



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:50 AM GMT

PDB ID : 2YJQ
Title : Structure of a Paenibacillus Polymyxa Xyloglucanase from Glycoside Hydrolase Family 44
Authors : Ariza, A.; Eklof, J.M.; Spadiut, O.; Offen, W.A.; Roberts, S.M.; Besenmatter, W.; Friis, E.P.; Skjot, M.; Wilson, K.S.; Brumer, H.; Davies, G.
Deposited on : 2011-05-23
Resolution : 2.25 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

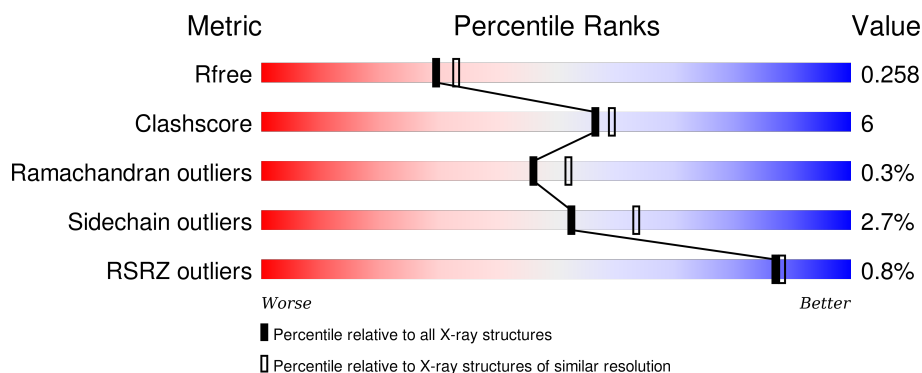
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	524	<div> <div></div> <div>85%</div> <div>12%</div> <div>.</div> </div>
1	B	524	<div> <div></div> <div>79%</div> <div>16%</div> <div>..</div> </div>

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
5	EDO	A	1525	-	-	-	X
7	SO4	B	1528[A]	-	-	-	X
8	PGE	A	1529[A]	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 8563 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 CEL44C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	5	0
			4022	2548	676	783	15			
1	B	506	Total	C	N	O	S	0	2	0
			3967	2512	666	775	14			

There are 30 discrepancies between the modelled and reference sequences:

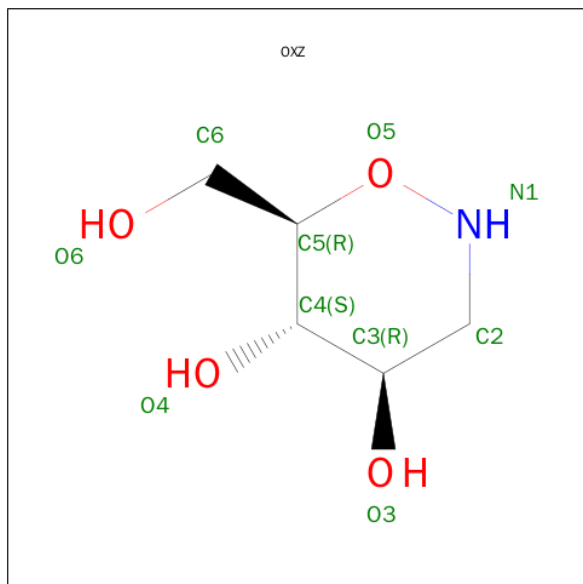
Chain	Residue	Modelled	Actual	Comment	Reference
A	17	PHE	SER	CONFLICT	UNP Q1A2D0
A	19	ASP	GLU	CONFLICT	UNP Q1A2D0
A	68	HIS	GLN	ENGINEERED MUTATION	UNP Q1A2D0
A	92	VAL	THR	ENGINEERED MUTATION	UNP Q1A2D0
A	118	ALA	LYS	ENGINEERED MUTATION	UNP Q1A2D0
A	129	ALA	LYS	ENGINEERED MUTATION	UNP Q1A2D0
A	144	ALA	THR	CONFLICT	UNP Q1A2D0
A	156	TYR	ARG	ENGINEERED MUTATION	UNP Q1A2D0
A	200	PRO	GLY	ENGINEERED MUTATION	UNP Q1A2D0
A	228	VAL	ILE	CONFLICT	UNP Q1A2D0
A	272	VAL	ALA	CONFLICT	UNP Q1A2D0
A	331	PHE	ASN	ENGINEERED MUTATION	UNP Q1A2D0
A	358	SER	GLU	ENGINEERED MUTATION	UNP Q1A2D0
A	403	ALA	PRO	CONFLICT	UNP Q1A2D0
A	473	ILE	SER	CONFLICT	UNP Q1A2D0
B	17	PHE	SER	CONFLICT	UNP Q1A2D0
B	19	ASP	GLU	CONFLICT	UNP Q1A2D0
B	68	HIS	GLN	ENGINEERED MUTATION	UNP Q1A2D0
B	92	VAL	THR	ENGINEERED MUTATION	UNP Q1A2D0
B	118	ALA	LYS	ENGINEERED MUTATION	UNP Q1A2D0
B	129	ALA	LYS	ENGINEERED MUTATION	UNP Q1A2D0
B	144	ALA	THR	CONFLICT	UNP Q1A2D0
B	156	TYR	ARG	ENGINEERED MUTATION	UNP Q1A2D0
B	200	PRO	GLY	ENGINEERED MUTATION	UNP Q1A2D0
B	228	VAL	ILE	CONFLICT	UNP Q1A2D0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	272	VAL	ALA	CONFLICT	UNP Q1A2D0
B	331	PHE	ASN	ENGINEERED MUTATION	UNP Q1A2D0
B	358	SER	GLU	ENGINEERED MUTATION	UNP Q1A2D0
B	403	ALA	PRO	CONFLICT	UNP Q1A2D0
B	473	ILE	SER	CONFLICT	UNP Q1A2D0

- Molecule 2 is TETRAHYDROOXAZINE (three-letter code: OXZ) (formula: $C_5H_{11}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total	C	O	0	0
			22	12	10		
3	B	2	Total	C	O	0	0
			22	12	10		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

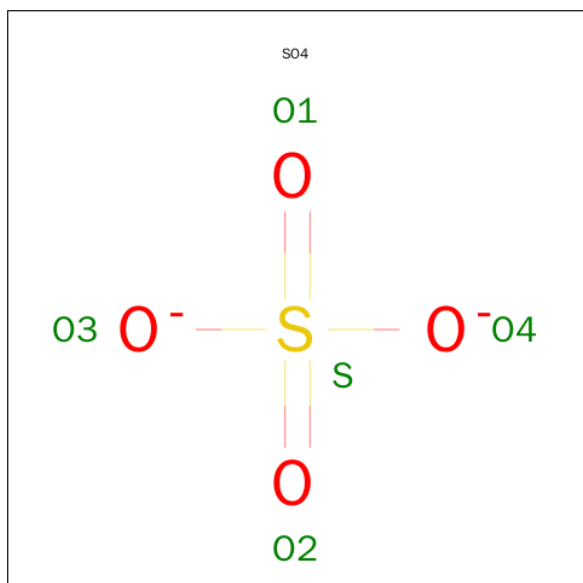


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	1
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

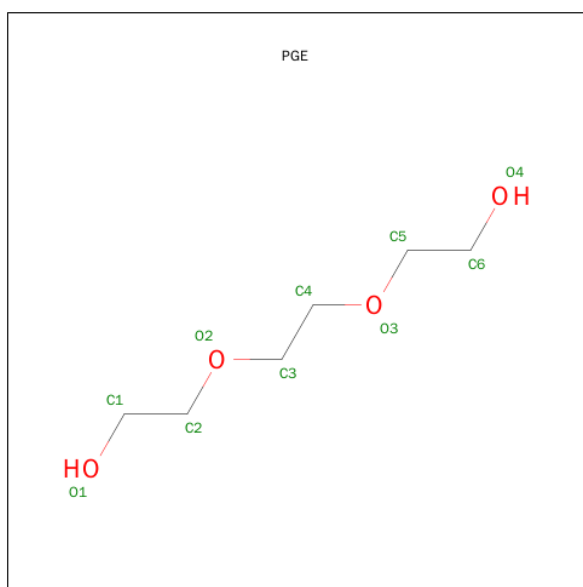
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Cl	0	0
			1	1		
6	A	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	1
			5	4	1		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	1
			10	6	4		

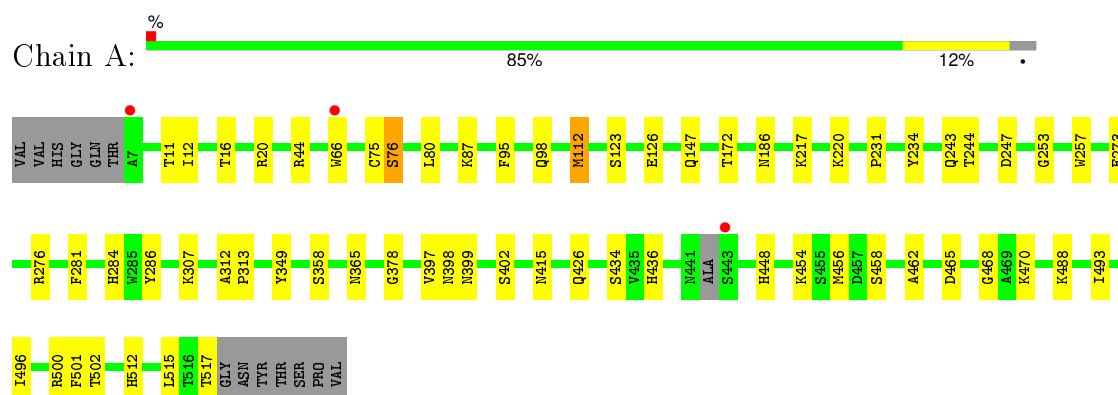
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	258	Total	O	0	4
			262	262		
9	B	181	Total	O	0	3
			184	184		

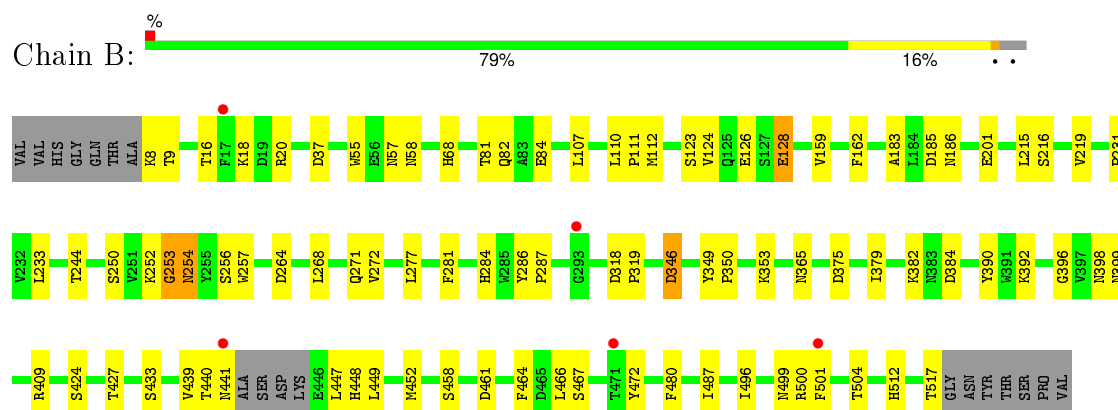
3 Residue-property plots [i](#)

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: CEL44C



• Molecule 1: CEL44C



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	84.20 Å 84.20 Å 320.05 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	106.68 – 2.25 66.36 – 2.25	Depositor EDS
% Data completeness (in resolution range)	98.2 (106.68-2.25) 93.2 (66.36-2.25)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.25 Å)	Xtriage
Refinement program	REFMAC 5.6.0086	Depositor
R, R_{free}	0.197 , 0.259 0.195 , 0.258	Depositor DCC
R_{free} test set	3026 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.4	EDS
Estimated twinning fraction	0.047 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 59601 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8563	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 50.54 % 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 6.3737e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, OXZ, CL, CA, EDO, BGC, SO4

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	0/4135	0.90	3/5618 (0.1%)
1	B	0.93	1/4072 (0.0%)	0.86	5/5534 (0.1%)
All	All	0.97	1/8207 (0.0%)	0.88	8/11152 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	128	GLU	CG-CD	5.81	1.60	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	37	ASP	CB-CG-OD1	6.70	124.33	118.30
1	A	20	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	B	264	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	112	MET	CG-SD-CE	5.81	109.50	100.20
1	B	409	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	247	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	264	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	346	ASP	CB-CG-OD1	5.06	122.85	118.30

There are no chirality outliers.

There are no planarity outliers.

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	4022	0	3864	43	0
1	B	3967	0	3806	56	0
2	A	10	0	10	1	0
2	B	10	0	10	0	0
3	A	22	0	19	0	0
3	B	22	0	19	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	20	0	30	5	0
5	B	20	0	30	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
8	A	10	0	14	3	0
9	A	262	0	0	3	0
9	B	184	0	0	10	0
All	All	8563	0	7802	96	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 6.

All (96) 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)
5:B:1529[B]:EDO:H12	9:B:2161:HOH:O	1.58	1.03
1:B:126[A]:GLU:CG	9:B:2073:HOH:O	2.15	0.93
1:B:396:GLY:H	5:B:1529[B]:EDO:H11	1.34	0.89
1:B:126[A]:GLU:OE2	9:B:2073:HOH:O	1.99	0.80
1:A:448:HIS:HD2	1:A:512:HIS:NE2	1.80	0.79
1:A:243:GLN:HE22	8:A:1529[A]:PGE:H22	1.48	0.79
1:A:415:ASN:HD21	1:B:82:GLN:HE22	1.29	0.78
1:A:243:GLN:HE22	8:A:1529[A]:PGE:C2	1.99	0.75
1:A:126[B]:GLU:OE2	9:A:2090:HOH:O	2.04	0.75
1:B:440:THR:HG22	1:B:441:ASN:H	1.52	0.73
1:B:126[A]:GLU:HG2	9:B:2073:HOH:O	1.83	0.72
1:B:254:ASN:H	1:B:254:ASN:ND2	1.93	0.66
1:A:488:LYS:NZ	1:B:123:SER:HB3	2.12	0.65
1:A:402:SER:HB2	5:A:1525:EDO:H22	1.79	0.64
1:B:448:HIS:HD2	1:B:512:HIS:NE2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:TYR:HA	1:B:517:THR:HG22	1.80	0.64
1:A:147:GLN:HA	5:A:1526:EDO:H11	1.82	0.62
1:A:273[B]:GLU:HG2	9:A:2165:HOH:O	2.00	0.61
5:B:1529[B]:EDO:C1	9:B:2161:HOH:O	2.31	0.61
1:B:231:PRO:HG2	1:B:233:LEU:HG	1.82	0.61
1:A:365:ASN:ND2	1:A:399:ASN:H	1.99	0.60
1:A:448:HIS:CD2	1:A:512:HIS:NE2	2.68	0.60
1:B:112:MET:HB2	1:B:185:ASP:HB2	1.84	0.60
1:B:353:LYS:HE2	9:B:2151:HOH:O	2.01	0.59
1:B:365:ASN:ND2	1:B:399:ASN:H	1.99	0.59
1:B:254:ASN:HD22	1:B:254:ASN:H	1.47	0.59
1:A:415:ASN:HD21	1:B:82:GLN:NE2	1.99	0.58
1:A:307:LYS:HE3	1:A:456:MET:HG3	1.84	0.58
1:B:439:VAL:HG23	1:B:440:THR:O	2.03	0.58
1:A:66[C]:TRP:CE3	1:A:66[C]:TRP:HA	2.39	0.56
1:A:16:THR:OG1	1:A:468:GLY:HA3	2.06	0.55
1:A:397:VAL:HB	5:A:1525:EDO:H12	1.88	0.55
1:A:234:TYR:OH	8:A:1529[A]:PGE:H42	2.07	0.55
1:B:346:ASP:HB2	9:B:2145:HOH:O	2.09	0.52
1:B:382:LYS:HE2	9:B:2159:HOH:O	2.10	0.51
1:B:286:TYR:O	1:B:287:PRO:C	2.49	0.51
1:A:76:SER:HB2	5:A:1522:EDO:H21	1.92	0.51
1:B:124:VAL:HG13	1:B:128:GLU:HB2	1.92	0.51
1:B:375:ASP:O	1:B:379:ILE:HG13	2.11	0.51
1:B:231:PRO:HG2	1:B:233:LEU:CG	2.41	0.50
1:A:365:ASN:HD22	1:A:399:ASN:HB2	1.77	0.49
1:B:55:TRP:CE2	1:B:162:PHE:HB2	2.48	0.49
1:B:392:LYS:HG2	1:B:398:ASN:ND2	2.28	0.49
1:A:470:LYS:HD3	1:A:517:THR:HG21	1.94	0.48
1:B:440:THR:HG22	1:B:441:ASN:N	2.24	0.48
1:B:81:THR:OG1	1:B:84:GLU:HG3	2.13	0.48
1:A:415:ASN:ND2	1:B:82:GLN:HE22	2.06	0.48
1:A:286:TYR:OH	2:A:1518:OXZ:N1	2.47	0.48
1:B:448:HIS:CD2	1:B:512:HIS:NE2	2.80	0.48
1:A:434:SER:OG	1:A:454:LYS:HE2	2.14	0.47
1:A:488:LYS:HZ1	1:B:123:SER:HB3	1.78	0.47
1:A:87:LYS:HB2	1:A:87:LYS:HE3	1.72	0.47
1:A:66[C]:TRP:HE3	1:A:66[C]:TRP:HA	1.80	0.47
1:A:365:ASN:HD21	1:A:399:ASN:H	1.61	0.47
1:B:186:ASN:HD21	1:B:284:HIS:HE1	1.63	0.47
1:B:159:VAL:HG11	1:B:215:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:THR:O	1:B:20:ARG:NH1	2.44	0.46
1:A:95:PHE:HA	1:A:98:GLN:OE1	2.14	0.46
1:A:496:ILE:HD11	1:A:515:LEU:HD22	1.97	0.46
1:B:353:LYS:CE	9:B:2151:HOH:O	2.61	0.46
1:B:346:ASP:HA	1:B:350:PRO:HA	1.98	0.46
1:A:172:THR:HB	9:A:2121:HOH:O	2.16	0.46
1:B:18:LYS:HG2	1:B:424:SER:HB2	1.98	0.45
1:A:462:ALA:O	1:A:502:THR:HA	2.17	0.45
1:A:217:LYS:HE2	1:A:273[B]:GLU:HG3	1.98	0.45
1:A:312:ALA:N	1:A:313:PRO:CD	2.80	0.45
1:B:107:LEU:HD11	1:B:183:ALA:HB2	1.99	0.44
1:B:472:TYR:O	1:B:496:ILE:HB	2.18	0.43
1:B:215:LEU:O	1:B:219:VAL:HG23	2.18	0.43
1:B:480:PHE:HD2	1:B:487:ILE:CD1	2.31	0.43
1:B:447:LEU:HD21	1:B:449:LEU:HD21	1.99	0.43
1:B:464:PHE:O	1:B:500:ARG:HA	2.19	0.43
1:B:110:LEU:HB3	1:B:111:PRO:HD2	2.01	0.43
1:B:466:LEU:HB2	1:B:499:ASN:HB3	2.01	0.42
1:A:231:PRO:HD3	1:A:281:PHE:CE1	2.54	0.42
1:B:244:THR:O	1:B:244:THR:HG22	2.19	0.42
1:B:68:HIS:HD2	9:B:2102:HOH:O	2.01	0.42
1:A:75:CYS:O	1:A:80:LEU:HB2	2.19	0.42
1:B:268:LEU:O	1:B:271:GLN:HB3	2.20	0.42
1:A:465:ASP:OD1	1:A:500:ARG:CZ	2.68	0.42
1:A:12:ILE:HA	1:A:426:GLN:O	2.20	0.42
1:A:378:GLY:HA3	1:A:436:HIS:CG	2.55	0.41
1:A:284:HIS:CG	1:A:358:SER:HB3	2.55	0.41
1:A:493:ILE:HD13	1:A:501:PHE:CE2	2.55	0.41
1:B:464:PHE:CG	1:B:501:PHE:CE1	3.09	0.41
1:B:318:ASP:HA	1:B:319:PRO:HD2	1.85	0.41
1:A:220:LYS:HE3	1:A:276:ARG:O	2.20	0.41
1:B:216:SER:OG	1:B:277:LEU:HB3	2.19	0.41
1:B:464:PHE:CD1	1:B:501:PHE:CE1	3.09	0.41
1:B:252:LYS:O	1:B:253:GLY:C	2.59	0.41
1:B:390:TYR:OH	1:B:398:ASN:ND2	2.54	0.40
1:B:231:PRO:HD3	1:B:281:PHE:CE1	2.56	0.40
1:B:268:LEU:O	1:B:272:VAL:HG23	2.22	0.40
1:A:398:ASN:H	5:A:1525:EDO:H21	1.87	0.40
1:B:57:ASN:O	1:B:58:ASN:HB2	2.21	0.40
1:A:44:ARG:HH22	1:A:186:ASN:HD22	1.68	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	511/524 (98%)	489 (96%)	21 (4%)	1 (0%)	52	61
1	B	504/524 (96%)	476 (94%)	26 (5%)	2 (0%)	39	43
All	All	1015/1048 (97%)	965 (95%)	47 (5%)	3 (0%)	46	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	253	GLY
1	B	250	SER
1	A	253	GLY

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	431/437 (99%)	423 (98%)	8 (2%)	65	75
1	B	425/437 (97%)	409 (96%)	16 (4%)	40	49
All	All	856/874 (98%)	832 (97%)	24 (3%)	52	62

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	THR
1	A	76	SER
1	A	112	MET

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Mol	Chain	Res	Type
1	A	123	SER
1	A	244	THR
1	A	257	TRP
1	A	349	TYR
1	A	458	SER
1	B	8	LYS
1	B	9	THR
1	B	201[A]	GLU
1	B	201[B]	GLU
1	B	254	ASN
1	B	256	SER
1	B	257	TRP
1	B	349	TYR
1	B	384	ASP
1	B	427	THR
1	B	433	SER
1	B	452	MET
1	B	458	SER
1	B	461	ASP
1	B	467	SER
1	B	504	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	68	HIS
1	A	136	ASN
1	A	186	ASN
1	A	243	GLN
1	A	298	ASN
1	A	343	GLN
1	A	365	ASN
1	A	389	ASN
1	A	448	HIS
1	A	486	GLN
1	B	68	HIS
1	B	82	GLN
1	B	121	ASN
1	B	137	GLN
1	B	186	ASN
1	B	254	ASN

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Mol	Chain	Res	Type
1	B	265	GLN
1	B	298	ASN
1	B	365	ASN
1	B	389	ASN
1	B	398	ASN
1	B	399	ASN
1	B	441	ASN
1	B	448	HIS
1	B	486	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 ⓘ

4 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	$\# Z > 2$
3	BGC	A	1519	3,2	11,11,12	0.74	1 (9%)	14,15,17	1.70	6 (42%)
3	BGC	A	1520	3	11,11,12	0.68	0	14,15,17	1.87	3 (21%)
3	BGC	B	1519	3,2	11,11,12	0.81	0	14,15,17	1.80	3 (21%)
3	BGC	B	1520	3	11,11,12	0.74	0	14,15,17	0.95	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGC	A	1519	3,2	-	0/2/19/22	0/1/1/1
3	BGC	A	1520	3	-	0/2/19/22	0/1/1/1
3	BGC	B	1519	3,2	-	0/2/19/22	0/1/1/1
3	BGC	B	1520	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1519	BGC	O4-C4	-2.12	1.37	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1519	BGC	C1-C2-C3	-3.92	104.90	109.54
3	A	1520	BGC	O5-C1-C2	-3.26	105.56	110.86
3	A	1519	BGC	O3-C3-C4	-2.75	104.14	110.34
3	A	1519	BGC	O4-C4-C5	-2.39	102.90	109.24
3	A	1519	BGC	O5-C1-C2	-2.37	107.02	110.86
3	A	1519	BGC	O6-C6-C5	-2.17	104.18	111.33
3	A	1520	BGC	C6-C5-C4	-2.16	107.69	113.02
3	A	1519	BGC	O3-C3-C2	-2.15	106.11	110.00
3	B	1519	BGC	C2-C3-C4	2.04	114.51	111.04
3	A	1519	BGC	C3-C4-C5	2.47	114.50	110.20
3	B	1519	BGC	C1-O5-C5	3.80	117.07	112.25
3	A	1520	BGC	O5-C5-C6	4.58	117.27	107.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	OXZ	A	1518	3	8,10,10	1.45	1 (12%)	10,13,13	1.54	3 (30%)
5	EDO	A	1522	-	3,3,3	0.46	0	2,2,2	0.77	0
5	EDO	A	1523	-	3,3,3	0.30	0	2,2,2	1.32	0
5	EDO	A	1525	-	3,3,3	0.56	0	2,2,2	0.13	0
5	EDO	A	1526	-	3,3,3	0.38	0	2,2,2	0.48	0
7	SO4	A	1528	-	4,4,4	0.25	0	6,6,6	0.61	0
8	PGE	A	1529[A]	-	9,9,9	0.55	0	8,8,8	0.48	0
5	EDO	A	1530[B]	-	3,3,3	0.49	0	2,2,2	0.45	0
2	OXZ	B	1518	3	8,10,10	0.69	0	10,13,13	1.62	3 (30%)
5	EDO	B	1522	-	3,3,3	0.54	0	2,2,2	0.53	0
5	EDO	B	1524	-	3,3,3	0.50	0	2,2,2	0.95	0
5	EDO	B	1526	-	3,3,3	0.35	0	2,2,2	0.61	0
5	EDO	B	1527	-	3,3,3	0.40	0	2,2,2	0.58	0
7	SO4	B	1528[A]	-	4,4,4	0.25	0	6,6,6	0.43	0
5	EDO	B	1529[B]	-	3,3,3	0.64	0	2,2,2	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OXZ	A	1518	3	-	0/2/16/16	0/1/1/1
5	EDO	A	1522	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1523	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1525	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1526	-	-	0/1/1/1	0/0/0/0
7	SO4	A	1528	-	-	0/0/0/0	0/0/0/0
8	PGE	A	1529[A]	-	-	0/7/7/7	0/0/0/0
5	EDO	A	1530[B]	-	-	0/1/1/1	0/0/0/0
2	OXZ	B	1518	3	-	0/2/16/16	0/1/1/1
5	EDO	B	1522	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1524	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1526	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1527	-	-	0/1/1/1	0/0/0/0
7	SO4	B	1528[A]	-	-	0/0/0/0	0/0/0/0
5	EDO	B	1529[B]	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1518	OXZ	C2-C3	3.36	1.56	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1518	OXZ	O5-C5-C4	-2.63	104.75	109.68
2	B	1518	OXZ	O3-C3-C2	-2.45	104.67	109.57
2	B	1518	OXZ	O5-C5-C4	-2.31	105.35	109.68
2	B	1518	OXZ	O4-C4-C5	-2.07	103.76	109.24
2	A	1518	OXZ	C2-C3-C4	2.13	112.73	110.29
2	A	1518	OXZ	C3-C4-C5	2.72	112.68	109.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1518	OXZ	1	0
5	A	1522	EDO	1	0
5	A	1525	EDO	3	0
5	A	1526	EDO	1	0
8	A	1529[A]	PGE	3	0
5	B	1529[B]	EDO	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	510/524 (97%)	-0.53	3 (0%) 90 91	14, 25, 42, 53	29 (5%)
1	B	506/524 (96%)	-0.34	5 (0%) 84 85	18, 31, 51, 61	67 (13%)
All	All	1016/1048 (96%)	-0.44	8 (0%) 87 88	14, 28, 48, 61	96 (9%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	441	ASN	3.6
1	B	17	PHE	2.6
1	B	293	GLY	2.6
1	B	471	THR	2.5
1	A	7	ALA	2.2
1	A	66[B]	TRP	2.2
1	B	501	PHE	2.1
1	A	443	SER	2.1

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(\AA^2)	Q<0.9
3	BGC	A	1519	11/12	0.98	0.09	-0.81	19,20,21,23	0
3	BGC	B	1519	11/12	0.95	0.08	-1.11	23,25,27,27	0
3	BGC	A	1520	11/12	0.98	0.08	-1.15	21,22,24,27	0
3	BGC	B	1520	11/12	0.97	0.08	-2.48	23,26,29,35	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(\AA^2)	Q<0.9
5	EDO	A	1525	4/4	0.94	0.19	7.83	38,38,38,41	0
8	PGE	A	1529[A]	10/10	0.83	0.18	7.39	30,32,33,33	10
7	SO4	B	1528[A]	5/5	0.99	0.13	5.51	34,34,36,36	5
5	EDO	B	1529[B]	4/4	0.99	0.10	1.30	25,27,27,27	4
5	EDO	A	1522	4/4	0.92	0.12	1.16	41,44,45,45	0
6	CL	B	1525	1/1	0.98	0.10	0.15	28,28,28,28	0
5	EDO	B	1522	4/4	0.96	0.10	0.03	46,46,47,49	0
2	OXZ	A	1518	10/10	0.97	0.09	-0.56	15,16,17,18	0
6	CL	A	1527	1/1	0.99	0.07	-1.27	18,18,18,18	0
2	OXZ	B	1518	10/10	0.97	0.08	-1.80	20,22,22,25	0
4	CA	B	1521	1/1	0.98	0.06	-2.57	25,25,25,25	0
4	CA	A	1521	1/1	1.00	0.06	-3.18	21,21,21,21	0
5	EDO	A	1526	4/4	0.96	0.20	-	38,40,41,41	1
7	SO4	A	1528	5/5	0.96	0.12	-	22,22,23,23	5
5	EDO	B	1524	4/4	0.94	0.20	-	45,47,47,50	0
5	EDO	A	1530[B]	4/4	0.91	0.20	-	51,52,52,52	4
5	EDO	A	1523	4/4	0.94	0.15	-	47,47,48,49	0
5	EDO	B	1526	4/4	0.91	0.24	-	18,19,19,20	4
5	EDO	B	1527	4/4	0.93	0.15	-	21,22,22,22	4

6.5 Other polymers [i](#)

There are no such residues in this entry.