



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:06 AM UTC

PDB ID : 4ZLF / pdb_00004zlf
Title : Cellobionic acid phosphorylase - cellobionic acid complex
Authors : Nam, Y.W.; Arakawa, T.; Fushinobu, S.
Deposited on : 2015-05-01
Resolution : 1.60 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

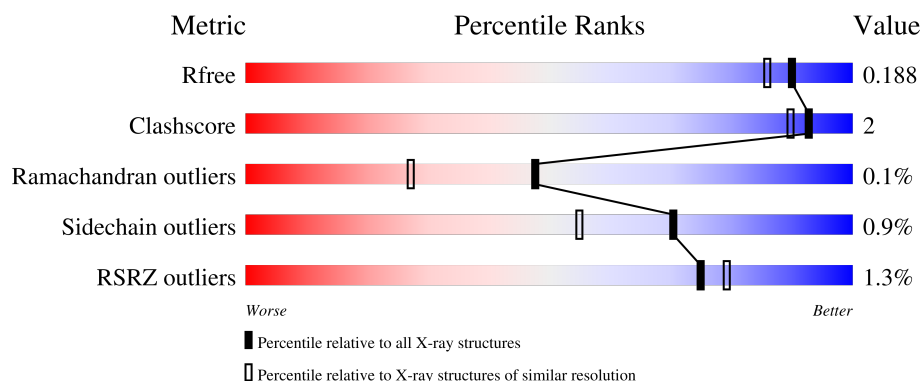
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 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	796	83% 15% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7117 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.

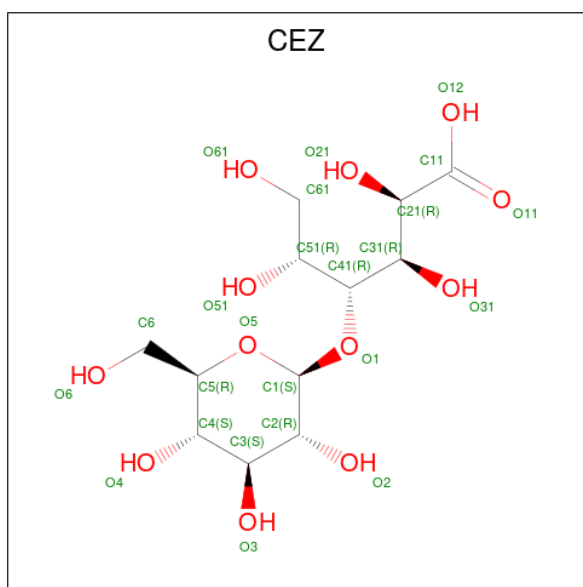
- Molecule 1 is a protein called Putative b-glycan phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	785	Total	C	N	O	S	0	2	0
			6244	3981	1060	1171	32			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	MET	engineered mutation	UNP Q21MB1
A	789	LEU	-	expression tag	UNP Q21MB1
A	790	GLU	-	expression tag	UNP Q21MB1
A	791	HIS	-	expression tag	UNP Q21MB1
A	792	HIS	-	expression tag	UNP Q21MB1
A	793	HIS	-	expression tag	UNP Q21MB1
A	794	HIS	-	expression tag	UNP Q21MB1
A	795	HIS	-	expression tag	UNP Q21MB1
A	796	HIS	-	expression tag	UNP Q21MB1

- Molecule 2 is 4-O-beta-D-glucopyranosyl-D-gluconic acid (CCD ID: CEZ) (formula: C₁₂H₂₂O₁₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			24	12	12		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

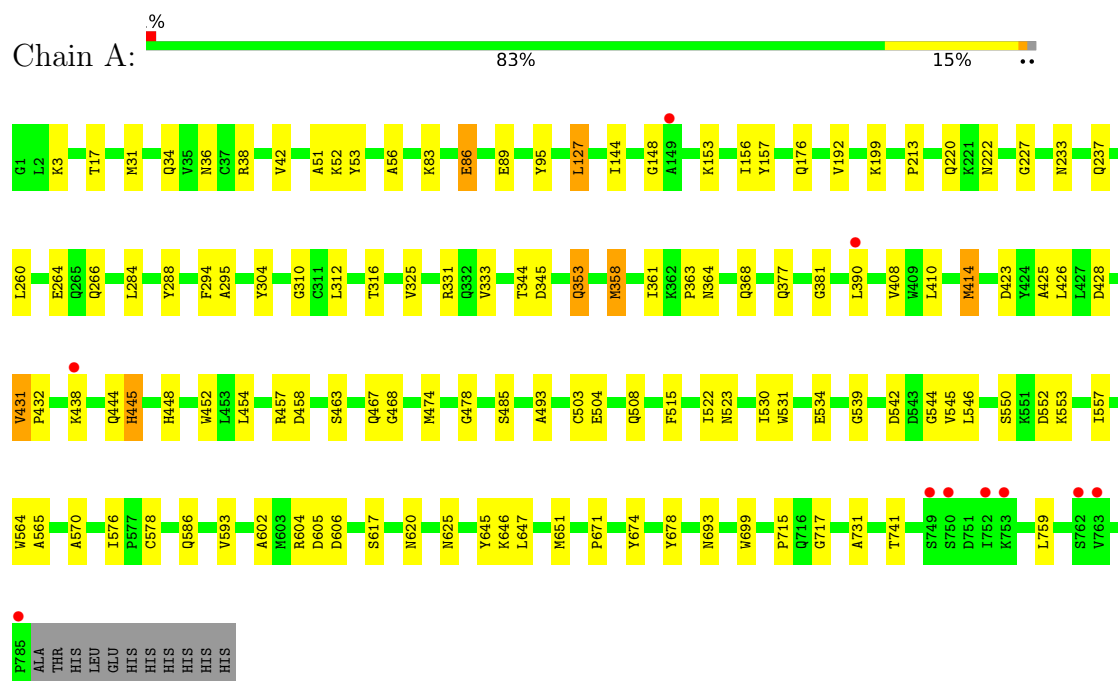
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	808	Total	O	0	0
			808	808		

3 Residue-property plots [i](#)

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: Putative b-glycan phosphorylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.19Å 107.19Å 186.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.14 – 1.60 31.14 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (31.14-1.60) 99.7 (31.14-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.156 , 0.177 0.169 , 0.188	Depositor DCC
R_{free} test set	8191 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7117	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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: CL, GOL, CEZ, 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	1.89	84/6417 (1.3%)	1.55	45/8715 (0.5%)

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	717	GLY	C-O	12.57	1.32	1.23
1	A	508	GLN	CD-OE1	11.91	1.46	1.23
1	A	31	MET	SD-CE	-10.68	1.52	1.79
1	A	414	MET	CB-CG	10.41	1.83	1.52
1	A	358	MET	SD-CE	-9.41	1.56	1.79
1	A	504	GLU	CA-C	7.67	1.62	1.52
1	A	148	GLY	N-CA	7.52	1.51	1.44
1	A	264	GLU	CA-C	7.42	1.62	1.52
1	A	304	TYR	N-CA	7.38	1.55	1.46
1	A	452	TRP	C-O	7.30	1.32	1.24
1	A	414	MET	CG-SD	-7.25	1.62	1.80
1	A	564	TRP	N-CA	-7.07	1.37	1.46
1	A	578	CYS	CA-C	6.88	1.61	1.52
1	A	593	VAL	CA-C	6.84	1.60	1.52
1	A	468	GLY	CA-C	6.72	1.58	1.51
1	A	625	ASN	CG-OD1	6.64	1.36	1.23
1	A	553	LYS	N-CA	-6.61	1.38	1.46
1	A	550	SER	C-O	-6.36	1.16	1.24
1	A	523	ASN	N-CA	-6.29	1.38	1.46
1	A	586	GLN	CA-CB	-6.26	1.44	1.53
1	A	671	PRO	CA-C	-6.14	1.46	1.52
1	A	674	TYR	N-CA	-6.13	1.38	1.46
1	A	199	LYS	C-O	-6.11	1.17	1.24
1	A	344	THR	N-CA	-6.11	1.38	1.46
1	A	333	VAL	CA-CB	6.10	1.61	1.54
1	A	353	GLN	CD-OE1	6.08	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	LEU	CB-CG	-6.08	1.41	1.53
1	A	368	GLN	CD-OE1	6.08	1.35	1.23
1	A	493	ALA	N-CA	6.04	1.53	1.46
1	A	546	LEU	CA-C	-6.01	1.45	1.52
1	A	312	LEU	CA-C	-5.96	1.45	1.52
1	A	545	VAL	N-CA	-5.95	1.39	1.46
1	A	552	ASP	C-O	5.94	1.31	1.24
1	A	457	ARG	CZ-NH2	-5.92	1.25	1.33
1	A	431	VAL	C-O	-5.92	1.20	1.24
1	A	410	LEU	N-CA	-5.91	1.42	1.46
1	A	503	CYS	CA-C	5.89	1.60	1.52
1	A	467	GLN	N-CA	5.88	1.52	1.46
1	A	478	GLY	CA-C	-5.88	1.43	1.51
1	A	157	TYR	CA-C	5.84	1.59	1.52
1	A	295	ALA	C-O	5.81	1.31	1.24
1	A	176	GLN	CD-NE2	-5.80	1.21	1.33
1	A	144	ILE	C-O	-5.78	1.18	1.24
1	A	645	TYR	N-CA	-5.72	1.39	1.46
1	A	325	VAL	CA-C	-5.69	1.45	1.52
1	A	620	ASN	CA-C	-5.67	1.47	1.53
1	A	570	ALA	C-O	5.67	1.31	1.24
1	A	316	THR	C-O	-5.64	1.19	1.24
1	A	363	PRO	C-O	5.60	1.31	1.24
1	A	222	ASN	CG-ND2	5.57	1.45	1.33
1	A	458	ASP	N-CA	5.57	1.52	1.46
1	A	153	LYS	CA-C	5.57	1.59	1.52
1	A	237	GLN	CA-CB	-5.56	1.44	1.53
1	A	531	TRP	N-CA	-5.55	1.39	1.46
1	A	534	GLU	CA-C	5.54	1.59	1.52
1	A	86	GLU	CA-C	-5.53	1.45	1.52
1	A	515	PHE	CA-C	-5.51	1.45	1.52
1	A	741	THR	C-O	5.48	1.30	1.24
1	A	731	ALA	CA-C	-5.47	1.46	1.52
1	A	213	PRO	N-CA	-5.45	1.41	1.46
1	A	364	ASN	CB-CG	5.37	1.65	1.52
1	A	565	ALA	N-CA	5.35	1.52	1.46
1	A	156	ILE	N-CA	5.33	1.52	1.46
1	A	53	TYR	CA-C	-5.32	1.45	1.52
1	A	345	ASP	CG-OD2	5.25	1.35	1.25
1	A	51	ALA	N-CA	-5.24	1.40	1.46
1	A	423	ASP	N-CA	-5.21	1.40	1.46
1	A	426	LEU	N-CA	5.20	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	604	ARG	C-O	5.16	1.29	1.24
1	A	260	LEU	CA-C	5.15	1.59	1.52
1	A	448	HIS	CA-CB	-5.15	1.45	1.53
1	A	617	SER	CA-C	-5.12	1.46	1.52
1	A	390	LEU	N-CA	5.08	1.52	1.46
1	A	474	MET	SD-CE	-5.07	1.66	1.79
1	A	602	ALA	CA-C	-5.07	1.46	1.52
1	A	294	PHE	N-CA	5.06	1.52	1.46
1	A	715	PRO	C-N	-5.06	1.26	1.33
1	A	604	ARG	CZ-NH1	-5.05	1.25	1.32
1	A	89	GLU	CA-C	5.04	1.59	1.52
1	A	83	LYS	C-O	-5.04	1.18	1.24
1	A	693	ASN	C-O	5.04	1.29	1.24
1	A	266	GLN	CA-C	5.04	1.58	1.52
1	A	544	GLY	CA-C	-5.02	1.44	1.51
1	A	425	ALA	C-O	-5.00	1.17	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	MET	N-CA-CB	10.03	125.67	110.22
1	A	605	ASP	N-CA-C	8.23	122.67	113.21
1	A	576	ILE	O-C-N	-7.30	115.75	120.42
1	A	539	GLY	CA-C-O	-7.28	114.45	121.87
1	A	414	MET	CB-CG-SD	-7.22	91.03	112.70
1	A	266	GLN	O-C-N	6.95	131.79	123.24
1	A	428	ASP	N-CA-C	6.74	121.33	113.18
1	A	522	ILE	O-C-N	-6.62	115.45	121.87
1	A	678	TYR	CA-C-O	-6.59	113.56	120.55
1	A	678	TYR	O-C-N	6.59	129.10	122.12
1	A	192	VAL	O-C-N	6.45	128.21	121.89
1	A	544	GLY	N-CA-C	6.37	124.89	115.08
1	A	542	ASP	O-C-N	6.25	129.53	122.22
1	A	381	GLY	CA-C-O	6.23	124.98	119.56
1	A	310	GLY	O-C-N	6.19	128.78	122.90
1	A	530	ILE	O-C-N	-6.04	115.02	122.57
1	A	651	MET	CG-SD-CE	-5.93	87.84	100.90
1	A	576	ILE	N-CA-C	5.89	120.03	112.67
1	A	576	ILE	CA-C-O	5.71	123.05	118.71
1	A	264	GLU	O-C-N	5.68	129.71	123.01
1	A	445	HIS	O-C-N	-5.67	116.11	122.12
1	A	646	LYS	O-C-N	5.66	127.90	122.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	PRO	O-C-N	-5.60	116.32	123.04
1	A	56	ALA	O-C-N	5.59	127.74	121.32
1	A	410	LEU	O-C-N	5.59	124.79	120.38
1	A	485	SER	CA-C-N	5.52	126.07	119.94
1	A	485	SER	C-N-CA	5.52	126.07	119.94
1	A	192	VAL	CA-C-O	-5.50	115.33	121.05
1	A	364	ASN	N-CA-CB	5.49	118.80	110.28
1	A	288	TYR	N-CA-C	5.46	120.59	113.88
1	A	220	GLN	N-CA-C	5.43	116.88	111.07
1	A	606	ASP	N-CA-C	-5.40	106.00	112.59
1	A	431	VAL	N-CA-CB	5.37	117.38	111.64
1	A	17	THR	N-CA-C	5.35	120.82	113.97
1	A	452	TRP	O-C-N	-5.35	116.56	122.07
1	A	463	SER	CA-C-O	-5.34	114.67	120.81
1	A	454	LEU	CA-C-O	-5.32	114.78	120.42
1	A	361	ILE	CA-C-N	5.28	126.92	122.28
1	A	361	ILE	C-N-CA	5.28	126.92	122.28
1	A	534	GLU	O-C-N	5.24	128.35	122.27
1	A	331	ARG	NE-CZ-NH2	-5.20	114.52	119.20
1	A	284	LEU	CA-C-O	5.18	126.04	120.55
1	A	578	CYS	N-CA-C	-5.17	105.65	111.28
1	A	557	ILE	O-C-N	5.07	128.68	123.05
1	A	3	LYS	N-CA-C	5.05	116.51	108.79

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	6244	0	6021	18	0
2	A	24	0	21	1	0
3	A	10	0	0	1	0
4	A	30	0	38	0	0
5	A	1	0	0	0	0
6	A	808	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7117	0	6080	19	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 2.

All (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:MET:CB	1:A:414:MET:CG	1.83	1.56
1:A:414:MET:CB	1:A:414:MET:SD	2.47	1.01
1:A:444:GLN:HG2	6:A:1525:HOH:O	1.80	0.81
1:A:353:GLN:HE21	1:A:699:TRP:HE1	1.30	0.80
1:A:42:VAL:HG13	6:A:1512:HOH:O	1.93	0.68
1:A:431:VAL:O	1:A:445:HIS:HE1	1.90	0.55
1:A:227:GLY:H	1:A:233:ASN:HD22	1.55	0.55
1:A:353:GLN:HE21	1:A:699:TRP:NE1	2.02	0.55
1:A:377:GLN:OE1	1:A:445:HIS:HD2	1.91	0.54
1:A:431:VAL:HG23	1:A:445:HIS:CE1	2.45	0.51
1:A:86:GLU:HG3	6:A:1638:HOH:O	2.10	0.51
1:A:431:VAL:HB	1:A:432:PRO:HD2	1.95	0.49
1:A:36:ASN:ND2	1:A:38:ARG:H	2.13	0.46
1:A:227:GLY:H	1:A:233:ASN:ND2	2.15	0.44
1:A:377:GLN:OE1	1:A:445:HIS:CD2	2.70	0.44
1:A:358:MET:HE3	1:A:358:MET:HB3	1.69	0.42
1:A:414:MET:SD	1:A:414:MET:HB2	2.52	0.42
1:A:759:LEU:HD21	6:A:1087:HOH:O	2.20	0.41
2:A:801:CEZ:H1	3:A:802:SO4:O3	2.21	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	785/796 (99%)	766 (98%)	18 (2%)	1 (0%)	48 27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	95	TYR

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	657/665 (99%)	651 (99%)	6 (1%)	70 55

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

Mol	Chain	Res	Type
1	A	34	GLN
1	A	52	LYS
1	A	127	LEU
1	A	408	VAL
1	A	438	LYS
1	A	647	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	36	ASN
1	A	103	ASN
1	A	108	ASN
1	A	222	ASN
1	A	233	ASN
1	A	302	GLN
1	A	313	GLN
1	A	340	ASN

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Mol	Chain	Res	Type
1	A	347	GLN
1	A	353	GLN
1	A	355	ASN
1	A	368	GLN
1	A	445	HIS
1	A	560	ASN
1	A	574	GLN
1	A	586	GLN
1	A	693	ASN
1	A	721	GLN
1	A	743	ASN
1	A	758	GLN
1	A	779	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	$\# Z > 2$
4	GOL	A	807	-	5,5,5	0.58	0	5,5,5	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	808	-	5,5,5	1.43	1 (20%)	5,5,5	0.71	0
3	SO4	A	803	-	4,4,4	0.68	0	6,6,6	0.65	0
3	SO4	A	802	-	4,4,4	0.64	0	6,6,6	0.80	0
2	CEZ	A	801	-	24,24,24	2.14	7 (29%)	32,34,34	2.84	15 (46%)
4	GOL	A	806	-	5,5,5	1.06	0	5,5,5	0.50	0
4	GOL	A	805	-	5,5,5	1.72	1 (20%)	5,5,5	0.40	0
4	GOL	A	804	-	5,5,5	0.80	0	5,5,5	1.13	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
4	GOL	A	807	-	-	0/4/4/4	-
4	GOL	A	808	-	-	0/4/4/4	-
2	CEZ	A	801	-	-	2/24/44/44	0/1/1/1
4	GOL	A	806	-	-	0/4/4/4	-
4	GOL	A	805	-	-	0/4/4/4	-
4	GOL	A	804	-	-	2/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	CEZ	O51-C51	5.31	1.54	1.43
2	A	801	CEZ	C51-C41	4.06	1.61	1.52
2	A	801	CEZ	C31-C21	3.72	1.61	1.53
4	A	805	GOL	O2-C2	-3.30	1.33	1.43
2	A	801	CEZ	C21-C11	-3.26	1.48	1.52
2	A	801	CEZ	O2-C2	3.09	1.50	1.43
2	A	801	CEZ	C31-C41	2.41	1.55	1.52
4	A	808	GOL	O3-C3	2.32	1.52	1.42
2	A	801	CEZ	O61-C61	2.30	1.52	1.42

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	CEZ	O11-C11-C21	-7.51	101.63	121.62
2	A	801	CEZ	O1-C41-C51	4.93	114.78	107.98
2	A	801	CEZ	O31-C31-C21	-4.41	101.38	109.29
2	A	801	CEZ	O12-C11-C21	4.23	125.07	113.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	CEZ	C4-C3-C2	-3.99	103.82	110.83
2	A	801	CEZ	O2-C2-C1	-3.88	100.82	110.08
2	A	801	CEZ	O61-C61-C51	-3.56	103.69	111.16
2	A	801	CEZ	C51-C41-C31	3.52	121.21	113.60
2	A	801	CEZ	O21-C21-C31	-3.23	103.37	110.38
2	A	801	CEZ	O21-C21-C11	3.18	117.48	110.69
2	A	801	CEZ	O1-C1-C2	-3.01	100.68	108.09
2	A	801	CEZ	O12-C11-O11	2.93	130.73	124.08
2	A	801	CEZ	O2-C2-C3	-2.87	103.60	110.38
2	A	801	CEZ	O5-C5-C4	-2.80	104.65	109.70
2	A	801	CEZ	O4-C4-C3	-2.34	104.86	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

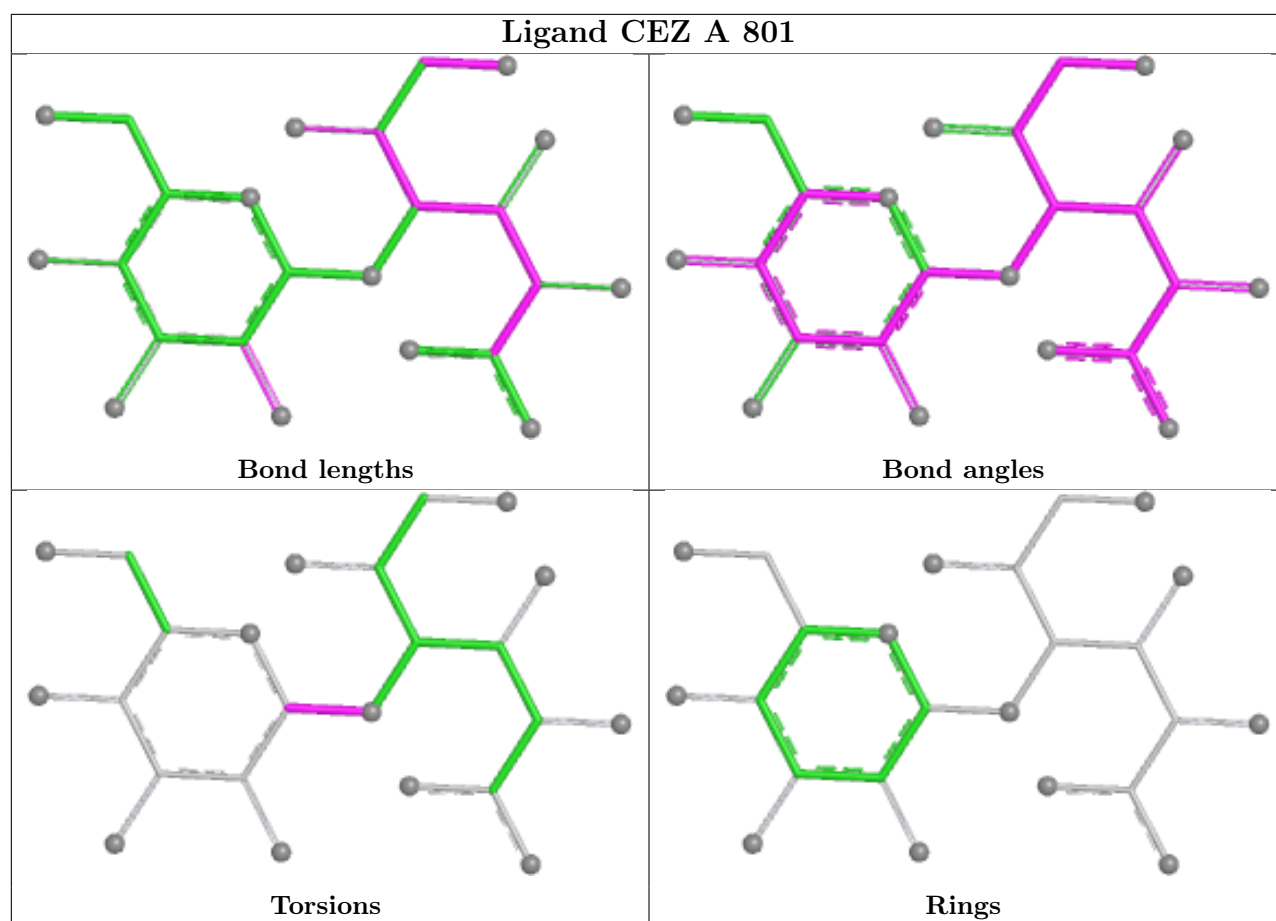
Mol	Chain	Res	Type	Atoms
4	A	804	GOL	C1-C2-C3-O3
4	A	804	GOL	O2-C2-C3-O3
2	A	801	CEZ	O5-C1-O1-C41
2	A	801	CEZ	C2-C1-O1-C41

There are no ring outliers.

2 monomers are involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	SO4	1	0
2	A	801	CEZ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	785/796 (98%)	-0.18	10 (1%) 75 79	10, 20, 35, 73	2 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	785	PRO	3.6
1	A	750	SER	3.5
1	A	752	ILE	3.4
1	A	753	LYS	2.7
1	A	390	LEU	2.7
1	A	749	SER	2.3
1	A	149	ALA	2.3
1	A	763	VAL	2.2
1	A	762	SER	2.2
1	A	438	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](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

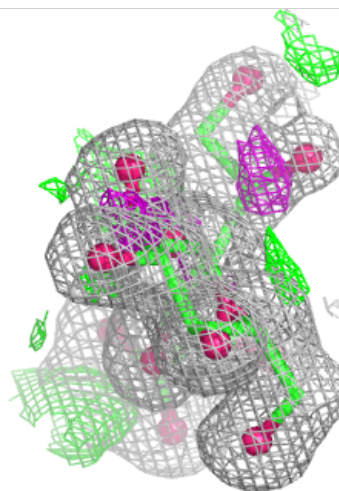
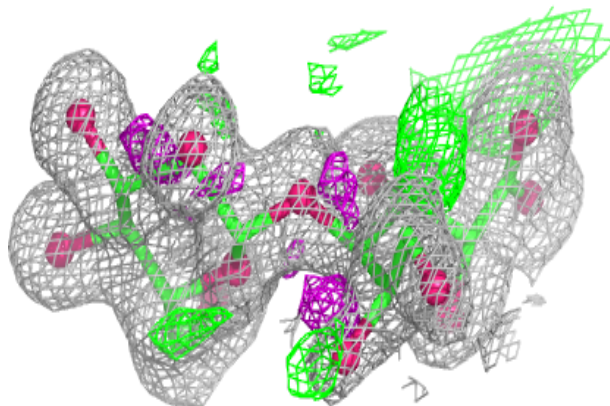
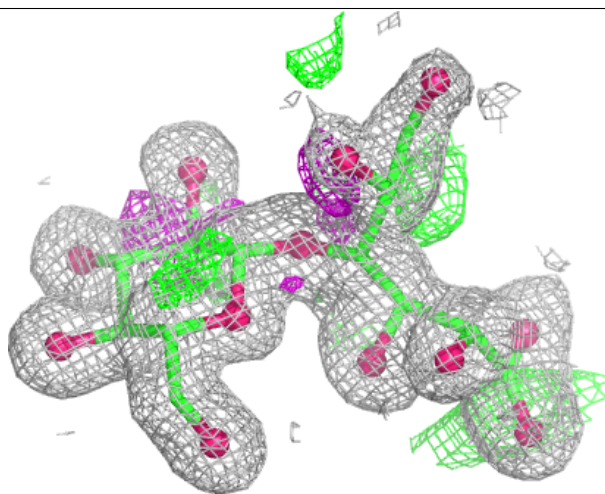
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
4	GOL	A	807	6/6	0.91	0.13	39,43,46,49	0
4	GOL	A	808	6/6	0.91	0.10	26,30,33,35	0
4	GOL	A	804	6/6	0.93	0.10	29,38,40,44	0
2	CEZ	A	801	24/24	0.94	0.09	17,24,35,40	0
4	GOL	A	805	6/6	0.94	0.09	26,30,35,37	0
4	GOL	A	806	6/6	0.96	0.10	22,24,24,26	0
3	SO4	A	803	5/5	0.98	0.11	28,29,30,32	0
3	SO4	A	802	5/5	0.99	0.04	19,20,22,26	0
5	CL	A	809	1/1	0.99	0.03	19,19,19,19	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around CEZ A 801:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.