



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:31 pm BST

PDB ID : 2JCH
Title : Structural and mechanistic basis of penicillin binding protein inhibition by lactivicins
Authors : Macheboeuf, P.; Fisher, D.S.; Brown, T.J.; Zervosen, A.; Luxen, A.; Joris, B.; Dessen, A.; Schofield, C.J.
Deposited on : 2006-12-23
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

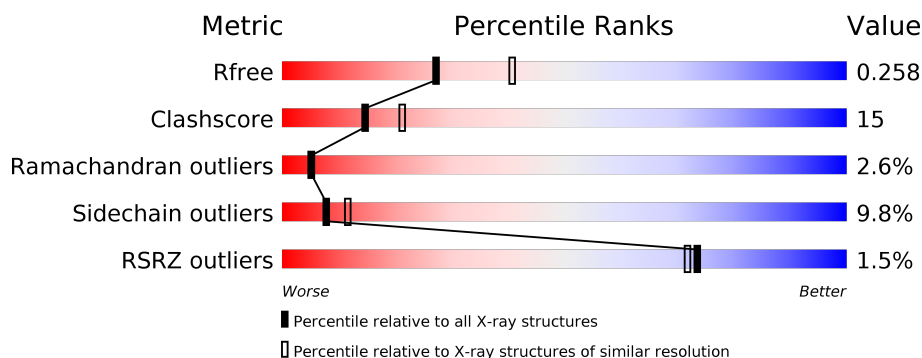
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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	720	<p>43% 16% 5% 36%</p>

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
4	EDO	A	1792	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3758 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 PENICILLIN-BINDING PROTEIN 1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	461	3575	2239	605	715	16	3	4	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	SER	ALA	engineered mutation	UNP O70038
A	123	MET	LEU	engineered mutation	UNP O70038
A	158	ASN	LYS	engineered mutation	UNP O70038
A	162	PRO	ARG	engineered mutation	UNP O70038
A	336	GLN	ARG	engineered mutation	UNP O70038
A	686	GLN	ARG	engineered mutation	UNP O70038
A	687	GLN	ARG	engineered mutation	UNP O70038

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

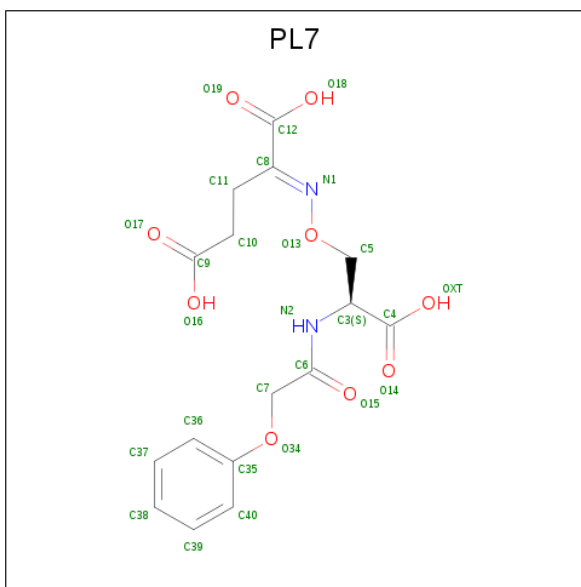
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is (2E)-2-({(2S)-2-CARBOXY-2-[(PHENOXYACETYL)AMINO]ETHOXY}IMINO)PENTANEDIOIC ACID (three-letter code: PL7) (formula: C₁₆H₁₈N₂O₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			26	16	2	8		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total	O	0	0
			147	147		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	105.84Å 143.58Å 97.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	85.13 – 2.40 19.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (85.13-2.40) 99.5 (19.90-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.203 , 0.262 0.202 , 0.258	Depositor DCC
R_{free} test set	1434 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	34.9	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3758	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% 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: PL7, CL, EDO, 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	1.47	11/3659 (0.3%)	1.20	18/4966 (0.4%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	GLN	CG-CD	34.86	2.31	1.51
1	A	411	TYR	CE1-CZ	6.55	1.47	1.38
1	A	346	GLU	CG-CD	6.30	1.61	1.51
1	A	522	TYR	CE1-CZ	5.88	1.46	1.38
1	A	409	TYR	CG-CD1	5.85	1.46	1.39
1	A	523	TRP	CE3-CZ3	5.52	1.47	1.38
1	A	459	ALA	CA-CB	5.38	1.63	1.52
1	A	408	ASP	CB-CG	5.28	1.62	1.51
1	A	717	PHE	CE2-CZ	5.17	1.47	1.37
1	A	586	ILE	CA-CB	5.08	1.66	1.54
1	A	445	GLU	CG-CD	5.03	1.59	1.51

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	GLN	CB-CG-CD	-10.67	83.85	111.60
1	A	626	SER	N-CA-CB	-10.18	95.23	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	456	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	A	456	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	716	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	111	SER	CA-CB-OG	-6.58	93.43	111.20
1	A	344	LEU	CB-CG-CD2	-6.55	99.87	111.00
1	A	716	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	647	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	534	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	529	ARG	CG-CD-NE	5.67	123.70	111.80
1	A	400	SER	N-CA-CB	5.64	118.96	110.50
1	A	466	LEU	CB-CG-CD1	5.62	120.55	111.00
1	A	506	MET	CG-SD-CE	5.49	108.98	100.20
1	A	669	ARG	CG-CD-NE	-5.17	100.94	111.80
1	A	112	ASP	CB-CG-OD1	5.13	122.91	118.30
1	A	627	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	778	ASP	CB-CG-OD1	5.03	122.83	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	ASP	Peptide
1	A	666	SER	Peptide

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	3575	0	3444	107	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0
4	A	4	0	6	4	1
5	A	26	0	15	4	0
6	A	147	0	0	3	0
All	All	3758	0	3465	108	1

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 15.

All (108) 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:628:VAL:HG22	4:A:1792:EDO:H11	1.12	1.12
1:A:656:ASN:HB3	5:A:1793:PL7:H7C2	1.33	1.06
1:A:780:GLN:HG3	6:A:2143:HOH:O	1.52	1.05
1:A:628:VAL:CG2	4:A:1792:EDO:H11	1.94	0.97
1:A:628:VAL:HG22	4:A:1792:EDO:C1	1.98	0.92
1:A:372:GLN:HG3	1:A:373:LYS:H	1.33	0.90
1:A:569:ASN:ND2	1:A:583:LYS:HG2	1.86	0.89
1:A:356:ALA:O	1:A:357:GLN:HG3	1.73	0.88
1:A:760:LYS:H	1:A:760:LYS:HD3	1.43	0.82
1:A:680:ASP:OD1	1:A:682:HIS:HD2	1.62	0.81
1:A:657:GLN:HB2	1:A:659:GLU:OE2	1.81	0.80
1:A:372:GLN:HG3	1:A:373:LYS:N	1.98	0.79
1:A:343:THR:HG21	1:A:392:THR:HG21	1.64	0.78
1:A:670:LEU:HD11	1:A:711:ILE:HG13	1.67	0.75
1:A:628:VAL:HG13	4:A:1792:EDO:H21	1.66	0.74
1:A:569:ASN:HD22	1:A:583:LYS:HG2	1.53	0.72
1:A:589:ILE:HG13	1:A:598:TYR:HB3	1.73	0.71
1:A:357:GLN:HA	1:A:360:ASN:O	1.92	0.70
1:A:711:ILE:HG22	6:A:2118:HOH:O	1.93	0.68
1:A:343:THR:HG21	1:A:392:THR:CG2	2.25	0.67
1:A:372:GLN:O	1:A:374:PHE:N	2.27	0.66
1:A:381:LYS:HD2	1:A:385:ASN:HD22	1.60	0.66
1:A:359:ASP:N	1:A:359:ASP:OD1	2.29	0.65
1:A:780:GLN:HG2	1:A:781:ASN:N	2.11	0.65
1:A:640:ASN:ND2	1:A:643:LEU:H	1.96	0.64
1:A:695:ASN:O	1:A:699:HIS:HD2	1.81	0.63
1:A:106:SER:HA	1:A:388:TYR:O	1.98	0.63
1:A:485:ASN:HD22	1:A:520:PRO:HD3	1.63	0.62
1:A:347:ALA:O	1:A:350:ARG:HB2	2.01	0.61
1:A:344:LEU:O	1:A:348:GLN:HG3	1.99	0.61
1:A:381:LYS:HD2	1:A:385:ASN:ND2	2.14	0.61
1:A:656:ASN:HB3	5:A:1793:PL7:C7	2.21	0.61
1:A:399:HIS:HD2	1:A:436:GLY:HA2	1.65	0.61
1:A:602:ASP:OD1	1:A:604:PRO:HD3	2.02	0.58
1:A:455:LYS:O	1:A:456:ARG:HG2	2.04	0.58
1:A:787:VAL:O	1:A:789:SER:N	2.36	0.58
1:A:732:THR:HG21	1:A:766:THR:HG21	1.85	0.58
1:A:569:ASN:ND2	1:A:583:LYS:CG	2.66	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:779:TYR:O	1:A:783:TRP:HB2	2.06	0.56
1:A:430:GLN:O	1:A:581:HIS:CD2	2.59	0.56
1:A:656:ASN:O	1:A:657:GLN:HG2	2.05	0.56
1:A:743:GLY:O	1:A:744:LYS:HB2	2.05	0.55
1:A:371:THR:HA	1:A:372:GLN:C	2.28	0.54
1:A:485:ASN:ND2	1:A:520:PRO:HD3	2.22	0.54
1:A:355:LEU:C	1:A:357:GLN:H	2.11	0.54
1:A:738:LYS:HB3	1:A:745:GLU:OE2	2.07	0.54
1:A:361:VAL:HG13	1:A:375:TYR:OH	2.08	0.54
1:A:371:THR:HA	1:A:372:GLN:HB3	1.90	0.53
1:A:110:TYR:CE2	1:A:396:GLN:HG3	2.44	0.52
1:A:458:PRO:HG2	1:A:462:THR:OG1	2.09	0.52
1:A:355:LEU:C	1:A:357:GLN:N	2.62	0.52
5:A:1793:PL7:H111	5:A:1793:PL7:H37	1.92	0.52
1:A:385:ASN:O	1:A:386:GLY:O	2.28	0.51
1:A:381:LYS:HG3	1:A:382:GLU:N	2.25	0.51
1:A:350:ARG:HD2	1:A:598:TYR:CZ	2.46	0.51
1:A:337:ASP:O	1:A:341:PHE:HD2	1.94	0.51
1:A:343:THR:HG22	1:A:586:ILE:HD11	1.93	0.51
1:A:371:THR:CA	1:A:372:GLN:HB3	2.40	0.51
1:A:442:ASN:ND2	1:A:445:GLU:HG2	2.26	0.50
1:A:787:VAL:HG12	1:A:788:GLY:N	2.27	0.50
1:A:345:ALA:O	1:A:349[A]:GLU:HG3	2.12	0.49
1:A:428:ASP:OD1	1:A:430:GLN:N	2.42	0.49
1:A:569:ASN:ND2	6:A:2076:HOH:O	2.44	0.49
1:A:787:VAL:C	1:A:789:SER:H	2.16	0.49
1:A:108:ILE:HG21	1:A:343:THR:HG21	1.94	0.48
1:A:371:THR:N	1:A:372:GLN:HB3	2.28	0.48
1:A:746:VAL:HG12	1:A:747:GLU:N	2.29	0.48
1:A:424:ASN:HD22	1:A:438:VAL:HB	1.79	0.48
1:A:482:ILE:HG21	1:A:770:PHE:HE2	1.78	0.48
1:A:107:GLU:HB3	1:A:117:ALA:O	2.14	0.47
1:A:457:SER:OG	1:A:557:GLY:O	2.24	0.47
1:A:346:GLU:HG2	1:A:586:ILE:HG12	1.96	0.47
1:A:611:ALA:O	1:A:615:ILE:HG13	2.15	0.47
1:A:656:ASN:CB	5:A:1793:PL7:H7C2	2.23	0.47
1:A:463:LYS:HG2	1:A:555:PRO:O	2.15	0.47
1:A:361:VAL:CG1	1:A:375:TYR:OH	2.63	0.46
1:A:602:ASP:CG	1:A:604:PRO:HD3	2.36	0.46
1:A:354:TYR:CE1	1:A:358:ARG:HB2	2.51	0.46
1:A:738:LYS:HA	1:A:746:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:TYR:O	1:A:499:ALA:HB3	2.15	0.46
1:A:361:VAL:HG12	1:A:362:SER:N	2.31	0.45
1:A:354:TYR:O	1:A:357:GLN:N	2.46	0.45
1:A:371:THR:HG22	1:A:372:GLN:O	2.17	0.45
1:A:568:THR:HG23	1:A:671:THR:HG22	2.00	0.44
1:A:734:GLN:HG2	1:A:764:PRO:HG2	1.99	0.44
1:A:486:TYR:CD1	1:A:778:ASP:HB3	2.53	0.44
1:A:388:TYR:HE1	1:A:597:VAL:HG21	1.82	0.44
1:A:432:GLY:O	1:A:583:LYS:HA	2.18	0.43
1:A:343:THR:CG2	1:A:392:THR:CG2	2.95	0.43
1:A:640:ASN:C	1:A:640:ASN:HD22	2.21	0.43
1:A:413:LEU:HD22	1:A:676:ILE:HG21	2.01	0.43
1:A:430:GLN:O	1:A:581:HIS:NE2	2.52	0.43
1:A:372:GLN:HE21	1:A:372:GLN:HB2	1.56	0.43
1:A:455:LYS:C	1:A:456:ARG:HG2	2.39	0.43
1:A:337:ASP:HB3	1:A:443:TYR:CE1	2.55	0.42
1:A:757:TRP:NE1	1:A:763:ALA:HB2	2.34	0.42
1:A:360:ASN:HD22	1:A:360:ASN:HA	1.67	0.42
1:A:371:THR:CG2	1:A:374:PHE:H	2.33	0.42
1:A:569:ASN:HD21	1:A:583:LYS:H	1.68	0.41
1:A:734:GLN:NE2	1:A:766:THR:HA	2.36	0.41
1:A:362:SER:HB3	1:A:363:ALA:H	1.65	0.41
1:A:616[A]:MET:HA	1:A:619:LEU:HD12	2.03	0.41
1:A:515:TYR:O	1:A:516:SER:CB	2.67	0.40
1:A:349[B]:GLU:OE1	1:A:376:ARG:NH2	2.55	0.40
1:A:357:GLN:CA	1:A:360:ASN:O	2.67	0.40
1:A:768:TYR:CE2	1:A:783:TRP:CD1	3.09	0.40

All (1) 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)
4:A:1792:EDO:O1	4:A:1792:EDO:O2[3_655]	1.96	0.24

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	459/720 (64%)	419 (91%)	28 (6%)	12 (3%)	5 5

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	ASN
1	A	361	VAL
1	A	373	LYS
1	A	386	GLY
1	A	657	GLN
1	A	744	LYS
1	A	788	GLY
1	A	356	ALA
1	A	743	GLY
1	A	745	GLU
1	A	591	ALA
1	A	646	ALA

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	381/590 (65%)	343 (90%)	38 (10%)	7 11

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	SER
1	A	107	GLU
1	A	111	SER
1	A	118	SER
1	A	119	ILE

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Mol	Chain	Res	Type
1	A	337	ASP
1	A	343	THR
1	A	350	ARG
1	A	359	ASP
1	A	371	THR
1	A	372	GLN
1	A	376	ARG
1	A	378	LEU
1	A	381	LYS
1	A	400	SER
1	A	506	MET
1	A	516	SER
1	A	567	HIS
1	A	583	LYS
1	A	585	VAL
1	A	589	ILE
1	A	595	ARG
1	A	601	GLN
1	A	603	LYS
1	A	640	ASN
1	A	656	ASN
1	A	681	ASN
1	A	706	GLN
1	A	716	ARG
1	A	719	LEU
1	A	727[A]	GLU
1	A	727[B]	GLU
1	A	742	GLU
1	A	749	THR
1	A	760	LYS
1	A	780	GLN
1	A	784	SER
1	A	789	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	348	GLN
1	A	360	ASN
1	A	372	GLN
1	A	385	ASN
1	A	399	HIS

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Mol	Chain	Res	Type
1	A	403	GLN
1	A	424	ASN
1	A	485	ASN
1	A	494	ASN
1	A	514	ASN
1	A	567	HIS
1	A	569	ASN
1	A	606	GLN
1	A	635	ASN
1	A	640	ASN
1	A	656	ASN
1	A	657	GLN
1	A	678	HIS
1	A	682	HIS
1	A	687	GLN
1	A	699	HIS
1	A	706	GLN
1	A	734	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	EDO	A	1792	-	3,3,3	0.90	0	2,2,2	0.52	0
5	PL7	A	1793	1	20,26,27	1.71	4 (20%)	22,32,34	1.71	4 (18%)
2	SO4	A	1790	-	4,4,4	0.71	0	6,6,6	0.62	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	EDO	A	1792	-	-	1/1/1/1	-
5	PL7	A	1793	1	-	6/18/26/28	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1793	PL7	C12-C8	-3.86	1.46	1.52
5	A	1793	PL7	O13-N1	-3.25	1.36	1.42
5	A	1793	PL7	C8-N1	-3.00	1.26	1.28
5	A	1793	PL7	C40-C35	2.31	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1793	PL7	C5-O13-N1	4.16	112.90	108.37
5	A	1793	PL7	C11-C10-C9	-3.96	106.03	112.67
5	A	1793	PL7	C10-C11-C8	-3.50	103.01	113.44
5	A	1793	PL7	O34-C7-C6	2.42	117.49	110.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1793	PL7	C5-C3-N2-C6
5	A	1793	PL7	C4-C3-N2-C6
5	A	1793	PL7	C40-C35-O34-C7
5	A	1793	PL7	C36-C35-O34-C7
4	A	1792	EDO	O1-C1-C2-O2

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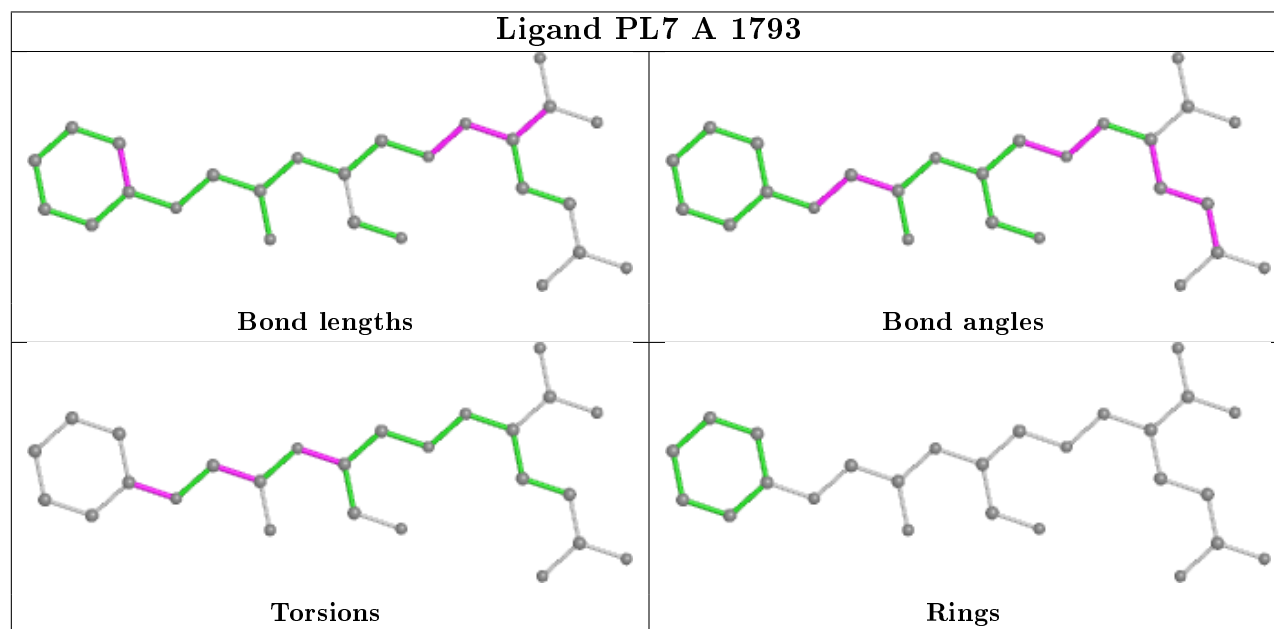
Mol	Chain	Res	Type	Atoms
5	A	1793	PL7	N2-C6-C7-O34
5	A	1793	PL7	O15-C6-C7-O34

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1792	EDO	4	1
5	A	1793	PL7	4	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 ⓘ

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 [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	461/720 (64%)	-0.40	7 (1%) 73 72	17, 33, 64, 89	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	360	ASN	5.4
1	A	359	ASP	3.3
1	A	743	GLY	2.6
1	A	361	VAL	2.3
1	A	596	VAL	2.2
1	A	788	GLY	2.1
1	A	387	GLY	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](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
4	EDO	A	1792	4/4	0.78	0.50	99,100,101,102	0

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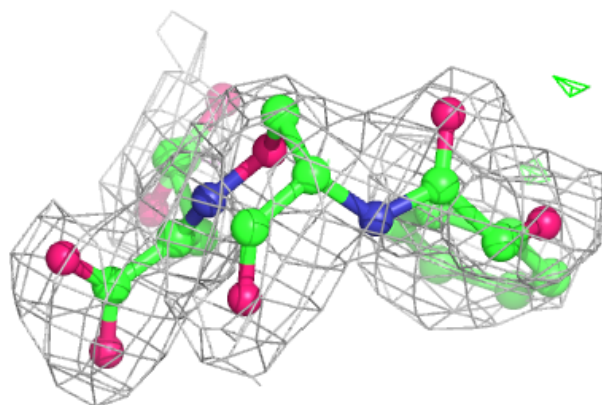
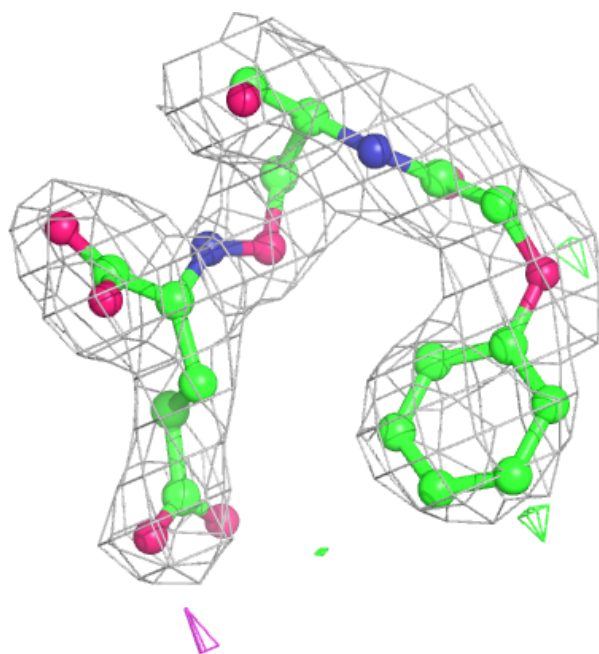
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PL7	A	1793	26/27	0.94	0.15	26,42,55,59	0
2	SO4	A	1790	5/5	0.98	0.17	40,41,45,48	0
3	CL	A	1791	1/1	0.99	0.10	26,26,26,26	1

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 PL7 A 1793:

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.