Full wwPDB X-ray Structure Validation Report (i)

Jun 10, 2025 – 12:43 PM JST

PDB ID	:	9J3Q / pdb_00009j3q
Title	:	Human Pigment Epithelium-Derived Factor with Zinc Ion Crystallized in P22(1)2(1) Space Group
Authors	:	Belousov, A.S.; Chistyakov, D.V.; Baksheeva, V.E.; Bulgakov, T.K.; Zamyatnin, A.A.; Zinchenko, D.V.; Wu, L.; Tsvetkov, P.O.; Permyakov, S.E.; Zernii, E.Y.; Borshchevskiy, V.I.
Deposited on	:	2024-08-08
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

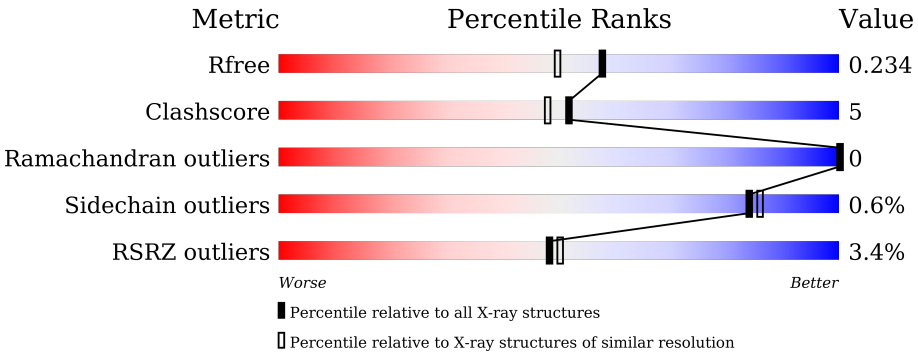
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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 <=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	398	3% 85% 10% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7244 atoms, of which 3618 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.

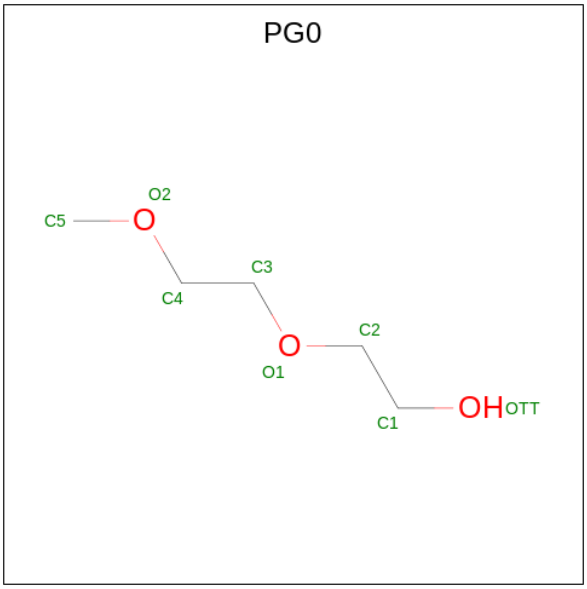
- Molecule 1 is a protein called Pigment epithelium-derived factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	378	6152	1958	3110	502	575	7	0	15	0

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is 2-(2-METHOXYETHOXY)ETHANOL (CCD ID: PG0) (formula: $C_5H_{12}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	20	5	12	3	0	0
			Total	C	H	O		
3	A	1	11	3	6	2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			15	4	9	2		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			12	3	7	2		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			15	4	9	2		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			18	5	11	2		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			18	5	11	2		
3	A	1	Total	C	H	O	0	0
			18	5	11	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			16	4	9	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			15	4	9	2		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			15	4	9	2		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			15	4	9	2		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		
3	A	1	Total	C	H	O	0	0
			20	5	12	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			20	5	12	3		

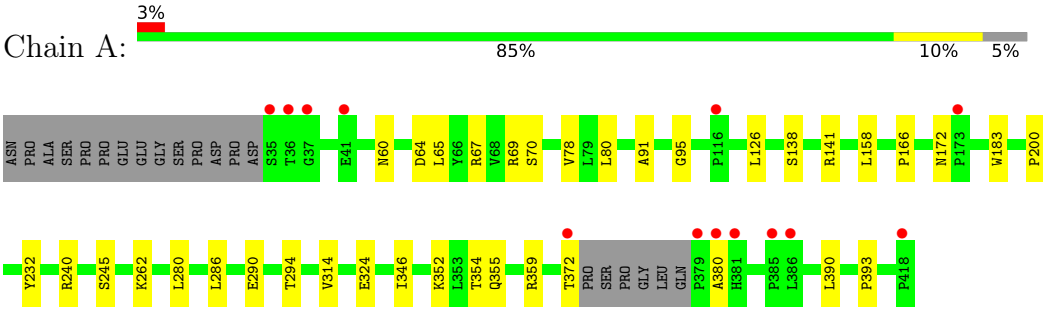
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	241	Total	O	0	3
			243	243		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Pigment epithelium-derived factor



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	174.97Å 61.60Å 44.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.23 – 1.90 36.23 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (36.23-1.90) 98.9 (36.23-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.03 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.189 , 0.233 0.191 , 0.234	Depositor DCC
R_{free} test set	1981 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	35.7	Xtriage
Anisotropy	0.342	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7244	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, PG0

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	0.41	0/3151	0.56	0/4276

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	240[A]	ARG	Sidechain
1	A	240[B]	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	3042	3110	3098	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	340	508	490	20	0
4	A	243	0	0	2	0
All	All	3626	3618	3588	35	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 (35) 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:126:LEU:HD22	3:A:522:PG0:H11	1.82	0.61
1:A:172:ASN:HD21	3:A:515:PG0:H51	1.64	0.61
1:A:158:LEU:HD23	1:A:166:PRO:HD3	1.84	0.60
1:A:262:LYS:HE2	3:A:520:PG0:H32	1.86	0.57
3:A:522:PG0:H52	4:A:792:HOH:O	2.05	0.56
1:A:172:ASN:ND2	3:A:515:PG0:H51	2.21	0.55
1:A:202:GLU:O	1:A:354[A]:THR:HG21	2.08	0.54
1:A:67:ARG:NH2	3:A:518:PG0:H52	2.25	0.52
1:A:380:ALA:HA	3:A:514:PG0:H53	1.91	0.52
1:A:60:ASN:HA	3:A:518:PG0:H51	1.93	0.51
1:A:67:ARG:HH22	3:A:518:PG0:H52	1.79	0.48
1:A:324:GLU:CD	1:A:355[A]:GLN:HE21	2.21	0.48
1:A:280:LEU:HA	3:A:520:PG0:H31	1.96	0.47
1:A:126:LEU:HD13	3:A:521:PG0:H32	1.97	0.47
1:A:314:VAL:HG22	1:A:390:LEU:HD12	1.96	0.47
1:A:232:TYR:O	1:A:393:PRO:HD3	2.15	0.47
1:A:245:SER:HB2	3:A:508:PG0:H42	1.98	0.46
1:A:95:GLY:HA3	1:A:346:ILE:HG13	1.98	0.46
1:A:294:THR:HG22	3:A:518:PG0:H41	1.98	0.46
1:A:70:SER:HA	1:A:78:VAL:HG21	1.99	0.45
1:A:65:LEU:O	1:A:69:ARG:HG2	2.18	0.43
3:A:521:PG0:H31	4:A:606:HOH:O	2.18	0.43
1:A:200:PRO:HG3	1:A:355[A]:GLN:HE22	1.83	0.43
1:A:69:ARG:HG3	1:A:80:LEU:HD11	2.00	0.43
3:A:502:PG0:H51	3:A:509:PG0:H21	2.01	0.42
1:A:324:GLU:CD	1:A:355[A]:GLN:HG3	2.45	0.42
1:A:64:ASP:OD1	3:A:507:PG0:H53	2.20	0.42
1:A:60:ASN:CA	3:A:518:PG0:H51	2.49	0.42
3:A:511:PG0:H51	3:A:513:PG0:H42	2.03	0.41
1:A:138:SER:O	3:A:522:PG0:H12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ALA:HB1	1:A:158:LEU:CD1	2.51	0.41
1:A:141:ARG:HB2	1:A:183:TRP:CH2	2.55	0.41
3:A:521:PG0:H52	3:A:522:PG0:H41	2.03	0.40
1:A:286:LEU:O	1:A:290:GLU:HG3	2.21	0.40
1:A:210:VAL:HA	1:A:359:ARG:O	2.22	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	389/398 (98%)	381 (98%)	8 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	346/354 (98%)	344 (99%)	2 (1%)	84 86

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

Mol	Chain	Res	Type
1	A	352	LYS

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Mol	Chain	Res	Type
1	A	372	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 46 ligands modelled in this entry, 1 is monoatomic - leaving 45 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	$\#\|Z\| > 2$
3	PG0	A	515	-	7,7,7	0.26	0	6,6,6	0.18	0
3	PG0	A	516	-	7,7,7	0.23	0	6,6,6	0.31	0
3	PG0	A	520	-	7,7,7	0.23	0	6,6,6	0.23	0
3	PG0	A	529	-	6,6,7	0.26	0	5,5,6	0.22	0
3	PG0	A	537	-	5,5,7	0.24	0	4,4,6	0.11	0
3	PG0	A	530	-	7,7,7	0.26	0	6,6,6	0.18	0
3	PG0	A	525	-	7,7,7	0.26	0	6,6,6	0.22	0
3	PG0	A	545	-	7,7,7	0.26	0	6,6,6	0.24	0
3	PG0	A	518	-	7,7,7	0.27	0	6,6,6	0.21	0
3	PG0	A	512	-	5,5,7	0.23	0	4,4,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PG0	A	533	-	7,7,7	0.24	0	6,6,6	0.23	0
3	PG0	A	509	-	7,7,7	0.27	0	6,6,6	0.22	0
3	PG0	A	502	-	7,7,7	0.26	0	6,6,6	0.18	0
3	PG0	A	528	-	7,7,7	0.26	0	6,6,6	0.19	0
3	PG0	A	507	-	7,7,7	0.25	0	6,6,6	0.19	0
3	PG0	A	511	-	7,7,7	0.25	0	6,6,6	0.18	0
3	PG0	A	544	-	7,7,7	0.25	0	6,6,6	0.22	0
3	PG0	A	513	-	7,7,7	0.26	0	6,6,6	0.16	0
3	PG0	A	504	-	5,5,7	0.33	0	4,4,6	0.24	0
3	PG0	A	535	-	7,7,7	0.26	0	6,6,6	0.26	0
3	PG0	A	541	-	7,7,7	0.26	0	6,6,6	0.14	0
3	PG0	A	508	-	7,7,7	0.26	0	6,6,6	0.22	0
3	PG0	A	510	-	4,4,7	0.23	0	3,3,6	0.24	0
3	PG0	A	536	-	7,7,7	0.26	0	6,6,6	0.22	0
3	PG0	A	503	-	4,4,7	0.22	0	3,3,6	0.28	0
3	PG0	A	523	-	6,6,7	0.32	0	5,5,6	0.18	0
3	PG0	A	539	-	5,5,7	0.33	0	4,4,6	0.26	0
3	PG0	A	531	-	7,7,7	0.25	0	6,6,6	0.35	0
3	PG0	A	526	-	7,7,7	0.27	0	6,6,6	0.14	0
3	PG0	A	514	-	7,7,7	0.26	0	6,6,6	0.21	0
3	PG0	A	524	-	6,6,7	0.32	0	5,5,6	0.13	0
3	PG0	A	532	-	5,5,7	0.24	0	4,4,6	0.09	0
3	PG0	A	543	-	7,7,7	0.27	0	6,6,6	0.17	0
3	PG0	A	519	-	7,7,7	0.27	0	6,6,6	0.20	0
3	PG0	A	546	-	7,7,7	0.25	0	6,6,6	0.19	0
3	PG0	A	538	-	7,7,7	0.25	0	6,6,6	0.28	0
3	PG0	A	534	-	7,7,7	0.25	0	6,6,6	0.21	0
3	PG0	A	506	-	7,7,7	0.25	0	6,6,6	0.22	0
3	PG0	A	517	-	7,7,7	0.27	0	6,6,6	0.16	0
3	PG0	A	542	-	7,7,7	0.26	0	6,6,6	0.22	0
3	PG0	A	521	-	6,6,7	0.32	0	5,5,6	0.12	0
3	PG0	A	527	-	7,7,7	0.24	0	6,6,6	0.29	0
3	PG0	A	505	-	7,7,7	0.25	0	6,6,6	0.22	0
3	PG0	A	540	-	7,7,7	0.26	0	6,6,6	0.16	0
3	PG0	A	522	-	7,7,7	0.27	0	6,6,6	0.28	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
3	PG0	A	515	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG0	A	516	-	-	4/5/5/5	-
3	PG0	A	520	-	-	2/5/5/5	-
3	PG0	A	529	-	-	1/4/4/5	-
3	PG0	A	537	-	-	1/3/3/5	-
3	PG0	A	530	-	-	1/5/5/5	-
3	PG0	A	525	-	-	2/5/5/5	-
3	PG0	A	545	-	-	1/5/5/5	-
3	PG0	A	518	-	-	1/5/5/5	-
3	PG0	A	512	-	-	3/3/3/5	-
3	PG0	A	533	-	-	3/5/5/5	-
3	PG0	A	509	-	-	2/5/5/5	-
3	PG0	A	502	-	-	3/5/5/5	-
3	PG0	A	528	-	-	2/5/5/5	-
3	PG0	A	507	-	-	2/5/5/5	-
3	PG0	A	511	-	-	2/5/5/5	-
3	PG0	A	544	-	-	2/5/5/5	-
3	PG0	A	513	-	-	0/5/5/5	-
3	PG0	A	504	-	-	1/3/3/5	-
3	PG0	A	535	-	-	3/5/5/5	-
3	PG0	A	541	-	-	2/5/5/5	-
3	PG0	A	508	-	-	3/5/5/5	-
3	PG0	A	510	-	-	1/2/2/5	-
3	PG0	A	536	-	-	2/5/5/5	-
3	PG0	A	503	-	-	1/2/2/5	-
3	PG0	A	523	-	-	2/4/4/5	-
3	PG0	A	539	-	-	2/3/3/5	-
3	PG0	A	531	-	-	3/5/5/5	-
3	PG0	A	526	-	-	3/5/5/5	-
3	PG0	A	514	-	-	3/5/5/5	-
3	PG0	A	524	-	-	2/4/4/5	-
3	PG0	A	532	-	-	1/3/3/5	-
3	PG0	A	543	-	-	1/5/5/5	-
3	PG0	A	519	-	-	1/5/5/5	-
3	PG0	A	546	-	-	3/5/5/5	-
3	PG0	A	538	-	-	3/5/5/5	-
3	PG0	A	534	-	-	3/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PG0	A	506	-	-	3/5/5/5	-
3	PG0	A	517	-	-	4/5/5/5	-
3	PG0	A	542	-	-	4/5/5/5	-
3	PG0	A	521	-	-	2/4/4/5	-
3	PG0	A	527	-	-	2/5/5/5	-
3	PG0	A	505	-	-	3/5/5/5	-
3	PG0	A	540	-	-	1/5/5/5	-
3	PG0	A	522	-	-	2/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (94) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	507	PG0	O1-C3-C4-O2
3	A	505	PG0	O1-C3-C4-O2
3	A	546	PG0	O1-C3-C4-O2
3	A	511	PG0	O1-C3-C4-O2
3	A	525	PG0	O1-C3-C4-O2
3	A	532	PG0	O1-C3-C4-O2
3	A	535	PG0	O1-C3-C4-O2
3	A	541	PG0	O1-C3-C4-O2
3	A	522	PG0	O1-C3-C4-O2
3	A	526	PG0	O1-C3-C4-O2
3	A	512	PG0	O1-C3-C4-O2
3	A	528	PG0	O1-C3-C4-O2
3	A	533	PG0	O1-C3-C4-O2
3	A	502	PG0	OTT-C1-C2-O1
3	A	522	PG0	OTT-C1-C2-O1
3	A	531	PG0	O1-C3-C4-O2
3	A	503	PG0	O1-C3-C4-O2
3	A	509	PG0	OTT-C1-C2-O1
3	A	536	PG0	OTT-C1-C2-O1
3	A	546	PG0	OTT-C1-C2-O1
3	A	527	PG0	O1-C3-C4-O2
3	A	542	PG0	O1-C3-C4-O2
3	A	529	PG0	OTT-C1-C2-O1
3	A	515	PG0	O1-C3-C4-O2

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Mol	Chain	Res	Type	Atoms
3	A	518	PG0	OTT-C1-C2-O1
3	A	506	PG0	O1-C3-C4-O2
3	A	509	PG0	O1-C3-C4-O2
3	A	508	PG0	OTT-C1-C2-O1
3	A	521	PG0	O1-C3-C4-O2
3	A	542	PG0	C4-C3-O1-C2
3	A	512	PG0	C4-C3-O1-C2
3	A	519	PG0	O1-C3-C4-O2
3	A	534	PG0	C3-C4-O2-C5
3	A	538	PG0	O1-C3-C4-O2
3	A	514	PG0	C4-C3-O1-C2
3	A	516	PG0	OTT-C1-C2-O1
3	A	517	PG0	OTT-C1-C2-O1
3	A	536	PG0	C4-C3-O1-C2
3	A	517	PG0	C4-C3-O1-C2
3	A	510	PG0	C3-C4-O2-C5
3	A	544	PG0	C1-C2-O1-C3
3	A	538	PG0	C4-C3-O1-C2
3	A	504	PG0	C4-C3-O1-C2
3	A	546	PG0	C1-C2-O1-C3
3	A	526	PG0	C1-C2-O1-C3
3	A	534	PG0	C1-C2-O1-C3
3	A	516	PG0	C4-C3-O1-C2
3	A	528	PG0	C4-C3-O1-C2
3	A	533	PG0	C4-C3-O1-C2
3	A	545	PG0	O1-C3-C4-O2
3	A	523	PG0	C4-C3-O1-C2
3	A	506	PG0	C4-C3-O1-C2
3	A	505	PG0	C1-C2-O1-C3
3	A	512	PG0	C3-C4-O2-C5
3	A	538	PG0	C1-C2-O1-C3
3	A	508	PG0	O1-C3-C4-O2
3	A	502	PG0	C3-C4-O2-C5
3	A	511	PG0	OTT-C1-C2-O1
3	A	525	PG0	C4-C3-O1-C2
3	A	535	PG0	C1-C2-O1-C3
3	A	524	PG0	C3-C4-O2-C5
3	A	542	PG0	C3-C4-O2-C5
3	A	524	PG0	O1-C3-C4-O2
3	A	521	PG0	C1-C2-O1-C3
3	A	542	PG0	C1-C2-O1-C3
3	A	535	PG0	C3-C4-O2-C5

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Mol	Chain	Res	Type	Atoms
3	A	540	PG0	C3-C4-O2-C5
3	A	526	PG0	C3-C4-O2-C5
3	A	520	PG0	C4-C3-O1-C2
3	A	533	PG0	C1-C2-O1-C3
3	A	516	PG0	O1-C3-C4-O2
3	A	541	PG0	C3-C4-O2-C5
3	A	539	PG0	OTT-C1-C2-O1
3	A	520	PG0	O1-C3-C4-O2
3	A	507	PG0	C4-C3-O1-C2
3	A	537	PG0	C4-C3-O1-C2
3	A	544	PG0	C3-C4-O2-C5
3	A	516	PG0	C1-C2-O1-C3
3	A	530	PG0	C3-C4-O2-C5
3	A	505	PG0	C4-C3-O1-C2
3	A	534	PG0	O1-C3-C4-O2
3	A	517	PG0	C3-C4-O2-C5
3	A	527	PG0	C1-C2-O1-C3
3	A	543	PG0	C3-C4-O2-C5
3	A	539	PG0	C1-C2-O1-C3
3	A	517	PG0	O1-C3-C4-O2
3	A	506	PG0	OTT-C1-C2-O1
3	A	523	PG0	O1-C3-C4-O2
3	A	531	PG0	C1-C2-O1-C3
3	A	514	PG0	C3-C4-O2-C5
3	A	514	PG0	O1-C3-C4-O2
3	A	508	PG0	C3-C4-O2-C5
3	A	502	PG0	C1-C2-O1-C3
3	A	531	PG0	OTT-C1-C2-O1

There are no ring outliers.

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	515	PG0	2	0
3	A	520	PG0	2	0
3	A	518	PG0	5	0
3	A	509	PG0	1	0
3	A	502	PG0	1	0
3	A	507	PG0	1	0
3	A	511	PG0	1	0
3	A	513	PG0	1	0
3	A	508	PG0	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	514	PG0	1	0
3	A	521	PG0	3	0
3	A	522	PG0	4	0

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, 95^{th} 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	378/398 (94%)	-0.03	13 (3%) 48 50	23, 44, 74, 120	14 (3%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	381[A]	HIS	8.5
1	A	418	PRO	5.0
1	A	379	PRO	4.6
1	A	380	ALA	4.5
1	A	372	THR	4.3
1	A	386	LEU	3.5
1	A	385	PRO	2.4
1	A	116	PRO	2.3
1	A	37	GLY	2.2
1	A	173	PRO	2.1
1	A	35	SER	2.1
1	A	36	THR	2.1
1	A	41	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides 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, 95^{th} 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	PG0	A	519	8/8	0.46	0.27	84,102,120,120	0
3	PG0	A	543	8/8	0.47	0.18	97,127,142,142	0
3	PG0	A	539	6/8	0.50	0.22	82,103,122,124	0
3	PG0	A	537	6/8	0.51	0.26	102,123,137,137	0
3	PG0	A	510	5/8	0.54	0.24	82,99,104,104	0
3	PG0	A	546	8/8	0.54	0.19	101,127,152,152	0
3	PG0	A	535	8/8	0.57	0.20	95,123,145,145	0
3	PG0	A	504	6/8	0.59	0.22	63,85,105,105	0
3	PG0	A	544	8/8	0.60	0.18	90,111,136,136	0
3	PG0	A	532	6/8	0.60	0.24	96,115,134,134	0
3	PG0	A	529	7/8	0.61	0.18	78,104,128,128	0
3	PG0	A	515	8/8	0.61	0.22	86,110,134,134	0
3	PG0	A	513	8/8	0.63	0.26	102,126,151,151	0
3	PG0	A	528	8/8	0.63	0.20	78,99,115,115	0
3	PG0	A	534	8/8	0.63	0.20	103,124,138,138	0
3	PG0	A	502	8/8	0.64	0.24	48,77,96,96	0
3	PG0	A	540	8/8	0.66	0.24	98,118,139,139	0
3	PG0	A	526	8/8	0.67	0.22	56,81,106,106	0
3	PG0	A	520	8/8	0.67	0.19	45,65,92,92	0
3	PG0	A	523	7/8	0.67	0.28	73,90,104,104	0
3	PG0	A	512	6/8	0.68	0.23	69,94,110,111	0
3	PG0	A	503	5/8	0.68	0.19	64,83,96,96	0
3	PG0	A	536	8/8	0.68	0.20	69,97,109,109	0
3	PG0	A	541	8/8	0.69	0.18	67,94,113,113	0
3	PG0	A	545	8/8	0.70	0.18	84,100,115,128	0
3	PG0	A	521	7/8	0.71	0.28	88,109,123,123	0
3	PG0	A	542	8/8	0.71	0.22	89,107,119,124	0
3	PG0	A	533	8/8	0.71	0.17	72,100,121,121	0
3	PG0	A	531	8/8	0.72	0.18	70,87,109,115	0
3	PG0	A	505	8/8	0.72	0.20	66,96,105,105	0
3	PG0	A	527	8/8	0.72	0.19	72,89,103,104	0
3	PG0	A	516	8/8	0.73	0.33	102,123,155,155	0
3	PG0	A	514	8/8	0.73	0.20	72,91,109,109	0
3	PG0	A	508	8/8	0.73	0.20	56,80,100,100	0
3	PG0	A	507	8/8	0.74	0.18	59,76,93,93	0
3	PG0	A	509	8/8	0.75	0.24	78,101,131,131	0
3	PG0	A	525	8/8	0.75	0.18	72,109,140,140	0

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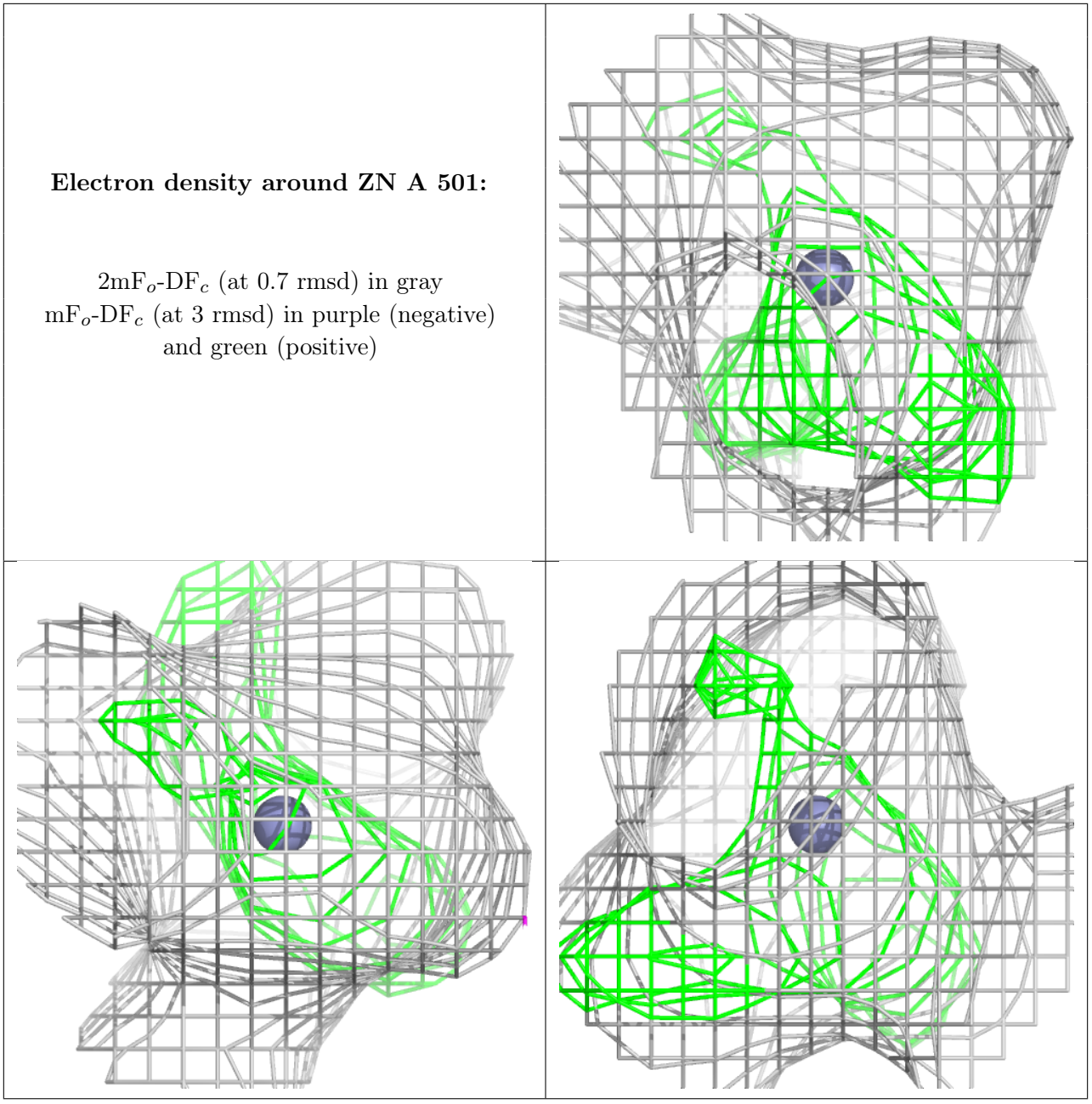
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PG0	A	530	8/8	0.75	0.18	77,104,136,136	0
3	PG0	A	524	7/8	0.76	0.23	77,95,112,112	0
3	PG0	A	522	8/8	0.78	0.21	47,81,94,97	0
3	PG0	A	506	8/8	0.79	0.18	73,95,112,115	0
3	PG0	A	517	8/8	0.79	0.19	69,86,105,105	0
3	PG0	A	511	8/8	0.79	0.19	58,97,116,116	0
3	PG0	A	538	8/8	0.79	0.19	74,97,117,117	0
3	PG0	A	518	8/8	0.81	0.17	29,62,78,84	0
2	ZN	A	501	1/1	0.99	0.07	44,44,44,44	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 ZN A 501:

$2mF_o$-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.