



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:29 PM GMT

PDB ID : 3RDK
Title : Protein crystal structure of xylanase A1 of Paenibacillus sp. JDR-2
Authors : Pozharski, E.; St John, F.J.
Deposited on : 2011-04-01
Resolution : 1.49 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

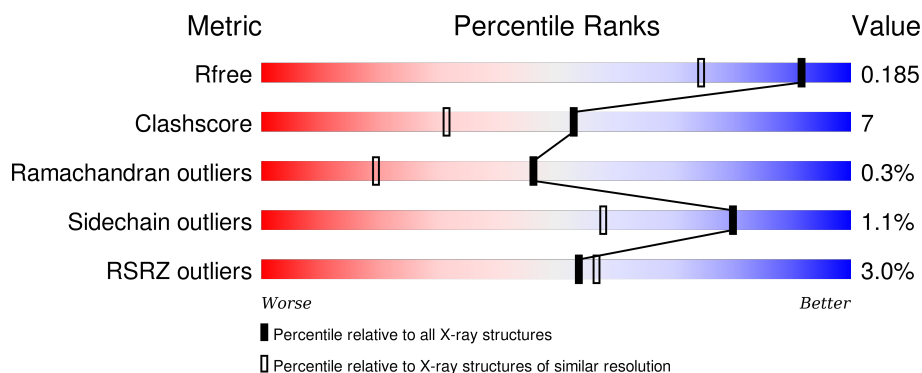
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


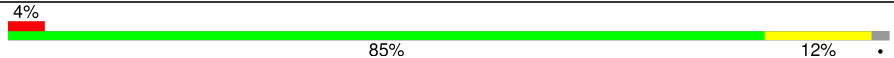
The reported resolution of this entry is 1.49 Å.

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}	91344	2072 (1.50-1.50)
Clashscore	102246	2274 (1.50-1.50)
Ramachandran outliers	100387	2218 (1.50-1.50)
Sidechain outliers	100360	2216 (1.50-1.50)
RSRZ outliers	91569	2075 (1.50-1.50)

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. 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	341	 2% 79% 16% . .
1	B	341	 4% 85% 12% .

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
2	GOL	A	347[A]	-	-	X	-
2	GOL	A	349	-	-	X	X
2	GOL	B	347[A]	-	-	X	-
2	GOL	B	347[B]	-	-	X	-
2	GOL	B	349	-	-	-	X
5	GCV	A	342	-	-	-	X
5	GCV	B	342	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6364 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 Endo-1,4-beta-xylanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	333	Total	C	N	O	S	0	14	0
			2735	1737	467	519	12			
1	B	334	Total	C	N	O	S	0	13	0
			2748	1736	470	529	13			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP C6CRV0
A	2	SER	-	EXPRESSION TAG	UNP C6CRV0
A	3	HIS	-	EXPRESSION TAG	UNP C6CRV0
A	4	MET	-	EXPRESSION TAG	UNP C6CRV0
A	339	ALA	-	EXPRESSION TAG	UNP C6CRV0
A	340	GLU	-	EXPRESSION TAG	UNP C6CRV0
A	341	GLN	-	EXPRESSION TAG	UNP C6CRV0
B	1	GLY	-	EXPRESSION TAG	UNP C6CRV0
B	2	SER	-	EXPRESSION TAG	UNP C6CRV0
B	3	HIS	-	EXPRESSION TAG	UNP C6CRV0
B	4	MET	-	EXPRESSION TAG	UNP C6CRV0
B	339	ALA	-	EXPRESSION TAG	UNP C6CRV0
B	340	GLU	-	EXPRESSION TAG	UNP C6CRV0
B	341	GLN	-	EXPRESSION TAG	UNP C6CRV0

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	1
			12	6	6		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	1
			12	6	6		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	1
			12	6	6		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Cl	0	0
			3	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total C O 41 22 19	0	0
5	B	4	Total C O 41 22 19	0	0

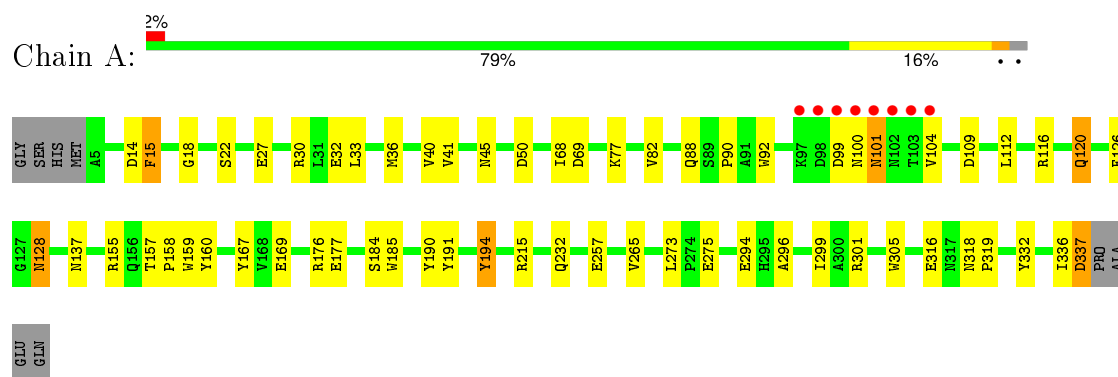
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	362	Total O 364 364	0	2
6	B	358	Total O 359 359	0	1

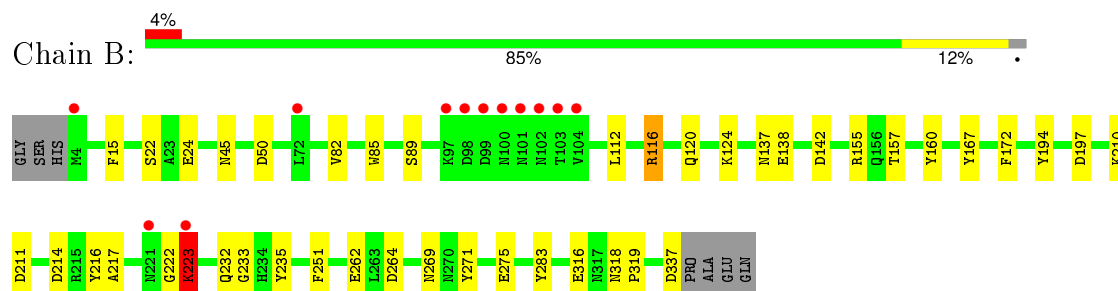
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Endo-1,4-beta-xylanase



• Molecule 1: Endo-1,4-beta-xylanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	165.11Å 165.11Å 66.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	117.04 – 1.49 42.36 – 1.49	Depositor EDS
% Data completeness (in resolution range)	99.7 (117.04-1.49) 99.7 (42.36-1.49)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.49Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.145 , 0.184 0.145 , 0.185	Depositor DCC
R_{free} test set	7447 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 148430 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6364	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: XYP, GOL, MG, XYS, CL, GCV

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	1.43	23/2831 (0.8%)	1.19	11/3845 (0.3%)
1	B	1.39	14/2829 (0.5%)	1.14	7/3845 (0.2%)
All	All	1.41	37/5660 (0.7%)	1.16	18/7690 (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	1

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	223	LYS	CE-NZ	7.43	1.67	1.49
1	A	177	GLU	CD-OE2	6.81	1.33	1.25
1	A	41	VAL	CB-CG2	-6.76	1.38	1.52
1	A	332	TYR	CD2-CE2	6.66	1.49	1.39
1	A	294	GLU	CG-CD	6.59	1.61	1.51
1	B	283	TYR	CD1-CE1	6.50	1.49	1.39
1	A	27	GLU	CB-CG	-6.39	1.40	1.52
1	A	294	GLU	CD-OE1	6.38	1.32	1.25
1	A	128	ASN	CB-CG	6.18	1.65	1.51
1	B	262	GLU	CD-OE1	6.07	1.32	1.25
1	A	169	GLU	CD-OE1	-5.94	1.19	1.25
1	A	32	GLU	CD-OE1	5.92	1.32	1.25
1	A	159	TRP	CG-CD1	5.88	1.45	1.36
1	A	15	PHE	CG-CD2	5.81	1.47	1.38
1	B	251	PHE	CE1-CZ	5.74	1.48	1.37
1	B	275	GLU	CB-CG	-5.68	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	167	TYR	CE2-CZ	5.68	1.46	1.38
1	A	265	VAL	CB-CG1	5.67	1.64	1.52
1	A	191	TYR	CD2-CE2	5.64	1.47	1.39
1	B	223	LYS	CB-CG	5.64	1.67	1.52
1	B	216	TYR	CD1-CE1	5.58	1.47	1.39
1	A	275	GLU	CB-CG	-5.48	1.41	1.52
1	B	269	ASN	CB-CG	-5.47	1.38	1.51
1	B	223	LYS	CD-CE	5.47	1.65	1.51
1	B	216	TYR	CE2-CZ	5.45	1.45	1.38
1	A	194	TYR	CE1-CZ	5.45	1.45	1.38
1	B	85	TRP	CG-CD1	5.35	1.44	1.36
1	A	77	LYS	CD-CE	5.27	1.64	1.51
1	B	271	TYR	CD1-CE1	5.27	1.47	1.39
1	A	194	TYR	CG-CD2	5.22	1.46	1.39
1	A	104	VAL	CB-CG1	5.22	1.63	1.52
1	B	275	GLU	CG-CD	5.20	1.59	1.51
1	A	120	GLN	CD-NE2	5.18	1.45	1.32
1	A	167	TYR	CG-CD1	5.17	1.45	1.39
1	A	316[A]	GLU	CG-CD	5.17	1.59	1.51
1	A	316[B]	GLU	CG-CD	5.17	1.59	1.51
1	A	257	GLU	CG-CD	5.11	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	30	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	B	197	ASP	CB-CG-OD1	7.27	124.85	118.30
1	B	116	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	112	LEU	CB-CG-CD1	6.59	122.21	111.00
1	A	176	ARG	NE-CZ-NH2	-6.55	117.03	120.30
1	A	301	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	B	264	ASP	CB-CG-OD2	6.43	124.08	118.30
1	A	273	LEU	CB-CG-CD2	-6.33	100.23	111.00
1	B	211	ASP	CB-CG-OD1	6.25	123.93	118.30
1	A	337	ASP	N-CA-CB	6.12	121.61	110.60
1	A	190	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	A	116[A]	ARG	NE-CZ-NH1	-5.59	117.51	120.30
1	A	116[B]	ARG	NE-CZ-NH1	-5.59	117.51	120.30
1	B	50	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	172	PHE	CB-CG-CD2	-5.32	117.08	120.80
1	A	69	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	69	ASP	CB-CG-OD2	-5.05	113.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	ASP	CB-CG-OD1	-5.03	113.77	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ILE	Peptide

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	2735	0	2681	35	0
1	B	2748	0	2654	27	0
2	A	42	0	53	19	0
2	B	30	0	38	15	0
3	A	3	0	0	0	1
4	A	1	0	0	0	0
5	A	41	0	32	1	0
5	B	41	0	32	1	0
6	A	364	0	0	10	0
6	B	359	0	0	16	1
All	All	6364	0	5490	74	2

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 7.

All (74) 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:223:LYS:NZ	1:B:223:LYS:CE	1.67	1.53
1:B:22:SER:HB2	2:B:347[B]:GOL:H12	1.19	1.12
1:A:22:SER:HB2	2:A:347[A]:GOL:H12	1.11	1.09
1:A:88:GLN:H	2:A:352[B]:GOL:H31	1.14	1.06
1:B:22:SER:HA	2:B:347[A]:GOL:H11	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:ASP:O	6:A:676[B]:HOH:O	1.86	0.93
1:A:22:SER:HB2	2:A:347[A]:GOL:C1	1.97	0.93
1:A:185:TRP:HE1	2:A:349:GOL:H12	1.34	0.92
2:A:347[A]:GOL:H11	6:A:708:HOH:O	1.74	0.88
1:B:22:SER:HB2	2:B:347[A]:GOL:H32	1.56	0.87
2:B:347[B]:GOL:H11	6:B:390:HOH:O	1.73	0.86
1:B:22:SER:HB2	2:B:347[B]:GOL:C1	2.08	0.80
1:A:82:VAL:HG21	1:A:137:ASN:HB2	1.66	0.77
1:A:88:GLN:N	2:A:352[B]:GOL:H31	1.97	0.76
1:A:22:SER:HB2	2:A:347[B]:GOL:H11	1.69	0.75
1:A:88:GLN:H	2:A:352[A]:GOL:H2	1.51	0.74
1:A:296:ALA:O	6:A:676[B]:HOH:O	2.06	0.72
1:A:185:TRP:NE1	2:A:349:GOL:H12	2.06	0.71
5:A:343:XYP:H4B	6:B:653:HOH:O	1.91	0.70
1:B:82:VAL:HG21	1:B:137:ASN:HB2	1.75	0.69
1:B:22:SER:CA	2:B:347[A]:GOL:H11	2.25	0.66
1:A:299:ILE:O	6:A:676[B]:HOH:O	2.14	0.65
2:B:347[B]:GOL:C1	6:B:390:HOH:O	2.39	0.65
1:B:22:SER:CB	2:B:347[A]:GOL:H32	2.30	0.62
1:B:210:LYS:HD2	6:B:447:HOH:O	2.01	0.60
2:A:347[B]:GOL:H31	6:A:708:HOH:O	2.01	0.60
1:A:68[B]:ILE:HD12	1:A:126:PHE:CE1	2.36	0.60
2:B:349:GOL:H11	6:B:683:HOH:O	2.03	0.59
1:A:45:ASN:HB2	2:A:347[A]:GOL:H31	1.84	0.58
1:B:120[B]:GLN:NE2	6:B:475:HOH:O	2.19	0.57
1:B:217:ALA:HB1	1:B:222:GLY:HA2	1.86	0.57
1:A:184:SER:OG	2:A:349:GOL:C3	2.54	0.56
1:A:337:ASP:HB3	6:A:593:HOH:O	2.05	0.56
1:B:155[A]:ARG:HD2	1:B:157:THR:CG2	2.37	0.55
1:A:109:ASP:HB2	2:A:353:GOL:H2	1.88	0.54
2:B:347[B]:GOL:C3	6:B:409:HOH:O	2.55	0.54
1:B:112[A]:LEU:HD21	6:B:663[A]:HOH:O	2.08	0.54
1:A:155[A]:ARG:HD2	1:A:157:THR:CG2	2.38	0.53
1:A:33[B]:LEU:HD23	1:A:36:MET:HE1	1.90	0.53
1:B:210:LYS:HE2	1:B:214:ASP:OD2	2.09	0.52
2:B:347[B]:GOL:H32	6:B:409:HOH:O	2.10	0.52
1:B:24[B]:GLU:OE2	6:B:359:HOH:O	2.19	0.50
1:A:184:SER:OG	2:A:349:GOL:H32	2.11	0.50
1:A:215:ARG:HG3	6:A:610:HOH:O	2.12	0.49
1:B:89:SER:H	2:B:349:GOL:H12	1.78	0.48
1:A:305:TRP:CD1	2:A:346:GOL:H12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33[B]:LEU:HD23	1:A:36:MET:CE	2.43	0.48
2:B:348:GOL:H32	6:B:713:HOH:O	2.14	0.48
1:B:116:ARG:HD2	6:B:663[A]:HOH:O	2.14	0.47
1:A:88:GLN:H	2:A:352[B]:GOL:C3	2.05	0.46
2:A:347[A]:GOL:H32	6:A:388:HOH:O	2.15	0.46
1:B:316:GLU:HG2	6:B:681:HOH:O	2.13	0.46
1:A:99:ASP:C	1:A:101:ASN:H	2.19	0.46
1:A:120:GLN:OE1	6:A:483:HOH:O	2.20	0.45
1:B:194:TYR:HB3	1:B:232:GLN:OE1	2.17	0.45
1:B:124:LYS:HE3	6:B:442:HOH:O	2.16	0.45
1:A:318:ASN:N	1:A:319:PRO:HD3	2.31	0.45
1:B:233:GLY:HA2	1:B:235:TYR:CZ	2.53	0.44
2:B:347[A]:GOL:H2	6:B:355:HOH:O	2.19	0.43
1:A:90:PRO:HB2	1:A:92:TRP:CD1	2.53	0.43
1:B:112[A]:LEU:CD2	6:B:663[A]:HOH:O	2.66	0.42
1:A:18:GLY:HA2	1:A:40:VAL:O	2.19	0.42
1:A:50:ASP:HA	1:A:90:PRO:HD3	2.02	0.42
1:B:318:ASN:N	1:B:319:PRO:HD3	2.35	0.42
1:A:194:TYR:HB3	1:A:232:GLN:OE1	2.19	0.42
2:A:349:GOL:H11	6:A:500:HOH:O	2.20	0.42
1:A:68[B]:ILE:HD12	1:A:126:PHE:CD1	2.56	0.41
1:B:155[B]:ARG:HG2	1:B:157:THR:HG23	2.02	0.41
1:A:185:TRP:HE1	2:A:349:GOL:C1	2.17	0.41
1:A:160:TYR:C	1:A:160:TYR:CD1	2.95	0.41
1:B:160:TYR:C	1:B:160:TYR:CD2	2.94	0.41
1:B:45:ASN:HB2	2:B:347[B]:GOL:H31	2.04	0.40
1:B:138:GLU:OE2	5:B:345:XYS:H1	2.22	0.40

All (2) 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)
3:A:351:CL:CL	3:A:351:CL:CL[7_555]	1.70	0.50
6:B:525:HOH:O	6:B:525:HOH:O[7_555]	2.09	0.11

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	345/341 (101%)	338 (98%)	5 (1%)	2 (1%)	30	8
1	B	345/341 (101%)	340 (99%)	5 (1%)	0	100	100
All	All	690/682 (101%)	678 (98%)	10 (1%)	2 (0%)	46	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASN
1	A	101	ASN

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	296/288 (103%)	293 (99%)	3 (1%)	82	62
1	B	296/288 (103%)	293 (99%)	3 (1%)	82	62
All	All	592/576 (103%)	586 (99%)	6 (1%)	80	62

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

Mol	Chain	Res	Type
1	A	15	PHE
1	A	128	ASN
1	A	158	PRO
1	B	15	PHE

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Mol	Chain	Res	Type
1	B	223	LYS
1	B	337	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	161	GLN

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 ⓘ

8 carbohydrates 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	$\# Z > 2$
5	GCV	A	342	5	11,14,14	1.31	2 (18%)	14,20,20	2.32	6 (42%)
5	XYP	A	343	5	9,9,10	3.17	5 (55%)	10,12,14	3.93	7 (70%)
5	XYP	A	344	5	9,9,10	1.49	1 (11%)	11,12,14	2.99	3 (27%)
5	XYS	A	345	5	9,9,10	2.39	3 (33%)	11,12,14	3.75	5 (45%)
5	GCV	B	342	5	11,14,14	1.79	3 (27%)	14,20,20	1.07	1 (7%)
5	XYP	B	343	5	9,9,10	1.92	3 (33%)	10,12,14	1.89	4 (40%)
5	XYP	B	344	5	9,9,10	1.62	3 (33%)	11,12,14	3.18	4 (36%)
5	XYS	B	345	5	9,9,10	2.06	3 (33%)	11,12,14	4.78	4 (36%)

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
5	GCV	A	342	5	-	0/2/26/26	0/1/1/1
5	XYP	A	343	5	-	0/0/13/17	0/1/1/1
5	XYP	A	344	5	-	0/0/14/17	0/1/1/1
5	XYS	A	345	5	-	0/0/14/17	0/1/1/1
5	GCV	B	342	5	-	0/2/26/26	0/1/1/1
5	XYP	B	343	5	-	0/0/13/17	0/1/1/1
5	XYP	B	344	5	-	0/0/14/17	0/1/1/1
5	XYS	B	345	5	-	0/0/14/17	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	342	GCV	O5-C5	-3.63	1.39	1.43
5	A	343	XYP	C2B-C3B	-3.61	1.46	1.52
5	B	343	XYP	O5B-C1B	-2.57	1.36	1.41
5	B	344	XYP	C4B-C3B	-2.25	1.48	1.52
5	B	342	GCV	C1-C2	2.04	1.56	1.52
5	A	345	XYS	C4-C3	2.23	1.55	1.52
5	B	343	XYP	O4A-C1B	2.24	1.44	1.39
5	A	345	XYS	O5-C5	2.29	1.49	1.44
5	A	342	GCV	O5-C1	2.41	1.47	1.43
5	A	343	XYP	O3B-C3B	2.44	1.48	1.43
5	B	344	XYP	C3B-C2B	2.51	1.56	1.52
5	B	344	XYP	O5B-C5B	2.59	1.50	1.44
5	B	345	XYS	C1-C2	2.65	1.58	1.52
5	A	342	GCV	O4-C7	2.89	1.53	1.42
5	B	342	GCV	O1-C1	3.01	1.50	1.39
5	B	345	XYS	C4-C3	3.25	1.56	1.52
5	A	344	XYP	C4B-C3B	3.56	1.57	1.52
5	A	343	XYP	O5B-C5B	3.72	1.50	1.43
5	B	343	XYP	C2B-C1B	3.86	1.59	1.51
5	B	345	XYS	O5-C1	3.89	1.48	1.43
5	A	343	XYP	O4A-C1B	3.95	1.48	1.39
5	A	343	XYP	C4B-C3B	5.90	1.60	1.52
5	A	345	XYS	O5-C1	6.35	1.52	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	345	XYS	C4-C3-C2	-11.60	98.55	111.39
5	B	345	XYS	O5-C5-C4	-8.79	96.99	110.76
5	A	345	XYS	O5-C5-C4	-8.21	97.89	110.76
5	A	345	XYS	C4-C3-C2	-7.44	103.16	111.39
5	A	343	XYP	O5B-C5B-C4B	-7.37	98.91	110.86
5	A	344	XYP	C4B-C3B-C2B	-6.96	103.68	111.39
5	A	344	XYP	O5B-C5B-C4B	-6.20	101.04	110.76
5	B	344	XYP	O5B-C5B-C4B	-6.16	101.11	110.76
5	A	342	GCV	C1-C2-C3	-5.97	101.55	110.43
5	A	343	XYP	C1B-C2B-C3B	-5.34	102.07	111.23
5	B	344	XYP	C4B-C3B-C2B	-5.24	105.59	111.39
5	A	343	XYP	C5B-O5B-C1B	-4.41	105.72	113.36
5	A	343	XYP	O4B-C4B-C5B	-3.96	101.26	109.21
5	B	343	XYP	C5B-O5B-C1B	-3.10	107.99	113.36
5	A	342	GCV	C7-O4-C4	-3.06	105.95	114.59
5	A	342	GCV	C2-C3-C4	-2.98	103.06	109.60
5	B	343	XYP	C1B-C2B-C3B	-2.92	106.22	111.23
5	A	343	XYP	O4A-C1B-O5B	-2.72	97.25	107.95
5	A	343	XYP	O3B-C3B-C2B	-2.63	103.63	110.06
5	B	345	XYS	O3-C3-C4	-2.51	104.24	109.93
5	B	343	XYP	O4A-C1B-O5B	-2.39	98.55	107.95
5	B	343	XYP	O3B-C3B-C2B	-2.38	104.22	110.06
5	A	345	XYS	O3-C3-C4	-2.38	104.54	109.93
5	B	342	GCV	O2-C2-C3	-2.22	105.35	110.34
5	A	342	GCV	O1-C1-O5	-2.09	104.52	110.25
5	A	344	XYP	O2B-C2B-C3B	-2.07	106.26	110.00
5	B	344	XYP	C1B-C2B-C3B	-2.05	107.38	110.43
5	A	342	GCV	O3-C3-C2	2.06	114.97	110.34
5	A	342	GCV	O1-C1-C2	2.11	114.87	109.21
5	A	345	XYS	C1-C2-C3	2.15	113.62	110.43
5	A	343	XYP	O4B-C4B-C3B	3.79	118.77	110.27
5	A	345	XYS	O1-C1-C2	3.94	119.76	109.21
5	B	345	XYS	C1-C2-C3	5.00	117.86	110.43
5	B	344	XYP	C5B-C4B-C3B	5.62	117.97	110.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	343	XYP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	345	XYS	1	0

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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
2	GOL	A	346	-	5,5,5	1.08	0	5,5,5	0.68	0
2	GOL	A	347[A]	4	5,5,5	1.58	2 (40%)	5,5,5	1.83	1 (20%)
2	GOL	A	347[B]	4	5,5,5	1.53	1 (20%)	5,5,5	1.75	1 (20%)
2	GOL	A	349	-	5,5,5	0.68	0	5,5,5	1.28	1 (20%)
2	GOL	A	352[A]	-	5,5,5	0.56	0	5,5,5	0.44	0
2	GOL	A	352[B]	-	5,5,5	0.55	0	5,5,5	0.54	0
2	GOL	A	353	-	5,5,5	1.11	0	5,5,5	0.51	0
2	GOL	B	346	-	5,5,5	0.98	0	5,5,5	0.64	0
2	GOL	B	347[A]	-	5,5,5	1.63	1 (20%)	5,5,5	1.88	2 (40%)
2	GOL	B	347[B]	-	5,5,5	2.30	1 (20%)	5,5,5	1.38	1 (20%)
2	GOL	B	348	-	5,5,5	0.80	0	5,5,5	0.92	0
2	GOL	B	349	-	5,5,5	1.00	0	5,5,5	1.71	1 (20%)

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	GOL	A	346	-	-	0/4/4/4	0/0/0/0
2	GOL	A	347[A]	4	-	0/4/4/4	0/0/0/0
2	GOL	A	347[B]	4	-	0/4/4/4	0/0/0/0
2	GOL	A	349	-	-	0/4/4/4	0/0/0/0
2	GOL	A	352[A]	-	-	0/4/4/4	0/0/0/0
2	GOL	A	352[B]	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	353	-	-	0/4/4/4	0/0/0/0
2	GOL	B	346	-	-	0/4/4/4	0/0/0/0
2	GOL	B	347[A]	-	-	0/4/4/4	0/0/0/0
2	GOL	B	347[B]	-	-	0/4/4/4	0/0/0/0
2	GOL	B	348	-	-	0/4/4/4	0/0/0/0
2	GOL	B	349	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	347[B]	GOL	O2-C2	-4.67	1.29	1.43
2	B	347[A]	GOL	O2-C2	-3.01	1.34	1.43
2	A	347[B]	GOL	O2-C2	-2.94	1.34	1.43
2	A	347[A]	GOL	O2-C2	-2.28	1.36	1.43
2	A	347[A]	GOL	O1-C1	2.53	1.53	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	349	GOL	O3-C3-C2	-2.95	95.86	110.18
2	B	347[B]	GOL	O3-C3-C2	-2.85	96.37	110.18
2	A	347[B]	GOL	O2-C2-C1	-2.71	96.24	108.65
2	B	347[A]	GOL	O3-C3-C2	-2.06	100.18	110.18
2	A	349	GOL	O2-C2-C1	2.05	118.04	108.65
2	B	347[A]	GOL	O1-C1-C2	2.59	122.77	110.18
2	A	347[A]	GOL	O2-C2-C3	3.14	123.07	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	346	GOL	1	0
2	A	347[A]	GOL	5	0
2	A	347[B]	GOL	2	0
2	A	349	GOL	6	0
2	A	352[A]	GOL	1	0
2	A	352[B]	GOL	3	0
2	A	353	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	347[A]	GOL	5	0
2	B	347[B]	GOL	7	0
2	B	348	GOL	1	0
2	B	349	GOL	2	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	333/341 (97%)	-0.41	8 (2%) 62 66	19, 27, 39, 77	0
1	B	334/341 (97%)	-0.19	12 (3%) 46 49	21, 28, 40, 72	1 (0%)
All	All	667/682 (97%)	-0.30	20 (2%) 54 57	19, 28, 40, 77	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	100	ASN	6.7
1	A	99	ASP	5.9
1	B	99	ASP	5.5
1	B	4	MET	5.1
1	B	100	ASN	4.8
1	A	102	ASN	4.5
1	B	102	ASN	4.3
1	B	101	ASN	3.8
1	B	98	ASP	3.2
1	B	103	THR	3.0
1	A	101	ASN	2.9
1	A	98	ASP	2.8
1	B	104	VAL	2.8
1	A	103	THR	2.5
1	B	72	LEU	2.4
1	A	104	VAL	2.3
1	B	97	LYS	2.1
1	B	223	LYS	2.1
1	B	221	ASN	2.0
1	A	97	LYS	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](#)

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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	GCV	A	342	14/14	0.92	0.11	3.04	35,44,51,53	0
5	GCV	B	342	14/14	0.94	0.10	2.28	35,45,59,60	0
5	XYS	B	345	9/10	0.99	0.10	0.64	21,22,24,25	0
5	XYS	A	345	9/10	0.98	0.09	0.39	20,22,24,26	0
5	XYP	A	344	9/10	0.99	0.08	-0.71	19,21,23,24	0
5	XYP	B	344	9/10	0.99	0.07	-1.18	20,22,24,24	0
5	XYP	A	343	9/10	0.97	0.09	-	22,31,44,45	0
5	XYP	B	343	9/10	0.97	0.09	-	24,31,40,42	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	GOL	A	349	6/6	0.84	0.26	40.72	38,46,47,53	0
2	GOL	B	349	6/6	0.88	0.21	7.79	39,55,61,61	0
2	GOL	B	348	6/6	0.93	0.11	1.20	44,55,60,62	0
2	GOL	B	347[B]	6/6	0.97	0.14	1.15	22,25,29,33	6
2	GOL	B	347[A]	6/6	0.97	0.14	0.82	26,29,32,33	6
2	GOL	A	347[A]	6/6	0.98	0.10	0.28	19,23,25,27	6
2	GOL	B	346	6/6	0.99	0.10	0.28	23,26,28,30	0
2	GOL	A	347[B]	6/6	0.98	0.10	0.10	25,28,33,37	6
2	GOL	A	346	6/6	0.98	0.06	-0.82	22,24,26,26	0
3	CL	A	348	1/1	1.00	0.03	-1.98	37,37,37,37	0
4	MG	A	354	1/1	0.99	0.06	-2.42	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CL	A	351	1/1	0.99	0.05	-	67,67,67,67	0
2	GOL	A	353	6/6	0.73	0.26	-	61,65,66,68	0
2	GOL	A	352[B]	6/6	0.92	0.17	-	26,38,40,41	6
3	CL	A	350	1/1	0.96	0.13	-	72,72,72,72	0
2	GOL	A	352[A]	6/6	0.92	0.17	-	32,36,42,42	6

6.5 Other polymers [i](#)

There are no such residues in this entry.