



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 10:07 am BST

PDB ID : 9RVA / pdb_00009rva
Title : Crystal structure of the extracellular part of human ACE2 in complex with the macrocyclic peptide WJL-63
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Deposited on : 2025-07-07
Resolution : 2.20 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	:	1.8.4, CSD as541be (2020)
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

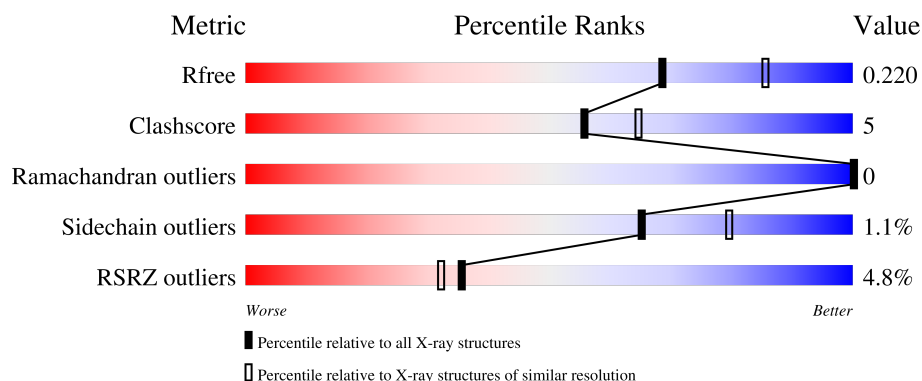
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	730	 4% 83% 9% 7%
2	C	24	 4% 63% 12% 25%

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
7	CL	A	822	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 11572 atoms, of which 5604 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 Angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	677	Total	C	H	N	O	S	243	2	0
			10852	3547	5308	924	1040	33			

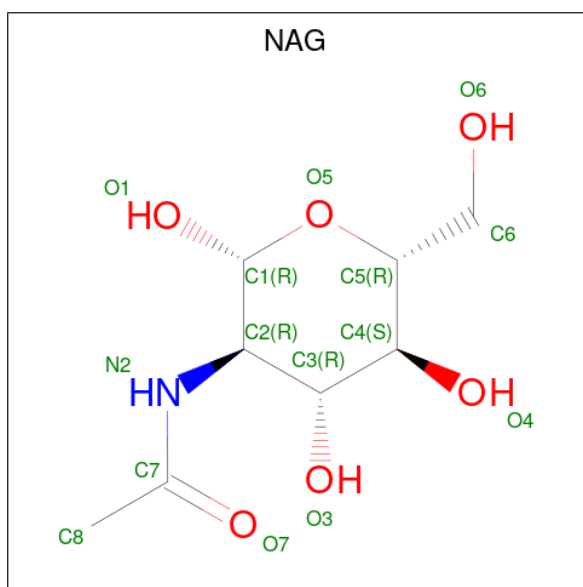
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	741	HIS	-	expression tag	UNP Q9BYF1
A	742	HIS	-	expression tag	UNP Q9BYF1
A	743	HIS	-	expression tag	UNP Q9BYF1
A	744	HIS	-	expression tag	UNP Q9BYF1
A	745	HIS	-	expression tag	UNP Q9BYF1
A	746	HIS	-	expression tag	UNP Q9BYF1
A	747	HIS	-	expression tag	UNP Q9BYF1
A	748	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called macrocyclic peptide WJL-63.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	18	Total	C	H	N	O	S	0	0	0
			255	79	121	27	27	1			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

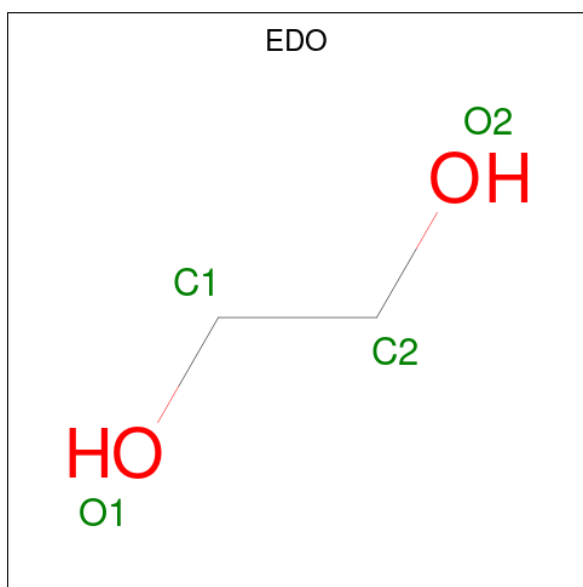


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
3	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

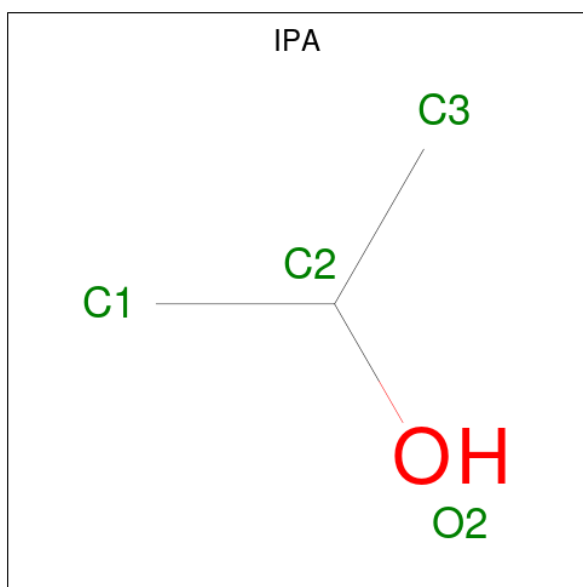
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	A	1	Total	C	H	O	0	0
			10	2	6	2		
5	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 6 is ISOPROPYL ALCOHOL (CCD ID: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			12	3	8	1		
6	A	1	Total	C	H	O	0	0
			12	3	8	1		

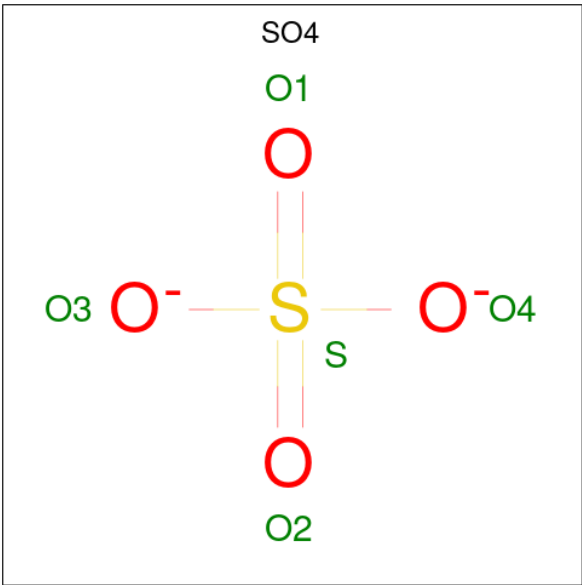
- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 8 is SODIUM ION (CCD ID: NA) (formula: Na).

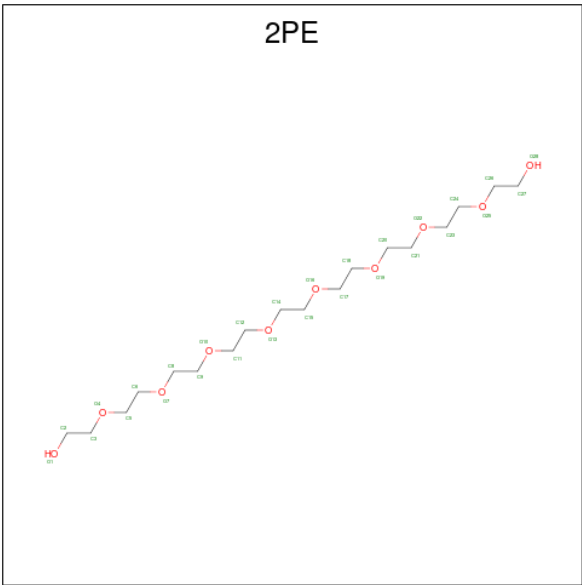
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Na	0	0
			1	1		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 10 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	H	O	0	0
			16	4	9	3		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	124	Total 124	O 124	0	0
11	C	4	Total 4	O 4	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.10Å 89.10Å 112.70Å 90.00° 108.30° 90.00°	Depositor
Resolution (Å)	46.64 – 2.20 46.64 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.2 (46.64-2.20) 98.7 (46.64-2.20)	Depositor EDS
R_{merge}	0.49	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.20_4459: ???)	Depositor
R, R_{free}	0.186 , 0.226 0.183 , 0.220	Depositor DCC
R_{free} test set	2430 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11572	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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: DTY, EDO, ZN, 2PE, IPA, NAG, SO4, CL, NA

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	0.51	0/5710	0.62	0/7749
2	C	0.50	0/121	0.62	0/157
All	All	0.51	0/5831	0.62	0/7906

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	ARG	Sidechain
1	A	559	ARG	Sidechain

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	5544	5308	5310	50	0
2	C	134	121	121	3	0
3	A	84	78	78	3	0
4	A	1	0	0	0	0
5	A	44	66	66	3	0
5	C	4	6	6	1	0
6	A	8	16	16	1	0
7	A	3	0	0	2	0
8	A	1	0	0	0	0
9	A	10	0	0	1	0
10	A	7	9	9	0	0
11	A	124	0	0	3	0
11	C	4	0	0	0	0
All	All	5968	5604	5606	53	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 (53) 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:416:LYS:NZ	7:A:822:CL:CL	2.49	0.80
1:A:294:THR:HG22	1:A:366:MET:H	1.58	0.67
1:A:635:TRP:HA	1:A:639:GLU:HG3	1.77	0.64
1:A:679:ILE:HG23	1:A:679:ILE:O	1.98	0.64
1:A:292:ASP:OD1	1:A:294:THR:HG23	1.96	0.64
1:A:557:MET:HB2	1:A:573:VAL:HG23	1.80	0.63
1:A:90:ASN:ND2	3:A:801:NAG:H83	2.18	0.59
1:A:82:MET:N	1:A:82:MET:HE2	2.20	0.57
1:A:535:HIS:ND1	7:A:822:CL:CL	2.77	0.55
1:A:456:LEU:C	1:A:456:LEU:HD23	2.33	0.53
1:A:35:GLU:OE1	6:A:820:IPA:H11	2.08	0.53
1:A:524:GLN:HE21	5:A:809:EDO:H11	1.74	0.53
1:A:20:THR:HG22	1:A:22:GLU:N	2.25	0.52
1:A:209:VAL:HG11	1:A:565:PRO:HB3	1.90	0.52
1:A:132:VAL:HG13	1:A:163:TRP:CZ2	2.45	0.52
1:A:693:ASP:HB2	3:A:805:NAG:O5	2.11	0.51
1:A:163:TRP:CD1	1:A:167[B]:SER:HG	2.29	0.50
1:A:374:HIS:C	1:A:374:HIS:CD2	2.90	0.50
1:A:584:LEU:HD23	1:A:584:LEU:C	2.37	0.49
1:A:675:LEU:HD13	1:A:681:PHE:HB3	1.94	0.49
1:A:298:VAL:O	1:A:300:GLN:O	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:ASN:ND2	3:A:805:NAG:H83	2.29	0.48
9:A:825:SO4:O2	9:A:826:SO4:O1	2.32	0.47
1:A:690:ASN:HD22	1:A:693:ASP:HB2	1.80	0.47
1:A:233:ILE:CG1	1:A:581:VAL:HG21	2.45	0.47
1:A:100:LEU:HG	1:A:391:LEU:HD11	1.97	0.46
1:A:402:GLU:HB2	1:A:518:ARG:HG3	1.97	0.46
1:A:230:PHE:HA	1:A:233:ILE:HD12	1.97	0.46
1:A:50:TYR:CE1	1:A:59:VAL:HG22	2.51	0.46
1:A:192:ARG:HH11	5:A:818:EDO:C1	2.29	0.45
1:A:20:THR:HG22	1:A:22:GLU:H	1.82	0.45
1:A:417:HIS:HB2	1:A:543:ASP:OD2	2.17	0.45
1:A:389:PRO:HG2	1:A:392:LEU:HD12	1.98	0.44
1:A:48:TRP:O	1:A:52:THR:HG22	2.17	0.44
1:A:621:ARG:O	1:A:679:ILE:HG12	2.18	0.43
1:A:187:LYS:NZ	11:A:913:HOH:O	2.51	0.43
1:A:499:ASP:N	1:A:500:PRO:CD	2.82	0.43
1:A:332:MET:HE1	1:A:342:ALA:HB1	1.99	0.43
1:A:474:MET:HE1	1:A:499:ASP:HB2	2.00	0.43
1:A:559:ARG:NE	11:A:914:HOH:O	2.52	0.43
1:A:560:LEU:HD11	1:A:572:ASN:ND2	2.35	0.42
1:A:336:PRO:HG2	1:A:340:GLN:O	2.19	0.42
11:A:992:HOH:O	2:C:5:ILE:HG12	2.18	0.42
1:A:132:VAL:CG2	1:A:167[B]:SER:HB3	2.50	0.42
1:A:440:LEU:C	1:A:440:LEU:HD13	2.45	0.42
1:A:545:SER:O	1:A:546:ASN:HB2	2.19	0.42
1:A:509:ASP:O	2:C:12:ASP:HB2	2.20	0.42
1:A:557:MET:CB	1:A:573:VAL:HG23	2.47	0.42
1:A:679:ILE:O	1:A:679:ILE:CG2	2.67	0.42
1:A:477:TRP:CE3	1:A:500:PRO:HG3	2.56	0.41
2:C:9:PHE:O	5:C:101:EDO:H22	2.21	0.41
1:A:192:ARG:HD3	5:A:818:EDO:O1	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	675/730 (92%)	654 (97%)	21 (3%)	0	100	100
2	C	15/24 (62%)	12 (80%)	3 (20%)	0	100	100
All	All	690/754 (92%)	666 (96%)	24 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	603/648 (93%)	596 (99%)	7 (1%)	63	78
2	C	13/17 (76%)	13 (100%)	0	100	100
All	All	616/665 (93%)	609 (99%)	7 (1%)	65	79

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	VAL
1	A	146	PRO
1	A	401	HIS
1	A	455	MET
1	A	559	ARG
1	A	562	LYS
1	A	667	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	139	GLN
1	A	552	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 5 are monoatomic - leaving 23 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	$\# Z > 2$
9	SO4	A	825	-	4,4,4	0.27	0	6,6,6	0.57	0
5	EDO	A	818	-	3,3,3	0.76	0	2,2,2	0.32	0
5	EDO	A	809	-	3,3,3	0.82	0	2,2,2	0.76	0
5	EDO	A	813	-	3,3,3	0.66	0	2,2,2	0.02	0
5	EDO	C	101	-	3,3,3	0.54	0	2,2,2	0.66	0
6	IPA	A	820	-	3,3,3	0.60	0	3,3,3	0.15	0
3	NAG	A	806	1	14,14,15	0.44	0	17,19,21	0.94	1 (5%)
5	EDO	A	814	-	3,3,3	0.71	0	2,2,2	0.17	0
5	EDO	A	817	-	3,3,3	0.45	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	812	-	3,3,3	0.64	0	2,2,2	0.15	0
3	NAG	A	805	1	14,14,15	0.82	1 (7%)	17,19,21	0.98	2 (11%)
3	NAG	A	802	1	14,14,15	0.83	2 (14%)	17,19,21	0.55	0
5	EDO	A	808	-	3,3,3	0.37	0	2,2,2	0.61	0
5	EDO	A	815	-	3,3,3	0.49	0	2,2,2	0.15	0
3	NAG	A	803	1	14,14,15	0.62	0	17,19,21	0.64	0
3	NAG	A	804	1	14,14,15	1.11	2 (14%)	17,19,21	0.86	1 (5%)
5	EDO	A	816	-	3,3,3	0.42	0	2,2,2	0.47	0
6	IPA	A	819	-	3,3,3	0.62	0	3,3,3	0.24	0
5	EDO	A	810	-	3,3,3	0.55	0	2,2,2	0.45	0
5	EDO	A	811	-	3,3,3	0.48	0	2,2,2	0.59	0
9	SO4	A	826	-	4,4,4	0.15	0	6,6,6	0.33	0
10	2PE	A	827	-	6,6,27	0.35	0	5,5,26	0.23	0
3	NAG	A	801	1	14,14,15	0.59	0	17,19,21	1.11	2 (11%)

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	EDO	A	818	-	-	0/1/1/1	-
5	EDO	A	809	-	-	1/1/1/1	-
5	EDO	A	813	-	-	0/1/1/1	-
5	EDO	C	101	-	-	1/1/1/1	-
3	NAG	A	806	1	-	4/6/23/26	0/1/1/1
5	EDO	A	814	-	-	1/1/1/1	-
5	EDO	A	817	-	-	0/1/1/1	-
5	EDO	A	812	-	-	1/1/1/1	-
3	NAG	A	805	1	-	2/6/23/26	0/1/1/1
3	NAG	A	802	1	-	1/6/23/26	0/1/1/1
5	EDO	A	808	-	-	0/1/1/1	-
5	EDO	A	815	-	-	0/1/1/1	-
3	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	NAG	A	804	1	-	0/6/23/26	0/1/1/1
5	EDO	A	816	-	-	0/1/1/1	-
5	EDO	A	810	-	-	0/1/1/1	-
5	EDO	A	811	-	-	1/1/1/1	-
10	2PE	A	827	-	-	2/4/4/25	-
3	NAG	A	801	1	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	NAG	O5-C1	3.20	1.48	1.43
3	A	805	NAG	O5-C1	2.70	1.48	1.43
3	A	804	NAG	C1-C2	2.37	1.55	1.52
3	A	802	NAG	C1-C2	2.21	1.55	1.52
3	A	802	NAG	O5-C1	2.06	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	NAG	C1-O5-C5	3.13	116.44	112.19
3	A	806	NAG	C1-O5-C5	3.06	116.33	112.19
3	A	805	NAG	C2-N2-C7	2.57	126.56	122.90
3	A	804	NAG	C1-O5-C5	2.36	115.40	112.19
3	A	801	NAG	C2-N2-C7	2.35	126.24	122.90
3	A	805	NAG	C1-O5-C5	2.30	115.31	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

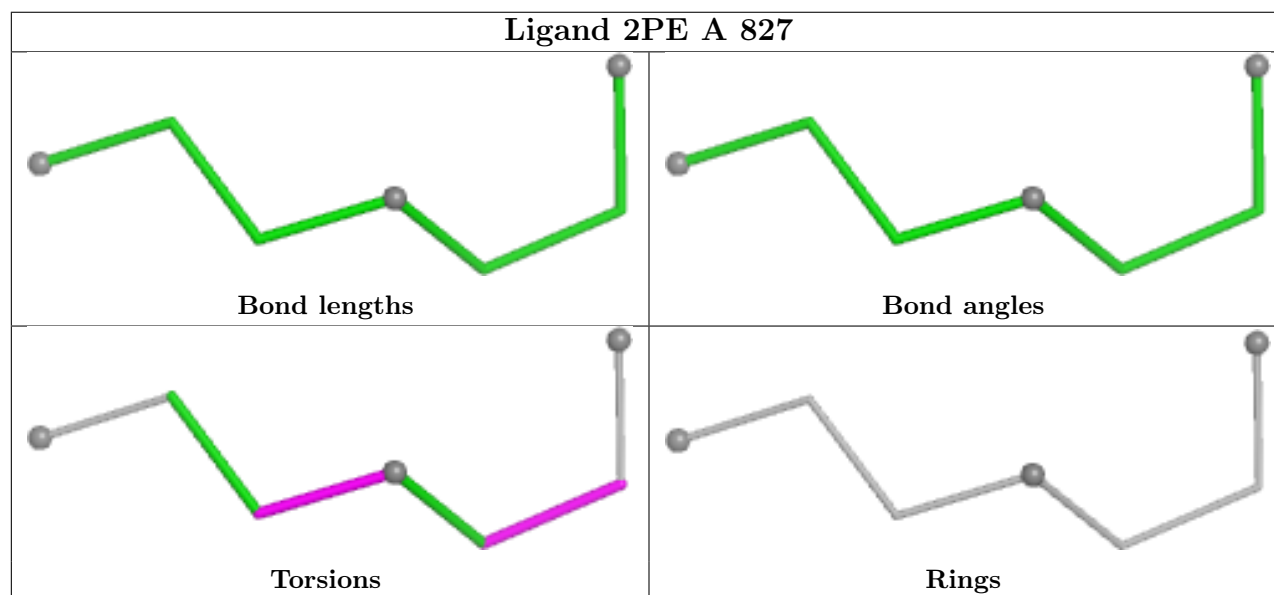
Mol	Chain	Res	Type	Atoms
3	A	806	NAG	C4-C5-C6-O6
3	A	806	NAG	O5-C5-C6-O6
3	A	801	NAG	C8-C7-N2-C2
3	A	801	NAG	O7-C7-N2-C2
3	A	805	NAG	C8-C7-N2-C2
3	A	805	NAG	O7-C7-N2-C2
3	A	806	NAG	C8-C7-N2-C2
3	A	806	NAG	O7-C7-N2-C2
3	A	801	NAG	O5-C5-C6-O6
5	A	809	EDO	O1-C1-C2-O2
5	A	811	EDO	O1-C1-C2-O2
3	A	801	NAG	C4-C5-C6-O6
3	A	802	NAG	O5-C5-C6-O6
5	A	812	EDO	O1-C1-C2-O2
10	A	827	2PE	O4-C5-C6-O7
10	A	827	2PE	C2-C3-O4-C5
5	A	814	EDO	O1-C1-C2-O2
5	C	101	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	825	SO4	1	0
5	A	818	EDO	2	0
5	A	809	EDO	1	0
5	C	101	EDO	1	0
6	A	820	IPA	1	0
3	A	805	NAG	2	0
9	A	826	SO4	1	0
3	A	801	NAG	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 ⓘ

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	677/730 (92%)	0.17	32 (4%) 36 33	22, 53, 86, 131	29 (4%)
2	C	17/24 (70%)	0.35	1 (5%) 28 25	48, 56, 70, 82	0
All	All	694/754 (92%)	0.18	33 (4%) 35 32	22, 53, 86, 131	29 (4%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	17	GLY	5.4
1	A	338	ASN	4.1
1	A	677	PRO	4.0
1	A	704	ILE	3.9
1	A	679	ILE	3.8
1	A	634	GLU	3.6
1	A	678	ARG	3.5
1	A	621	ARG	3.3
1	A	662	MET	3.0
1	A	635	TRP	2.9
1	A	339	VAL	2.9
1	A	289	PRO	2.9
1	A	707	SER	2.8
1	A	658	VAL	2.8
1	A	618	ILE	2.8
1	A	676	LYS	2.6
1	A	700	VAL	2.6
1	A	656	LEU	2.6
1	A	663	ILE	2.5
1	A	657	LYS	2.5
1	A	553	LYS	2.4
1	A	620	VAL	2.4
1	A	619	LYS	2.3
1	A	428	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	675	LEU	2.2
1	A	665	PHE	2.2
1	A	655	PHE	2.2
1	A	650	ALA	2.2
1	A	427	ASP	2.1
1	A	19	SER	2.1
1	A	341	LYS	2.1
1	A	703	ALA	2.1
1	A	87	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	DTY	C	1	12/13	0.90	0.10	47,58,70,70	0

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(Å ²)	Q<0.9
3	NAG	A	805	14/15	0.52	0.18	76,89,107,116	0
3	NAG	A	806	14/15	0.66	0.14	73,89,107,114	0
3	NAG	A	802	14/15	0.71	0.17	78,96,113,116	0
9	SO4	A	825	5/5	0.74	0.15	59,78,97,100	0
3	NAG	A	801	14/15	0.80	0.13	61,80,94,99	0
5	EDO	C	101	4/4	0.81	0.16	63,76,85,88	0
6	IPA	A	819	4/4	0.81	0.28	46,68,82,90	0
3	NAG	A	803	14/15	0.81	0.12	65,89,110,111	0

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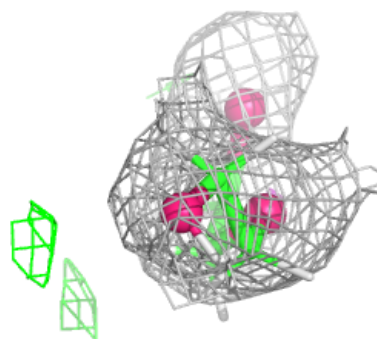
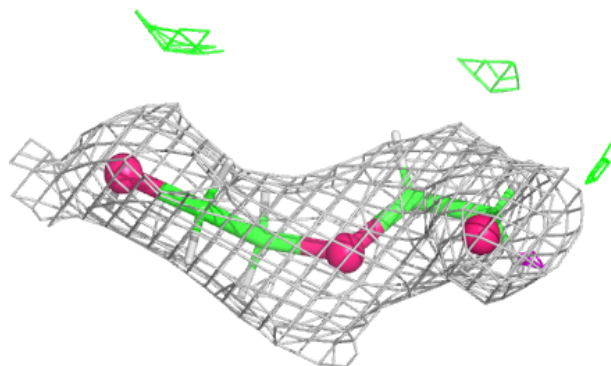
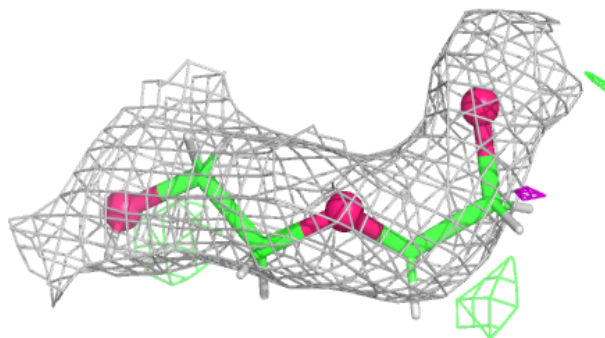
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	IPA	A	820	4/4	0.83	0.18	46,58,69,80	0
5	EDO	A	812	4/4	0.83	0.16	57,68,79,89	0
5	EDO	A	816	4/4	0.85	0.20	48,69,76,84	0
5	EDO	A	817	4/4	0.85	0.16	65,78,81,85	0
5	EDO	A	815	4/4	0.87	0.12	56,70,85,85	0
3	NAG	A	804	14/15	0.88	0.10	63,80,91,101	0
5	EDO	A	809	4/4	0.88	0.14	45,56,64,77	0
5	EDO	A	814	4/4	0.89	0.14	50,63,76,76	0
5	EDO	A	818	4/4	0.89	0.11	54,65,73,76	0
10	2PE	A	827	7/28	0.89	0.14	54,65,74,74	0
5	EDO	A	813	4/4	0.90	0.12	56,68,88,89	0
5	EDO	A	811	4/4	0.91	0.15	52,67,78,94	0
7	CL	A	822	1/1	0.92	0.10	75,75,75,75	0
5	EDO	A	810	4/4	0.93	0.12	42,53,67,81	0
7	CL	A	823	1/1	0.95	0.09	54,54,54,54	0
9	SO4	A	826	5/5	0.96	0.06	61,66,68,82	0
8	NA	A	824	1/1	0.97	0.06	44,44,44,44	0
5	EDO	A	808	4/4	0.97	0.08	54,65,76,76	0
7	CL	A	821	1/1	0.99	0.04	44,44,44,44	0
4	ZN	A	807	1/1	1.00	0.03	45,45,45,45	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 2PE A 827:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.