

Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2022 – 06:16 pm GMT

PDB ID	:	7ZHX
Title	:	Leishmania donovani Glucose 6-Phosphate Dehydrogenase (N-terminal dele-
		tion variant) complexed with NADP(H)
Authors	:	Fritz-Wolf, K.; Berneburg, I.
Deposited on	:	2022-04-07
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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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 $(#Entries, resolution range(Å))$		
Rfree	130704	6207 (1.90-1.90)		
Clashscore	141614	6847 (1.90-1.90)		
Ramachandran outliers	138981	6760 (1.90-1.90)		
Sidechain outliers	138945	6760 (1.90-1.90)		
RSRZ outliers	127900	6082 (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	Quality of chain					
			24%						
1	A	503	86%	9%	•				

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	PG4	А	602	_	_	Х	-



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	А	609	-	-	Х	Х



7ZHX

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4306 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 Glucose-6-phosphate 1-dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	481	Total 3826	C 2435	N 658	0 716	S 17	0	4	0

• Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0
2	А	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 7 4 3 \end{array}$	0	0

• Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



PG4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	А	1	Total 13	C 8	O 5	0	0

• Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
Б	Δ	1	Total	С	Ν	Ο	Р	0	0
5 A	L	48	21	7	17	3	U	U	

• Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	381	Total O 381 381	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: Glucose-6-phosphate 1-dehydrogenase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants	75.75Å 229.66Å 83.55 Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{accolution}}(\hat{\mathbf{A}})$	47.30 - 1.90	Depositor
Resolution (A)	47.32 - 1.89	EDS
% Data completeness	99.6 (47.30-1.90)	Depositor
(in resolution range)	99.7 (47.32-1.89)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.47 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
D D.	0.182 , 0.210	Depositor
Π, Π_{free}	0.179 , 0.207	DCC
R_{free} test set	4692 reflections $(8.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	33.2	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	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	4306	wwPDB-VP
Average B, all atoms $(Å^2)$	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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: PEG, EDO, NDP, PG4 $\,$

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).

Mal	Chain	Bond	lengths	Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.44	0/3916	0.62	0/5295

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	А	3826	0	3813	42	0
2	А	14	0	20	2	0
3	А	13	0	18	9	0
4	А	24	0	35	6	0
5	А	48	0	26	5	0
6	А	381	0	0	8	1
All	All	4306	0	3912	47	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 6.

All (47) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:387:ARG:HE	1:A:389:ASN:HD21	1.29	0.81	
1:A:456:LEU:HA	1:A:458:GLY:N	1.99	0.78	
1:A:106:ASN:ND2	6:A:705:HOH:O	2.24	0.70	
1:A:502:LYS:NZ	6:A:703:HOH:O	2.20	0.69	
1:A:68:LYS:NZ	6:A:706:HOH:O	2.25	0.69	
1:A:215:ARG:HH12	3:A:602:PG4:H32	1.58	0.69	
1:A:549:LYS:NZ	6:A:702:HOH:O	2.09	0.66	
1:A:213:TRP:HE1	3:A:602:PG4:H62	1.64	0.61	
1:A:87:LYS:NZ	5:A:610:NDP:H71N	2.01	0.59	
1:A:62:LYS:N	6:A:716:HOH:O	2.36	0.59	
1:A:68:LYS:HD3	1:A:103:PRO:HD2	1.86	0.57	
1:A:132:ASN:HB2	1:A:136:ARG:HD2	1.86	0.57	
5:A:610:NDP:H5N	6:A:1011:HOH:O	2.05	0.57	
1:A:387:ARG:HE	1:A:389:ASN:ND2	2.00	0.56	
1:A:455:GLY:O	1:A:456:LEU:HD12	2.06	0.55	
1:A:362:ASP:OD1	1:A:364:SER:N	2.40	0.54	
1:A:87:LYS:HZ1	5:A:610:NDP:H71N	1.55	0.54	
1:A:371:ASP:HB3	1:A:374:VAL:HG23	1.89	0.54	
1:A:164:ASP:OD2	1:A:168[B]:ARG:NH1	2.42	0.53	
1:A:432:ARG:CZ	1:A:549:LYS:HG2	2.40	0.52	
1:A:420:ARG:HD3	2:A:608:PEG:H42	1.93	0.51	
1:A:215:ARG:HH12	3:A:602:PG4:C3	2.25	0.49	
1:A:87:LYS:HZ2	5:A:610:NDP:H42N	1.78	0.48	
1:A:168[B]:ARG:HE	1:A:208:GLN:HG2	1.78	0.48	
1:A:389:ASN:HB2	4:A:609:EDO:C2	2.44	0.47	
1:A:322:MET:HB2	1:A:336:GLU:HB3	1.97	0.47	
1:A:383:PHE:CE1	1:A:385:VAL:HG23	2.51	0.46	
3:A:602:PG4:H71	6:A:898:HOH:O	2.16	0.46	
3:A:602:PG4:H61	6:A:794:HOH:O	2.16	0.46	
1:A:213:TRP:HE1	3:A:602:PG4:C6	2.29	0.45	
1:A:389:ASN:HB2	4:A:609:EDO:H21	1.99	0.45	
1:A:493:LEU:C	3:A:602:PG4:H31	2.36	0.45	
1:A:387:ARG:NE	1:A:389:ASN:HD21	2.05	0.44	
1:A:362:ASP:OD2	1:A:364:SER:HB3	2.18	0.43	
1:A:220:LYS:HB2	1:A:221:PRO:HA	2.00	0.43	
1:A:345:GLU:HB2	4:A:609:EDO:C2	2.48	0.43	
1:A:356:GLN:O	1:A:528:PRO:HA	2.18	0.43	
1:A:347:ILE:HA	4:A:605:EDO:H22	2.01	0.43	
1:A:213:TRP:NE1	3:A:602:PG4:H62	2.34	0.42	
1:A:338:VAL:HG22	1:A:504:GLU:HB2	2.02	0.42	
1:A:548:PHE:HE2	1:A:550:HIS:CD2	2.37	0.42	
1:A:159:ASP:OD1	2:A:601:PEG:H32	2.19	0.42	



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:389:ASN:CB	4:A:609:EDO:H21	2.50	0.41
1:A:271:SER:HB3	4:A:606:EDO:H22	2.02	0.41
5:A:610:NDP:H2N	5:A:610:NDP:H2D	1.82	0.40
3:A:602:PG4:H72	3:A:602:PG4:O1	2.22	0.40
1:A:459:ASP:OD2	1:A:461[A]:ARG:NE	2.50	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)
6:A:1036:HOH:O	6:A:1036:HOH:O[3_655]	2.03	0.17

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	Perce	entiles
1	А	481/503~(96%)	471 (98%)	10 (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	А	414/431~(96%)	412 (100%)	2~(0%)	88 89	



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

Mol	Chain	Res	Type
1	А	138	CYS
1	А	139	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	389	ASN
1	А	465	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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 T	Turne	Chain	Dec	Link	В	Bond lengths			Bond angles		
	Type	Ullalli	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2	
4	EDO	A	604	-	$3,\!3,\!3$	0.46	0	2,2,2	0.29	0	
2	PEG	А	608	-	$6,\!6,\!6$	0.82	0	$5,\!5,\!5$	0.40	0	
4	EDO	А	606	-	$3,\!3,\!3$	0.46	0	2,2,2	0.17	0	
2	PEG	А	601	-	$6,\!6,\!6$	0.90	0	$5,\!5,\!5$	0.57	0	



Mol Type (Chain	Dog	Link	B	ond leng	gths	Bond angles		
Moi Type Cham	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2		
4	EDO	А	603	-	3,3,3	0.51	0	2,2,2	0.47	0
4	EDO	А	605	-	$3,\!3,\!3$	0.43	0	2,2,2	0.19	0
4	EDO	А	607	-	$3,\!3,\!3$	0.48	0	2,2,2	0.33	0
3	PG4	А	602	-	12,12,12	0.50	0	11,11,11	0.40	0
5	NDP	А	610	-	45,52,52	3.85	17 (37%)	53,80,80	2.06	6 (11%)
4	EDO	А	609	-	3,3,3	0.47	0	2,2,2	0.35	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	А	604	-	-	0/1/1/1	-
2	PEG	А	608	-	-	3/4/4/4	-
4	EDO	А	606	-	-	0/1/1/1	-
2	PEG	А	601	-	-	4/4/4/4	-
4	EDO	А	603	-	-	0/1/1/1	-
4	EDO	А	605	-	-	1/1/1/1	-
4	EDO	А	607	-	-	0/1/1/1	-
3	PG4	А	602	-	-	4/10/10/10	-
5	NDP	А	610	-	-	6/30/77/77	0/5/5/5
4	EDO	А	609	_	_	1/1/1/1	_

All	(17)	bond	length	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	А	610	NDP	O4B-C1B	12.81	1.58	1.41
5	А	610	NDP	C6N-C5N	11.93	1.54	1.33
5	А	610	NDP	O4D-C1D	7.53	1.59	1.42
5	А	610	NDP	C2D-C1D	-6.82	1.31	1.53
5	А	610	NDP	O4D-C4D	-6.22	1.31	1.45
5	А	610	NDP	O4B-C4B	-5.80	1.32	1.45
5	А	610	NDP	P2B-O2B	4.96	1.68	1.59
5	А	610	NDP	C2N-C3N	4.89	1.48	1.34
5	А	610	NDP	O2D-C2D	4.22	1.52	1.43
5	А	610	NDP	C4N-C3N	4.01	1.57	1.49
5	А	610	NDP	C6N-N1N	3.93	1.47	1.37
5	A	610	NDP	C2A-N3A	3.86	1.38	1.32
5	A	610	NDP	C7N-N7N	3.30	1.42	1.33
5	A	610	NDP	C6A-N6A	3.17	1.45	1.34



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
5	А	610	NDP	C4N-C5N	2.80	1.56	1.48
5	А	610	NDP	C5D-C4D	2.79	1.60	1.51
5	А	610	NDP	C5A-C4A	-2.62	1.34	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
5	А	610	NDP	C5A-C6A-N6A	8.37	133.07	120.35
5	А	610	NDP	C1B-N9A-C4A	-6.25	115.67	126.64
5	А	610	NDP	N6A-C6A-N1A	-5.99	106.14	118.57
5	А	610	NDP	N3A-C2A-N1A	-5.96	119.36	128.68
5	А	610	NDP	PN-O3-PA	-2.50	124.24	132.83
5	А	610	NDP	C3B-C2B-C1B	2.27	107.16	102.89

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	А	610	NDP	C2B-O2B-P2B-O1X
3	А	602	PG4	O3-C5-C6-O4
3	А	602	PG4	O1-C1-C2-O2
2	А	601	PEG	O1-C1-C2-O2
2	А	608	PEG	O2-C3-C4-O4
5	А	610	NDP	C2D-C1D-N1N-C6N
2	А	601	PEG	C4-C3-O2-C2
3	А	602	PG4	C4-C3-O2-C2
2	А	601	PEG	C1-C2-O2-C3
5	А	610	NDP	O4D-C1D-N1N-C6N
2	А	601	PEG	O2-C3-C4-O4
5	А	610	NDP	PN-O3-PA-O2A
2	А	608	PEG	O1-C1-C2-O2
5	А	610	NDP	C2D-C1D-N1N-C2N
3	А	602	PG4	C6-C5-O3-C4
5	А	610	NDP	PN-O3-PA-O1A
4	А	609	EDO	O1-C1-C2-O2
2	А	608	PEG	C4-C3-O2-C2
4	А	605	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 22 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	А	608	PEG	1	0
4	А	606	EDO	1	0
2	А	601	PEG	1	0
4	А	605	EDO	1	0
3	А	602	PG4	9	0
5	А	610	NDP	5	0
4	А	609	EDO	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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, 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	$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q<0.9
1	А	481/503~(95%)	1.57	119 (24%) 0 0	27, 36, 71, 89	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	456	LEU	12.6
1	А	362	ASP	9.1
1	А	359	ALA	9.1
1	А	372	VAL	8.1
1	А	63	VAL	7.9
1	А	455	GLY	7.7
1	А	369	LEU	7.0
1	А	374	VAL	6.6
1	А	289	THR	6.2
1	А	292	THR	6.2
1	А	62	LYS	5.9
1	А	363	GLY	5.7
1	А	365	ILE	5.6
1	А	457	SER	5.4
1	А	373	THR	5.4
1	А	364	SER	5.3
1	А	375	PRO	4.8
1	А	480	LEU	4.8
1	А	296	GLY	4.7
1	А	210	VAL	4.7
1	A	360	SER	4.6
1	А	528	PRO	4.6
1	A	298	TYR	4.6
1	А	297	GLY	4.6
1	А	358	THR	4.4
1	А	454	PRO	4.1
1	A	471	THR	4.0



Mol	Chain	Res	Type	RSRZ
1	А	66	GLU	4.0
1	А	68	LYS	3.9
1	А	361	ALA	3.8
1	А	64	LYS	3.8
1	А	132	ASN	3.8
1	А	531	ALA	3.8
1	А	65	ASP	3.8
1	А	379	THR	3.7
1	А	548	PHE	3.7
1	А	532	GLY	3.5
1	А	295	ARG	3.5
1	А	69	SER	3.5
1	А	408	VAL	3.4
1	А	370	GLU	3.4
1	А	366	PRO	3.4
1	А	462	GLN	3.3
1	А	209	GLU	3.2
1	А	465	GLN	3.2
1	А	537	LYS	3.2
1	А	453	VAL	3.2
1	А	487	LEU	3.2
1	А	290	ILE	3.1
1	А	527	ILE	3.0
1	А	458	GLY	3.0
1	А	134	SER	2.9
1	А	218	ILE	2.9
1	А	217	ILE	2.9
1	А	139	HIS	2.9
1	А	77	PHE	2.9
1	А	299	PHE	2.8
1	А	216	VAL	2.8
1	А	526	PRO	2.8
1	А	175	LYS	2.7
1	Ā	83	LEU	2.7
1	А	371	ASP	2.7
1	Ā	136	ARG	2.7
1	А	376	GLU	2.7
1	A	138	CYS	2.6
1	A	533	THR	2.6
1	A	550	HIS	2.5
1	A	341	LEU	2.5
1	Ā	137	GLY	2.5



Mol	Chain	Res	Type	RSRZ	
1	А	248	ILE	2.5	
1	А	151	CYS	2.5	
1	А	390	ILE	2.5	
1	А	281[A]	CYS	2.5	
1	А	368	TYR	2.5	
1	А	274	TRP	2.4	
1	А	133	LEU	2.4	
1	А	186	TYR	2.4	
1	А	486	SER	2.4	
1	А	521	SER	2.4	
1	А	318	ALA	2.4	
1	A	67	GLN	2.4	
1	А	300	ASP	2.4	
1	A	470	LEU	2.4	
1	А	189	LEU	2.3	
1	А	108	ILE	2.3	
1	А	413	VAL	2.3	
1	А	330	ALA	2.3	
1	А	378	SER	2.3	
1	A	499	PHE	2.3	
1	А	78	GLY	2.3	
1	А	111	ALA	2.3	
1	A	415	ILE	2.3	
1	A	525	LYS	2.2	
1	A	251	TYR	2.2	
1	A	198	CYS	2.2	
1	A	367	GLY	2.2	
1	A	76	VAL	2.2	
1	A	319	LEU	2.2	
1	A	147	ILE	2.1	
1	A	505	LEU	2.1	
1	A	153	ALA	2.1	
1	A	536	PRO	2.1	
1	A	301	ASN	2.1	
1	A	276	ALA	2.1	
1	A	395	TRP	2.1	
1	A	118	VAL	2.1	
1	A	107	ILE	2.1	
1	A	524	ILE	2.1	
1	A	467	GLU	2.1	
1	A	75		2.1	
1	A	333	I ILE	2.1	



Mol	Chain	Res	Type	RSRZ	
1	А	488	ILE	2.1	
1	А	332	CYS	2.1	
1	А	377	GLY	2.1	
1	А	172	ASN	2.0	
1	А	257	VAL	2.0	
1	А	140	ALA	2.0	
1	А	103	PRO	2.0	
1	А	339	SER	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 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	PG4	А	602	13/13	0.59	0.31	42,64,79,85	0
2	PEG	А	601	7/7	0.64	0.35	29,31,37,40	7
2	PEG	А	608	7/7	0.69	0.22	41,45,59,61	0
4	EDO	А	603	4/4	0.73	0.20	38, 39, 43, 47	0
4	EDO	А	609	4/4	0.78	0.45	47,51,59,64	0
4	EDO	А	605	4/4	0.83	0.22	40,40,47,50	0
4	EDO	А	606	4/4	0.85	0.30	29,32,33,35	0
4	EDO	А	604	4/4	0.86	0.23	39,41,44,44	0
5	NDP	А	610	48/48	0.90	0.14	$29,\!36,\!45,\!53$	0
4	EDO	А	607	4/4	0.91	0.16	43,45,46,46	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.





6.5 Other polymers (i)

There are no such residues in this entry.

