

# Full wwPDB X-ray Structure Validation Report (i)

#### Oct 19, 2023 – 04:15 PM EDT

PDB ID	:	8EI7
Title	:	Crystal structure of the WWP2 HECT domain in complex with H304, a He-
		licon Polypeptide
Authors	:	Li, K.; Tokareva, O.S.; Thomson, T.M.; Verdine, G.L.; McGee, J.H.
Deposited on	:	2022-09-14
Resolution	:	2.22  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:

:	4.02b-467
:	1.8.5 (274361), CSD as541be (2020)
:	1.13
:	2.36
:	20191225.v01 (using entries in the PDB archive December 25th 2019)
:	5.8.0158
:	7.0.044 (Gargrove)
:	Engh & Huber $(2001)$
:	Parkinson et al. (1996)
:	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 2.22 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.



Motria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries},  { m resolution}  { m range}({ m \AA}))$
R <sub>free</sub>	130704	5912(2.24-2.20)
Clashscore	141614	$6646 \ (2.24-2.20)$
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	376	3%	18%	•
1	В	376	9%	19%	••
2	С	19	89%	1	1%



# 2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6764 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 NEDD4-like E3 ubiquitin-protein ligase WWP2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	А	375	Total	С	Ν	0	$\mathbf{S}$	0	5	0
1	11	010	3198	2061	541	576	20	Ŭ	9	
1	Р	270	Total	С	Ν	Ο	$\mathbf{S}$	0	9	
	D	370	3140	2027	527	566	20	U	J	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	490	GLY	-	expression tag	UNP 000308
А	491	PRO	-	expression tag	UNP 000308
В	490	GLY	-	expression tag	UNP 000308
В	491	PRO	-	expression tag	UNP 000308

• Molecule 2 is a protein called H304.

Mol	Chain	Residues		Ate	$\mathbf{oms}$			ZeroOcc	AltConf	Trace
2	С	19	Total 147	C 94	N 24	O 25	$\begin{array}{c} \mathrm{S} \\ 4 \end{array}$	0	0	1

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	А	1	$\begin{array}{ccc} \text{Total}  \text{C}  \text{O} \\ 6  3  3 \end{array}$	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



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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
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total Zn 1 1	0	0
5	В	1	Total Zn 1 1	0	0

• Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	В	1	Total 10	$\begin{array}{c} \mathrm{C} \\ \mathrm{6} \end{array}$	0 4	0	0

• Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{C} \\ 7 & 4 & 3 \end{array}$	) ;	0	0

• Molecule 8 is N,N'-(1,4-phenylene) diacetamide (three-letter code: WHL) (formula:  $\rm C_{10}H_{12}N_2O_2).$ 





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	С	1	Total 14	C 10	N 2	0 2	0	0

• Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	А	110	Total O 110 110	0	0
9	В	77	Total O 77 77	0	0
9	С	7	Total O 7 7	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: NEDD4-like E3 ubiquitin-protein ligase WWP2



Chain C: 89%



11%

# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	62.16Å 64.30Å 103.69Å	Deneriten
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.90^{\circ}$ $90.00^{\circ}$	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	40.12 - 2.22	Depositor
Resolution (A)	40.12 - 2.22	EDS
% Data completeness	98.5 (40.12-2.22)	Depositor
(in resolution range)	98.5(40.12-2.22)	EDS
R <sub>merge</sub>	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.71 (at 2.22 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
B B.	0.200 , $0.264$	Depositor
II, IIfree	0.200 , $0.262$	DCC
$R_{free}$ test set	2013 reflections $(5.03%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	38.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	0.36 , $46.3$	EDS
L-test for $twinning^2$	$< L >=0.50, < L^2>=0.33$	Xtriage
	0.009 for -k,-h,-l	
Estimated twinning fraction	0.007 for k,h,-l	Xtriage
	0.024 for h,-k,-l	
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6764	wwPDB-VP
Average B, all atoms $(Å^2)$	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.88% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities 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: NH2, GOL, PGE, WHL, PEG, ZN, EDO, ACE

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	
	Unam	RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	А	0.58	0/3283	0.72	0/4426
1	В	0.51	0/3224	0.71	0/4346
2	С	0.57	0/149	0.69	0/200
All	All	0.55	0/6656	0.71	0/8972

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	3198	0	3128	45	0
1	В	3140	0	3066	56	0
2	С	147	0	125	3	0
3	А	12	0	15	2	0
4	А	24	0	36	4	0
4	В	16	0	24	0	0
5	А	1	0	0	0	0
5	В	1	0	0	0	0
6	В	10	0	14	1	0
7	В	7	0	10	2	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	С	14	0	0	0	0
9	А	110	0	0	3	0
9	В	77	0	0	1	0
9	С	7	0	0	0	0
All	All	6764	0	6418	103	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 8.

All (103) 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:B:561:ARG:O	1:B:562:GLU:HB3	1.73	0.87
1:B:659:LYS:HG2	1:B:660:GLU:H	1.42	0.84
1:A:548:MET:HG2	1:A:559:ILE:HD11	1.63	0.79
1:A:556:TYR:HA	1:A:559:ILE:HG22	1.70	0.72
1:A:521[B]:ARG:NH1	1:A:551:GLU:OE2	2.24	0.71
1:A:686:GLU:OE2	1:A:692:GLU:HB2	1.90	0.71
1:B:518[B]:SER:O	1:B:531:GLN:NE2	2.28	0.66
1:B:824:ASP:HB2	1:B:841:ARG:HD2	1.77	0.65
1:B:518[A]:SER:O	1:B:531:GLN:NE2	2.28	0.65
1:B:556:TYR:HA	1:B:559:ILE:HG22	1.78	0.65
1:A:753:GLN:HG2	1:A:804:LEU:HD23	1.80	0.63
1:B:525:PHE:HE1	1:B:571:VAL:HG12	1.64	0.63
1:B:546:ILE:HD13	1:B:560:ALA:HA	1.82	0.62
1:A:650:GLU:HG3	1:A:651:PHE:N	2.16	0.61
1:B:527:ASP:OD2	1:B:549:ARG:NH2	2.32	0.61
1:B:658:ILE:O	1:B:701:LYS:NZ	2.33	0.61
1:A:581:TYR:CG	1:A:586:ASN:HA	2.35	0.60
1:B:656:VAL:O	1:B:659:LYS:HB3	2.02	0.59
1:B:774:LYS:HD2	1:B:778:TRP:NE1	2.19	0.57
1:B:794:LEU:HA	1:B:861:ILE:HD12	1.86	0.57
1:B:541:ARG:HH12	7:B:902:PEG:H42	1.69	0.56
1:A:794:LEU:HA	1:A:861:ILE:HD12	1.87	0.56
1:B:579:PHE:HB3	1:B:589:LEU:HD11	1.87	0.56
1:B:659:LYS:CG	1:B:660:GLU:H	2.17	0.56
1:A:565:PHE:HZ	2:C:0:ACE:H2	1.71	0.55
1:A:588:CYS:HA	3:A:901:GOL:H31	1.88	0.55
1:B:773:SER:O	1:B:775:GLN:N	2.39	0.55
1:B:690:GLY:O	1:B:694:ILE:HD13	2.06	0.55
1:B:514:HIS:CE1	6:B:901:PGE:H62	2.41	0.55



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance $(\text{\AA})$	overlap (Å)
1:B:770:THR:OG1	1:B:772:ASN:O	2.24	0.55
1:B:784:LYS:HA	1:B:791:ARG:HH21	1.72	0.54
1:B:774:LYS:H	1:B:777:GLN:NE2	2.06	0.54
1:A:697:THR:H	1:A:700:ASN:HB2	1.71	0.54
1:A:541:ARG:HH12	4:A:908:EDO:C2	2.21	0.54
1:B:657:TRP:O	1:B:661:ASN:HB3	2.08	0.53
1:B:616:LEU:HD12	1:B:728:PHE:HZ	1.73	0.53
1:A:518:SER:O	1:A:531:GLN:NE2	2.40	0.53
1:A:767:ARG:HD3	1:A:822:CYS:SG	2.49	0.53
1:B:774:LYS:H	1:B:777:GLN:HE21	1.56	0.52
1:A:857:LEU:O	1:A:861:ILE:HG12	2.10	0.52
1:B:738:ARG:NH1	1:B:739:TYR:OH	2.42	0.51
1:B:561:ARG:O	1:B:562:GLU:CB	2.44	0.51
1:A:567:LEU:HD23	1:A:611:PHE:CE1	2.46	0.51
1:B:521:ARG:HB2	1:B:522:GLN:NE2	2.26	0.50
1:B:778:TRP:CD1	1:B:850:TYR:HB2	2.47	0.50
1:B:541:ARG:HH12	7:B:902:PEG:C4	2.25	0.49
3:A:901:GOL:H32	9:A:1076:HOH:O	2.13	0.49
1:B:786:MET:HB3	1:B:790:LYS:HB2	1.95	0.49
1:A:548:MET:CG	1:A:559:ILE:HD11	2.38	0.49
1:A:565:PHE:CZ	2:C:0:ACE:H2	2.47	0.48
1:A:847:TYR:CE1	1:A:856:LYS:HD2	2.48	0.48
1:B:556:TYR:O	1:B:559:ILE:HG22	2.13	0.48
1:A:769:TYR:CE1	1:A:825:LYS:HD2	2.48	0.48
1:B:704:TYR:CZ	1:B:708:LEU:HD12	2.48	0.48
1:A:606[B]:ARG:HD2	4:A:903:EDO:H12	1.96	0.48
1:A:525:PHE:HB2	1:A:570:GLU:HG3	1.95	0.47
1:B:542:ARG:O	1:B:618:HIS:HE1	1.97	0.47
1:A:499:TYR:HD1	1:A:748:MET:SD	2.36	0.47
1:A:638:ARG:NH1	1:A:706:MET:O	2.47	0.47
1:A:750:CYS:O	2:C:8:ARG:HD2	2.15	0.47
1:A:554:LEU:HB3	1:A:555:ASP:H	1.55	0.47
1:B:781:GLN:HG3	1:B:850:TYR:HE2	1.79	0.47
1:B:561:ARG:HG2	9:B:1024:HOH:O	2.14	0.47
1:B:774:LYS:HD2	1:B:778:TRP:CE2	2.50	0.47
1:A:541:ARG:HH12	4:A:908:EDO:H21	1.79	0.46
1:A:793:ARG:CG	1:A:861:ILE:HG22	2.45	0.46
1:B:672:PHE:CE2	1:B:696:VAL:HG22	2.50	0.46
1:A:499:TYR:CD1	1:A:748:MET:SD	3.09	0.46
1:B:660:GLU:O	1:B:661:ASN:HB2	2.15	0.46
1:B:562:GLU:HA	1:B:565:PHE:HB3	1.97	0.46



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:793:ARG:HG2	1:A:861:ILE:HG22	1.96	0.46
1:A:612:ILE:HD12	1:A:622:ILE:HD13	1.98	0.45
1:B:559:ILE:HD13	1:B:559:ILE:O	2.17	0.45
1:A:499:TYR:CZ	1:A:503:ARG:HD3	2.51	0.45
1:B:544:LEU:HG	1:B:618:HIS:CE1	2.51	0.45
1:A:505:LEU:HD13	1:A:736:TRP:CD1	2.52	0.45
1:A:606[B]:ARG:NH2	9:A:1001:HOH:O	2.26	0.45
1:B:755:ILE:HG21	1:B:760:TRP:CE3	2.52	0.45
1:B:493:ARG:HD2	1:B:493:ARG:HA	1.77	0.44
1:B:567:LEU:HD23	1:B:611:PHE:CE1	2.53	0.44
1:A:610:ARG:O	1:A:614:MET:HG3	2.18	0.44
4:A:905:EDO:H11	9:A:1086:HOH:O	2.19	0.43
1:B:572:LEU:HD21	1:B:624:THR:HG23	2.00	0.43
1:A:608:ILE:O	1:A:612:ILE:HG12	2.19	0.43
1:B:672:PHE:HE2	1:B:704:TYR:HB2	1.83	0.43
1:B:573:ASN:HB3	1:B:576:TYR:CD2	2.54	0.43
1:A:726:ASP:O	1:A:730:GLU:HG3	2.18	0.42
1:B:769:TYR:CE2	1:B:825:LYS:HB2	2.54	0.42
1:B:515:VAL:HG13	1:B:542:ARG:HD2	2.00	0.42
1:A:673:ILE:HG22	1:A:686:GLU:HA	2.01	0.42
1:A:676:MET:SD	1:A:678:ILE:HD11	2.59	0.42
1:B:673:ILE:HD13	1:B:692:GLU:HG2	2.01	0.42
1:A:668:LEU:HD13	1:A:670:LEU:HD11	2.03	0.41
1:A:695:ARG:O	1:A:700:ASN:ND2	2.54	0.41
1:B:546:ILE:O	1:B:559:ILE:HD12	2.19	0.41
1:A:847:TYR:CZ	1:A:856:LYS:HD2	2.56	0.41
1:B:672:PHE:CD2	1:B:696:VAL:HG22	2.56	0.41
1:A:761:GLN:HG3	1:A:780:TRP:CE2	2.57	0.40
1:B:525:PHE:CE1	1:B:571:VAL:HG12	2.50	0.40
1:A:521[A]:ARG:H	1:A:521[A]:ARG:HG2	1.66	0.40
1:A:803:ARG:HH21	1:A:803:ARG:HD2	1.71	0.40
1:B:703:GLU:O	1:B:707:LEU:HD13	2.20	0.40
1:B:781:GLN:HG3	1:B:850:TYR:CE2	2.55	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	378/376~(100%)	366~(97%)	9~(2%)	3~(1%)	19 18
1	В	369/376~(98%)	358~(97%)	8 (2%)	3~(1%)	19 18
2	С	17/19~(90%)	17 (100%)	0	0	100 100
All	All	764/771~(99%)	741 (97%)	17 (2%)	6 (1%)	22 18

All (6) Ramachandran outliers are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	А	552	GLU
1	В	659	LYS
1	В	774	LYS
1	А	521[A]	ARG
1	А	521[B]	ARG
1	В	562	GLU

#### 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	nalysed Rotameric Outliers		Percentiles		
1	А	348/344~(101%)	335~(96%)	13 (4%)	34	42	
1	В	342/344~(99%)	332~(97%)	10 (3%)	42	53	
2	С	14/14 (100%)	14 (100%)	0	100	100	
All	All	704/702~(100%)	681 (97%)	23 (3%)	41	47	



Mol	Chain	Res	Type
1	А	520[A]	SER
1	А	520[B]	SER
1	А	521[A]	ARG
1	А	521[B]	ARG
1	А	554	LEU
1	А	561	ARG
1	А	601	HIS
1	А	666	CYS
1	А	668	LEU
1	А	699	GLU
1	А	701	LYS
1	А	834	ARG
1	А	848	LYS
1	В	559	ILE
1	В	561	ARG
1	В	562	GLU
1	В	638	ARG
1	В	692	GLU
1	В	693	SER
1	В	735	GLU
1	В	753	GLN
1	В	758	SER
1	В	848	LYS

All (23) residues with a non-rotameric sidechain are listed below:

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such side chains are listed below:

Mol	Chain	Res	Type
1	В	514	HIS
1	В	674	GLN
1	В	772	ASN
1	В	777	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)

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	Tuno	Chain	Dog	Link	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z  > 2
4	EDO	В	905	-	3,3,3	0.53	0	$2,\!2,\!2$	0.12	0
4	EDO	А	904	-	3,3,3	0.47	0	2,2,2	0.54	0
4	EDO	А	907	-	3,3,3	0.53	0	$2,\!2,\!2$	0.33	0
4	EDO	А	908	-	3,3,3	0.45	0	$2,\!2,\!2$	0.95	0
4	EDO	В	904	-	3,3,3	0.52	0	$2,\!2,\!2$	0.39	0
4	EDO	А	905	-	3,3,3	0.58	0	$2,\!2,\!2$	0.25	0
3	GOL	А	901	-	$5,\!5,\!5$	1.00	0	$5,\!5,\!5$	1.25	1 (20%)
4	EDO	А	906	-	3,3,3	0.58	0	2,2,2	0.16	0
6	PGE	В	901	-	9,9,9	0.31	0	8,8,8	0.70	0
8	WHL	С	101	2	14,14,14	2.36	6 (42%)	18,18,18	2.42	9 (50%)
4	EDO	В	903	-	3,3,3	0.46	0	2,2,2	0.45	0
4	EDO	А	903	-	3,3,3	0.62	0	2,2,2	0.25	0
7	PEG	В	902	-	6,6,6	0.49	0	5, 5, 5	0.69	0
4	EDO	В	906	-	3,3,3	0.49	0	2,2,2	0.42	0
3	GOL	А	902	-	$5,\!5,\!5$	0.94	0	$5,\!5,\!5$	0.98	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	В	905	-	-	0/1/1/1	-
4	EDO	А	904	-	-	1/1/1/1	-
4	EDO	А	907	-	-	1/1/1/1	-
4	EDO	А	908	-	-	1/1/1/1	-



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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	В	904	-	-	1/1/1/1	-
4	EDO	А	905	-	-	1/1/1/1	-
3	GOL	А	901	-	-	0/4/4/4	-
4	EDO	А	906	-	-	1/1/1/1	-
6	PGE	В	901	-	-	4/7/7/7	-
8	WHL	С	101	2	-	0/8/8/8	0/1/1/1
4	EDO	В	903	-	-	1/1/1/1	-
4	EDO	А	903	-	-	0/1/1/1	-
7	PEG	В	902	-	-	3/4/4/4	-
4	EDO	В	906	-	-	1/1/1/1	-
3	GOL	А	902	-	-	4/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
8	С	101	WHL	CJ-NB	4.45	1.44	1.36
8	С	101	WHL	CG-NA	4.13	1.43	1.36
8	С	101	WHL	CF-NA	3.34	1.48	1.41
8	С	101	WHL	OB-CG	-2.47	1.17	1.23
8	С	101	WHL	CB-CA	2.29	1.42	1.38
8	С	101	WHL	CC-NB	2.21	1.46	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	С	101	WHL	CH-CG-NA	5.72	123.38	114.98
8	С	101	WHL	OB-CG-NA	-3.88	117.94	123.04
8	С	101	WHL	CB-CC-NB	3.19	131.13	120.40
8	С	101	WHL	CD-CC-NB	-2.95	110.50	120.40
8	С	101	WHL	CD-CE-CF	2.87	123.61	120.30
8	С	101	WHL	CA-CF-NA	2.71	129.51	120.40
8	С	101	WHL	OA-CJ-NB	-2.21	120.13	123.04
8	С	101	WHL	CE-CF-NA	-2.15	113.18	120.40
8	С	101	WHL	CF-NA-CG	-2.02	124.32	127.99
3	А	901	GOL	C3-C2-C1	-2.02	103.85	111.70

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	А	902	GOL	C1-C2-C3-O3

Mol	Chain	$\mathbf{Res}$	Type	Atoms
3	А	902	GOL	O1-C1-C2-O2
6	В	901	PGE	O2-C3-C4-O3
3	А	902	GOL	O1-C1-C2-C3
6	В	901	PGE	O1-C1-C2-O2
3	А	902	GOL	O2-C2-C3-O3
4	В	903	EDO	O1-C1-C2-O2
4	В	904	EDO	O1-C1-C2-O2
7	В	902	PEG	C1-C2-O2-C3
6	В	901	PGE	C6-C5-O3-C4
7	В	902	PEG	C4-C3-O2-C2
4	А	904	EDO	O1-C1-C2-O2
4	А	905	EDO	O1-C1-C2-O2
4	А	908	EDO	O1-C1-C2-O2
6	В	901	PGE	C4-C3-O2-C2
4	В	906	EDO	O1-C1-C2-O2
7	В	902	PEG	01-C1-C2-O2
4	А	906	EDO	O1-C1-C2-O2
4	А	907	EDO	O1-C1-C2-O2

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There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	А	908	EDO	2	0
4	А	905	EDO	1	0
3	А	901	GOL	2	0
6	В	901	PGE	1	0
4	А	903	EDO	1	0
7	В	902	PEG	2	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 (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	375/376~(99%)	0.02	10 (2%) 54 52	24, 39, 66, 115	0
1	В	370/376~(98%)	0.34	32 (8%) 10 9	26, 49, 90, 118	0
2	С	17/19~(89%)	-0.27	0 100 100	26, 32, 38, 40	0
All	All	762/771~(98%)	0.17	42 (5%) 25 23	24, 42, 85, 118	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	553	GLY	10.0
1	А	556	TYR	9.2
1	В	668	LEU	5.8
1	В	660	GLU	5.7
1	А	554	LEU	5.6
1	В	657	TRP	5.5
1	В	658	ILE	5.4
1	А	555	ASP	5.3
1	В	659	LYS	4.5
1	В	669	GLU	4.1
1	В	693	SER	3.8
1	В	753	GLN	3.8
1	А	681	LYS	3.7
1	В	673	ILE	3.6
1	В	670	LEU	3.5
1	В	685	HIS	3.5
1	В	762	LYS	3.5
1	В	767	ARG	3.4
1	В	826	VAL	3.3
1	А	680	GLY	3.3
1	В	699	GLU	3.2
1	В	770	THR	3.2
1	В	768	HIS	3.0



Mol	Chain	Res	Type	RSRZ
1	А	550	GLY	3.0
1	В	694	ILE	2.9
1	В	772	ASN	2.9
1	В	656	VAL	2.7
1	В	696	VAL	2.6
1	В	766	TYR	2.5
1	В	707	LEU	2.5
1	В	681	LYS	2.4
1	В	765	ILE	2.4
1	В	763	SER	2.3
1	А	685	HIS	2.3
1	В	692	GLU	2.3
1	В	754	GLU	2.2
1	А	557	GLY	2.2
1	А	684	THR	2.1
1	В	784	LYS	2.1
1	В	769	TYR	2.1
1	В	757	MET	2.0
1	В	758	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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
4	EDO	В	906	4/4	0.67	0.23	$56,\!63,\!69,\!74$	0
4	EDO	А	903	4/4	0.76	0.17	48,48,51,61	0
4	EDO	В	903	4/4	0.77	0.18	47,53,57,65	0
4	EDO	А	904	4/4	0.77	0.24	58,60,61,66	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q<0.9
4	EDO	А	907	4/4	0.81	0.17	$46,\!47,\!48,\!51$	0
7	PEG	В	902	7/7	0.84	0.14	50,54,59,60	0
4	EDO	В	905	4/4	0.85	0.16	$51,\!53,\!56,\!58$	0
5	ZN	А	909	1/1	0.87	0.14	79,79,79,79	0
5	ZN	В	907	1/1	0.88	0.06	$98,\!98,\!98,\!98$	0
4	EDO	А	905	4/4	0.88	0.16	44,46,48,52	0
8	WHL	С	101	14/14	0.89	0.18	30,40,48,65	0
3	GOL	А	901	6/6	0.90	0.16	37,40,42,42	0
4	EDO	В	904	4/4	0.90	0.12	41,43,44,54	0
4	EDO	А	908	4/4	0.91	0.10	47,51,55,55	0
4	EDO	А	906	4/4	0.92	0.13	43,45,50,55	0
3	GOL	А	902	6/6	0.94	0.11	38,42,45,52	0
6	PGE	В	901	10/10	0.95	0.14	40,43,49,50	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

