



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:25 AM UTC

PDB ID : 8EI7 / pdb_00008ei7
Title : Crystal structure of the WWP2 HECT domain in complex with H304, a Helicon 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 ⓘ 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 ⓘ](#)) 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

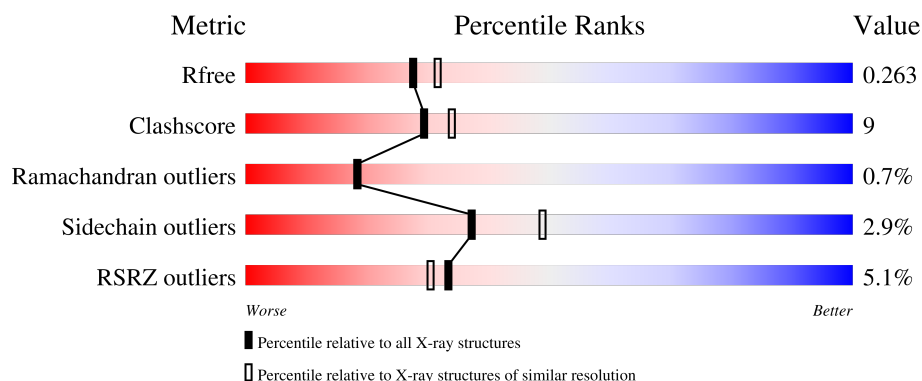
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-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.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (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 $\leq 5\%$. 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	376	3% 80% 18% ..
1	B	376	8% 77% 20% ..
2	C	19	89% 11%

2 Entry composition

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	A	375	Total	C	N	O	S	0	5	0
			3198	2061	541	576	20			
1	B	370	Total	C	N	O	S	0	3	0
			3140	2027	527	566	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	490	GLY	-	expression tag	UNP O00308
A	491	PRO	-	expression tag	UNP O00308
B	490	GLY	-	expression tag	UNP O00308
B	491	PRO	-	expression tag	UNP O00308

- Molecule 2 is a protein called H304.

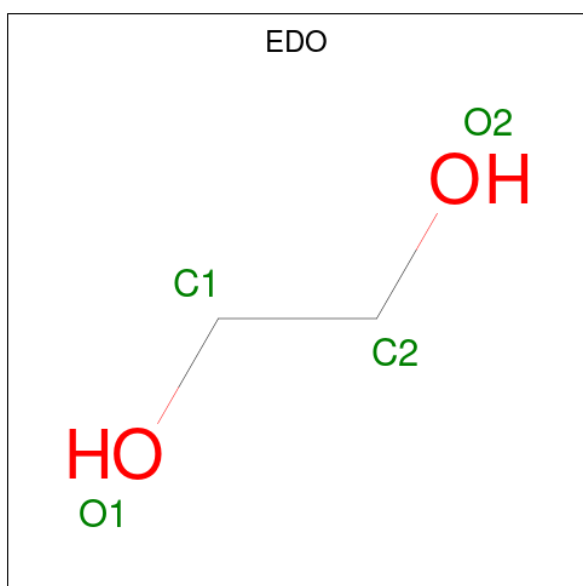
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	19	Total	C	N	O	S	0	0	1
			147	94	24	25	4			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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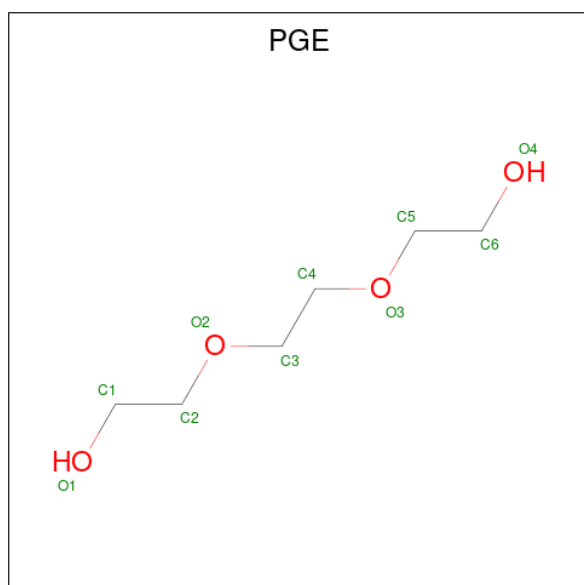
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

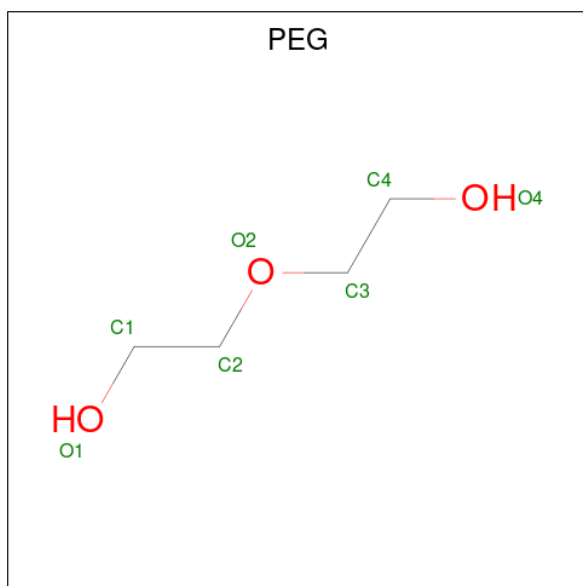
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	B	1	Total Zn 1 1	0	0

- Molecule 6 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



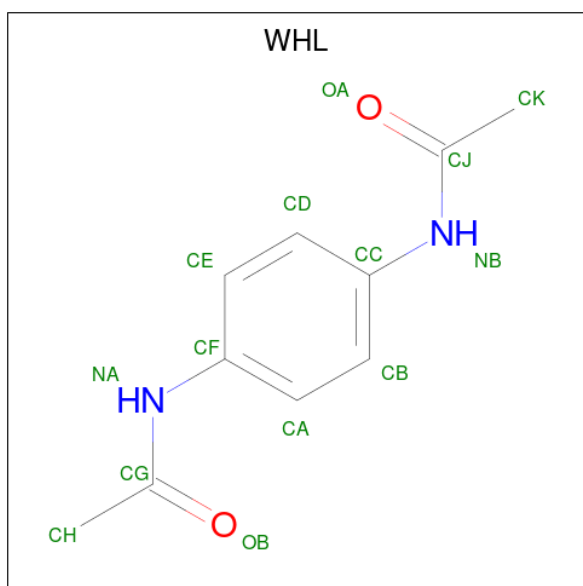
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is N,N'-(1,4-phenylene)diacetamide (CCD ID: WHL) (formula: $C_{10}H_{12}N_2O_2$).



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

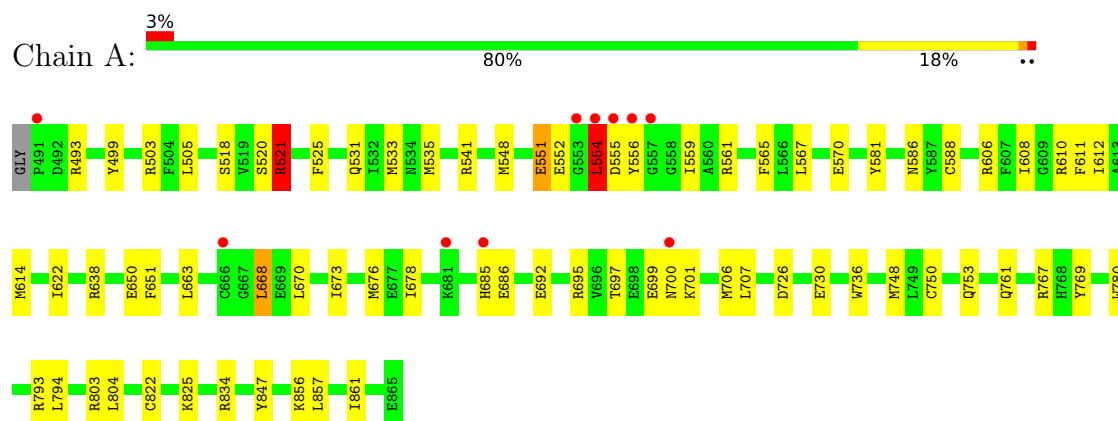
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	110	Total	O	0	0
			110	110		
9	B	77	Total	O	0	0
			77	77		
9	C	7	Total	O	0	0
			7	7		

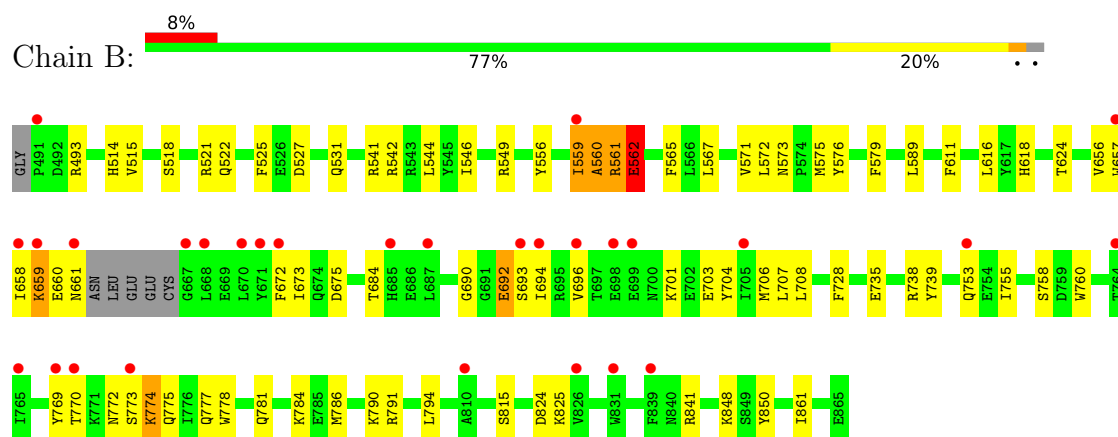
3 Residue-property plots [i](#)

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.

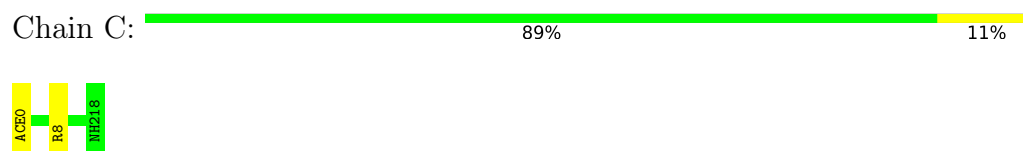
- Molecule 1: NEDD4-like E3 ubiquitin-protein ligase WWP2



- Molecule 1: NEDD4-like E3 ubiquitin-protein ligase WWP2



- Molecule 2: H304



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.16Å 64.30Å 103.69Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	40.12 – 2.22 40.12 – 2.22	Depositor EDS
% Data completeness (in resolution range)	98.5 (40.12-2.22) 98.5 (40.12-2.22)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.200 , 0.264 0.202 , 0.263	Depositor DCC
R_{free} test set	2015 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -k,-h,-l 0.007 for k,h,-l 0.024 for h,-k,-l	Xtriage
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.*

¹Intensities estimated from amplitudes.

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.

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: ZN, ACE, PEG, EDO, NH2, PGE, GOL, WHL

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	0.54	0/3283	0.73	2/4426 (0.0%)
1	B	0.46	1/3224 (0.0%)	0.73	1/4346 (0.0%)
2	C	0.52	0/149	0.58	0/200
All	All	0.50	1/6656 (0.0%)	0.73	3/8972 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	815	SER	CA-C	-5.15	1.45	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	560	ALA	N-CA-C	-6.75	104.00	111.36
1	A	554	LEU	CB-CA-C	-5.70	109.99	116.54
1	A	551	GLU	N-CA-C	5.64	115.86	108.07

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	3198	0	3128	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3140	0	3066	60	0
2	C	147	0	125	3	0
3	A	12	0	15	2	0
4	A	24	0	36	4	0
4	B	16	0	24	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	B	10	0	14	1	0
7	B	7	0	10	2	0
8	C	14	0	0	0	0
9	A	110	0	0	3	0
9	B	77	0	0	1	0
9	C	7	0	0	0	0
All	All	6764	0	6418	112	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 9.

All (112) 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: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:706:MET:HE3	1:B:707:LEU:HD12	1.81	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:521[B]:ARG:NH1	1:A:548:MET:HE2	2.27	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:675:ASP:OD1	1:B:684:THR:OG1	2.24	0.48
1:B:704:TYR:CZ	1:B:708:LEU:HD12	2.48	0.48
1:A:533:MET:HE1	1:A:606[A]:ARG:HG2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:676:MET:HE2	1:A:685:HIS:NE2	2.29	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:B:575:MET:HA	1:B:575:MET:HE2	1.95	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
1:B:706:MET:HE3	1:B:707:LEU:CD1	2.46	0.46
1:A:793:ARG:HG2	1:A:861:ILE:HG22	1.96	0.46
1:A:531:GLN:O	1:A:535:MET:HE3	2.16	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:767:ARG:C	1:A:769:TYR:H	2.28	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

5.3.1 Protein backbone

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	378/376 (100%)	366 (97%)	9 (2%)	3 (1%)	16	15
1	B	369/376 (98%)	358 (97%)	8 (2%)	3 (1%)	16	15
2	C	17/19 (90%)	17 (100%)	0	0	100	100
All	All	764/771 (99%)	741 (97%)	17 (2%)	6 (1%)	18	15

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	552	GLU
1	B	659	LYS
1	B	774	LYS
1	A	521[A]	ARG
1	A	521[B]	ARG
1	B	562	GLU

5.3.2 Protein sidechains ⓘ

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	348/344 (101%)	335 (96%)	13 (4%)	30	39
1	B	342/344 (99%)	333 (97%)	9 (3%)	40	53
2	C	14/14 (100%)	14 (100%)	0	100	100
All	All	704/702 (100%)	682 (97%)	22 (3%)	37	46

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	493	ARG
1	A	520[A]	SER
1	A	520[B]	SER
1	A	521[A]	ARG
1	A	521[B]	ARG
1	A	554	LEU
1	A	561	ARG
1	A	663	LEU
1	A	668	LEU
1	A	699	GLU
1	A	701	LYS
1	A	707	LEU
1	A	834	ARG
1	B	559	ILE
1	B	561	ARG
1	B	562	GLU
1	B	692	GLU
1	B	693	SER
1	B	735	GLU
1	B	753	GLN
1	B	758	SER
1	B	848	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	522	GLN
1	A	819	GLN
1	B	514	HIS
1	B	585	ASN
1	B	586	ASN
1	B	772	ASN
1	B	777	GLN
1	B	781	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	EDO	A	907	-	3,3,3	0.50	0	2,2,2	0.36	0
3	GOL	A	902	-	5,5,5	0.96	0	5,5,5	1.05	0
4	EDO	A	908	-	3,3,3	0.42	0	2,2,2	0.96	0
8	WHL	C	101	2	14,14,14	2.38	6 (42%)	18,18,18	2.39	8 (44%)
6	PGE	B	901	-	9,9,9	0.32	0	8,8,8	0.69	0
4	EDO	A	903	-	3,3,3	0.60	0	2,2,2	0.18	0
4	EDO	A	904	-	3,3,3	0.44	0	2,2,2	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	A	905	-	3,3,3	0.55	0	2,2,2	0.22	0
4	EDO	B	903	-	3,3,3	0.44	0	2,2,2	0.49	0
4	EDO	B	904	-	3,3,3	0.50	0	2,2,2	0.43	0
4	EDO	B	905	-	3,3,3	0.50	0	2,2,2	0.18	0
7	PEG	B	902	-	6,6,6	0.51	0	5,5,5	0.69	0
3	GOL	A	901	-	5,5,5	1.01	0	5,5,5	1.35	1 (20%)
4	EDO	B	906	-	3,3,3	0.46	0	2,2,2	0.46	0
4	EDO	A	906	-	3,3,3	0.55	0	2,2,2	0.21	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	A	907	-	-	1/1/1/1	-
3	GOL	A	902	-	-	4/4/4/4	-
4	EDO	A	908	-	-	1/1/1/1	-
8	WHL	C	101	2	-	0/8/8/8	0/1/1/1
6	PGE	B	901	-	-	4/7/7/7	-
4	EDO	A	903	-	-	0/1/1/1	-
4	EDO	A	904	-	-	1/1/1/1	-
4	EDO	A	905	-	-	1/1/1/1	-
4	EDO	B	903	-	-	1/1/1/1	-
4	EDO	B	904	-	-	1/1/1/1	-
4	EDO	B	905	-	-	0/1/1/1	-
7	PEG	B	902	-	-	3/4/4/4	-
3	GOL	A	901	-	-	0/4/4/4	-
4	EDO	B	906	-	-	1/1/1/1	-
4	EDO	A	906	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	101	WHL	CJ-NB	4.41	1.44	1.36
8	C	101	WHL	CG-NA	4.09	1.43	1.36
8	C	101	WHL	CF-NA	3.35	1.48	1.41
8	C	101	WHL	CB-CA	2.54	1.42	1.38
8	C	101	WHL	OB-CG	-2.50	1.17	1.23
8	C	101	WHL	CC-NB	2.21	1.46	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	101	WHL	CH-CG-NA	5.60	123.38	114.95
8	C	101	WHL	OB-CG-NA	-3.73	117.94	123.06
8	C	101	WHL	CB-CC-NB	3.19	131.13	120.41
8	C	101	WHL	CD-CC-NB	-2.95	110.50	120.41
8	C	101	WHL	CD-CE-CF	2.88	123.61	120.30
8	C	101	WHL	CA-CF-NA	2.71	129.51	120.41
3	A	901	GOL	C3-C2-C1	-2.17	103.85	111.80
8	C	101	WHL	CE-CF-NA	-2.16	113.18	120.41
8	C	101	WHL	OA-CJ-NB	-2.13	120.13	123.06

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	GOL	C1-C2-C3-O3
3	A	902	GOL	O1-C1-C2-O2
3	A	902	GOL	O1-C1-C2-C3
6	B	901	PGE	O2-C3-C4-O3
3	A	902	GOL	O2-C2-C3-O3
6	B	901	PGE	O1-C1-C2-O2
4	B	903	EDO	O1-C1-C2-O2
4	B	904	EDO	O1-C1-C2-O2
7	B	902	PEG	C1-C2-O2-C3
6	B	901	PGE	C6-C5-O3-C4
7	B	902	PEG	C4-C3-O2-C2
4	A	908	EDO	O1-C1-C2-O2
6	B	901	PGE	C4-C3-O2-C2
4	A	904	EDO	O1-C1-C2-O2
4	A	905	EDO	O1-C1-C2-O2
4	A	906	EDO	O1-C1-C2-O2
4	A	907	EDO	O1-C1-C2-O2
7	B	902	PEG	O1-C1-C2-O2
4	B	906	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	908	EDO	2	0
6	B	901	PGE	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	903	EDO	1	0
4	A	905	EDO	1	0
7	B	902	PEG	2	0
3	A	901	GOL	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	375/376 (99%)	-0.01	10 (2%) 56 53	16, 39, 66, 115	5 (1%)
1	B	370/376 (98%)	0.51	29 (7%) 19 16	20, 49, 90, 118	3 (0%)
2	C	17/19 (89%)	-0.49	0 100 100	26, 32, 38, 40	0
All	All	762/771 (98%)	0.23	39 (5%) 33 30	16, 42, 85, 118	8 (1%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	667	GLY	4.7
1	A	491	PRO	3.9
1	B	658	ILE	3.7
1	A	554	LEU	3.6
1	B	559	ILE	3.3
1	A	556	TYR	3.3
1	A	557	GLY	3.1
1	B	661	ASN	3.1
1	B	668	LEU	3.1
1	B	694	ILE	3.0
1	B	699	GLU	2.8
1	A	553	GLY	2.8
1	B	491	PRO	2.6
1	B	670	LEU	2.6
1	B	753	GLN	2.6
1	A	700	ASN	2.6
1	B	657	TRP	2.6
1	B	696	VAL	2.6
1	B	659	LYS	2.6
1	B	839	PHE	2.5
1	B	693	SER	2.5
1	A	555	ASP	2.5
1	B	831	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	810	ALA	2.4
1	A	681	LYS	2.4
1	B	770	THR	2.4
1	B	698	GLU	2.4
1	B	826	VAL	2.3
1	A	666	CYS	2.3
1	B	773	SER	2.3
1	B	765	ILE	2.3
1	B	769	TYR	2.3
1	B	671	TYR	2.2
1	B	685	HIS	2.1
1	B	672	PHE	2.1
1	B	687	LEU	2.1
1	B	705	ILE	2.0
1	B	764	THR	2.0
1	A	685	HIS	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	EDO	A	904	4/4	0.62	0.19	58,60,61,66	0
4	EDO	B	906	4/4	0.77	0.13	56,63,69,74	0
7	PEG	B	902	7/7	0.78	0.15	50,54,59,60	0
4	EDO	A	906	4/4	0.79	0.13	43,45,50,55	0
4	EDO	A	903	4/4	0.81	0.14	48,48,51,61	0
4	EDO	A	908	4/4	0.82	0.12	47,51,55,55	0
4	EDO	A	907	4/4	0.85	0.11	46,47,48,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	B	903	4/4	0.86	0.14	47,53,57,65	0
4	EDO	B	905	4/4	0.86	0.12	51,53,56,58	0
5	ZN	B	907	1/1	0.87	0.13	98,98,98,98	0
3	GOL	A	901	6/6	0.88	0.12	37,40,42,42	0
4	EDO	B	904	4/4	0.88	0.11	41,43,44,54	0
8	WHL	C	101	14/14	0.88	0.12	30,40,48,65	0
4	EDO	A	905	4/4	0.89	0.11	44,46,48,52	0
3	GOL	A	902	6/6	0.90	0.09	38,42,45,52	0
5	ZN	A	909	1/1	0.92	0.18	79,79,79,79	0
6	PGE	B	901	10/10	0.94	0.09	40,43,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.