



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:40 PM UTC

PDB ID : 2JCH / pdb_00002jch
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 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

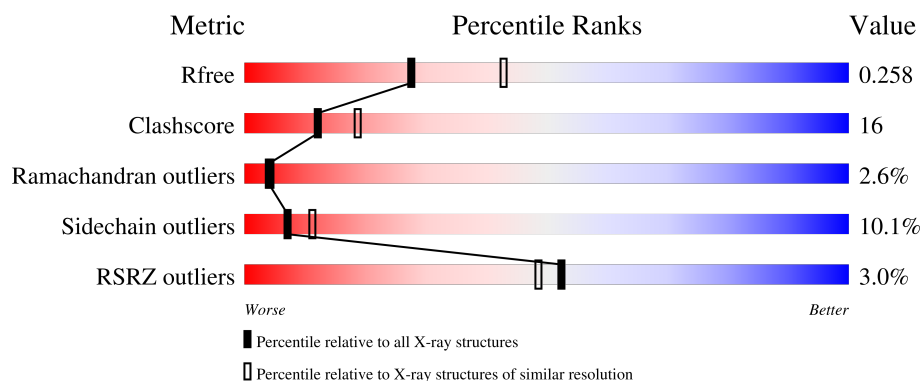
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 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	720	

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	-

2 Entry composition [i](#)

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.

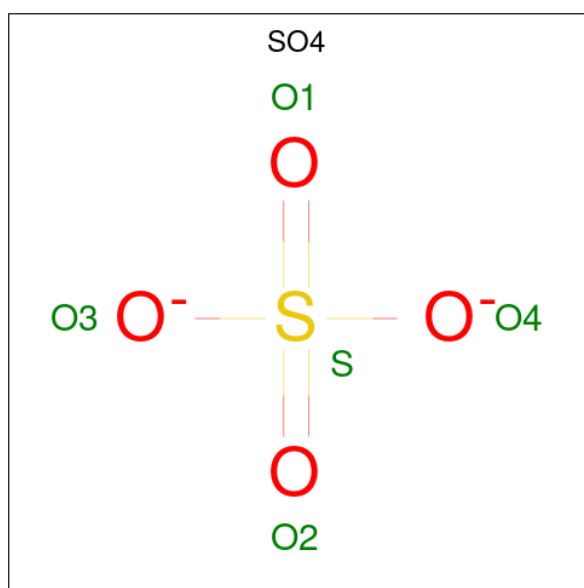
- Molecule 1 is a protein called PENICILLIN-BINDING PROTEIN 1B.

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 (CCD ID: SO4) (formula: O₄S).

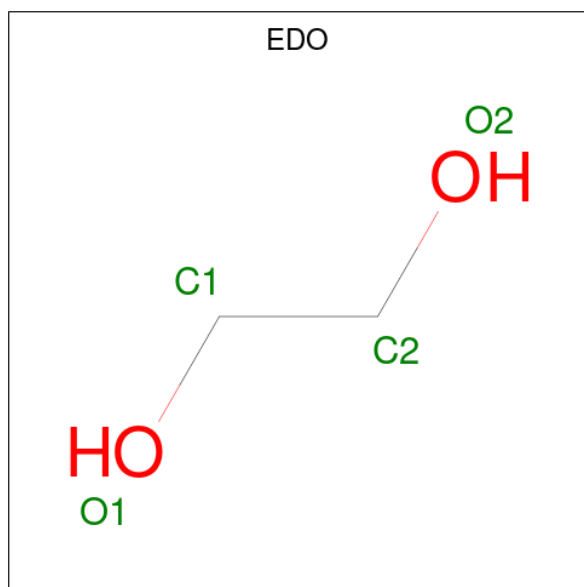


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

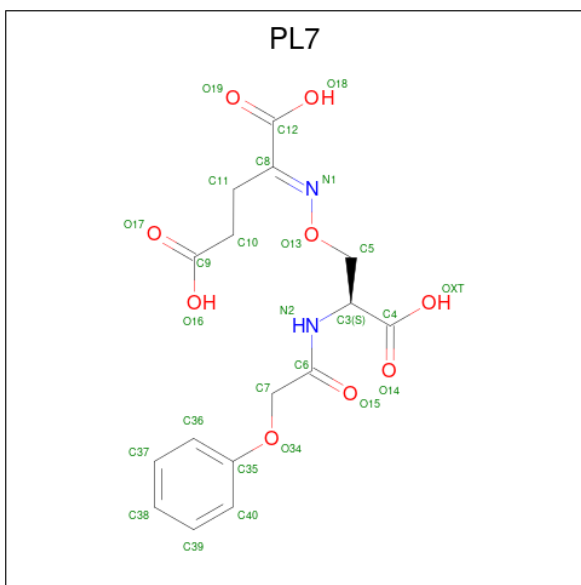
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: 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 (CCD ID: 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		

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.

Chain A:

Category	Value	Category	Value	Category	Value	Category	Value	Category	Value
Q706	K610	N485	D377	SER	GLN	PRO	SER	GLY	GLN
I711	A611	Y486	L378	TYR	THR	THR	TYR	GLU	THR
F717	I615	T488	A379	LYS	VAL	ALA	LYS	ASN	GLY
A718	M616	Y498	K381	ASP	PRO	ARG	ASP	LYS	ILE
L719	Q617	A499	E382	TYR	GLN	LYS	TYR	LYS	ALA
I727	L619	M506	I383	LEU	ALA	ALA	LEU	ILE	TYR
T732	L624	S606	E384	ASP	PHE	GLU	GLY	ILE	GLY
G733	S625	L513	G387	GLN	ALA	ILE	GLN	ALA	VAL
Q734	S626	H514	Y388	ASP	GLY	VAL	ASP	THR	ALA
K735	R627	Y515	K389	PHE	LEU	ALA	LEU	LEU	LEU
K738	V628	S516	I390	PRO	PRO	GLU	ASP	PHE	VAL
E742	T631	I519	T392	SER	SER	LEU	GLY	LYS	ARG
G743	F632	P620	Q396	THR	ILE	GLU	VAL	GLU	VAL
K744	K633	A521	K397	VAL	THR	ARG	THR	PRO	VAL
E745	T637	Y522	I398	GLY	TYR	ALA	GLN	HIS	PRO
V746	M640	R529	H399	ILE	SER	GLY	TYR	GLY	GLN
E747	N640	M639	S400	SER	PRO	VAL	GLY	VAL	THR
T748	L643	E749	Y406	GLN	TYR	ASP	THR	GLU	GLU
G750	A646	E552	A407	D337	GLU	GLU	GLY	LEU	LEU
S755	M656	P555	D408	F341	ASN	ILE	VAL	ASN	VAL
Y756	K656	M556	L413	T342	THR	THR	THR	ASN	ASN
W757	Q657	G557	L413	L343	GLY	THR	GLY	GLY	GLN
K760	D658	E559	N424	A345	LEU	LEU	TYR	LYS	VAL
A763	R669	S666	D428	E346	LYS	LEU	LEU	PRO	VAL
P764	E669	T667	N429	A347	SER	ASN	ASN	ILE	ALA
A765	R669	T568	Q430	Q348	GLU	VAL	GLY	LEU	THR
T766	L670	M569	T431	R350	ASP	ALA	ASP	LYS	ILE
G767	W675	E579	G432	K351	LEU	PHE	PHE	ILE	ILE
D778	H678	Y580	G436	Y354	GLY	GLY	GLY	VAL	GLY
Y779	D679	H581	V438	L355	ILE	ARG	ARG	GLY	VAL
Q780	D680	K582	H584	A356	GLY	ASN	ASN	LEU	LEU
N781	N681	K588	Y443	R358	ARG	ALA	ALA	GLY	GLY
A782	H682	I589	Q444	D359	ALA	LYS	ILE	GLY	GLY
W783	S683	E590	E445	V361	VAL	ALA	ALA	THR	THR
G784	A688	A591	D453	A363	LEU	LEU	ALA	LEU	GLU
T786	N692	R595	T454	LYS	TYR	ALA	ALA	THR	SER
G788	N695	Y596	R456	GLU	MET	GLN	GLN	GLN	ASP
S789	Q601	V597	S457	LEU	TYR	ARG	ALA	GLN	GLY
LEU	D602	Y598	P458	ASN	THR	GLY	ALA	ILE	ASP
PRO	K603	Q604	A459	GLY	ALA	ILE	GLY	GLN	THR
	A703		S460	A370	ALA	THR	GLY	GLN	SER
			T461	T371	LEU	PHE	GLY	ILE	ILE
			K463	Q372	SER	GLY	VAL	SER	SER
			K463	K373	LYS	VAL	VAL	SER	GLY
				F374	ASP	ASP	GLY	GLU	ASP
				X375	ALA	ALA	ALA	THR	THR
				P376	THR	SER	THR	THR	THR

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 85.13 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (85.13-2.40) 99.6 (85.13-2.40)	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 (4.86%)	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 , 40.2	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	0.94	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: CL, PL7, 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	1.75	37/3659 (1.0%)	1.54	44/4966 (0.9%)

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 (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	GLN	CG-CD	31.67	2.31	1.52
1	A	519	ILE	CA-CB	12.02	1.60	1.54
1	A	586	ILE	CA-CB	9.80	1.66	1.54
1	A	390	ILE	CA-CB	8.18	1.64	1.54
1	A	383	ILE	CA-CB	7.65	1.64	1.54
1	A	116	ILE	CA-CB	6.63	1.61	1.54
1	A	675	TRP	CA-C	6.55	1.60	1.52
1	A	371	THR	CA-C	6.29	1.59	1.53
1	A	624	LEU	C-O	-6.27	1.16	1.24
1	A	643	LEU	N-CA	6.09	1.54	1.46
1	A	391	THR	CA-CB	6.02	1.61	1.53
1	A	107	GLU	N-CA	6.01	1.53	1.45
1	A	520	PRO	CA-C	5.98	1.62	1.52
1	A	667	THR	N-CA	5.94	1.52	1.46
1	A	579	VAL	CA-CB	5.78	1.61	1.53
1	A	688	ALA	CA-C	5.77	1.60	1.52
1	A	610	LYS	C-O	-5.73	1.17	1.24
1	A	656	ASN	CA-CB	5.67	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	459	ALA	CA-CB	5.67	1.63	1.52
1	A	770	PHE	CA-C	5.66	1.60	1.52
1	A	488	THR	C-O	-5.62	1.17	1.23
1	A	591	ALA	CA-C	5.60	1.60	1.52
1	A	585	VAL	CA-C	5.58	1.59	1.52
1	A	637	THR	N-CA	5.58	1.53	1.46
1	A	679	ASP	N-CA	5.54	1.53	1.46
1	A	643	LEU	CA-C	5.46	1.60	1.52
1	A	453	ASP	CA-C	5.43	1.57	1.52
1	A	587	SER	N-CA	5.41	1.53	1.46
1	A	115	VAL	CA-CB	5.39	1.60	1.53
1	A	703	ALA	CA-CB	-5.38	1.44	1.53
1	A	580	TYR	N-CA	5.33	1.52	1.46
1	A	560	ILE	C-O	-5.31	1.18	1.24
1	A	755	SER	C-O	-5.21	1.18	1.24
1	A	513	LEU	CA-C	5.18	1.59	1.52
1	A	589	ILE	CA-C	5.18	1.58	1.52
1	A	618	GLY	N-CA	5.07	1.52	1.45
1	A	108	ILE	CA-CB	5.01	1.60	1.54

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	GLN	CB-CG-CD	-16.91	83.85	112.60
1	A	735	LYS	CA-C-N	-9.89	110.73	120.52
1	A	735	LYS	C-N-CA	-9.89	110.73	120.52
1	A	625	SER	N-CA-C	9.23	120.95	111.07
1	A	626	SER	N-CA-CB	-9.13	95.23	110.39
1	A	111	SER	CA-CB-OG	-8.84	93.43	111.10
1	A	513	LEU	N-CA-C	8.41	120.45	111.28
1	A	107	GLU	N-CA-C	7.78	120.74	109.14
1	A	406	VAL	N-CA-C	7.57	118.34	110.62
1	A	396	GLN	N-CA-C	6.68	118.36	111.14
1	A	519	ILE	CA-C-N	-6.62	112.81	119.56
1	A	519	ILE	C-N-CA	-6.62	112.81	119.56
1	A	698	ALA	N-CA-C	-6.54	103.99	112.23
1	A	780	GLN	N-CA-C	-6.25	104.39	111.14
1	A	461	THR	N-CA-C	-6.21	105.56	113.01
1	A	625	SER	CA-CB-OG	-6.20	98.70	111.10
1	A	408	ASP	N-CA-C	6.13	117.96	111.28
1	A	783	TRP	N-CA-C	6.11	118.74	111.71
1	A	619	LEU	N-CA-C	5.87	117.36	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	552	GLU	N-CA-C	5.83	118.39	111.33
1	A	381	LYS	N-CA-C	-5.82	104.31	111.40
1	A	400	SER	N-CA-CB	5.60	118.96	110.28
1	A	711	ILE	N-CA-C	5.59	116.33	110.62
1	A	746	VAL	N-CA-C	5.55	117.20	109.55
1	A	522	TYR	N-CA-C	5.53	117.74	111.11
1	A	785	SER	N-CA-C	-5.47	107.25	114.31
1	A	625	SER	CB-CA-C	-5.47	102.30	110.88
1	A	656	ASN	N-CA-C	5.45	117.80	109.62
1	A	750	GLY	N-CA-C	5.43	118.68	110.97
1	A	670	LEU	N-CA-C	5.37	118.03	109.81
1	A	529	ARG	CG-CD-NE	5.32	123.70	112.00
1	A	683	SER	N-CA-C	5.31	117.73	110.24
1	A	656	ASN	N-CA-CB	5.26	116.94	110.53
1	A	717	PHE	N-CA-C	-5.21	102.57	110.28
1	A	692	ASN	N-CA-C	5.16	116.71	111.14
1	A	516	SER	N-CA-CB	-5.15	104.64	112.47
1	A	631	THR	CA-C-N	5.14	127.49	120.54
1	A	631	THR	C-N-CA	5.14	127.49	120.54
1	A	631	THR	N-CA-C	5.13	119.26	113.15
1	A	656	ASN	CA-C-N	5.12	131.32	121.54
1	A	656	ASN	C-N-CA	5.12	131.32	121.54
1	A	379	ALA	N-CA-C	5.11	117.25	111.11
1	A	539	MET	N-CA-C	5.07	116.81	111.28
1	A	669	ARG	CG-CD-NE	-5.03	100.94	112.00

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	109	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	110	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 16.

All (110) 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:HD3	1:A:760:LYS:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:355:LEU:C	1:A:357:GLN:H	2.11	0.58
1:A:371:THR:HA	1:A:372:GLN:C	2.28	0.58
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
1:A:355:LEU:C	1:A:357:GLN:N	2.62	0.56
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:485:ASN:ND2	1:A:520:PRO:HD3	2.22	0.54
1:A:738:LYS:HB3	1:A:745:GLU:OE2	2.07	0.54
1:A:787:VAL:C	1:A:789:SER:H	2.16	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:351:MET:HE3	1:A:382:GLU:HG3	1.91	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:602:ASP:CG	1:A:604:PRO:HD3	2.36	0.51
1:A:350:ARG:HD2	1:A:598:TYR:CZ	2.46	0.51
1:A:381:LYS:HG3	1:A:382:GLU:N	2.25	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: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:640:ASN:C	1:A:640:ASN:HD22	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:455:LYS:C	1:A:456:ARG:HG2	2.39	0.47
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:463:LYS:HG2	1:A:555:PRO:O	2.15	0.47
1:A:656:ASN:CB	5:A:1793:PL7:H7C2	2.23	0.47
1:A:361:VAL:CG1	1:A:375:TYR:OH	2.63	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
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:388:TYR:HE1	1:A:597:VAL:HG21	1.82	0.44
1:A:486:TYR:CD1	1:A:778:ASP:HB3	2.53	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: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: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:787:VAL:C	1:A:789:SER:N	2.78	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 [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	459/720 (64%)	419 (91%)	28 (6%)	12 (3%)	4 4

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 [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	381/590 (65%)	342 (90%)	39 (10%)	7 11

All (39) 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
1	A	337	ASP
1	A	343	THR
1	A	350	ARG
1	A	359	ASP
1	A	371	THR
1	A	376	ARG
1	A	378	LEU
1	A	381	LYS
1	A	397	LYS
1	A	400	SER
1	A	506	MET
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	610	LYS
1	A	633	LYS
1	A	640	ASN
1	A	656	ASN
1	A	681	ASN
1	A	706	GLN
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	787	VAL

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Mol	Chain	Res	Type
1	A	789	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) 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
1	A	403	GLN
1	A	424	ASN
1	A	449	ASN
1	A	485	ASN
1	A	494	ASN
1	A	531	ASN
1	A	567	HIS
1	A	569	ASN
1	A	640	ASN
1	A	657	GLN
1	A	678	HIS
1	A	682	HIS
1	A	699	HIS
1	A	734	GLN
1	A	781	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
5	PL7	A	1793	1	23,26,27	1.42	3 (13%)	25,32,34	3.49	7 (28%)
4	EDO	A	1792	-	3,3,3	0.85	0	2,2,2	0.44	0
2	SO4	A	1790	-	4,4,4	0.78	0	6,6,6	0.61	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
5	PL7	A	1793	1	-	12/25/26/28	0/1/1/1
4	EDO	A	1792	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1793	PL7	O13-N1	-3.28	1.36	1.42
5	A	1793	PL7	C8-N1	-2.78	1.26	1.28
5	A	1793	PL7	C40-C35	2.42	1.43	1.38

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1793	PL7	O13-N1-C8	15.31	134.34	111.47
5	A	1793	PL7	C5-O13-N1	4.21	112.90	108.33
5	A	1793	PL7	C10-C11-C8	-3.46	103.01	113.51
5	A	1793	PL7	C11-C10-C9	-2.88	106.03	113.67
5	A	1793	PL7	O17-C9-C10	-2.76	114.35	123.09
5	A	1793	PL7	O34-C7-C6	2.43	117.49	110.80
5	A	1793	PL7	C37-C36-C35	2.04	122.07	118.98

There are no chirality outliers.

All (13) torsion outliers are listed below:

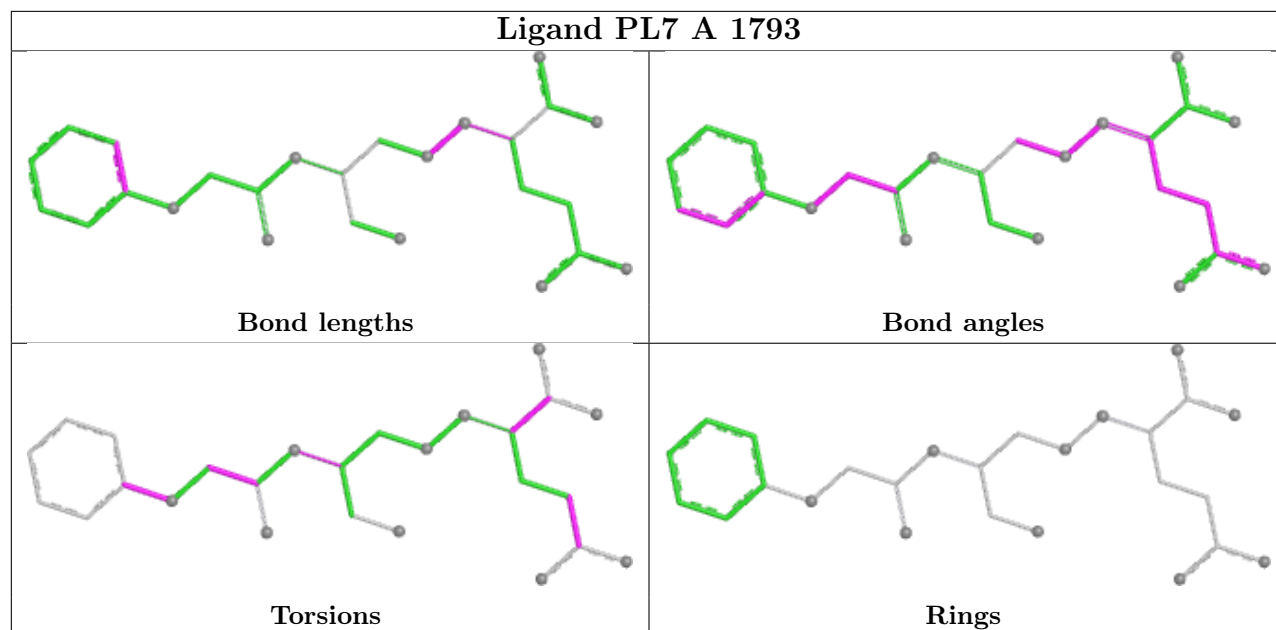
Mol	Chain	Res	Type	Atoms
5	A	1793	PL7	O18-C12-C8-C11
5	A	1793	PL7	O19-C12-C8-N1
5	A	1793	PL7	O18-C12-C8-N1
5	A	1793	PL7	C5-C3-N2-C6
5	A	1793	PL7	C4-C3-N2-C6
5	A	1793	PL7	C40-C35-O34-C7
5	A	1793	PL7	C36-C35-O34-C7
4	A	1792	EDO	O1-C1-C2-O2
5	A	1793	PL7	O19-C12-C8-C11
5	A	1793	PL7	N2-C6-C7-O34
5	A	1793	PL7	O15-C6-C7-O34
5	A	1793	PL7	C11-C10-C9-O17
5	A	1793	PL7	C11-C10-C9-O16

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1793	PL7	4	0
4	A	1792	EDO	4	1

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	461/720 (64%)	-0.18	14 (3%)	52 48	15, 33, 64, 89	5 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	ALA	6.1
1	A	360	ASN	4.4
1	A	370	ALA	3.5
1	A	361	VAL	3.2
1	A	386	GLY	3.2
1	A	359	ASP	2.9
1	A	387	GLY	2.4
1	A	375	TYR	2.3
1	A	358	ARG	2.3
1	A	591	ALA	2.2
1	A	383	ILE	2.2
1	A	356	ALA	2.1
1	A	385	ASN	2.1
1	A	371	THR	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

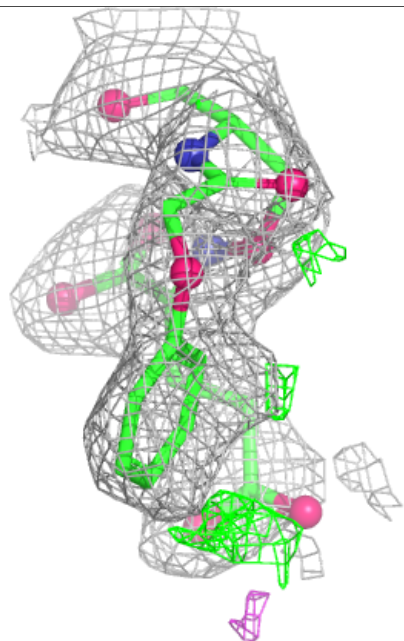
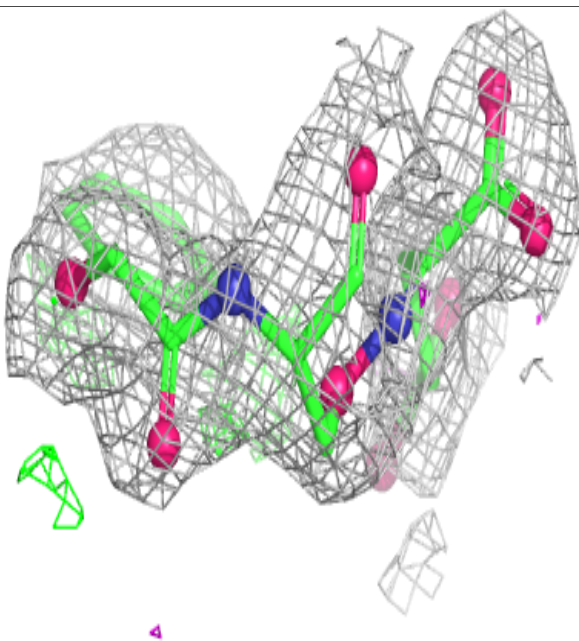
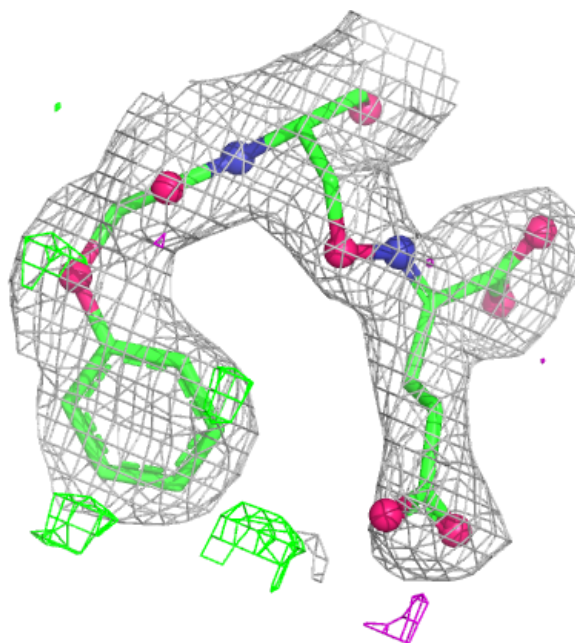
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	A	1792	4/4	0.81	0.31	99,100,101,102	0
5	PL7	A	1793	26/27	0.90	0.11	26,42,55,59	0
2	SO4	A	1790	5/5	0.97	0.13	40,41,45,48	0
3	CL	A	1791	1/1	0.98	0.03	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 [i](#)

There are no such residues in this entry.