



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:01 AM UTC

PDB ID : 7SS8 / pdb_00007ss8
Title : Human P300 complexed with a proline-based inhibitor
Authors : Shewchuk, L.M.; Reid, R.A.
Deposited on : 2021-11-10
Resolution : 2.15 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

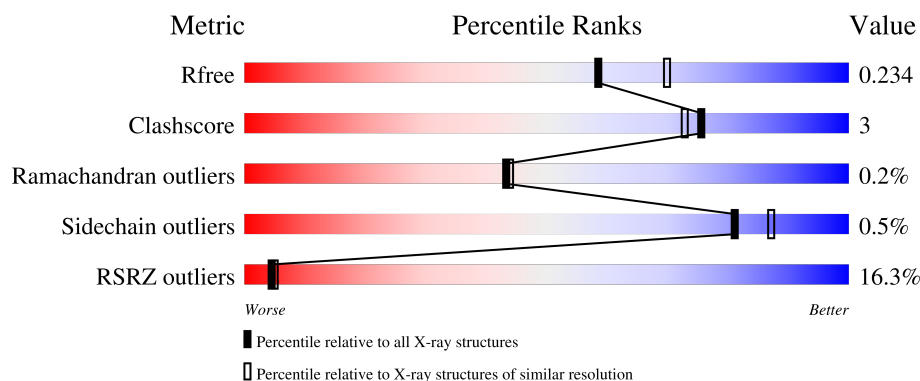
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	569	

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
3	EDO	A	1704	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4103 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 Histone acetyltransferase p300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	4	0
			3855	2496	636	694	29			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1039	GLY	-	expression tag	UNP Q09472
A	1040	GLY	-	expression tag	UNP Q09472
A	1041	HIS	-	expression tag	UNP Q09472
A	1042	HIS	-	expression tag	UNP Q09472
A	1043	HIS	-	expression tag	UNP Q09472
A	1044	HIS	-	expression tag	UNP Q09472
A	1045	HIS	-	expression tag	UNP Q09472
A	1046	HIS	-	expression tag	UNP Q09472
A	1047	GLY	-	expression tag	UNP Q09472
A	1467	PHE	TYR	engineered mutation	UNP Q09472
A	1577	SER	-	linker	UNP Q09472
A	1578	GLY	-	linker	UNP Q09472
A	1579	GLY	-	linker	UNP Q09472
A	1580	SER	-	linker	UNP Q09472
A	1581	GLY	-	linker	UNP Q09472

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

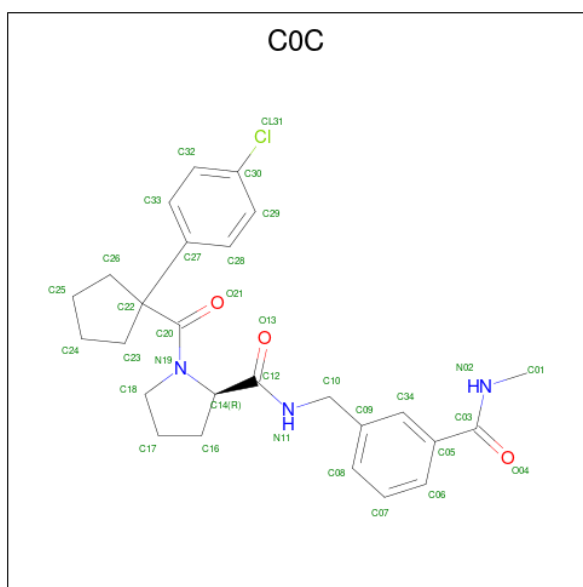
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 4 is 1-[1-(4-chlorophenyl)cyclopentane-1-carbonyl]-N-{[3-(methylcarbamoyl)phenyl]methyl}-D-prolinamide (CCD ID: C0C) (formula: $C_{26}H_{30}ClN_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	0	0
			33	26	1	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	205	Total 205	O 205	0	0

- Molecule 1: Histone acetyltransferase p300



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.85Å 49.50Å 110.60Å 90.00° 102.27° 90.00°	Depositor
Resolution (Å)	38.81 – 2.15 38.81 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.7 (38.81-2.15) 94.7 (38.81-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.200 , 0.230 0.206 , 0.234	Depositor DCC
R_{free} test set	1671 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.443	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4103	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, EDO, C0C

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	1.08	3/3976 (0.1%)	1.33	0/5402

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1381	TYR	C-O	6.46	1.31	1.24
1	A	1464	GLN	C-O	5.93	1.30	1.24
1	A	1430	TYR	C-O	5.74	1.30	1.24

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3855	0	3655	23	0
2	A	2	0	0	0	0
3	A	8	0	12	5	0
4	A	33	0	0	0	0
5	A	205	0	0	0	0
All	All	4103	0	3667	23	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 3.

All (23) 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:1105:LYS:NZ	3:A:1704:EDO:H11	1.84	0.92
1:A:1105:LYS:HZ1	3:A:1704:EDO:H11	1.31	0.92
1:A:1105:LYS:NZ	3:A:1704:EDO:C1	2.55	0.68
1:A:1105:LYS:HZ1	3:A:1704:EDO:C1	2.11	0.60
1:A:1105:LYS:CE	3:A:1704:EDO:H11	2.34	0.57
1:A:1508:PHE:CE2	1:A:1512:VAL:HG21	2.42	0.55
1:A:1308:ASP:OD1	1:A:1311:ARG:NH2	2.40	0.54
1:A:1440:PRO:HB3	1:A:1446:TYR:CD1	2.46	0.51
1:A:1508:PHE:CZ	1:A:1512:VAL:HG21	2.47	0.49
1:A:1339:MET:HE3	1:A:1513:LEU:HB3	1.96	0.46
1:A:1054:LEU:HD23	1:A:1054:LEU:HA	1.85	0.46
1:A:1163:CYS:HB2	1:A:1258:CYS:HB3	2.00	0.44
1:A:1444:ASP:OD2	1:A:1627:ARG:NH2	2.50	0.44
1:A:1501:LEU:HD23	1:A:1501:LEU:HA	1.91	0.44
1:A:1463:LEU:HD11	1:A:1467:PHE:CE2	2.52	0.44
1:A:1471:LEU:O	1:A:1475:VAL:HG23	2.18	0.43
1:A:1154:ASP:HB3	1:A:1155:PRO:CD	2.49	0.43
1:A:1079:VAL:HG13	1:A:1084:LEU:HD12	2.02	0.41
1:A:1631:LEU:HD23	1:A:1631:LEU:HA	1.98	0.40
1:A:1419:ILE:HG12	1:A:1474:ALA:HB2	2.02	0.40
1:A:1651:THR:HA	1:A:1654:MET:HG2	2.02	0.40
1:A:1154:ASP:HB3	1:A:1155:PRO:HD3	2.02	0.40
1:A:1360:LEU:HD21	1:A:1376:MET:HE2	2.04	0.40

There are no symmetry-related clashes.

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	480/569 (84%)	467 (97%)	12 (2%)	1 (0%)	43 44

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1446	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	401/515 (78%)	399 (100%)	2 (0%)	81 87

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1106	LEU
1	A	1627	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1638	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are 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	C0C	A	1705	-	36,36,36	1.06	3 (8%)	47,51,51	1.19	3 (6%)
3	EDO	A	1703	-	3,3,3	0.17	0	2,2,2	0.11	0
3	EDO	A	1704	-	3,3,3	0.58	0	2,2,2	0.14	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	C0C	A	1705	-	-	2/31/50/50	0/4/4/4
3	EDO	A	1703	-	-	0/1/1/1	-
3	EDO	A	1704	-	-	1/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1705	C0C	C03-N02	4.02	1.38	1.33
4	A	1705	C0C	C20-N19	2.80	1.39	1.34
4	A	1705	C0C	C12-N11	2.11	1.38	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1705	C0C	C26-C22-C27	5.01	121.23	113.28
4	A	1705	C0C	C23-C22-C27	-2.46	109.37	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1705	C0C	O21-C20-C22	-2.04	118.22	121.57

There are no chirality outliers.

All (3) torsion outliers are listed below:

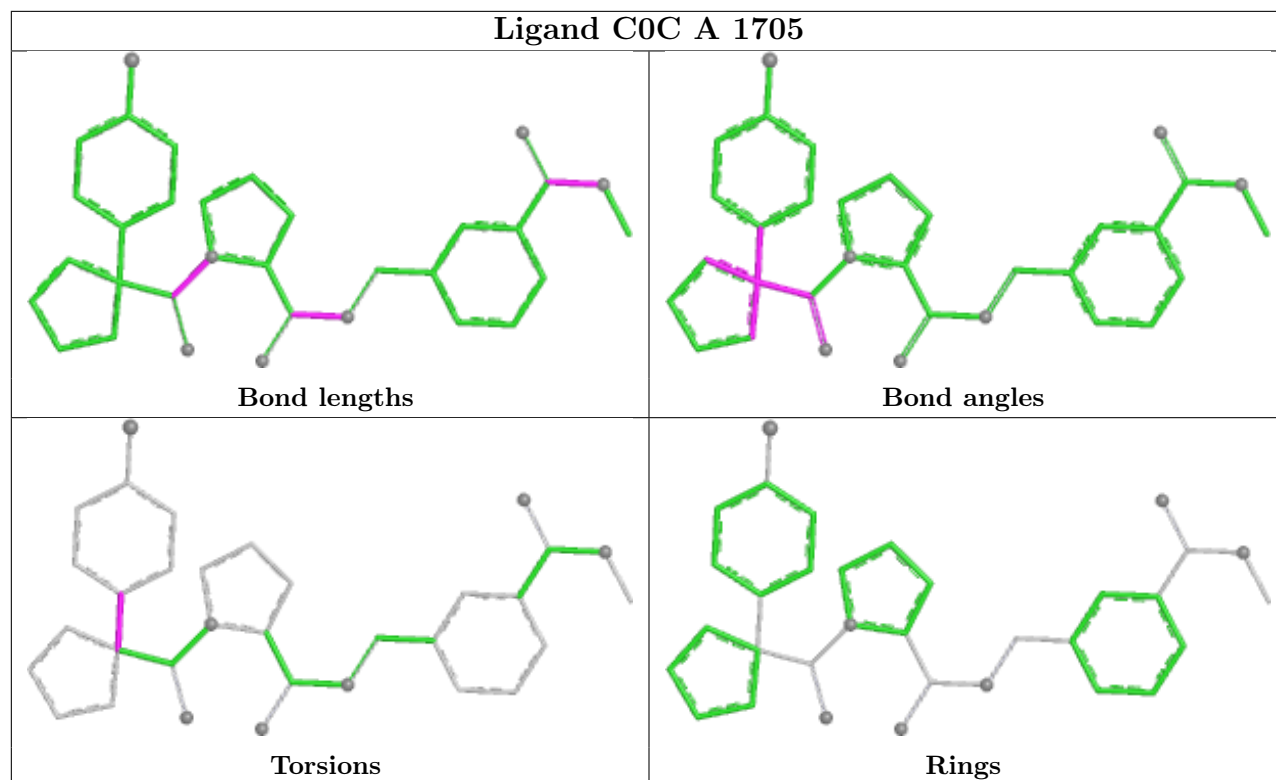
Mol	Chain	Res	Type	Atoms
3	A	1704	EDO	O1-C1-C2-O2
4	A	1705	C0C	C23-C22-C27-C28
4	A	1705	C0C	C23-C22-C27-C33

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1704	EDO	5	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 ⓘ

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	484/569 (85%)	0.76	79 (16%) 4 5	12, 36, 107, 139	4 (0%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1513	LEU	5.8
1	A	1586	ALA	5.2
1	A	1509	TRP	4.8
1	A	1585	TYR	4.5
1	A	1341	ALA	4.5
1	A	1517	ILE	4.3
1	A	1595	PHE	4.3
1	A	1497	SER	4.2
1	A	1347	GLY	4.0
1	A	1344	VAL	3.8
1	A	1353	PHE	3.8
1	A	1511	ASN	3.8
1	A	1596	PHE	3.7
1	A	1605	ALA	3.7
1	A	1047	GLY	3.7
1	A	1339	MET	3.7
1	A	1483	TYR	3.6
1	A	1512	VAL	3.6
1	A	1604	PRO	3.6
1	A	1589	GLU	3.4
1	A	1336	LYS	3.3
1	A	1516	SER	3.3
1	A	1584	LEU	3.2
1	A	1598	ILE	3.2
1	A	1345	ASP	3.2
1	A	1515	GLU	3.1
1	A	1500	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1485	ASP	3.0
1	A	1503	TYR	3.0
1	A	1348	GLU	2.9
1	A	1441	SER	2.9
1	A	1238	THR	2.9
1	A	1436	TRP	2.9
1	A	1437	ALA	2.9
1	A	1488	LYS	2.9
1	A	1591	HIS	2.9
1	A	1588	MET	2.8
1	A	1501	LEU	2.8
1	A	1603	GLY	2.8
1	A	1486	ILE	2.8
1	A	1498	ALA	2.7
1	A	1237	ASP	2.7
1	A	1487	PHE	2.7
1	A	1280	ALA	2.7
1	A	1613	VAL	2.6
1	A	1594	VAL	2.6
1	A	1349	MET	2.6
1	A	1636	ASP	2.6
1	A	1083	LEU	2.6
1	A	1443	GLY	2.5
1	A	1343	PHE	2.5
1	A	1590	LYS	2.5
1	A	1494	ARG	2.5
1	A	1342	ARG	2.5
1	A	1608	SER	2.4
1	A	1048	ILE	2.4
1	A	1476	SER	2.4
1	A	1661	GLN	2.3
1	A	1491	THR	2.3
1	A	1382	GLY	2.3
1	A	1454	ASP	2.3
1	A	1337	PRO	2.3
1	A	1137	ARG	2.3
1	A	1350	ALA	2.2
1	A	1236	ASN	2.2
1	A	1354	PRO	2.2
1	A	1435	ILE	2.2
1	A	1489	GLN	2.2
1	A	1602	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1351	GLU	2.1
1	A	1593	GLU	2.1
1	A	1438	CYS	2.1
1	A	1334	GLU	2.1
1	A	1481	HIS	2.1
1	A	1466	TRP	2.1
1	A	1508	PHE	2.1
1	A	1490	ALA	2.1
1	A	1606	ALA	2.1
1	A	1408	CYS	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](#)

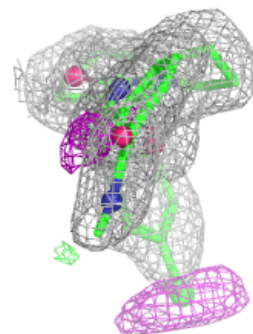
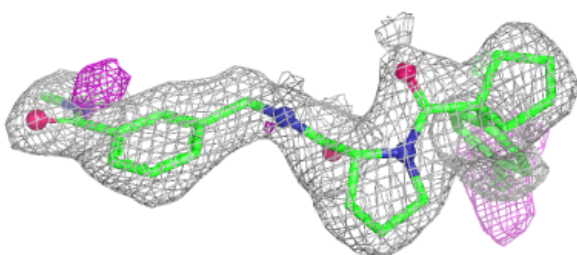
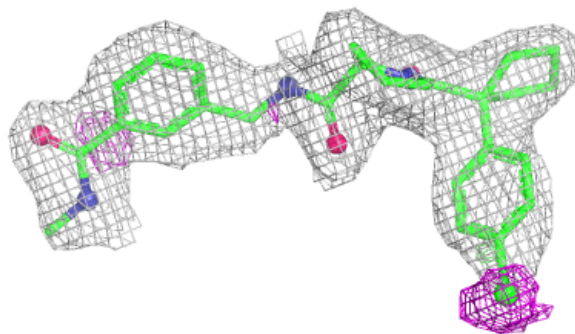
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	EDO	A	1704	4/4	0.86	0.17	42,45,45,47	0
4	C0C	A	1705	33/33	0.88	0.12	32,37,55,74	0
3	EDO	A	1703	4/4	0.94	0.08	22,27,27,27	0
2	ZN	A	1701	1/1	0.99	0.01	16,16,16,16	0
2	ZN	A	1702	1/1	1.00	0.02	24,24,24,24	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 C0C A 1705:

$2mF_o-DF_c$ (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.