Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2026 – 06:34 AM UTC

PDB ID	:	8SW0 / pdb_00008sw0
Title	:	Puromycin sensitive aminopeptidase
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Deposited on	:	2023-05-17
Resolution	:	2.30 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:

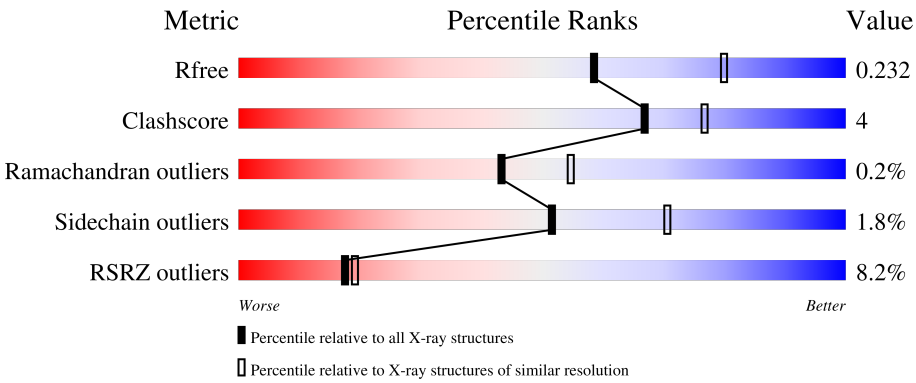
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	902	8% 85% 11% •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7055 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 Puromycin-sensitive aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	864	6856	4388	1144	1293	31	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	initiating methionine	UNP P55786
A	19	SER	-	expression tag	UNP P55786
A	20	TYR	-	expression tag	UNP P55786
A	21	TYR	-	expression tag	UNP P55786
A	22	HIS	-	expression tag	UNP P55786
A	23	HIS	-	expression tag	UNP P55786
A	24	HIS	-	expression tag	UNP P55786
A	25	HIS	-	expression tag	UNP P55786
A	26	HIS	-	expression tag	UNP P55786
A	27	HIS	-	expression tag	UNP P55786
A	28	ASP	-	expression tag	UNP P55786
A	29	TYR	-	expression tag	UNP P55786
A	30	ASP	-	expression tag	UNP P55786
A	31	ILE	-	expression tag	UNP P55786
A	32	PRO	-	expression tag	UNP P55786
A	33	THR	-	expression tag	UNP P55786
A	34	THR	-	expression tag	UNP P55786
A	35	GLU	-	expression tag	UNP P55786
A	36	ASN	-	expression tag	UNP P55786
A	37	LEU	-	expression tag	UNP P55786
A	38	TYR	-	expression tag	UNP P55786
A	39	PHE	-	expression tag	UNP P55786
A	40	GLN	-	expression tag	UNP P55786
A	41	GLY	-	expression tag	UNP P55786
A	42	ALA	-	expression tag	UNP P55786
A	43	MET	-	expression tag	UNP P55786
A	44	GLY	-	expression tag	UNP P55786

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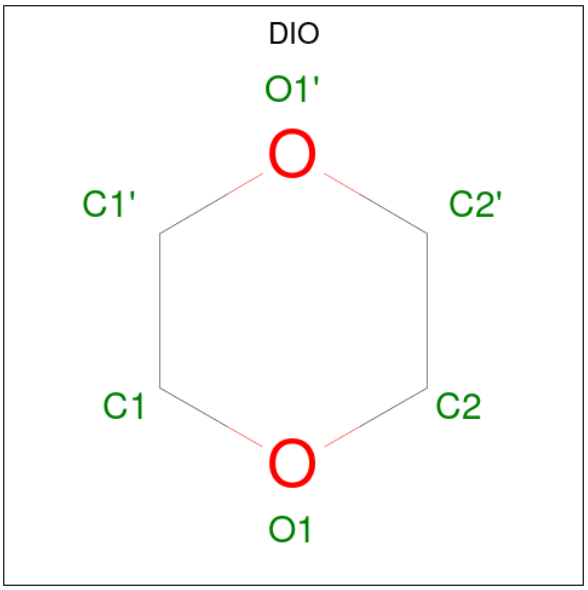
Chain	Residue	Modelled	Actual	Comment	Reference
A	45	SER	-	expression tag	UNP P55786

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

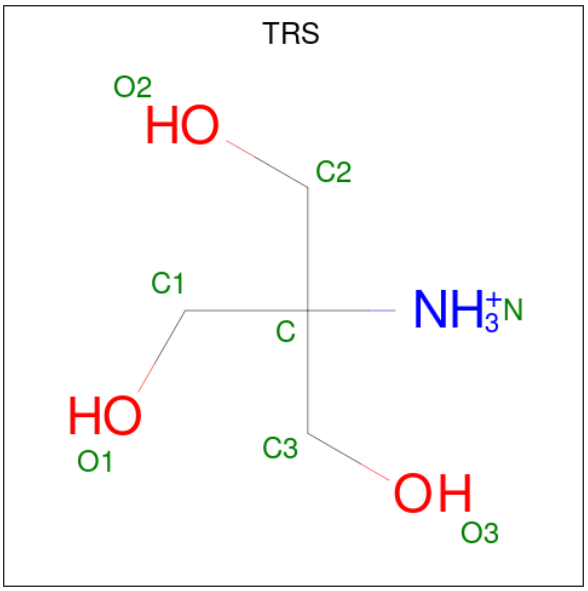
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (CCD ID: DIO) (formula: $C_4H_8O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	4	2	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	8	4	1	3	0	0

- Molecule 5 is water.

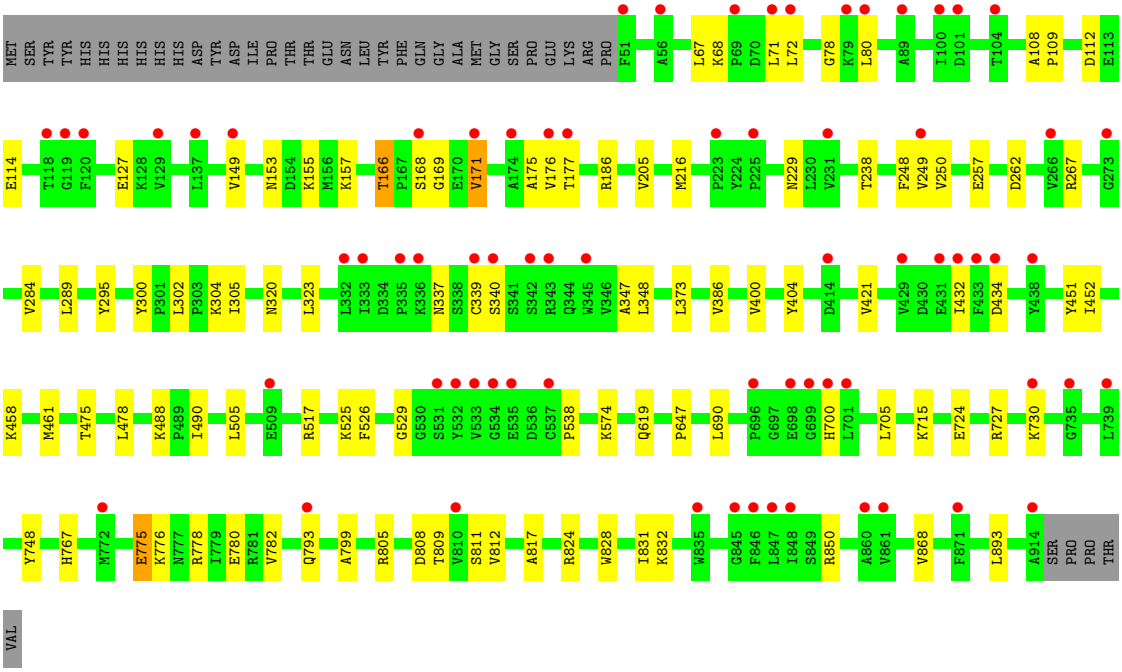
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	184	184	184	0	0

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: Puromycin-sensitive aminopeptidase

Chain A: 8% 85% 11%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	70.68Å 257.71Å 60.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.20 – 2.30 45.20 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.7 (45.20-2.30) 95.7 (45.20-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.52 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.20	Depositor
R, R_{free}	0.223 , 0.241 0.227 , 0.232	Depositor DCC
R_{free} test set	2121 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7055	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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 (i)

5.1 Standard geometry (i)

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

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	0.08	0/7017	0.25	0/9523

There are no bond length outliers.

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	6856	0	6773	50	0
2	A	1	0	0	0	0
3	A	6	0	8	0	0
4	A	8	0	12	0	0
5	A	184	0	0	2	0
All	All	7055	0	6793	50	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 4.

All (50) 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:109:PRO:HG2	1:A:112:ASP:HB2	1.75	0.67
1:A:805:ARG:NH2	1:A:808:ASP:OD2	2.32	0.62
1:A:525:LYS:HD2	1:A:538:PRO:HG2	1.81	0.62
1:A:177:THR:HG21	1:A:248:PHE:H	1.64	0.61
1:A:517:ARG:NH2	1:A:574:LYS:O	2.35	0.59
1:A:421:VAL:HB	1:A:432:ILE:HD13	1.87	0.56
1:A:811:SER:OG	1:A:850:ARG:NH2	2.41	0.53
1:A:68:LYS:HG3	1:A:205:VAL:HB	1.91	0.52
1:A:529:GLY:HA2	1:A:893:LEU:HD21	1.91	0.52
1:A:67:LEU:HD13	1:A:78:GLY:HA3	1.91	0.51
1:A:175:ALA:HB3	1:A:250:VAL:HB	1.93	0.51
1:A:339:CYS:SG	1:A:340:SER:N	2.83	0.51
1:A:289:LEU:HD11	1:A:305:ILE:HG21	1.92	0.50
1:A:690:LEU:HD11	1:A:705:LEU:HG	1.92	0.50
1:A:216:MET:HG2	1:A:238:THR:HG22	1.93	0.49
1:A:108:ALA:HB2	1:A:114:GLU:HB3	1.95	0.47
1:A:216:MET:HE1	1:A:302:LEU:HD22	1.95	0.47
1:A:775:GLU:HG2	1:A:778:ARG:HH12	1.79	0.47
1:A:767:HIS:O	1:A:776:LYS:NZ	2.48	0.46
1:A:373:LEU:HD22	1:A:475:THR:HG23	1.97	0.46
1:A:249:VAL:HG12	1:A:323:LEU:HD21	1.98	0.45
1:A:715:LYS:NZ	5:A:1118:HOH:O	2.45	0.45
1:A:127:GLU:OE2	1:A:186:ARG:NH2	2.51	0.44
1:A:461:MET:HE1	1:A:478:LEU:HD11	1.99	0.44
1:A:828:TRP:CE2	1:A:832:LYS:HD2	2.52	0.44
1:A:451:TYR:CZ	1:A:488:LYS:HD3	2.53	0.44
1:A:400:VAL:HA	1:A:404:TYR:HB3	1.99	0.44
1:A:828:TRP:CE3	1:A:831:ILE:HD11	2.53	0.44
1:A:799:ALA:HB1	1:A:809:THR:HG23	1.99	0.43
1:A:295:TYR:HA	1:A:458:LYS:HE3	2.00	0.43
1:A:452:ILE:HD11	1:A:490:ILE:HD11	2.00	0.43
1:A:320:ASN:HB2	1:A:323:LEU:O	2.18	0.43
1:A:166:THR:OG1	1:A:169:GLY:O	2.36	0.43
1:A:176:VAL:HG22	1:A:249:VAL:HG23	2.01	0.43
1:A:257:GLU:HB3	1:A:267:ARG:HG2	2.00	0.43
1:A:153:ASN:ND2	5:A:1108:HOH:O	2.40	0.42
1:A:155:LYS:HB2	1:A:157:LYS:HG2	2.01	0.42
1:A:780:GLU:HB3	1:A:812:VAL:HG22	2.01	0.42
1:A:340:SER:HB3	1:A:700:HIS:HB2	2.01	0.42
1:A:505:LEU:HB2	1:A:526:PHE:HB2	2.01	0.41
1:A:724:GLU:HA	1:A:727:ARG:HE	1.84	0.41
1:A:71:LEU:HG	1:A:72:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:VAL:HG11	1:A:347:ALA:HA	2.03	0.41
1:A:169:GLY:C	1:A:171:VAL:H	2.27	0.41
1:A:748:TYR:HB3	1:A:782:VAL:HG21	2.01	0.41
1:A:434:ASP:N	1:A:434:ASP:OD1	2.53	0.41
1:A:828:TRP:HE3	1:A:831:ILE:HD11	1.86	0.41
1:A:817:ALA:HA	1:A:824:ARG:HA	2.01	0.41
1:A:348:LEU:HD23	1:A:386:VAL:HG21	2.03	0.40
1:A:300:TYR:CE2	1:A:302:LEU:HB2	2.57	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	862/902 (96%)	824 (96%)	36 (4%)	2 (0%)	43 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	VAL
1	A	647	PRO

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	742/777 (96%)	729 (98%)	13 (2%)	51 70

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LEU
1	A	149	VAL
1	A	166	THR
1	A	168	SER
1	A	229	ASN
1	A	262	ASP
1	A	304	LYS
1	A	337	ASN
1	A	619	GLN
1	A	730	LYS
1	A	775	GLU
1	A	793	GLN
1	A	868	VAL

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

Mol	Chain	Res	Type
1	A	388	HIS
1	A	539	GLN
1	A	875	HIS

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	DIO	A	1002	-	6,6,6	0.47	0	6,6,6	0.58	0
4	TRS	A	1003	-	7,7,7	0.36	0	9,9,9	0.39	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	DIO	A	1002	-	-	-	0/1/1/1
4	TRS	A	1003	-	-	0/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 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	864/902 (95%)	0.71	71 (8%) 17 19	30, 63, 115, 177	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	433	PHE	5.4
1	A	137	LEU	4.5
1	A	71	LEU	4.3
1	A	432	ILE	4.1
1	A	846	PHE	4.0
1	A	533	VAL	3.9
1	A	914	ALA	3.7
1	A	223	PRO	3.7
1	A	249	VAL	3.6
1	A	696	PRO	3.6
1	A	225	PRO	3.5
1	A	534	GLY	3.4
1	A	339	CYS	3.4
1	A	72	LEU	3.3
1	A	699	GLY	3.3
1	A	429	VAL	3.2
1	A	860	ALA	3.2
1	A	345	TRP	3.0
1	A	340	SER	3.0
1	A	735	GLY	2.9
1	A	171	VAL	2.9
1	A	438	TYR	2.9
1	A	535	GLU	2.8
1	A	51	PHE	2.8
1	A	120	PHE	2.8
1	A	772	MET	2.8
1	A	333	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	56	ALA	2.8
1	A	431	GLU	2.7
1	A	231	VAL	2.7
1	A	176	VAL	2.6
1	A	532	TYR	2.6
1	A	342	SER	2.6
1	A	118	THR	2.6
1	A	69	PRO	2.5
1	A	335	PRO	2.5
1	A	847	LEU	2.5
1	A	698	GLU	2.4
1	A	739	LEU	2.4
1	A	531	SER	2.4
1	A	273	GLY	2.3
1	A	149	VAL	2.3
1	A	101	ASP	2.3
1	A	845	GLY	2.3
1	A	89	ALA	2.3
1	A	848	ILE	2.3
1	A	861	VAL	2.3
1	A	79	LYS	2.3
1	A	537	CYS	2.3
1	A	835	TRP	2.3
1	A	434	ASP	2.2
1	A	730	LYS	2.2
1	A	129	VAL	2.2
1	A	336	LYS	2.2
1	A	80	LEU	2.2
1	A	414	ASP	2.2
1	A	810	VAL	2.2
1	A	793	GLN	2.2
1	A	332	LEU	2.1
1	A	266	VAL	2.1
1	A	168	SER	2.1
1	A	174	ALA	2.1
1	A	343	ARG	2.1
1	A	104	THR	2.1
1	A	701	LEU	2.1
1	A	871	PHE	2.1
1	A	700	HIS	2.1
1	A	100	ILE	2.1
1	A	119	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	177	THR	2.0
1	A	509	GLU	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)

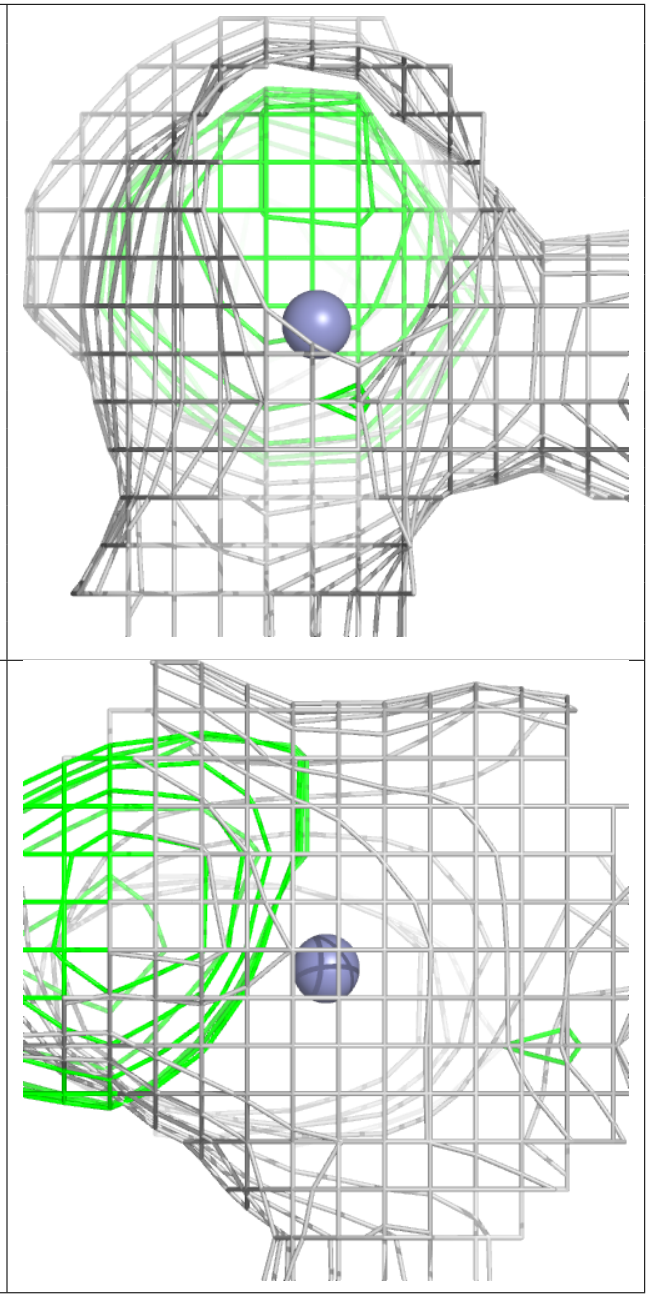
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TRS	A	1003	8/8	0.79	0.28	82,82,82,83	0
3	DIO	A	1002	6/6	0.89	0.18	51,52,53,54	0
2	ZN	A	1001	1/1	0.98	0.04	37,37,37,37	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 ZN A 1001:

$2mF_o$-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.