



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:04 AM GMT

PDB ID : 1ZIW
Title : Human Toll-like Receptor 3 extracellular domain structure
Authors : Wilson, I.A.; Choe, J.
Deposited on : 2005-04-27
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

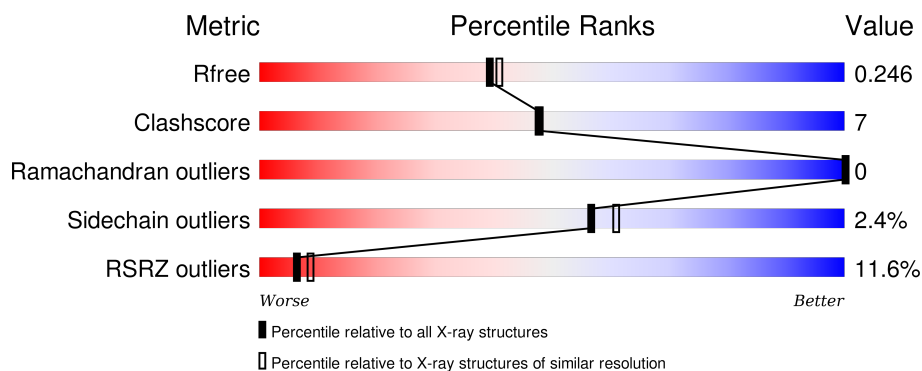
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	680	<div> <div>11%</div> <div>79%</div> <div>12%</div> <div>8%</div> </div>

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
2	NDG	A	1	-	-	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	2	-	-	-	X
3	NAG	A	5	-	-	-	X
3	NAG	A	9	-	-	-	X
5	SO4	A	777	-	-	-	X
6	GOL	A	779	-	-	-	X
6	GOL	A	782	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5628 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.

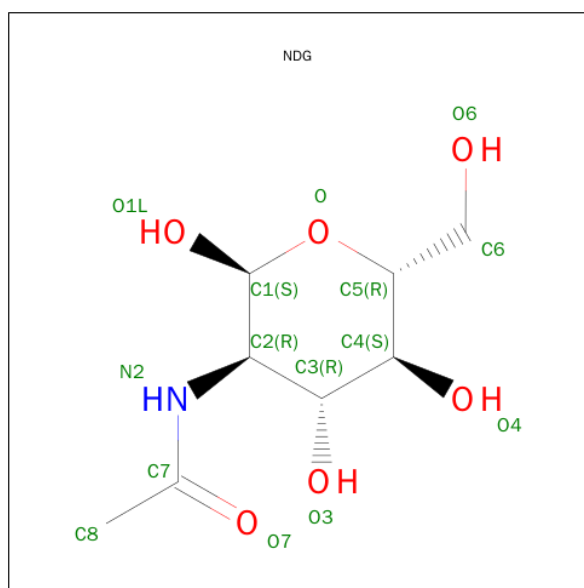
- Molecule 1 is a protein called Toll-like receptor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	629	5052	3232	856	948	16	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	701	HIS	-	EXPRESSION TAG	UNP O15455
A	702	HIS	-	EXPRESSION TAG	UNP O15455
A	703	HIS	-	EXPRESSION TAG	UNP O15455
A	704	HIS	-	EXPRESSION TAG	UNP O15455
A	705	HIS	-	EXPRESSION TAG	UNP O15455
A	706	HIS	-	EXPRESSION TAG	UNP O15455

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).

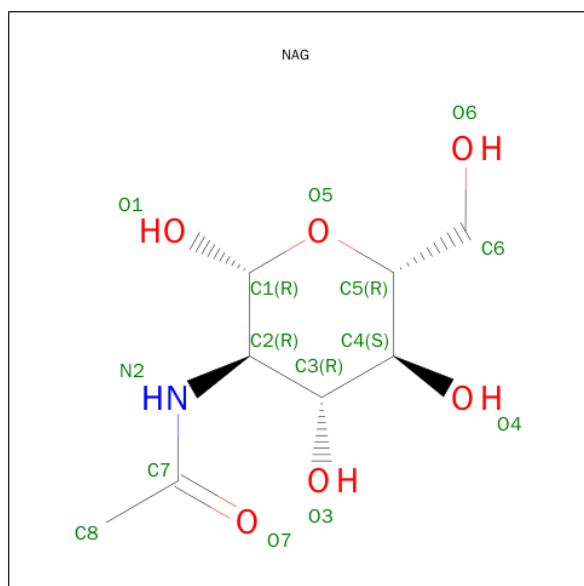


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

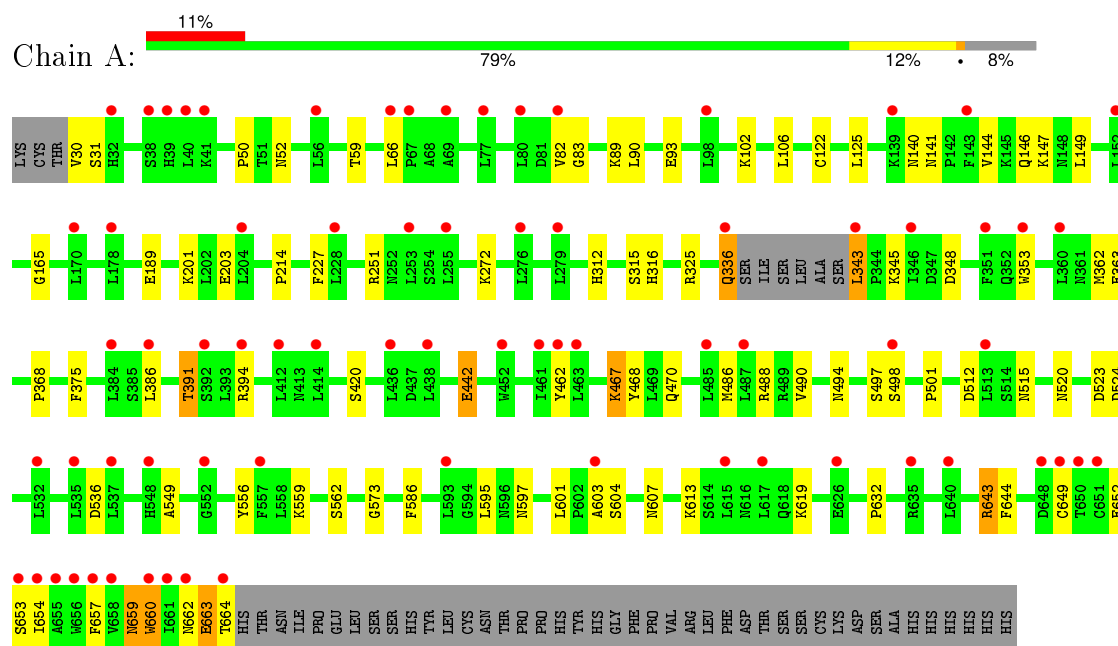
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	362	Total	O	0	0
			362	362		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Toll-like receptor 3



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	138.50Å 155.12Å 119.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 19.98 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.10) 99.7 (19.98-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0013	Depositor
R, R_{free}	0.208 , 0.248 0.207 , 0.246	Depositor DCC
R_{free} test set	3795 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 61.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 74866 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5628	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG, NDG, SO4

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	0.74	3/5152 (0.1%)	0.74	2/6987 (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	A	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	549	ALA	CA-CB	6.64	1.66	1.52
1	A	467	LYS	CE-NZ	6.30	1.64	1.49
1	A	442	GLU	CG-CD	5.35	1.59	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	467	LYS	CD-CE-NZ	8.40	131.02	111.70
1	A	643	ARG	N-CA-C	5.51	125.87	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	391	THR	Peptide
1	A	498	SER	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	654	ILE	Peptide

5.2 Too-close contacts ⓘ

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	5052	0	5081	74	1
2	A	28	0	26	2	0
3	A	112	0	100	2	0
4	A	28	0	26	0	0
5	A	10	0	0	0	0
6	A	36	0	47	5	0
7	A	362	0	0	25	1
All	All	5628	0	5280	78	2

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 7.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:524:ASP:HB3	7:A:1070:HOH:O	1.14	1.30
1:A:442:GLU:OE1	1:A:467:LYS:HE2	1.43	1.17
6:A:780:GOL:O3	7:A:1125:HOH:O	1.77	1.02
1:A:523:ASP:HB3	7:A:1103:HOH:O	1.61	1.01
1:A:644:PHE:N	7:A:1055:HOH:O	1.75	0.97
1:A:315:SER:O	1:A:353:TRP:CZ3	2.18	0.97
1:A:315:SER:O	1:A:353:TRP:HZ3	1.47	0.96
1:A:556:TYR:O	1:A:559:LYS:HE2	1.68	0.94
1:A:362:MET:HE3	1:A:386:LEU:CD2	1.97	0.93
1:A:394:ARG:HB2	7:A:1076:HOH:O	1.77	0.84
1:A:31:SER:HB2	7:A:797:HOH:O	1.76	0.84
1:A:362:MET:CE	1:A:386:LEU:HD21	2.09	0.83
1:A:512:ASP:OD2	6:A:782:GOL:H31	1.81	0.81
1:A:562:SER:HB3	7:A:1098:HOH:O	1.84	0.78
1:A:348:ASP:OD2	7:A:1112:HOH:O	2.03	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLN:O	1:A:343:LEU:HD12	1.84	0.77
1:A:362:MET:CE	1:A:386:LEU:CD2	2.62	0.76
1:A:660:TRP:HE3	1:A:664:THR:HA	1.59	0.68
1:A:362:MET:HE3	1:A:386:LEU:HD23	1.74	0.67
1:A:442:GLU:CD	1:A:467:LYS:HE2	2.14	0.67
1:A:573:GLY:C	7:A:1130:HOH:O	2.33	0.67
3:A:3:NAG:O6	7:A:971:HOH:O	2.12	0.67
1:A:520:ASN:HB3	7:A:1054:HOH:O	1.97	0.64
1:A:660:TRP:CE3	1:A:664:THR:HA	2.35	0.61
1:A:597:ASN:N	7:A:1130:HOH:O	2.27	0.60
1:A:343:LEU:HD23	1:A:368:PRO:HG3	1.82	0.60
1:A:325:ARG:CZ	7:A:1096:HOH:O	2.49	0.59
1:A:607:ASN:ND2	1:A:632:PRO:HG3	2.18	0.58
1:A:595:LEU:N	1:A:595:LEU:HD12	2.19	0.58
1:A:251:ARG:NH2	7:A:1013:HOH:O	2.37	0.57
1:A:659:ASN:OD1	1:A:659:ASN:N	2.35	0.57
1:A:442:GLU:OE1	1:A:467:LYS:CE	2.36	0.57
1:A:90:LEU:HD11	1:A:106:LEU:HD11	1.86	0.56
1:A:59:THR:HA	1:A:83:GLY:O	2.06	0.56
1:A:147:LYS:HE3	7:A:992:HOH:O	2.05	0.55
1:A:523:ASP:HB2	1:A:559:LYS:HE3	1.87	0.54
1:A:315:SER:O	1:A:353:TRP:CH2	2.59	0.54
6:A:778:GOL:O3	7:A:1049:HOH:O	0.53	0.53
1:A:660:TRP:CE3	1:A:664:THR:HG22	2.43	0.53
1:A:603:ALA:O	1:A:604:SER:HB2	2.09	0.53
1:A:523:ASP:CB	7:A:1103:HOH:O	2.34	0.53
1:A:343:LEU:HD11	1:A:391:THR:HG21	1.91	0.52
1:A:363:GLU:CD	7:A:924:HOH:O	2.47	0.52
1:A:497:SER:HB2	1:A:501:PRO:HD3	1.91	0.52
1:A:442:GLU:CD	1:A:467:LYS:CE	2.79	0.51
3:A:2:NAG:H82	7:A:793:HOH:O	2.11	0.50
1:A:536:ASP:OD2	6:A:782:GOL:O3	2.22	0.50
1:A:146:GLN:HB3	1:A:149:LEU:HB2	1.95	0.49
1:A:512:ASP:OD2	6:A:782:GOL:C3	2.58	0.48
1:A:102:LYS:HE2	2:A:1:NDG:O7	2.14	0.48
1:A:586:PHE:HB2	7:A:1085:HOH:O	2.14	0.48
1:A:189:GLU:CD	7:A:841:HOH:O	2.51	0.48
1:A:643:ARG:O	1:A:663:GLU:O	2.32	0.47
1:A:660:TRP:CD1	1:A:660:TRP:N	2.82	0.47
1:A:93:GLU:HG3	7:A:949:HOH:O	2.15	0.47
1:A:660:TRP:HE3	1:A:664:THR:CA	2.27	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:CG1	7:A:1026:HOH:O	2.63	0.47
1:A:30:VAL:HG11	7:A:1026:HOH:O	2.14	0.46
1:A:316:HIS:HA	1:A:353:TRP:CZ3	2.50	0.46
1:A:201:LYS:HG3	1:A:227:PHE:CE2	2.50	0.46
1:A:604:SER:HA	1:A:607:ASN:ND2	2.31	0.46
1:A:66:LEU:HD11	1:A:82:VAL:HG21	1.98	0.46
1:A:89:LYS:HB2	7:A:1036:HOH:O	2.15	0.45
1:A:442:GLU:HA	1:A:467:LYS:HG2	1.98	0.45
1:A:102:LYS:HE2	2:A:1:NDG:C7	2.46	0.45
1:A:140:ASN:O	1:A:165:GLY:HA2	2.17	0.44
1:A:470:GLN:HG3	1:A:494:ASN:OD1	2.18	0.44
1:A:488:ARG:NH1	1:A:515:ASN:ND2	2.66	0.44
1:A:362:MET:HE2	1:A:375:PHE:CE1	2.54	0.43
1:A:50:PRO:HB2	1:A:52:ASN:HB2	2.01	0.42
1:A:462:TYR:CD1	1:A:486:MET:HG3	2.53	0.42
1:A:619:LYS:HG2	1:A:644:PHE:HB2	2.01	0.41
1:A:141:ASN:HB3	1:A:144:VAL:HB	2.01	0.41
1:A:312:HIS:CE1	1:A:345:LYS:HD3	2.55	0.41
1:A:122:CYS:HB3	1:A:125:LEU:HG	2.02	0.41
1:A:468:TYR:HA	1:A:490:VAL:O	2.20	0.41
1:A:613:LYS:HA	1:A:613:LYS:HD2	1.95	0.40
1:A:601:LEU:HA	1:A:601:LEU:HD23	1.89	0.40

All (2) 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)
1:A:467:LYS:NZ	1:A:467:LYS:NZ[4_555]	1.07	1.13
7:A:841:HOH:O	7:A:841:HOH:O[3_555]	1.84	0.36

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	625/680 (92%)	578 (92%)	47 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	586/634 (92%)	572 (98%)	14 (2%)	57	61

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	GLU
1	A	214	PRO
1	A	272	LYS
1	A	336	GLN
1	A	343	LEU
1	A	420	SER
1	A	649	CYS
1	A	652	GLU
1	A	653	SER
1	A	657	PHE
1	A	659	ASN
1	A	660	TRP
1	A	662	ASN
1	A	663	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	218	HIS
1	A	515	ASN
1	A	563	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	607	ASN

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 ⓘ

8 carbohydrates 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	NAG	A	10	3	14,14,15	0.60	0	15,19,21	2.98	2 (13%)
3	NAG	A	11	1,3	14,14,15	0.64	0	15,19,21	2.28	3 (20%)
3	NAG	A	12	3	14,14,15	0.58	0	15,19,21	1.35	2 (13%)
3	NAG	A	2	1,3	14,14,15	0.58	0	15,19,21	1.17	1 (6%)
3	NAG	A	3	3	14,14,15	0.58	0	15,19,21	0.87	0
3	NAG	A	5	1,3	14,14,15	0.82	1 (7%)	15,19,21	0.99	1 (6%)
3	NAG	A	6	3	14,14,15	0.64	0	15,19,21	1.21	1 (6%)
3	NAG	A	9	1,3	14,14,15	0.90	1 (7%)	15,19,21	1.82	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	10	3	-	0/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	11	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	12	3	-	0/6/23/26	0/1/1/1
3	NAG	A	2	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3	3	-	0/6/23/26	0/1/1/1
3	NAG	A	5	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	6	3	-	0/6/23/26	0/1/1/1
3	NAG	A	9	1,3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	9	NAG	C1-C2	2.02	1.55	1.52
3	A	5	NAG	C1-C2	2.05	1.55	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	9	NAG	C2-N2-C7	-3.74	118.23	123.04
3	A	11	NAG	C2-N2-C7	-3.63	118.37	123.04
3	A	10	NAG	C3-C4-C5	-3.28	104.48	110.20
3	A	2	NAG	O4-C4-C3	-2.77	104.10	110.34
3	A	9	NAG	O6-C6-C5	-2.72	102.35	111.33
3	A	11	NAG	C6-C5-C4	-2.51	106.83	113.02
3	A	5	NAG	O7-C7-C8	-2.03	118.34	122.06
3	A	12	NAG	C3-C4-C5	2.49	114.54	110.20
3	A	6	NAG	C1-O5-C5	3.48	116.66	112.25
3	A	12	NAG	C4-C3-C2	3.79	117.12	111.23
3	A	9	NAG	C1-O5-C5	4.25	117.65	112.25
3	A	11	NAG	C1-O5-C5	7.05	121.19	112.25
3	A	10	NAG	C1-O5-C5	10.45	125.51	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2	NAG	1	0
3	A	3	NAG	1	0

5.6 Ligand geometry

12 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NDG	A	1	1	14,14,15	0.56	0	15,19,21	2.14	4 (26%)
4	NAG	A	4	1	14,14,15	0.40	0	15,19,21	2.81	4 (26%)
2	NDG	A	7	1	14,14,15	0.71	0	15,19,21	0.83	0
5	SO4	A	776	-	4,4,4	0.99	0	6,6,6	0.76	0
5	SO4	A	777	-	4,4,4	0.25	0	6,6,6	0.21	0
6	GOL	A	778	-	5,5,5	1.45	1 (20%)	5,5,5	0.70	0
6	GOL	A	779	-	5,5,5	0.48	0	5,5,5	0.77	0
6	GOL	A	780	-	5,5,5	0.42	0	5,5,5	0.44	0
6	GOL	A	781	-	5,5,5	0.38	0	5,5,5	0.35	0
6	GOL	A	782	-	5,5,5	0.42	0	5,5,5	0.79	0
6	GOL	A	783	-	5,5,5	0.45	0	5,5,5	0.49	0
4	NAG	A	8	1	14,14,15	0.45	0	15,19,21	1.80	3 (20%)

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	NDG	A	1	1	-	0/6/23/26	0/1/1/1
4	NAG	A	4	1	-	0/6/23/26	0/1/1/1
2	NDG	A	7	1	-	0/6/23/26	0/1/1/1
5	SO4	A	776	-	-	0/0/0/0	0/0/0/0
5	SO4	A	777	-	-	0/0/0/0	0/0/0/0
6	GOL	A	778	-	-	0/4/4/4	0/0/0/0
6	GOL	A	779	-	-	0/4/4/4	0/0/0/0
6	GOL	A	780	-	-	0/4/4/4	0/0/0/0
6	GOL	A	781	-	-	0/4/4/4	0/0/0/0
6	GOL	A	782	-	-	0/4/4/4	0/0/0/0
6	GOL	A	783	-	-	0/4/4/4	0/0/0/0
4	NAG	A	8	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	778	GOL	O3-C3	-3.14	1.28	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	4	NAG	C4-C3-C2	-3.37	105.99	111.23
4	A	8	NAG	O7-C7-C8	-2.09	118.22	122.06
4	A	4	NAG	C3-C2-N2	2.55	116.66	110.56
4	A	4	NAG	C2-N2-C7	2.96	126.84	123.04
2	A	1	NDG	C4-C3-C2	3.00	115.89	111.23
4	A	8	NAG	C3-C4-C5	3.65	116.56	110.20
2	A	1	NDG	C2-N2-C7	3.69	127.77	123.04
4	A	8	NAG	C1-O5-C5	3.95	117.27	112.25
2	A	1	NDG	C3-C4-C5	4.23	117.56	110.20
2	A	1	NDG	C1-O-C5	4.28	117.68	112.25
4	A	4	NAG	C1-O5-C5	8.81	123.43	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	NDG	2	0
6	A	778	GOL	1	0
6	A	780	GOL	1	0
6	A	782	GOL	3	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	629/680 (92%)	0.58	73 (11%) 6 9	30, 40, 60, 87	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	649	CYS	8.4
1	A	656	TRP	7.0
1	A	664	THR	6.3
1	A	39	HIS	5.5
1	A	654	ILE	5.2
1	A	498	SER	5.2
1	A	660	TRP	5.1
1	A	32	HIS	4.5
1	A	635	ARG	4.4
1	A	617	LEU	3.8
1	A	655	ALA	3.7
1	A	661	ILE	3.6
1	A	657	PHE	3.6
1	A	41	LYS	3.6
1	A	56	LEU	3.6
1	A	343	LEU	3.6
1	A	648	ASP	3.5
1	A	139	LYS	3.4
1	A	255	LEU	3.4
1	A	452	TRP	3.3
1	A	537	LEU	3.3
1	A	80	LEU	3.2
1	A	548	HIS	3.1
1	A	658	VAL	3.1
1	A	650	THR	3.1
1	A	412	LEU	3.0
1	A	651	CYS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	438	LEU	3.0
1	A	662	ASN	3.0
1	A	535	LEU	2.9
1	A	615	LEU	2.9
1	A	436	LEU	2.9
1	A	69	ALA	2.9
1	A	82	VAL	2.8
1	A	351	PHE	2.8
1	A	461	ILE	2.8
1	A	336	GLN	2.6
1	A	626	GLU	2.6
1	A	253	LEU	2.6
1	A	414	LEU	2.6
1	A	513	LEU	2.6
1	A	487	LEU	2.5
1	A	394	ARG	2.5
1	A	392	SER	2.5
1	A	386	LEU	2.5
1	A	653	SER	2.5
1	A	77	LEU	2.4
1	A	152	LEU	2.4
1	A	640	LEU	2.4
1	A	463	LEU	2.3
1	A	603	ALA	2.3
1	A	532	LEU	2.3
1	A	593	LEU	2.3
1	A	276	LEU	2.3
1	A	38	SER	2.2
1	A	204	LEU	2.2
1	A	279	LEU	2.2
1	A	40	LEU	2.2
1	A	178	LEU	2.2
1	A	228	LEU	2.2
1	A	360	LEU	2.2
1	A	170	LEU	2.1
1	A	462	TYR	2.1
1	A	66	LEU	2.1
1	A	485	LEU	2.1
1	A	143	PHE	2.1
1	A	67	PRO	2.1
1	A	557	PHE	2.1
1	A	353	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	346	ILE	2.1
1	A	384	LEU	2.0
1	A	552	GLY	2.0
1	A	98	LEU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	5	14/15	0.84	0.35	24.19	38,61,73,89	0
3	NAG	A	2	14/15	0.91	0.28	9.63	46,49,54,55	0
3	NAG	A	9	14/15	0.94	0.16	2.51	25,32,44,53	0
3	NAG	A	3	14/15	0.75	0.42	-	65,70,72,73	0
3	NAG	A	10	14/15	0.76	0.44	-	48,64,80,83	0
3	NAG	A	11	14/15	0.94	0.24	-	33,45,65,74	0
3	NAG	A	6	14/15	0.55	0.52	-	98,99,99,99	0
3	NAG	A	12	14/15	0.80	0.46	-	79,87,91,93	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	NDG	A	1	14/15	0.76	0.48	17.07	80,90,96,98	0
6	GOL	A	779	6/6	0.67	0.53	9.47	56,69,76,77	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	SO4	A	777	5/5	0.99	0.27	6.87	53,59,61,65	0
6	GOL	A	782	6/6	0.71	0.18	3.28	50,65,72,74	0
6	GOL	A	783	6/6	0.82	0.17	-0.09	33,51,62,65	0
6	GOL	A	778	6/6	0.97	0.14	-0.41	9,44,50,59	0
6	GOL	A	780	6/6	0.82	0.21	-	31,58,69,69	0
5	SO4	A	776	5/5	0.99	0.15	-	34,34,35,39	0
6	GOL	A	781	6/6	0.56	0.32	-	71,78,85,90	0
2	NDG	A	7	14/15	0.87	0.28	-	64,77,81,83	0
4	NAG	A	4	14/15	0.78	0.33	-	65,76,85,85	0
4	NAG	A	8	14/15	0.87	0.36	-	71,75,79,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.