614:THR:CG2	2.47	0.44
1:A:1079:ARG:HD3	1:A:1079:ARG:HA	1.85	0.44
1:A:562:VAL:HG22	1:A:585:HIS:HB2	1.99	0.44
1:A:697:ALA:HB3	1:A:700:VAL:HB	1.98	0.44
1:B:648:SER:HA	1:B:687:ASP:HB3	2.00	0.44
1:B:987:VAL:O	1:B:987:VAL:HG23	2.17	0.44
1:A:647:VAL:O	1:A:647:VAL:HG13	2.18	0.43
1:A:881:TYR:CE2	1:A:883:ASP:HB3	2.53	0.43
1:B:1193:ASP:O	1:B:1194:LYS:C	2.55	0.43
1:A:582:LYS:HA	1:A:921:TYR:CD1	2.53	0.43
1:A:966:LYS:HE2	1:A:1023:SER:O	2.18	0.43
1:A:1302:ALA:O	1:A:1373:ASP:HB2	2.19	0.43
1:B:1147:ALA:HB1	1:B:1196:ASN:HB3	2.00	0.43
1:A:1231:TYR:CE1	1:A:1235:VAL:HG21	2.53	0.43
1:B:817:SER:HB3	1:B:849:LEU:HD11	2.01	0.43
1:A:1349:TYR:HB2	1:A:1358:TYR:CE1	2.53	0.43
1:A:945:MET:HA	1:A:945:MET:HE2	2.01	0.43
1:B:767:ASP:CG	1:B:818:ARG:HH11	2.21	0.43
1:B:847:SER:HB3	1:B:911:SER:HA	2.01	0.42
1:B:646:LEU:HD23	1:B:646:LEU:H	1.83	0.42
1:A:1333:THR:HB	1:A:1400:GLN:HB3	2.01	0.42
1:A:583:PHE:CE1	1:A:586:LEU:HD12	2.55	0.42
1:B:589:ALA:HA	1:B:590:PHE:HA	1.82	0.42
1:B:1016:VAL:HB	1:B:1038:VAL:HG23	2.01	0.42
1:A:989:ASN:N	1:A:989:ASN:HD22	2.18	0.42
1:B:767:ASP:OD1	1:B:816:TYR:OH	2.38	0.42
1:A:1359:LEU:HB2	1:A:1370:ILE:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1305:ALA:O	1:B:1331:THR:HA	2.20	0.42
1:A:1298:VAL:HG11	1:A:1394:MET:HB2	2.01	0.41
1:B:728:THR:O	1:B:728:THR:HG22	2.20	0.41
1:B:670:PHE:O	1:B:673:SER:OG	2.36	0.41
1:B:767:ASP:OD2	2:B:1502:NAG:O6	2.35	0.41
1:A:1115:ASN:O	1:A:1119:LEU:HG	2.20	0.41
1:B:691:GLU:HA	1:B:692:TYR:CG	2.55	0.41
1:B:1318:LEU:HD22	1:B:1319:PHE:CD2	2.55	0.41
1:A:662:LEU:HA	1:A:710:ASN:ND2	2.36	0.41
1:A:661:ALA:O	1:A:710:ASN:HB3	2.21	0.41
1:A:870:PRO:HD2	1:A:881:TYR:O	2.21	0.41
1:A:731:LYS:NZ	1:B:1325:GLN:O	2.53	0.41
1:B:1065:VAL:HB	1:B:1122:LEU:HD11	2.02	0.41
1:A:1147:ALA:HB1	1:A:1196:ASN:HB3	2.02	0.41
1:B:652:TRP:O	1:B:653:GLU:HG2	2.21	0.41
1:A:1397:ASP:C	1:A:1397:ASP:OD1	2.59	0.40
1:A:691:GLU:HA	1:A:692:TYR:CD1	2.56	0.40
1:A:738:ALA:HA	1:A:762:ASN:HB2	2.03	0.40
1:B:1268:VAL:HG13	1:B:1355:LYS:HB2	2.04	0.40
1:A:1309:VAL:HG12	1:A:1368:THR:HG22	2.03	0.40
1:B:1063:TYR:CD2	1:B:1402:ILE:HG22	2.56	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	861/885 (97%)	805 (94%)	53 (6%)	3 (0%)	44	68
1	B	858/885 (97%)	763 (89%)	83 (10%)	12 (1%)	13	24
All	All	1719/1770 (97%)	1568 (91%)	136 (8%)	15 (1%)	20	38

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1180	VAL
1	B	595	ASN
1	B	614	THR
1	B	694	VAL
1	B	1023	SER
1	B	1148	LEU
1	B	1258	TRP
1	B	724	ALA
1	B	801	ASN
1	B	945	MET
1	B	806	ALA
1	A	1342	PHE
1	B	576	ARG
1	A	613	ILE
1	B	1312	PRO

### 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	710/730 (97%)	664 (94%)	46 (6%)	20	38
1	B	707/730 (97%)	654 (92%)	53 (8%)	16	30
All	All	1417/1460 (97%)	1318 (93%)	99 (7%)	18	34

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	565	ILE
1	A	573	LYS
1	A	574	ASP
1	A	575	GLU
1	A	576	ARG
1	A	599	VAL
1	A	602	LYS
1	A	613	ILE

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Mol	Chain	Res	Type
1	A	646	LEU
1	A	662	LEU
1	A	703	SER
1	A	704	ARG
1	A	706	GLU
1	A	743	LYS
1	A	752	THR
1	A	777	SER
1	A	818	ARG
1	A	902	PHE
1	A	906	GLU
1	A	922	SER
1	A	927	LYS
1	A	930	THR
1	A	945	MET
1	A	960	LEU
1	A	972	SER
1	A	977	SER
1	A	989	ASN
1	A	1025	VAL
1	A	1031	THR
1	A	1032	ASP
1	A	1083	ASN
1	A	1104	ARG
1	A	1145	ASP
1	A	1175	ASP
1	A	1180	VAL
1	A	1195	GLN
1	A	1217	LYS
1	A	1233	ASN
1	A	1265	GLN
1	A	1289	LYS
1	A	1318	LEU
1	A	1347	THR
1	A	1363	ASP
1	A	1371	THR
1	A	1379	LYS
1	A	1397	ASP
1	B	600	THR
1	B	608	THR
1	B	614	THR
1	B	615	GLU

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Mol	Chain	Res	Type
1	B	619	ILE
1	B	644	LYS
1	B	646	LEU
1	B	665	GLU
1	B	686	ILE
1	B	725	GLN
1	B	729	THR
1	B	757	TYR
1	B	779	HIS
1	B	896	GLN
1	B	902	PHE
1	B	903[A]	MET
1	B	903[B]	MET
1	B	906	GLU
1	B	913	SER
1	B	923	ARG
1	B	927	LYS
1	B	930	THR
1	B	943	VAL
1	B	949	THR
1	B	955	THR
1	B	984	THR
1	B	986	THR
1	B	1002	ASN
1	B	1009	ASN
1	B	1023	SER
1	B	1031	THR
1	B	1038	VAL
1	B	1048	LEU
1	B	1083	ASN
1	B	1120	LYS
1	B	1124	GLN
1	B	1125	GLN
1	B	1143	PHE
1	B	1175	ASP
1	B	1186	VAL
1	B	1192	GLU
1	B	1195	GLN
1	B	1217	LYS
1	B	1261	LYS
1	B	1265	GLN
1	B	1268	VAL

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Mol	Chain	Res	Type
1	B	1289	LYS
1	B	1318	LEU
1	B	1344	LYS
1	B	1347	THR
1	B	1352	ASN
1	B	1365	ASN
1	B	1371	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	787	ASN
1	A	802	ASN
1	A	821	GLN
1	A	822	ASN
1	A	857	ASN
1	A	989	ASN
1	A	1009	ASN
1	A	1060	ASN
1	A	1124	GLN
1	A	1215	HIS
1	A	1265	GLN
1	A	1320	GLN
1	A	1325	GLN
1	A	1328	ASN
1	A	1335	ASN
1	A	1365	ASN
1	B	624	ASN
1	B	725	GLN
1	B	787	ASN
1	B	802	ASN
1	B	822	ASN
1	B	896	GLN
1	B	989	ASN
1	B	1009	ASN
1	B	1060	ASN
1	B	1083	ASN
1	B	1126	ASN
1	B	1215	HIS
1	B	1242	GLN
1	B	1265	GLN
1	B	1320	GLN

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Mol	Chain	Res	Type
1	B	1325	GLN
1	B	1328	ASN
1	B	1335	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 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	NAG	A	3001	2	14,14,15	0.87	0	15,19,21	1.70	3 (20%)
2	NAG	A	3002	2	15,15,15	0.74	0	21,21,21	2.74	5 (23%)
3	PO4	A	3003	-	4,4,4	1.45	0	6,6,6	1.09	0
2	NAG	B	1501	2	14,14,15	0.59	0	15,19,21	2.38	3 (20%)
2	NAG	B	1502	2	15,15,15	0.87	0	21,21,21	2.58	7 (33%)
3	PO4	B	1503	-	4,4,4	0.79	0	6,6,6	1.36	1 (16%)

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	NAG	A	3001	2	-	0/6/23/26	0/1/1/1
2	NAG	A	3002	2	-	0/6/26/26	0/1/1/1
3	PO4	A	3003	-	-	0/0/0/0	0/0/0/0
2	NAG	B	1501	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1502	2	-	0/6/26/26	0/1/1/1
3	PO4	B	1503	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	NAG	O4-C4-C3	-4.24	101.14	110.36
2	B	1502	NAG	O3-C3-C4	-3.39	102.98	110.36
2	B	1502	NAG	O7-C7-C8	-3.16	116.31	122.06
2	A	3002	NAG	O7-C7-C8	-2.65	117.24	122.06
2	A	3002	NAG	O1-C1-O5	-2.44	102.99	110.20
3	B	1503	PO4	O4-P-O3	-2.23	99.71	107.90
2	A	3001	NAG	O7-C7-N2	2.02	125.81	121.92
2	B	1502	NAG	C2-N2-C7	2.03	128.32	123.19
2	A	3002	NAG	O7-C7-N2	2.11	125.97	121.92
2	A	3001	NAG	O3-C3-C2	2.73	115.24	109.39
2	B	1501	NAG	C2-N2-C7	2.75	126.95	122.94
2	B	1502	NAG	C8-C7-N2	2.85	121.26	116.11
2	B	1501	NAG	C8-C7-N2	3.08	121.67	116.11
2	A	3002	NAG	C1-C2-C3	4.12	116.16	110.54
2	B	1502	NAG	C1-C2-C3	4.19	116.26	110.54
2	B	1502	NAG	O5-C1-C2	5.84	115.38	109.52
2	B	1502	NAG	C1-O5-C5	5.85	123.94	113.39
2	B	1501	NAG	C1-O5-C5	7.22	122.11	112.17
2	A	3002	NAG	O5-C1-C2	10.42	119.98	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1501	NAG	3	0
2	B	1502	NAG	3	0

## 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	860/885 (97%)	-0.13	21 (2%) 59 52	17, 40, 76, 104	0
1	B	859/885 (97%)	-0.03	23 (2%) 55 48	16, 41, 81, 109	0
All	All	1719/1770 (97%)	-0.08	44 (2%) 56 50	16, 41, 79, 109	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	929	GLY	7.8
1	B	1003	GLY	5.9
1	A	927	LYS	4.6
1	A	662	LEU	4.3
1	B	619	ILE	3.4
1	B	927	LYS	3.3
1	A	928	SER	3.3
1	B	803	GLY	3.2
1	B	663	THR	3.2
1	B	1005	THR	3.2
1	B	1002	ASN	3.1
1	A	660	ALA	2.9
1	A	931	PRO	2.9
1	A	929	GLY	2.9
1	B	705	PRO	2.9
1	B	928	SER	2.8
1	A	665	GLU	2.7
1	B	664	PRO	2.7
1	A	1360	TYR	2.7
1	A	558	GLN	2.7
1	B	662	LEU	2.6
1	A	1349	TYR	2.6
1	A	1342	PHE	2.5
1	A	1314	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	627	GLU	2.4
1	B	932	LEU	2.4
1	B	576	ARG	2.4
1	B	926	ALA	2.4
1	A	573	LYS	2.4
1	B	1313	ASN	2.3
1	A	1180	VAL	2.3
1	A	1363	ASP	2.2
1	A	930	THR	2.2
1	A	1192	GLU	2.2
1	B	704	ARG	2.2
1	A	1364	ALA	2.1
1	B	1059	THR	2.1
1	A	1148	LEU	2.0
1	A	1368	THR	2.0
1	B	665	GLU	2.0
1	A	1003	GLY	2.0
1	B	986	THR	2.0
1	B	609	GLU	2.0
1	B	622	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 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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	3002	15/15	0.96	0.18	1.54	33,35,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	3001	14/15	0.94	0.18	1.42	26,31,35,38	0
2	NAG	B	1502	15/15	0.95	0.20	0.72	33,37,52,62	0
3	PO4	B	1503	5/5	0.97	0.14	0.07	41,43,48,54	0
3	PO4	A	3003	5/5	0.99	0.13	-0.34	30,31,40,43	0
2	NAG	B	1501	14/15	0.96	0.14	-0.92	28,36,38,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.