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

May 3, 2018 – 04:22 PM EDT

Deposition ID : D_1000234324
PDB ID : *(not yet assigned)*

This is a Preliminary Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB Deposition System during initial deposition but before annotation of the structure.

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 following versions of software and data (see references (1)) were used in the production of this report:

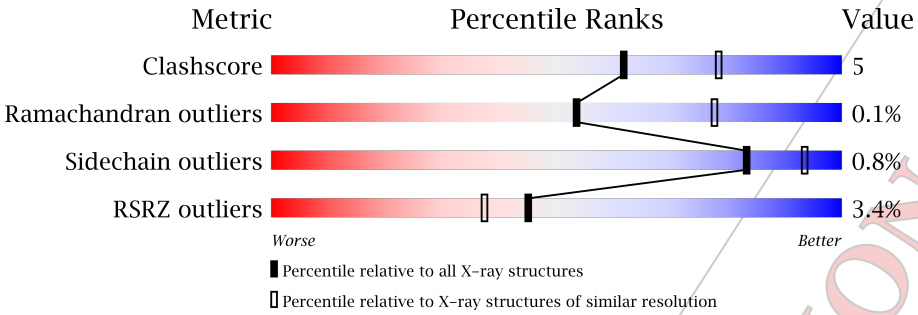
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	rb-20031021
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031021

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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 <=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	522	3% 87% 12%
2	C	522	4% 87% 13%
3	B	522	3% 88% 12%

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	NAG	C	3347	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11975 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	522	3956	2470	669	788	29	0	0	0

- Molecule 2 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	522	3962	2473	668	792	29	0	0	0

- Molecule 3 is a protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	522	3962	2473	668	792	29	0	0	0

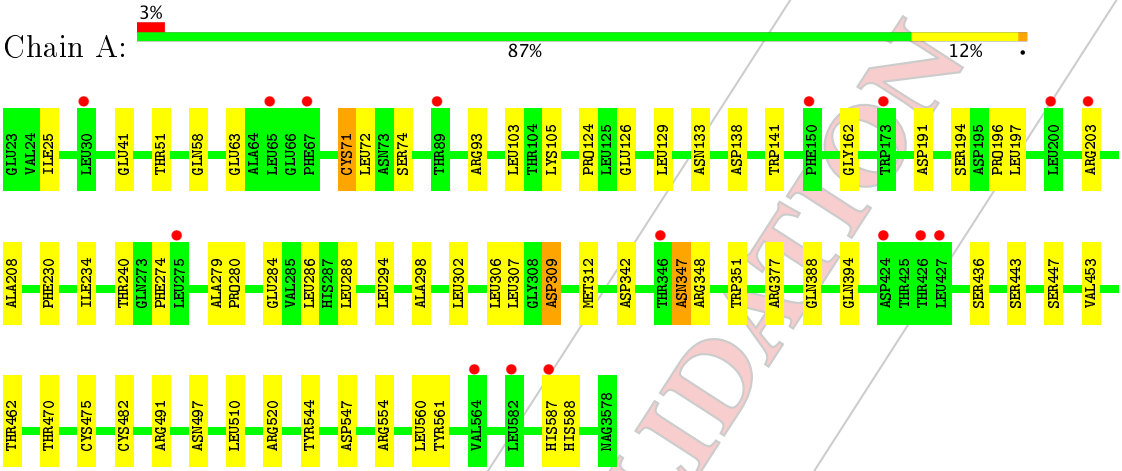
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	W	95	95	95	0	0

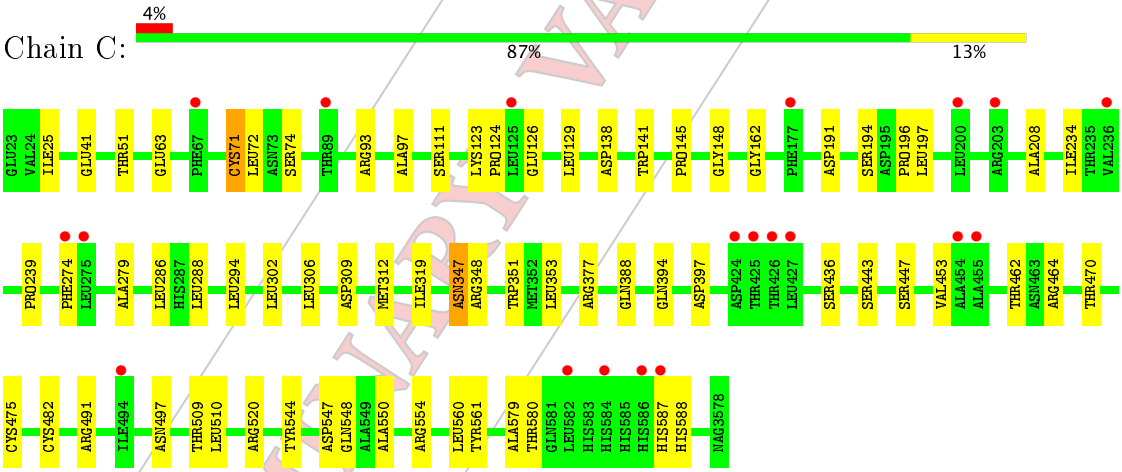
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometryand 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.

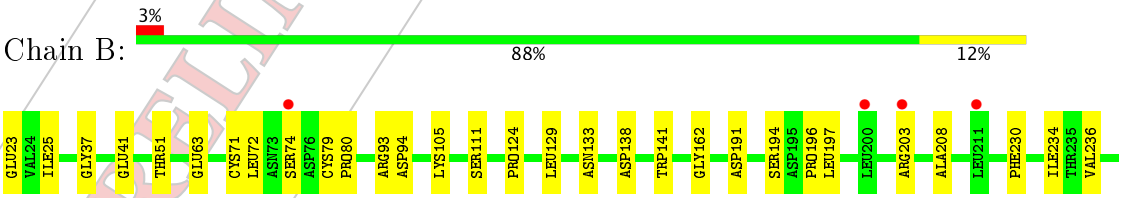
- Molecule 1:

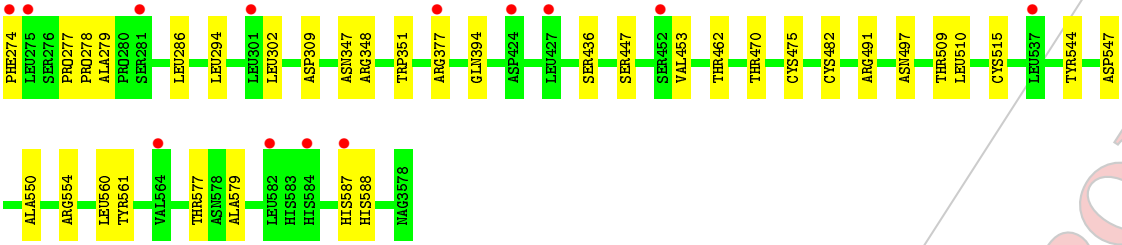


- Molecule 2:



- Molecule 3:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	198.22Å 117.60Å 115.21Å 90.00° 123.79° 90.00°	Depositor
Resolution (Å)	48.99 – 2.60 48.99 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (48.99-2.60) 97.1 (48.99-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.237 , 0.276 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	88.7	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 79.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -1/2*h+3/2*k-l,1/2*h+1/2*k+l,1/2*h-1/2*k 0.000 for 1/2*h-1/2*k+2*l,-1/2*h+1/2*k,-1/2*h-1/2*k-l 0.000 for -h-k-l,l,k 0.000 for -h+k-l,-l,-k 0.000 for -1/2*h-3/2*k-l,-1/2*h+1/2*k-l,1/2*h+1/2*k 0.000 for 1/2*h+1/2*k+2*l,1/2*h+1/2*k,-1/2*h+1/2*k-l 0.460 for -1/2*h+1/2*k+l,1/2*h-1/2*k+l,1/2*h+1/2*k 0.468 for -1/2*h-1/2*k+l,-1/2*h-1/2*k-l,1/2*h-1/2*k 0.000 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.000 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l 0.000 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11975	wwPDB-VP
Average B, all atoms (Å^2)	120.0	wwPDB-VP

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, MAN

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	0.25	0/3955	0.46	0/5387
2	C	0.25	0/3950	0.45	0/5380
3	B	0.25	0/3950	0.46	0/5380
All	All	0.25	0/11855	0.46	0/16147

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	1
2	C	0	1
3	B	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	ALA	Peptide
3	B	279	ALA	Peptide
2	C	279	ALA	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 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	3956	0	3830	43	0
2	C	3962	0	3834	44	0
3	B	3962	0	3834	42	0
4	W	95	0	0	6	0
All	All	11975	0	11498	113	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 5.

All (113) 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)
2:C:348:ARG:NH1	2:C:436:SER:O	2.14	0.79
1:A:348:ARG:NH1	1:A:436:SER:O	2.17	0.76
3:B:348:ARG:NH1	3:B:436:SER:O	2.18	0.75
3:B:129:LEU:HB2	3:B:208:ALA:HB3	1.68	0.74
3:B:515:CYS:SG	4:W:50:HOH:O	2.48	0.72
1:A:129:LEU:HB2	1:A:208:ALA:HB3	1.72	0.71
3:B:162:GLY:O	3:B:377:ARG:NH1	2.26	0.69
2:C:129:LEU:HB2	2:C:208:ALA:HB3	1.75	0.68
1:A:162:GLY:O	1:A:377:ARG:NH1	2.28	0.67
1:A:280:PRO:O	4:W:96:HOH:O	2.13	0.66
2:C:162:GLY:O	2:C:377:ARG:NH1	2.30	0.64
3:B:138:ASP:HB2	3:B:377:ARG:HH12	1.61	0.64
3:B:302:LEU:HD13	3:B:453:VAL:HG22	1.82	0.62
1:A:138:ASP:HB2	1:A:377:ARG:HH12	1.63	0.61
2:C:138:ASP:HB2	2:C:377:ARG:HH12	1.63	0.61
2:C:312:MET:HE3	2:C:443:SER:HB3	1.83	0.61
2:C:302:LEU:HD13	2:C:453:VAL:HG22	1.84	0.58
1:A:274:PHE:HB3	2:C:41:GLU:HG3	1.84	0.58
1:A:133:ASN:O	1:A:203:ARG:NH2	2.31	0.58
1:A:312:MET:HE3	1:A:443:SER:HB3	1.85	0.56
3:B:234:ILE:HB	3:B:286:LEU:HB2	1.88	0.55
3:B:196:PRO:HG2	3:B:197:LEU:HD12	1.88	0.55
1:A:510:LEU:HD13	1:A:560:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLU:HG2	1:A:462:THR:HG23	1.89	0.54
2:C:274:PHE:HB3	3:B:41:GLU:HG3	1.88	0.54
1:A:196:PRO:HG2	1:A:197:LEU:HD12	1.89	0.54
2:C:234:ILE:HB	2:C:286:LEU:HB2	1.89	0.53
1:A:342:ASP:N	4:W:33:HOH:O	2.41	0.53
1:A:41:GLU:HG3	3:B:274:PHE:HB3	1.90	0.53
2:C:510:LEU:HD13	2:C:560:LEU:HD13	1.91	0.53
2:C:196:PRO:HG2	2:C:197:LEU:HD12	1.90	0.52
1:A:191:ASP:O	1:A:194:SER:OG	2.25	0.51
3:B:63:GLU:HG2	3:B:462:THR:HG23	1.92	0.51
2:C:63:GLU:HG2	2:C:462:THR:HG23	1.92	0.51
3:B:510:LEU:HD13	3:B:560:LEU:HD13	1.92	0.51
3:B:547:ASP:OD2	3:B:554:ARG:NH2	2.43	0.51
1:A:74:SER:HB2	1:A:93:ARG:HE	1.76	0.51
2:C:124:PRO:HD2	2:C:394:GLN:HG3	1.94	0.50
2:C:74:SER:HB2	2:C:93:ARG:HE	1.77	0.50
1:A:274:PHE:HB2	2:C:41:GLU:HA	1.94	0.50
2:C:123:LYS:NZ	2:C:397:ASP:OD2	2.44	0.50
1:A:25:ILE:HG23	2:C:51:THR:HG21	1.94	0.49
1:A:309:ASP:HA	1:A:447:SER:HA	1.95	0.49
2:C:274:PHE:HB2	3:B:41:GLU:HA	1.94	0.49
1:A:41:GLU:HA	3:B:274:PHE:HB2	1.95	0.48
1:A:51:THR:HG21	3:B:25:ILE:HG23	1.95	0.48
1:A:284:GLU:OE2	1:A:298:ALA:N	2.47	0.48
2:C:191:ASP:O	2:C:194:SER:OG	2.27	0.48
1:A:302:LEU:HD13	1:A:453:VAL:HG22	1.96	0.48
1:A:547:ASP:OD2	1:A:554:ARG:NH2	2.47	0.48
2:C:72:LEU:O	2:C:93:ARG:HB3	2.14	0.48
1:A:348:ARG:HA	1:A:351:TRP:CD1	2.50	0.47
2:C:580:THR:N	4:W:66:HOH:O	2.31	0.47
1:A:240:THR:HG22	4:W:96:HOH:O	2.15	0.47
3:B:124:PRO:HD2	3:B:394:GLN:HG3	1.96	0.47
2:C:547:ASP:OD2	2:C:554:ARG:NH2	2.47	0.47
1:A:124:PRO:HD2	1:A:394:GLN:HG3	1.95	0.47
2:C:548:GLN:O	4:W:66:HOH:O	2.20	0.46
3:B:309:ASP:HA	3:B:447:SER:HA	1.98	0.46
1:A:491:ARG:HD3	1:A:544:TYR:CE2	2.51	0.46
3:B:133:ASN:O	3:B:203:ARG:NH2	2.37	0.46
2:C:288:LEU:HD23	2:C:306:LEU:HB2	1.97	0.46
1:A:520:ARG:NH2	2:C:111:SER:O	2.49	0.46
3:B:470:THR:N	3:B:497:ASN:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:191:ASP:O	3:B:194:SER:OG	2.27	0.45
3:B:72:LEU:O	3:B:93:ARG:HB3	2.17	0.45
1:A:561:TYR:CD2	2:C:294:LEU:HD11	2.51	0.45
2:C:97:ALA:HB1	2:C:239:PRO:HG2	1.98	0.45
1:A:470:THR:N	1:A:497:ASN:O	2.50	0.44
2:C:587:HIS:O	2:C:588:HIS:ND1	2.51	0.44
3:B:79:CYS:HB3	3:B:80:PRO:HD3	1.99	0.44
2:C:348:ARG:HA	2:C:351:TRP:CD1	2.52	0.44
1:A:105:LYS:HE3	1:A:230:PHE:CD2	2.53	0.44
1:A:491:ARG:HD3	1:A:544:TYR:CZ	2.52	0.44
1:A:475:CYS:HA	1:A:482:CYS:HA	2.00	0.44
2:C:309:ASP:HA	2:C:447:SER:HA	2.00	0.44
2:C:470:THR:N	2:C:497:ASN:O	2.48	0.44
3:B:509:THR:HB	3:B:561:TYR:HB2	1.99	0.44
1:A:72:LEU:O	1:A:93:ARG:HB3	2.17	0.44
1:A:234:ILE:HB	1:A:286:LEU:HB2	1.99	0.43
3:B:72:LEU:HB2	3:B:94:ASP:HB2	2.01	0.43
2:C:491:ARG:HD3	2:C:544:TYR:CE2	2.53	0.43
2:C:561:TYR:CD2	3:B:294:LEU:HD11	2.53	0.43
1:A:288:LEU:HD23	1:A:306:LEU:HB2	2.00	0.43
2:C:520:ARG:NH2	3:B:111:SER:O	2.52	0.43
1:A:587:HIS:O	1:A:588:HIS:ND1	2.52	0.43
3:B:475:CYS:HA	3:B:482:CYS:HA	2.00	0.43
3:B:587:HIS:O	3:B:588:HIS:ND1	2.52	0.42
1:A:294:LEU:HD11	3:B:561:TYR:CD2	2.54	0.42
2:C:319:ILE:HB	2:C:353:LEU:HD21	2.02	0.42
3:B:348:ARG:HA	3:B:351:TRP:CD1	2.54	0.42
2:C:126:GLU:HB3	2:C:388:GLN:OE1	2.20	0.42
2:C:475:CYS:HA	2:C:482:CYS:HA	2.00	0.42
3:B:491:ARG:HD3	3:B:544:TYR:CZ	2.54	0.42
3:B:550:ALA:HB2	3:B:579:ALA:HB2	2.01	0.42
3:B:554:ARG:HH11	3:B:577:THR:HG21	1.85	0.42
1:A:347:ASN:HB3	1:A:348:ARG:H	1.77	0.41
2:C:550:ALA:HB2	2:C:579:ALA:HB2	2.02	0.41
2:C:464:ARG:O	3:B:37:GLY:N	2.43	0.41
3:B:236:VAL:HG21	3:B:302:LEU:HD23	2.02	0.41
3:B:491:ARG:HD3	3:B:544:TYR:CE2	2.55	0.41
2:C:491:ARG:HD3	2:C:544:TYR:CZ	2.56	0.41
2:C:509:THR:HB	2:C:561:TYR:HB2	2.02	0.41
2:C:25:ILE:HG23	3:B:51:THR:HG21	2.02	0.41
3:B:74:SER:HB2	3:B:93:ARG:HE	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:PRO:HG2	2:C:148:GLY:H	1.86	0.41
2:C:347:ASN:HB3	2:C:348:ARG:H	1.45	0.41
1:A:126:GLU:HB3	1:A:388:GLN:OE1	2.21	0.40
1:A:309:ASP:OD1	1:A:447:SER:HB3	2.21	0.40
1:A:58:GLN:NE2	1:A:103:LEU:O	2.54	0.40
1:A:307:LEU:HD21	3:B:23:GLU:HG2	2.03	0.40
3:B:277:PRO:HA	3:B:278:PRO:HD3	1.97	0.40
3:B:105:LYS:HE3	3:B:230:PHE:CD2	2.56	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	A	505/522 (97%)	477 (94%)	27 (5%)	1 (0%)	49	74
2	C	504/522 (97%)	476 (94%)	27 (5%)	1 (0%)	49	74
3	B	504/522 (97%)	476 (94%)	28 (6%)	0	100	100
All	All	1513/1566 (97%)	1429 (94%)	82 (5%)	2 (0%)	53	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	CYS
2	C	71	CYS

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	A	430/430 (100%)	426 (99%)	4 (1%)	81 92
2	C	430/430 (100%)	427 (99%)	3 (1%)	85 95
3	B	430/430 (100%)	427 (99%)	3 (1%)	85 95
All	All	1290/1290 (100%)	1280 (99%)	10 (1%)	83 93

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	CYS
1	A	141	TRP
1	A	309	ASP
1	A	347	ASN
2	C	71	CYS
2	C	141	TRP
2	C	347	ASN
3	B	71	CYS
3	B	141	TRP
3	B	347	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

20 non-standard protein/DNA/RNA residues 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	$\#\|Z\|>2$
1	NAG	A	3347	1	14,14,15	0.28	0	17,19,21	0.51	0
1	NAG	A	3497	1	14,14,15	0.28	0	17,19,21	0.46	0
1	NAG	A	3498	1	14,14,15	0.24	0	17,19,21	0.49	0
1	BMA	A	3499	1	11,11,12	0.56	0	15,15,17	0.75	0
1	NAG	A	3514	1	14,14,15	0.26	0	17,19,21	0.39	0
1	NAG	A	3578	1	14,14,15	0.47	0	17,19,21	0.53	0
3	NAG	B	3347	3	14,14,15	0.29	0	17,19,21	0.53	0
3	NAG	B	3497	3	14,14,15	0.28	0	17,19,21	0.46	0
3	NAG	B	3498	3	14,14,15	0.25	0	17,19,21	0.47	0
3	BMA	B	3499	3	11,11,12	0.57	0	15,15,17	0.91	0
3	MAN	B	3500	3	11,11,12	0.74	0	15,15,17	1.20	2 (13%)
3	NAG	B	3514	3	14,14,15	0.23	0	17,19,21	0.42	0
3	NAG	B	3578	3	14,14,15	0.40	0	17,19,21	0.53	0
2	NAG	C	3347	2	14,14,15	0.34	0	17,19,21	0.49	0
2	NAG	C	3497	2	14,14,15	0.31	0	17,19,21	0.45	0
2	NAG	C	3498	2	14,14,15	0.26	0	17,19,21	0.50	0
2	BMA	C	3499	2	11,11,12	0.56	0	15,15,17	0.89	0
2	MAN	C	3500	2	11,11,12	0.72	0	15,15,17	1.19	2 (13%)
2	NAG	C	3514	2	14,14,15	0.24	0	17,19,21	0.45	0
2	NAG	C	3578	2	14,14,15	0.44	0	17,19,21	0.55	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
1	NAG	A	3347	1	-	0/6/23/26	0/1/1/1
1	NAG	A	3497	1	-	0/6/23/26	0/1/1/1
1	NAG	A	3498	1	-	0/6/23/26	0/1/1/1
1	BMA	A	3499	1	-	0/2/19/22	0/1/1/1
1	NAG	A	3514	1	-	0/6/23/26	0/1/1/1
1	NAG	A	3578	1	-	0/6/23/26	0/1/1/1
3	NAG	B	3347	3	-	0/6/23/26	0/1/1/1
3	NAG	B	3497	3	-	0/6/23/26	0/1/1/1
3	NAG	B	3498	3	-	0/6/23/26	0/1/1/1
3	BMA	B	3499	3	-	0/2/19/22	0/1/1/1
3	MAN	B	3500	3	-	0/2/19/22	1/1/1/1
3	NAG	B	3514	3	-	0/6/23/26	0/1/1/1
3	NAG	B	3578	3	-	0/6/23/26	0/1/1/1
2	NAG	C	3347	2	-	0/6/23/26	0/1/1/1
2	NAG	C	3497	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	3498	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3499	2	-	0/2/19/22	0/1/1/1
2	MAN	C	3500	2	-	0/2/19/22	1/1/1/1
2	NAG	C	3514	2	-	0/6/23/26	0/1/1/1
2	NAG	C	3578	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3500	MAN	O2-C2-C3	-2.29	105.72	110.19
3	B	3500	MAN	O2-C2-C3	-2.27	105.77	110.19
2	C	3500	MAN	C1-O5-C5	3.40	116.87	112.19
3	B	3500	MAN	C1-O5-C5	3.45	116.93	112.19

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	3500	MAN	C1-C2-C3-C4-C5-O5
2	C	3500	MAN	C1-C2-C3-C4-C5-O5

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	B	9
1	A	9
2	C	9

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	588:HIS	C	3347:NAG	O4	59.82
1	A	588:HIS	C	3497:NAG	O4	53.89
1	C	588:HIS	C	3497:NAG	O4	53.85
1	A	3514:NAG	C1	3347:NAG	O4	48.37
1	C	3514:NAG	C1	3347:NAG	O4	48.17
1	B	3500:MAN	C1	3514:NAG	O4	39.45
1	C	3500:MAN	C1	3514:NAG	O4	38.62
1	A	3347:NAG	C1	3578:NAG	O4	38.11
1	C	3347:NAG	C1	3578:NAG	O4	38.11
1	A	3499:BMA	C1	3514:NAG	O4	35.99
1	B	3514:NAG	C1	3578:NAG	O4	27.74
1	B	3347:NAG	C1	3497:NAG	O4	24.57
1	B	240:THR	C	273:GLN	N	22.62
1	A	240:THR	C	273:GLN	N	22.49
1	A	331:ALA	C	342:ASP	N	22.08
1	C	240:THR	C	273:GLN	N	21.94
1	B	330:PRO	C	342:ASP	N	19.74
1	C	330:PRO	C	342:ASP	N	19.61
1	C	83:CYS	C	89:THR	N	9.79
1	A	83:CYS	C	89:THR	N	9.67
1	B	83:CYS	C	89:THR	N	9.58
1	C	76:ASP	C	79:CYS	N	8.63
1	B	76:ASP	C	79:CYS	N	8.47
1	A	76:ASP	C	79:CYS	N	8.29
1	A	74:SER	C	76:ASP	N	4.41
1	C	74:SER	C	76:ASP	N	4.39
1	B	74:SER	C	76:ASP	N	4.37

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, 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	OWAB(Å^2)	Q<0.9
1	A	516/522 (98%)	0.07	16 (3%) 49 41	77, 110, 189, 270	0
2	C	515/522 (98%)	0.11	20 (3%) 39 31	80, 110, 186, 277	0
3	B	515/522 (98%)	0.05	17 (3%) 46 39	78, 110, 189, 291	0
All	All	1546/1566 (98%)	0.08	53 (3%) 45 37	77, 110, 189, 291	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	275	LEU	8.6
3	B	274	PHE	8.2
1	A	275	LEU	7.6
2	C	274	PHE	7.2
3	B	275	LEU	6.9
3	B	424	ASP	5.5
2	C	424	ASP	5.3
1	A	200	LEU	5.0
1	A	582	LEU	4.9
3	B	452	SER	4.8
2	C	200	LEU	4.7
2	C	89	THR	4.5
2	C	426	THR	4.3
2	C	454	ALA	4.3
2	C	584	HIS	3.8
2	C	587	HIS	3.6
2	C	427	LEU	3.4
3	B	211	LEU	3.4
2	C	67	PHE	3.3
3	B	587	HIS	3.3
2	C	582	LEU	3.2
1	A	424	ASP	3.1
2	C	455	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	67	PHE	2.9
2	C	425	THR	2.8
3	B	582	LEU	2.6
1	A	89	THR	2.6
1	A	587	HIS	2.6
2	C	125	LEU	2.6
1	A	564	VAL	2.5
1	A	346	THR	2.5
1	A	203	ARG	2.4
3	B	427	LEU	2.4
3	B	301	LEU	2.4
2	C	586	HIS	2.4
1	A	426	THR	2.3
3	B	203	ARG	2.3
1	A	173	TRP	2.3
3	B	200	LEU	2.3
1	A	30	LEU	2.3
1	A	427	LEU	2.2
3	B	564	VAL	2.2
3	B	584	HIS	2.2
3	B	74	SER	2.1
2	C	494	ILE	2.1
1	A	150	PHE	2.1
1	A	65	LEU	2.1
3	B	537	LEU	2.0
3	B	281	SER	2.0
2	C	236	VAL	2.0
2	C	177	PHE	2.0
2	C	203	ARG	2.0
3	B	377	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	NAG	A	3514	14/?	0.56	0.26	129,157,178,181	0
1	NAG	A	3347	14/?	0.70	0.38	150,177,207,208	0
2	NAG	C	3347	14/?	0.75	0.43	139,181,195,195	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MAN	B	3500	11/?	0.81	0.22	221,227,230,232	0
2	NAG	C	3514	14/?	0.81	0.13	127,151,162,164	0
2	NAG	C	3578	14/?	0.81	0.16	113,131,150,153	0
3	NAG	B	3347	14/?	0.82	0.30	136,164,190,193	0
3	NAG	B	3578	14/?	0.82	0.16	109,126,140,141	0
3	NAG	B	3514	14/?	0.85	0.20	142,160,172,174	0
1	BMA	A	3499	11/?	0.87	0.14	175,186,198,199	0
1	NAG	A	3578	14/?	0.87	0.17	106,128,147,148	0
2	MAN	C	3500	11/?	0.90	0.23	237,243,246,246	0
3	NAG	B	3498	14/?	0.91	0.14	132,161,171,186	0
1	NAG	A	3498	14/?	0.91	0.17	132,160,165,173	0
3	BMA	B	3499	11/?	0.92	0.10	199,206,216,219	0
2	NAG	C	3498	14/?	0.92	0.15	136,164,174,189	0
3	NAG	B	3497	14/?	0.93	0.15	84,117,150,151	0
2	BMA	C	3499	11/?	0.93	0.11	204,213,222,230	0
1	NAG	A	3497	14/?	0.94	0.13	90,122,150,152	0
2	NAG	C	3497	14/?	0.97	0.11	79,113,154,158	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.