

Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 06:25 pm GMT

PDB ID	:	8C4W
Title	:	Crystal structure of rat autotaxin and compound MEY-002
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Deposited on	:	2023-01-05
Resolution	:	1.95 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	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.95 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678(1.96-1.96)
Sidechain outliers	138945	2678(1.96-1.96)
RSRZ outliers	127900	2539(1.96-1.96)

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	А	862	10%	18%	·	10%		
2	В	2	50%	50%				

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	IOD	А	915	-	-	Х	-



2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 6840 atoms, of which 88 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 Ectonucleotide pyrophosphatase/phosphodiesterase family member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	А	779	Total 6287	C 3985	N 1082	0 1171	S 49	0	0	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	53	ALA	ASN	engineered mutation	UNP Q64610
А	410	ALA	ASN	engineered mutation	UNP Q64610
А	?	-	GLU	deletion	UNP Q64610
А	?	-	ALA	deletion	UNP Q64610
А	?	-	GLU	deletion	UNP Q64610
А	?	-	THR	deletion	UNP Q64610
А	?	-	GLY	deletion	UNP Q64610
А	?	-	LYS	deletion	UNP Q64610
А	?	-	PHE	deletion	UNP Q64610
А	?	-	ARG	deletion	UNP Q64610
А	?	-	GLY	deletion	UNP Q64610
А	?	-	SER	deletion	UNP Q64610
А	?	-	LYS	deletion	UNP Q64610
А	?	-	HIS	deletion	UNP Q64610
А	?	-	GLU	deletion	UNP Q64610
А	?	-	ASN	deletion	UNP Q64610
А	?	-	LYS	deletion	UNP Q64610
А	?	-	LYS	deletion	UNP Q64610
А	?	-	ASN	deletion	UNP Q64610
А	?	-	LEU	deletion	UNP Q64610
A	?	-	ASN	deletion	UNP Q64610
A	?	-	GLY	deletion	UNP Q64610
A	?	_	SER	deletion	UNP Q64610
A	?	_	VAL	deletion	UNP Q64610
A	?		GLU	deletion	UNP Q64610
A	?	-	PRO	deletion	UNP Q64610

There are 27 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
А	?	_	ARG	deletion	UNP Q64610

• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	ŀ	Aton	ns		ZeroOcc	AltConf	Trace
2	В	2	Total 28	C 16	N 2	O 10	0	0	0

• Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	2	Total Zn 2 2	0	0

• Molecule 4 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	9	Total I 9 9	0	0

• Molecule 5 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	Δ	1	Total C N S	0	0
0	11	1	3 1 1 1	0	0
5	Δ	1	Total C N S	0	0
0	11	1	3 1 1 1	0	0
5	Δ	1	Total C N S	0	0
0	11	1	3 1 1 1	0	0
5	Δ	1	Total C N S	0	0
0	11	1	3 1 1 1	0	0
5	Δ	1	Total C N S	0	0
0	11	1	3 1 1 1	0	0
5	Δ	1	Total C N S	0	0
0	А		3 1 1 1	0	0

• Molecule 6 is 7alpha-hydroxycholesterol (three-letter code: 5JK) (formula: $C_{27}H_{46}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	А	1	Total 75	C 27	H 46	0	0	0
			15	21	40	\angle		

• Molecule 7 is 5,7-bis(oxidanyl)-2-[1-(phenylmethyl)indol-3-yl]chromen-4-one (three-letter code: TIJ) (formula: $C_{24}H_{17}NO_4$) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	А	1	Total	C	N	0	0	0
			29	24	T	4		

• Molecule 8 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	А	1	Total	C 10	H	07	0	0
			45	12	26	(

• Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf			
9	А	1	Total	C	Н	0	0	0			
			14	3	8	3					
0	А	Δ	Δ	Δ	1	Total	\mathbf{C}	Η	Ο	0	0
9		1	14	3	8	3	0	0			

• Molecule 10 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	А	1	Total Ca 1 1	0	0

• Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	А	318	Total O 318 318	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.

 \bullet Molecule 1: Ectonucleotide pyrophosphatase/phosphodiesterase family member 2



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B:

50%

50%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants	53.23Å 62.86Å 70.15Å	Deperitor
a, b, c, α , β , γ	98.99° 106.57° 99.51°	Depositor
Bosolution(A)	47.65 - 1.95	Depositor
Resolution (A)	47.65 - 1.95	EDS
% Data completeness	97.2 (47.65-1.95)	Depositor
(in resolution range)	$97.2 \ (47.65 - 1.95)$	EDS
R_{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.25 (at 1.95 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
P. P.	0.196 , 0.236	Depositor
Λ, Λ_{free}	0.195 , 0.235	DCC
R_{free} test set	2000 reflections $(3.34%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	27.7	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.38, 56.0	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	0.95	EDS
Total number of atoms	6840	wwPDB-VP
Average B, all atoms $(Å^2)$	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.78% 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: TIJ, NAG, ZN, 5JK, SCN, IOD, GOL, CA, P6G

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	Bo	nd angles
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.42	0/6465	0.63	2/8771~(0.0%)

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	А	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	213	LEU	CA-CB-CG	5.77	128.57	115.30
1	А	201	MET	CG-SD-CE	-5.56	91.30	100.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	394	ALA	Peptide
1	А	86	CYS	Peptide
1	А	87	HIS	Peptide

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	6287	0	6027	176	0
2	В	28	0	25	2	0
3	А	2	0	0	0	0
4	А	9	0	0	5	0
5	А	18	0	0	1	0
6	А	29	46	0	1	0
7	А	29	0	0	1	0
8	А	19	26	26	0	0
9	А	12	16	16	0	0
10	А	1	0	0	0	0
11	А	318	0	0	15	0
All	All	6752	88	6094	179	0

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.

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 14.

All (179) 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 (\AA)	overlap (Å)	
1:A:79:CYS:SG	11:A:1184:HOH:O	2.13	1.03	
1:A:62:CYS:HA	1:A:89:PHE:CE1	2.02	0.94	
1:A:62:CYS:HA	1:A:89:PHE:HE1	1.30	0.93	
1:A:85:CYS:HB2	1:A:89:PHE:HD2	1.34	0.92	
1:A:58:CYS:HB3	1:A:61:ARG:HB2	1.52	0.91	
1:A:180:LYS:HE3	1:A:180:LYS:HA	1.52	0.89	
1:A:86:CYS:O	1:A:89:PHE:N	2.05	0.89	
5:A:905:SCN:S	11:A:1265:HOH:O	2.32	0.88	
1:A:178:MET:CE	1:A:192:ARG:HD3	2.04	0.87	
1:A:52:THR:HB	1:A:71:PRO:HB3	1.56	0.86	
1:A:53:ALA:HB3	1:A:72:ASP:HA	1.58	0.85	
1:A:405:LYS:HE3	1:A:405:LYS:HA	1.60	0.83	
1:A:199:PRO:HG2	1:A:502:PRO:HG3	1.59	0.83	
1:A:63:PHE:O	1:A:291:TRP:NE1	2.12	0.81	
1:A:52:THR:OG1	1:A:70:PRO:HB2	1.81	0.80	
1:A:94:LEU:HD23	1:A:94:LEU:O	1.82	0.80	
1:A:757:GLU:OE1	11:A:1002:HOH:O	2.00	0.78	
1:A:52:THR:N	1:A:71:PRO:HA	1.99	0.78	
1:A:85:CYS:HB2	1:A:89:PHE:CD2	2.18	0.78	
1:A:546:GLU:OE1	1:A:600:ARG:NH2	2.17	0.78	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:296:ASP:HB3	1:A:299:ARG:HH22	1.50	0.77	
1:A:85:CYS:SG	11:A:1012:HOH:O	2.44	0.75	
1:A:68:VAL:HG12	1:A:69:GLY:H	1.52	0.75	
1:A:178:MET:HE3	1:A:192:ARG:HD3	1.68	0.75	
1:A:496:TYR:CE2	1:A:497:ARG:HD2	2.22	0.74	
1:A:178:MET:HE2	1:A:192:ARG:HD3	1.68	0.74	
1:A:468:CYS:HB2	11:A:1005:HOH:O	1.87	0.74	
1:A:210:PHE:CD1	1:A:243:LEU:HD11	2.23	0.73	
1:A:296:ASP:HB3	1:A:299:ARG:NH2	2.04	0.73	
1:A:536:THR:O	1:A:538:THR:N	2.22	0.73	
1:A:481:ASN:OD1	11:A:1003:HOH:O	2.05	0.73	
1:A:381:ASP:HB3	1:A:399:ASN:ND2	2.04	0.73	
1:A:535:ARG:HG2	1:A:536:THR:CG2	2.19	0.73	
1:A:479:LYS:O	1:A:859:GLU:HG3	1.89	0.72	
1:A:793:PHE:CD1	1:A:795:LEU:HG	2.25	0.71	
1:A:65:LEU:O	1:A:66:GLN:HG2	1.92	0.70	
1:A:182:SER:O	11:A:1004:HOH:O	2.09	0.70	
1:A:716:GLN:OE1	4:A:920:IOD:I	2.80	0.70	
1:A:52:THR:HB	1:A:71:PRO:CB	2.23	0.69	
1:A:535:ARG:HG2	1:A:536:THR:HG22	1.74	0.69	
1:A:61:ARG:HD3	1:A:75:CYS:SG	2.34	0.68	
1:A:90:ASP:O	1:A:93:CYS:N	2.24	0.68	
1:A:93:CYS:O	1:A:94:LEU:HB2	1.95	0.67	
1:A:682:PRO:HB3	1:A:716:GLN:HB3	1.75	0.67	
1:A:53:ALA:HB3	1:A:72:ASP:CA	2.25	0.66	
1:A:496:TYR:CZ	1:A:497:ARG:HD2	2.30	0.66	
1:A:381:ASP:HB3	1:A:399:ASN:HD22	1.60	0.65	
1:A:74:ARG:NH1	1:A:74:ARG:HA	2.10	0.65	
1:A:367:ASP:OD2	11:A:1005:HOH:O	2.15	0.65	
1:A:73:CYS:O	1:A:74:ARG:NH1	2.31	0.63	
1:A:87:HIS:HA	11:A:1012:HOH:O	1.98	0.63	
1:A:497:ARG:HH11	1:A:497:ARG:HG2	1.64	0.62	
1:A:90:ASP:HB2	11:A:1012:HOH:O	1.99	0.62	
1:A:180:LYS:HA	1:A:180:LYS:CE	2.29	0.61	
1:A:558:LEU:HD12	1:A:561:GLU:HG3	1.82	0.61	
1:A:562:PHE:CD1	1:A:660:PRO:HG3	2.36	0.61	
1:A:65:LEU:HD22	1:A:65:LEU:N	2.16	0.60	
1:A:75:CYS:HA	1:A:89:PHE:CE2	2.36	0.60	
1:A:180:LYS:HG3	1:A:320:PHE:CE1	2.35	0.60	
1:A:550:PRO:HB2	1:A:611:ILE:HG12	1.82	0.59	
1:A:52:THR:HG23	4:A:915:IOD:I	2.72	0.59	



		Interatomic Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:665:ASN:HD22	1:A:667:LEU:H	1.50	0.58	
1:A:70:PRO:HA	1:A:71:PRO:O	2.03	0.58	
1:A:74:ARG:HA	1:A:74:ARG:CZ	2.34	0.58	
1:A:371:PHE:CE1	1:A:457:PRO:HA	2.39	0.57	
1:A:222:PRO:HA	1:A:225:HIS:CE1	2.39	0.57	
1:A:52:THR:HB	1:A:71:PRO:CA	2.35	0.57	
1:A:65:LEU:C	1:A:66:GLN:HG2	2.24	0.56	
1:A:844:SER:OG	1:A:847:GLU:HB3	2.04	0.56	
11:A:1310:HOH:O	2:B:2:NAG:N2	2.22	0.56	
1:A:67:GLU:HA	1:A:74:ARG:HH21	1.70	0.56	
1:A:85:CYS:O	1:A:87:HIS:N	2.39	0.56	
1:A:550:PRO:HB3	1:A:609:TYR:CZ	2.41	0.56	
2:B:2:NAG:H3	2:B:2:NAG:O7	2.04	0.56	
1:A:52:THR:CB	1:A:71:PRO:HA	2.37	0.55	
1:A:58:CYS:SG	1:A:86:CYS:HB2	2.46	0.55	
1:A:91:GLU:OE2	1:A:94:LEU:HB3	2.06	0.55	
1:A:245:GLY:HA2	1:A:246:ARG:NH1	2.22	0.55	
1:A:65:LEU:HD21	1:A:291:TRP:CD1	2.42	0.55	
1:A:557:TYR:O	1:A:656:VAL:HB	2.08	0.54	
1:A:77:ASN:ND2	11:A:1014:HOH:O	2.41	0.54	
1:A:54:THR:O	1:A:54:THR:HG22	2.07	0.54	
1:A:281:HIS:NE2	1:A:308:GLU:OE2	2.36	0.54	
1:A:543:MET:HG2	1:A:845:TYR:CE1	2.42	0.54	
1:A:497:ARG:HG2	1:A:497:ARG:NH1	2.24	0.53	
1:A:210:PHE:CE1	1:A:243:LEU:HD11	2.43	0.53	
1:A:67:GLU:HB3	1:A:74:ARG:HE	1.72	0.53	
1:A:85:CYS:H	1:A:87:HIS:CE1	2.26	0.53	
1:A:535:ARG:HG2	1:A:536:THR:HG23	1.90	0.52	
1:A:471:GLN:HB3	11:A:1011:HOH:O	2.10	0.52	
1:A:665:ASN:ND2	1:A:668:ALA:H	2.07	0.52	
1:A:52:THR:HG22	1:A:52:THR:O	2.10	0.52	
1:A:63:PHE:CD1	1:A:77:ASN:HB3	2.45	0.51	
1:A:312:PHE:CZ	1:A:316:LYS:HD2	2.46	0.51	
1:A:553:PRO:HB3	1:A:556:MET:HE1	1.93	0.51	
1:A:58:CYS:O	1:A:60:GLY:N	2.44	0.51	
1:A:57:SER:O	1:A:59:LYS:N	2.44	0.51	
1:A:76:ASP:N	1:A:76:ASP:OD1	2.44	0.50	
1:A:68:VAL:HG12	1:A:69:GLY:N	2.22	0.50	
1:A:246:ARG:CD	1:A:246:ARG:N	2.74	0.50	
1:A:458:LEU:HD23	11:A:1285:HOH:O	2.12	0.50	
1:A:704:MET:HA	1:A:797:HIS:NE2	2.26	0.50	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:654:PRO:HG3	4:A:916:IOD:I	2.82	0.49	
1:A:246:ARG:N	1:A:246:ARG:HD3	2.27	0.49	
1:A:839:ARG:O	1:A:840:LYS:HD3	2.13	0.49	
1:A:77:ASN:HD21	1:A:291:TRP:HH2	1.60	0.48	
1:A:540:ARG:HA	1:A:540:ARG:HD2	1.69	0.48	
1:A:92:LEU:H	1:A:92:LEU:HD23	1.78	0.48	
1:A:326:ASN:HB2	1:A:327:PRO:HD3	1.95	0.48	
1:A:52:THR:CA	1:A:71:PRO:HA	2.43	0.48	
1:A:64:GLU:OE1	1:A:64:GLU:HA	2.14	0.48	
1:A:398:ASN:O	1:A:399:ASN:HB2	2.14	0.48	
1:A:843:ARG:HB3	1:A:847:GLU:CG	2.44	0.48	
1:A:531:ASN:ND2	1:A:538:THR:HB	2.29	0.48	
1:A:329:ARG:HH11	1:A:329:ARG:HG2	1.79	0.47	
1:A:673:LYS:HG2	11:A:1002:HOH:O	2.12	0.47	
1:A:213:LEU:HB3	7:A:909:TIJ:C18	2.44	0.47	
1:A:52:THR:HB	1:A:71:PRO:HA	1.93	0.47	
1:A:329:ARG:HG2	1:A:329:ARG:NH1	2.30	0.47	
1:A:180:LYS:HE3	1:A:180:LYS:CA	2.23	0.47	
1:A:240:SER:O	1:A:247:GLU:HG2	2.14	0.47	
1:A:383:THR:OG1	1:A:395:LYS:HG3	2.15	0.47	
1:A:243:LEU:HA	1:A:243:LEU:HD12	1.50	0.46	
1:A:783:LYS:CG	1:A:783:LYS:O	2.63	0.46	
1:A:88:ASP:O	1:A:92:LEU:HD21	2.14	0.46	
1:A:322:PRO:HD2	1:A:323:GLU:OE1	2.14	0.46	
1:A:73:CYS:HB2	1:A:86:CYS:N	2.30	0.45	
1:A:85:CYS:SG	1:A:87:HIS:CE1	3.09	0.45	
1:A:61:ARG:HB3	1:A:75:CYS:CB	2.47	0.45	
1:A:86:CYS:O	1:A:88:ASP:N	2.49	0.45	
1:A:63:PHE:HD1	1:A:77:ASN:HB3	1.80	0.45	
1:A:568:CYS:SG	1:A:569:ASP:N	2.90	0.45	
1:A:536:THR:OG1	1:A:537:ASN:N	2.46	0.45	
1:A:565:GLY:HA3	1:A:667:LEU:HG	1.98	0.45	
1:A:405:LYS:HE3	1:A:405:LYS:CA	2.36	0.45	
1:A:53:ALA:HB3	1:A:72:ASP:N	2.32	0.44	
1:A:86:CYS:O	1:A:89:PHE:HB3	2.17	0.44	
1:A:76:ASP:N	1:A:89:PHE:CZ	2.84	0.44	
1:A:621:TYR:HA	1:A:628:PRO:HA	2.00	0.44	
1:A:90:ASP:OD1	1:A:90:ASP:C	2.55	0.44	
1:A:169:SER:HA	1:A:356:VAL:O	2.18	0.44	
1:A:625:PHE:HE2	1:A:752:ILE:CD1	2.31	0.44	
1:A:843:ARG:HB3	1:A:847:GLU:HG2	1.99	0.44	



	A i a	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:217:ALA:O	1:A:258:PRO:HA	2.17	0.44	
1:A:394:ALA:HB2	1:A:402:TYR:CG	2.53	0.44	
1:A:555:ILE:HD13	1:A:555:ILE:N	2.33	0.43	
1:A:559:GLN:H	1:A:559:GLN:HG3	1.61	0.43	
1:A:92:LEU:H	1:A:92:LEU:CD2	2.31	0.43	
1:A:205:TYR:CD1	1:A:206:PRO:HA	2.53	0.43	
1:A:79:CYS:HB2	1:A:85:CYS:HB3	1.53	0.43	
1:A:58:CYS:HB2	1:A:89:PHE:HB2	2.01	0.43	
1:A:124:LEU:N	1:A:129:CYS:SG	2.92	0.43	
1:A:626:LEU:O	1:A:627:MET:HB3	2.18	0.43	
1:A:769:SER:HB2	1:A:793:PHE:CZ	2.53	0.43	
1:A:665:ASN:ND2	1:A:667:LEU:HB2	2.35	0.42	
1:A:540:ARG:HH12	1:A:846:SER:HB3	1.84	0.42	
1:A:740:TYR:OH	1:A:754:GLN:HB2	2.20	0.42	
1:A:61:ARG:HB3	1:A:75:CYS:SG	2.60	0.42	
1:A:250:ASN:HB3	4:A:906:IOD:I	2.89	0.42	
1:A:827:ARG:HD2	1:A:827:ARG:HA	1.88	0.42	
1:A:359:HIS:NE2	1:A:474:HIS:CE1	2.87	0.42	
1:A:83:SER:O	1:A:84:SER:HB3	2.20	0.42	
1:A:95:LYS:HB2	1:A:95:LYS:HE3	1.84	0.42	
1:A:681:PHE:CD1	1:A:682:PRO:HD2	2.55	0.42	
1:A:118:HIS:O	1:A:129:CYS:HA	2.20	0.42	
1:A:680:LEU:O	1:A:716:GLN:NE2	2.53	0.41	
1:A:89:PHE:CD1	1:A:89:PHE:O	2.73	0.41	
1:A:155:GLU:O	1:A:350:CYS:HB2	2.21	0.41	
1:A:553:PRO:HB2	1:A:556:MET:HE2	2.01	0.41	
1:A:399:ASN:OD1	1:A:401:LYS:HG3	2.20	0.41	
1:A:52:THR:CG2	4:A:915:IOD:I	3.38	0.41	
1:A:670:LYS:HD3	1:A:670:LYS:HA	1.74	0.41	
1:A:65:LEU:HD22	1:A:65:LEU:H	1.85	0.41	
1:A:780:PRO:HD2	1:A:783:LYS:HD2	2.02	0.41	
1:A:698:VAL:O	1:A:701:MET:HG2	2.20	0.41	
1:A:249:PHE:HZ	6:A:908:5JK:C26	2.33	0.40	
1:A:550:PRO:HB3	1:A:609:TYR:CE2	2.56	0.40	
1:A:206:PRO:HD3	1:A:434:TYR:CE1	2.57	0.40	
1:A:95:LYS:HE3	1:A:283:ARG:NH2	2.36	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	А	773/862~(90%)	719~(93%)	44 (6%)	10 (1%)	12 3

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	58	CYS
1	А	59	LYS
1	А	71	PRO
1	А	72	ASP
1	А	94	LEU
1	А	537	ASN
1	А	73	CYS
1	А	86	CYS
1	А	69	GLY
1	А	84	SER

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	705/778~(91%)	688~(98%)	17~(2%)	49 40

All (17) residues with a non-rotameric sidechain are listed below:

IVIOI	Chain	Res	Type
1	А	73	CYS



Mol	Chain	Res	Type
1	А	125	SER
1	А	213	LEU
1	А	244	ARG
1	А	246	ARG
1	А	296	ASP
1	А	346	ARG
1	А	380	ASP
1	А	389	LEU
1	А	401	LYS
1	А	469	PHE
1	А	479	LYS
1	A	539	PHE
1	А	549	ARG
1	A	558	LEU
1	A	559	GLN
1	А	783	LYS

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

Mol	Chain	Res	Type
1	А	665	ASN

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)

2 monosaccharides 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



Mol	Tuno	Chain	Dog	Link	Bo	ond leng	ths	В	ond ang	jles
	туре	Ullaili	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NAG	В	1	1,2	$14,\!14,\!15$	0.40	0	$17,\!19,\!21$	0.65	0
2	NAG	В	2	2	14,14,15	1.21	1 (7%)	17,19,21	0.91	1 (5%)

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).

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
2	NAG	В	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	В	2	2	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	2	NAG	O5-C1	-3.97	1.37	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	2	NAG	C1-O5-C5	2.26	115.25	112.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	2	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	В	2	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 12 are monoatomic - leaving 11 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).

Mal	Turne	Chain	Dec	Tinle	B	ond leng	gths	Bond angles		
	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
7	TIJ	А	909	-	31,33,33	2.03	9 (29%)	41,48,48	1.62	6 (14%)
9	GOL	А	922	-	5,5,5	1.05	0	5,5,5	1.67	1 (20%)
5	SCN	А	913	-	1,2,2	0.72	0	0,1,1	-	-



Mal	Turne	Chain	Dec	Tink	B	ond leng	gths	Bond angles		
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
5	SCN	А	905	-	1,2,2	0.54	0	0,1,1	-	-
5	SCN	А	911	-	1,2,2	0.92	0	$0,\!1,\!1$	-	-
6	5JK	А	908	-	32,32,32	3.97	14 (43%)	47,50,50	2.94	15 (31%)
8	P6G	А	910	-	18,18,18	0.55	0	17,17,17	0.33	0
5	SCN	А	907	-	1,2,2	1.15	0	0,1,1	-	-
5	SCN	А	914	-	$1,\!2,\!2$	1.02	0	$0,\!1,\!1$	-	-
9	GOL	A	921	-	$5,\!5,\!5$	1.15	0	$5,\!5,\!5$	1.52	1 (20%)
5	SCN	А	912	-	1,2,2	0.84	0	0,1,1	-	-

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
7	TIJ	А	909	-	-	3/4/8/8	0/5/5/5
9	GOL	А	922	-	-	2/4/4/4	-
6	5JK	А	908	-	-	0/10/71/71	0/4/4/4
8	P6G	А	910	-	-	7/16/16/16	-
9	GOL	А	921	-	-	0/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	А	908	5JK	C6-C5	14.00	1.58	1.33
6	А	908	5JK	C8-C7	8.16	1.62	1.53
7	А	909	TIJ	O01-C02	7.24	1.40	1.24
6	А	908	5JK	C20-C17	-6.39	1.43	1.54
6	А	908	5JK	C16-C15	6.13	1.70	1.54
6	А	908	5JK	C15-C14	5.49	1.65	1.54
6	А	908	5JK	C13-C17	4.56	1.63	1.55
6	А	908	5JK	C12-C13	-4.28	1.46	1.54
7	А	909	TIJ	C06-N07	-4.24	1.33	1.38
7	А	909	TIJ	O21-C04	-3.73	1.31	1.36
6	А	908	5JK	C12-C11	3.61	1.61	1.53
6	А	908	5JK	O2-C7	-3.55	1.36	1.43
6	А	908	5JK	C10-C9	3.05	1.61	1.56
6	А	908	5JK	C8-C9	3.04	1.59	1.53
6	А	908	5JK	C8-C14	-3.03	1.48	1.53
6	А	908	5JK	C10-C5	-2.72	1.47	1.52
7	A	909	TIJ	O21-C22	-2.61	1.34	1.38



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
7	А	909	TIJ	C23-C22	2.45	1.43	1.38
7	А	909	TIJ	C29-C22	-2.41	1.36	1.40
6	А	908	5JK	C22-C20	2.39	1.60	1.54
7	А	909	TIJ	C08-N07	-2.39	1.45	1.49
7	А	909	TIJ	C15-N07	-2.32	1.36	1.39
7	А	909	TIJ	O28-C27	2.18	1.40	1.36

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	А	908	5JK	C7-C6-C5	-16.20	114.88	125.42
7	А	909	TIJ	O21-C04-C05	6.09	117.89	110.57
7	А	909	TIJ	C04-C03-C02	-4.71	117.17	122.25
6	А	908	5JK	C1-C10-C5	3.65	115.44	108.75
6	А	908	5JK	C17-C13-C14	3.65	104.39	100.07
6	А	908	5JK	C19-C10-C9	-3.43	107.59	111.68
9	А	922	GOL	C3-C2-C1	-3.29	98.90	111.70
6	А	908	5JK	C18-C13-C12	-3.15	105.62	110.59
6	А	908	5JK	C16-C15-C14	-3.12	98.96	105.13
9	А	921	GOL	C3-C2-C1	-2.88	100.50	111.70
6	А	908	5JK	C12-C13-C14	2.88	111.74	107.27
6	А	908	5JK	C15-C14-C8	2.86	122.33	118.33
7	А	909	TIJ	C22-O21-C04	2.86	122.97	119.53
6	А	908	5JK	C11-C9-C10	-2.79	109.40	113.08
6	А	908	5JK	C16-C17-C20	-2.77	107.86	112.15
6	А	908	5JK	C10-C5-C6	-2.57	118.97	122.81
7	А	909	TIJ	C19-C20-C05	-2.39	132.22	135.63
6	А	908	5JK	C21-C20-C17	-2.37	109.30	112.92
7	А	909	TIJ	C14-C09-C10	2.35	121.86	118.17
6	А	908	5JK	O1-C3-C4	-2.26	104.82	109.68
6	А	908	5JK	C16-C17-C13	2.26	106.57	103.84
6	А	908	5JK	C2-C3-C4	2.19	113.31	110.31
7	А	909	TIJ	C27-C29-C22	2.19	119.57	117.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	А	922	GOL	O1-C1-C2-C3
8	А	910	P6G	O16-C17-C18-O19
9	А	922	GOL	O1-C1-C2-O2
8	А	910	P6G	C15-C14-O13-C12



Mol	Chain	Res	Type	Atoms
8	А	910	P6G	O4-C5-C6-O7
7	А	909	TIJ	N07-C08-C09-C10
7	А	909	TIJ	N07-C08-C09-C14
8	А	910	P6G	O13-C14-C15-O16
7	А	909	TIJ	C09-C08-N07-C06
8	А	910	P6G	C8-C9-O10-C11
8	А	910	P6G	C5-C6-O7-C8
8	А	910	P6G	O7-C8-C9-O10

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	А	909	TIJ	1	0
5	А	905	SCN	1	0
6	А	908	5JK	1	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 sufficient 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	779/862~(90%)	0.66	82 (10%) 6 10	19, 31, 89, 185	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	59	LYS	25.3
1	А	75	CYS	21.0
1	А	68	VAL	20.4
1	А	69	GLY	18.4
1	А	55	SER	17.8
1	А	85	CYS	16.1
1	А	397	ILE	15.1
1	А	60	GLY	13.5
1	А	57	SER	13.3
1	А	52	THR	13.2
1	А	537	ASN	12.8
1	А	70	PRO	12.8
1	А	54	THR	12.5
1	А	58	CYS	11.0
1	А	71	PRO	10.4
1	А	73	CYS	9.8
1	А	65	LEU	9.8
1	А	92	LEU	8.9
1	А	86	CYS	8.8
1	А	89	PHE	8.7
1	А	53	ALA	8.6
1	А	458	LEU	8.5
1	А	74	ARG	8.5
1	А	557	TYR	7.0
1	А	61	ARG	6.7
1	А	398	ASN	6.5
1	А	562	PHE	6.4



Mol	Chain	Res	Type	RSRZ
1	А	558	LEU	6.3
1	А	459	ASP	6.0
1	А	66	GLN	5.7
1	А	571	LYS	5.7
1	А	181	GLY	5.3
1	А	87	HIS	5.3
1	А	62	CYS	5.0
1	А	56	GLY	4.8
1	А	180	LYS	4.8
1	А	72	ASP	4.5
1	А	90	ASP	4.3
1	А	569	ASP	4.3
1	А	567	THR	4.3
1	А	84	SER	4.0
1	А	667	LEU	3.9
1	А	570	ASP	3.5
1	А	399	ASN	3.3
1	А	63	PHE	3.3
1	А	88	ASP	3.3
1	А	566	CYS	3.3
1	А	556	MET	3.2
1	А	64	GLU	3.2
1	А	110	VAL	3.2
1	А	320	PHE	3.1
1	А	538	THR	3.0
1	А	563	ASP	3.0
1	А	183	LYS	3.0
1	А	650	ASN	3.0
1	А	757	GLU	2.9
1	А	568	CYS	2.9
1	А	395	LYS	2.7
1	А	378	ASN	2.7
1	A	179	LYS	2.6
1	А	644	ILE	2.6
1	A	93	CYS	2.5
1	А	559	GLN	2.5
1	А	67	GLU	2.4
1	А	536	THR	2.4
1	А	647	HIS	2.4
1	А	432	LEU	2.3
1	А	402	TYR	2.2
1	А	645	PRO	2.2



		1	1 0	
Mol	Chain	Res	Type	RSRZ
1	А	182	SER	2.1
1	А	137	CYS	2.1
1	А	111	ARG	2.1
1	А	758	GLY	2.1
1	А	555	ILE	2.1
1	А	564	LEU	2.1
1	А	469	PHE	2.1
1	А	79	CYS	2.1
1	А	127	GLY	2.1
1	А	468	CYS	2.1
1	А	124	LEU	2.0
1	А	648	LEU	2.0
1	А	646	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)

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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
2	NAG	В	2	14/15	0.77	0.17	30,37,43,47	0
2	NAG	В	1	14/15	0.98	0.10	16,23,27,27	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





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
5	SCN	А	912	3/3	0.48	0.34	56, 56, 57, 61	0
5	SCN	А	905	3/3	0.59	0.21	36,36,37,58	0
9	GOL	А	922	6/6	0.68	0.15	47,57,67,67	0
4	IOD	А	915	1/1	0.74	0.19	198,198,198,198	0
5	SCN	А	911	3/3	0.75	0.15	52,52,54,77	0
9	GOL	А	921	6/6	0.78	0.14	34,48,57,57	0
8	P6G	А	910	19/19	0.80	0.13	37,49,62,66	0
5	SCN	А	913	3/3	0.87	0.12	57,57,61,65	0
5	SCN	А	914	3/3	0.90	0.12	40,40,44,49	0
6	5JK	A	908	29/29	0.90	0.14	22,32,49,53	75
7	TIJ	A	909	29/29	0.90	0.12	26,29,32,32	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	B -factors (A^2)	Q < 0.9		
4	IOD	А	917	1/1	0.98	0.14	87,87,87,87	0		
4	IOD	А	920	1/1	0.99	0.11	75,75,75,75	0		
3	ZN	А	901	1/1	0.99	0.10	$25,\!25,\!25,\!25$	0		
5	SCN	А	907	3/3	0.99	0.11	29,29,35,41	0		
4	IOD	А	916	1/1	0.99	0.11	79,79,79,79	0		
4	IOD	А	906	1/1	0.99	0.10	61,61,61,61	0		
4	IOD	А	918	1/1	0.99	0.09	$65,\!65,\!65,\!65$	0		
4	IOD	А	904	1/1	1.00	0.03	$53,\!53,\!53,\!53$	0		
3	ZN	А	902	1/1	1.00	0.04	28,28,28,28	0		
4	IOD	А	903	1/1	1.00	0.08	29,29,29,29	0		
4	IOD	А	919	1/1	1.00	0.08	52,52,52,52	0		
10	CA	A	923	1/1	1.00	0.07	22,22,22,22	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.

