



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:25 PM BST

PDB ID : 6APB
Title : Crystal Structure of Non-Neutralizing Infant Antibody ADI-14359 in Complex with Postfusion RSV F Glycoprotein
Authors : Gilman, M.S.A.; McLellan, J.S.
Deposited on : 2017-08-17
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

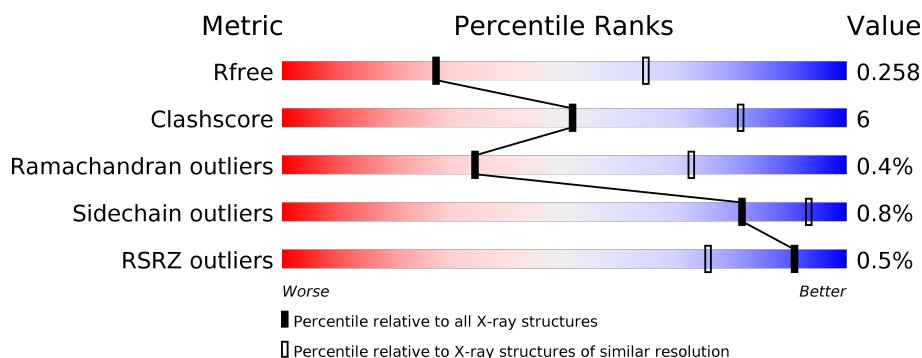
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	510	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 13%, green 70%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 70% 13% 16% </div> </div>
1	B	510	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 68%, yellow 16%, orange 1%, grey 16%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 68% 16% • 16% </div> </div>
1	C	510	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 70%, yellow 13%, grey 17%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 70% 13% 17% </div> </div>
2	H	230	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 89%, yellow 6%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 89% 6% 5% </div> </div>
3	L	214	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 93%, yellow 6%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 93% 6% • </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13306 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 Fusion glycoprotein F0,Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3330	2102	549	658	21			
1	B	429	Total	C	N	O	S	0	0	0
			3339	2110	549	659	21			
1	C	425	Total	C	N	O	S	0	0	0
			3307	2088	545	653	21			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	514	GLY	-	expression tag	UNP A0A1P8J9V4
A	515	LEU	-	expression tag	UNP A0A1P8J9V4
A	516	GLU	-	expression tag	UNP A0A1P8J9V4
A	517	VAL	-	expression tag	UNP A0A1P8J9V4
A	518	LEU	-	expression tag	UNP A0A1P8J9V4
A	519	PHE	-	expression tag	UNP A0A1P8J9V4
A	520	GLN	-	expression tag	UNP A0A1P8J9V4
B	514	GLY	-	expression tag	UNP A0A1P8J9V4
B	515	LEU	-	expression tag	UNP A0A1P8J9V4
B	516	GLU	-	expression tag	UNP A0A1P8J9V4
B	517	VAL	-	expression tag	UNP A0A1P8J9V4
B	518	LEU	-	expression tag	UNP A0A1P8J9V4
B	519	PHE	-	expression tag	UNP A0A1P8J9V4
B	520	GLN	-	expression tag	UNP A0A1P8J9V4
C	514	GLY	-	expression tag	UNP A0A1P8J9V4
C	515	LEU	-	expression tag	UNP A0A1P8J9V4
C	516	GLU	-	expression tag	UNP A0A1P8J9V4
C	517	VAL	-	expression tag	UNP A0A1P8J9V4
C	518	LEU	-	expression tag	UNP A0A1P8J9V4
C	519	PHE	-	expression tag	UNP A0A1P8J9V4
C	520	GLN	-	expression tag	UNP A0A1P8J9V4

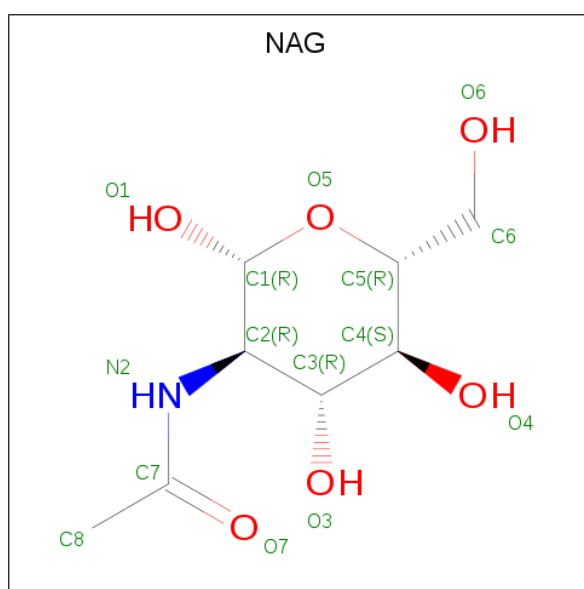
- Molecule 2 is a protein called IgG H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	0	0
			1668	1059	269	332	8			

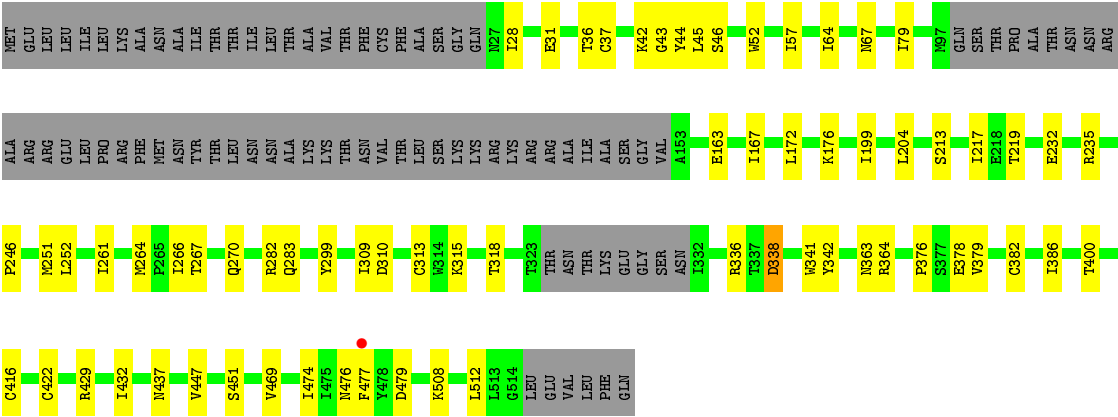
- Molecule 3 is a protein called ADI-14359 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1620	1013	270	332	5			

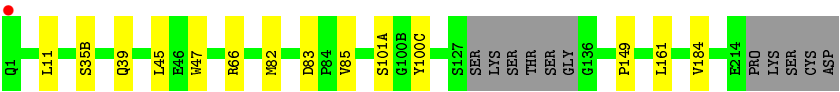
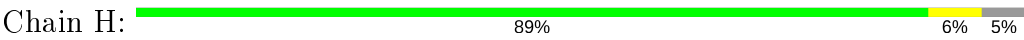
- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



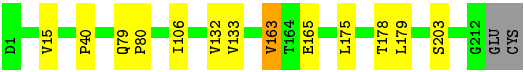
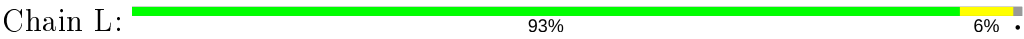
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		



● Molecule 2: IgG H chain



● Molecule 3: ADI-14359 Fab Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.45Å 99.04Å 323.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.11 – 3.00 51.11 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (51.11-3.00) 99.9 (51.11-3.00)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.222 , 0.255 0.228 , 0.258	Depositor DCC
R_{free} test set	2881 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.974	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 30.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13306	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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

5.1 Standard geometry

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

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	0.26	0/3376	0.47	0/4573
1	B	0.28	0/3385	0.51	0/4585
1	C	0.27	0/3353	0.48	0/4541
2	H	0.24	0/1709	0.42	0/2337
3	L	0.25	0/1655	0.43	0/2247
All	All	0.27	0/13478	0.47	0/18283

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

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	3330	0	3374	50	1
1	B	3339	0	3387	57	0
1	C	3307	0	3350	50	0
2	H	1668	0	1638	8	0
3	L	1620	0	1574	6	1
4	A	14	0	13	0	0
4	B	14	0	13	2	0
4	C	14	0	13	0	0
All	All	13306	0	13362	148	1

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 6.

All (148) 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:C:252:LEU:O	1:C:282:ARG:NH1	2.11	0.84
1:B:310:ASP:OD1	1:B:364:ARG:NH2	2.16	0.78
1:A:310:ASP:OD1	1:A:364:ARG:NH2	2.17	0.77
1:B:252:LEU:O	1:B:282:ARG:NH1	2.20	0.75
1:B:246:PRO:HB3	1:B:283:GLN:HA	1.67	0.75
1:A:252:LEU:O	1:A:282:ARG:NH1	2.19	0.74
1:C:310:ASP:OD1	1:C:364:ARG:NH2	2.20	0.73
1:C:28:ILE:HD11	1:C:363:ASN:HA	1.70	0.72
1:A:232:GLU:OE2	1:C:235:ARG:NH1	2.27	0.68
1:C:338:ASP:OD1	1:C:338:ASP:N	2.29	0.65
1:B:37:CYS:HB2	1:B:321:LEU:HD13	1.79	0.65
1:A:312:PRO:HG2	1:A:344:ASP:OD2	1.97	0.63
1:C:432:ILE:HD11	1:C:447:VAL:HG22	1.80	0.62
1:A:28:ILE:HD11	1:A:363:ASN:HA	1.79	0.62
1:B:67:ASN:HB2	1:C:476:ASN:ND2	2.16	0.61
1:C:318:THR:HG21	1:C:336:ARG:HB2	1.82	0.61
1:B:270:GLN:HG2	1:B:309:ILE:HD13	1.82	0.60
1:C:246:PRO:HB3	1:C:283:GLN:HA	1.81	0.60
1:A:246:PRO:HB3	1:A:283:GLN:HA	1.81	0.60
1:B:338:ASP:N	1:B:338:ASP:OD1	2.33	0.59
1:A:200:ASP:OD1	1:B:483:PHE:HB3	2.01	0.59
1:A:376:PRO:HB2	1:A:378:GLU:HG2	1.84	0.59
1:B:316:LEU:HD11	1:B:336:ARG:NH1	2.18	0.58
1:A:46:SER:HB3	1:A:313:CYS:SG	2.44	0.57
1:A:57:ILE:HD11	1:A:252:LEU:HD13	1.85	0.57
1:B:57:ILE:HD11	1:B:252:LEU:HD13	1.86	0.57
1:A:235:ARG:NH1	1:B:232:GLU:OE2	2.39	0.56
1:A:36:THR:HG22	1:A:386:ILE:HG12	1.87	0.56
1:B:318:THR:O	1:B:406:VAL:HG21	2.05	0.56
1:B:416:CYS:O	1:B:437:ASN:HA	2.06	0.56
1:B:322:CYS:HB2	1:B:417:TYR:CD1	2.42	0.55
1:B:427:LYS:HG2	1:B:448:ASP:OD2	2.07	0.55
1:C:31:GLU:OE1	2:H:100(C):TYR:OH	2.24	0.55
1:B:379:VAL:O	1:B:382:CYS:HB2	2.07	0.55
1:B:28:ILE:HD11	1:B:363:ASN:HA	1.89	0.55
1:B:496:ASN:O	1:B:500:ASN:HB2	2.06	0.54
1:A:318:THR:HG21	1:A:336:ARG:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:ILE:O	1:B:210:GLN:HG3	2.07	0.54
1:C:46:SER:HB3	1:C:313:CYS:SG	2.48	0.54
1:C:57:ILE:HD11	1:C:252:LEU:HD13	1.90	0.54
1:B:376:PRO:HB2	1:B:378:GLU:HG2	1.89	0.53
1:B:261:ILE:HA	1:B:264:MET:HE2	1.91	0.53
1:C:376:PRO:HB2	1:C:378:GLU:HG2	1.90	0.53
1:C:270:GLN:HG2	1:C:309:ILE:HD13	1.89	0.53
1:A:378:GLU:OE2	1:B:400:THR:HG21	2.09	0.53
1:B:235:ARG:NH1	1:C:232:GLU:OE2	2.41	0.53
1:C:251:MET:HG3	1:C:299:TYR:CE2	2.44	0.52
3:L:132:VAL:HB	3:L:179:LEU:HB3	1.91	0.52
2:H:11:LEU:HB2	2:H:149:PRO:HG3	1.92	0.52
1:A:243:VAL:HG22	1:A:288:ILE:HG23	1.93	0.51
1:C:261:ILE:HA	1:C:264:MET:HE2	1.93	0.51
1:A:426:ASN:OD1	1:A:427:LYS:N	2.43	0.51
2:H:35(B):SER:HG	2:H:47:TRP:HE1	1.59	0.51
3:L:80:PRO:HA	3:L:106:ILE:HD13	1.93	0.50
1:B:318:THR:HG21	1:B:336:ARG:HB2	1.92	0.50
1:A:199:ILE:O	1:A:204:LEU:HB2	2.12	0.50
1:B:497:GLU:HG3	4:B:800:NAG:H81	1.93	0.50
3:L:133:VAL:HG22	3:L:178:THR:HG23	1.94	0.50
1:A:167:ILE:HG12	1:C:167:ILE:HD11	1.93	0.50
1:A:267:THR:OG1	1:A:270:GLN:HG3	2.11	0.50
1:A:407:ILE:HD11	1:A:457:TYR:HB3	1.94	0.50
1:B:199:ILE:O	1:B:204:LEU:HB2	2.12	0.49
1:A:79:ILE:HD11	1:A:219:THR:HB	1.95	0.49
1:B:163:GLU:O	1:B:167:ILE:HG22	2.13	0.49
1:B:219:THR:OG1	1:C:476:ASN:HB3	2.13	0.49
1:B:45:LEU:HB3	1:B:364:ARG:NH1	2.28	0.48
1:C:422:CYS:HA	1:C:451:SER:O	2.14	0.48
1:B:67:ASN:HB2	1:C:476:ASN:HD21	1.76	0.48
2:H:35(B):SER:OG	2:H:47:TRP:NE1	2.42	0.48
1:A:270:GLN:HG2	1:A:309:ILE:HD13	1.96	0.48
1:C:199:ILE:O	1:C:204:LEU:HB2	2.13	0.48
1:C:508:LYS:O	1:C:512:LEU:HD13	2.14	0.48
3:L:40:PRO:HB3	3:L:165:GLU:HG3	1.96	0.48
1:B:199:ILE:HD11	1:C:199:ILE:HD11	1.96	0.47
1:A:416:CYS:O	1:A:437:ASN:HA	2.14	0.47
1:A:167:ILE:HD11	1:B:167:ILE:HG12	1.94	0.47
1:C:163:GLU:O	1:C:167:ILE:HG22	2.14	0.47
1:A:261:ILE:HA	1:A:264:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LYS:HG2	1:C:52:TRP:HB2	1.96	0.47
1:B:59:ILE:HG12	1:C:469:VAL:HB	1.97	0.47
1:C:379:VAL:O	1:C:382:CYS:HB2	2.15	0.47
1:B:312:PRO:HG2	1:B:344:ASP:OD2	2.15	0.46
1:A:338:ASP:HB2	1:A:342:TYR:OH	2.15	0.46
1:A:90:VAL:HG13	1:A:292:ILE:HG12	1.98	0.46
1:B:36:THR:HB	1:B:386:ILE:HD11	1.98	0.46
1:A:476:ASN:ND2	1:C:67:ASN:HB2	2.31	0.46
1:C:315:LYS:HD2	1:C:341:TRP:CE2	2.50	0.46
1:B:32:PHE:CD1	1:B:441:TYR:HB2	2.51	0.46
1:B:46:SER:HB3	1:B:313:CYS:SG	2.55	0.46
1:A:163:GLU:O	1:A:167:ILE:HG22	2.15	0.46
1:C:36:THR:HG22	1:C:386:ILE:HG12	1.98	0.46
1:C:44:TYR:HB2	1:C:313:CYS:HB2	1.99	0.45
1:A:476:ASN:HB3	1:C:219:THR:OG1	2.16	0.45
1:A:379:VAL:HG12	1:A:391:TYR:CE2	2.51	0.45
1:B:294:GLU:N	1:B:294:GLU:OE1	2.48	0.45
1:A:476:ASN:OD1	1:A:476:ASN:N	2.48	0.45
1:B:66:GLU:HA	1:B:79:ILE:HG21	1.98	0.45
1:B:379:VAL:HG12	1:B:391:TYR:CE1	2.52	0.45
1:C:64:ILE:HD12	1:C:79:ILE:HG23	1.98	0.45
1:C:476:ASN:N	1:C:476:ASN:OD1	2.50	0.44
1:A:199:ILE:HD11	1:C:199:ILE:HD11	2.00	0.44
1:C:266:ILE:HD12	1:C:270:GLN:HB2	1.99	0.44
1:C:416:CYS:O	1:C:437:ASN:HA	2.17	0.44
1:C:213:SER:O	1:C:217:ILE:HG13	2.17	0.44
2:H:66:ARG:O	2:H:82:MET:HA	2.18	0.44
2:H:161:LEU:HD21	2:H:184:VAL:HG21	2.00	0.43
1:C:45:LEU:HB3	1:C:364:ARG:NH1	2.34	0.43
1:C:508:LYS:HD2	1:C:508:LYS:HA	1.70	0.43
1:A:37:CYS:HB2	1:A:321:LEU:HD13	2.01	0.43
1:B:261:ILE:HG12	1:B:264:MET:HE1	2.00	0.43
1:A:379:VAL:O	1:A:382:CYS:HB2	2.19	0.42
1:B:77:LYS:O	1:B:81:GLN:HG3	2.19	0.42
1:C:172:LEU:O	1:C:176:LYS:HG3	2.18	0.42
1:B:64:ILE:HG22	1:C:474:ILE:HB	2.00	0.42
3:L:15:VAL:HG13	3:L:79:GLN:HA	2.00	0.42
1:A:290:SER:HB3	1:A:299:TYR:HA	2.01	0.42
1:C:508:LYS:HE2	1:C:512:LEU:HD11	2.01	0.42
1:C:267:THR:OG1	1:C:270:GLN:HG3	2.18	0.42
3:L:163:VAL:HG22	3:L:175:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ASN:HB2	1:A:460:ASN:OD1	2.19	0.42
1:A:57:ILE:HG12	1:B:467:LEU:HB2	2.01	0.42
1:A:476:ASN:HD21	1:C:67:ASN:HB2	1.84	0.42
2:H:83:ASP:HB3	2:H:85:VAL:HG12	2.02	0.42
1:A:414:VAL:HG22	1:A:450:VAL:HG11	2.02	0.42
1:B:203:LEU:O	1:B:207:VAL:HG23	2.19	0.41
1:C:477:PHE:CE2	1:C:479:ASP:HB2	2.54	0.41
1:A:27:ASN:HB3	1:A:28:ILE:H	1.70	0.41
1:C:338:ASP:HB2	1:C:342:TYR:OH	2.20	0.41
2:H:39:GLN:HB2	2:H:45:LEU:HD23	2.03	0.41
1:A:30:GLU:HB2	1:A:410:LEU:HD12	2.02	0.41
1:B:261:ILE:HA	1:B:264:MET:CE	2.51	0.41
1:B:267:THR:OG1	1:B:270:GLN:HG3	2.21	0.41
1:B:82:GLU:HG2	1:B:220:VAL:HG13	2.02	0.41
1:A:379:VAL:HG12	1:A:391:TYR:CZ	2.55	0.41
1:A:199:ILE:HD11	1:B:199:ILE:HD11	2.03	0.41
1:A:31:GLU:HG2	1:A:33:TYR:CZ	2.56	0.41
1:B:315:LYS:HD2	1:B:341:TRP:CE2	2.56	0.41
1:B:315:LYS:HD2	1:B:341:TRP:CZ2	2.56	0.41
1:B:360:VAL:HG22	1:B:365:VAL:HG22	2.03	0.41
1:A:508:LYS:O	1:A:512:LEU:HD13	2.21	0.40
1:A:67:ASN:HB2	1:B:476:ASN:ND2	2.36	0.40
1:C:42:LYS:HG2	1:C:43:GLY:N	2.36	0.40
1:A:251:MET:HG3	1:A:299:TYR:CE2	2.56	0.40
1:A:318:THR:O	1:A:406:VAL:HG21	2.22	0.40
1:B:378:GLU:OE2	1:C:400:THR:HG21	2.22	0.40
1:B:228:ASN:O	1:B:232:GLU:HG2	2.21	0.40
1:B:496:ASN:HB3	4:B:800:NAG:H82	2.03	0.40
1:B:251:MET:HG3	1:B:299:TYR:CE1	2.56	0.40

All (1) 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:385:ASP:OD2	3:L:203:SER:OG[1_565]	2.00	0.20

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	422/510 (83%)	407 (96%)	14 (3%)	1 (0%)	47	82
1	B	423/510 (83%)	396 (94%)	23 (5%)	4 (1%)	17	55
1	C	419/510 (82%)	407 (97%)	11 (3%)	1 (0%)	47	82
2	H	215/230 (94%)	208 (97%)	7 (3%)	0	100	100
3	L	210/214 (98%)	202 (96%)	8 (4%)	0	100	100
All	All	1689/1974 (86%)	1620 (96%)	63 (4%)	6 (0%)	34	72

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	CYS
1	B	162	GLY
1	C	37	CYS
1	B	346	ALA
1	B	362	SER
1	B	517	VAL

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	395/465 (85%)	394 (100%)	1 (0%)	92	97
1	B	396/465 (85%)	388 (98%)	8 (2%)	55	83
1	C	392/465 (84%)	390 (100%)	2 (0%)	88	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	H	193/203 (95%)	192 (100%)	1 (0%)	88	96
3	L	186/188 (99%)	185 (100%)	1 (0%)	88	96
All	All	1562/1786 (88%)	1549 (99%)	13 (1%)	81	93

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	ASP
1	B	319	SER
1	B	338	ASP
1	B	401	ASP
1	B	405	SER
1	B	416	CYS
1	B	442	VAL
1	B	448	ASP
1	B	500	ASN
1	C	338	ASP
1	C	429	ARG
2	H	101(A)	SER
3	L	163	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	210	GLN
1	B	279	GLN
1	C	210	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 monosaccharides in this entry.

5.6 Ligand geometry

3 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$
4	NAG	B	800	1	14,14,15	1.40	1 (7%)	17,19,21	1.32	2 (11%)
4	NAG	C	800	1	14,14,15	1.53	4 (28%)	17,19,21	0.95	0
4	NAG	A	800	1	14,14,15	1.47	3 (21%)	17,19,21	1.09	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	NAG	B	800	1	-	0/6/23/26	0/1/1/1
4	NAG	C	800	1	-	3/6/23/26	0/1/1/1
4	NAG	A	800	1	-	1/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	800	NAG	O5-C1	3.36	1.49	1.43
4	A	800	NAG	O5-C1	3.24	1.48	1.43
4	B	800	NAG	O5-C1	2.94	1.48	1.43
4	C	800	NAG	O5-C5	2.15	1.47	1.43
4	A	800	NAG	O5-C5	2.13	1.47	1.43
4	C	800	NAG	C3-C2	-2.11	1.48	1.52
4	A	800	NAG	C7-N2	2.10	1.41	1.34
4	C	800	NAG	C7-N2	2.04	1.41	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	800	NAG	C1-O5-C5	-3.24	107.81	112.19
4	B	800	NAG	C4-C3-C2	2.38	114.50	111.02

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	800	NAG	C4-C5-C6-O6
4	C	800	NAG	C3-C2-N2-C7
4	A	800	NAG	C3-C2-N2-C7
4	C	800	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	800	NAG	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, 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	428/510 (83%)	-0.14	4 (0%) 84 63	19, 35, 65, 82	0
1	B	429/510 (84%)	-0.17	2 (0%) 91 75	19, 35, 66, 93	0
1	C	425/510 (83%)	-0.28	1 (0%) 95 87	16, 31, 58, 82	0
2	H	219/230 (95%)	-0.10	1 (0%) 91 75	22, 37, 67, 90	0
3	L	212/214 (99%)	-0.19	0 100 100	26, 39, 54, 65	0
All	All	1713/1974 (86%)	-0.18	8 (0%) 91 75	16, 35, 63, 93	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	ASN	3.9
1	B	477	PHE	3.4
2	H	1	GLN	3.1
1	A	65	LYS	3.0
1	A	429	ARG	2.8
1	C	477	PHE	2.1
1	A	67	ASN	2.0
1	B	428	ASN	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, 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	NAG	B	800	14/15	0.82	0.40	52,58,60,61	0
4	NAG	A	800	14/15	0.86	0.34	50,55,56,57	0
4	NAG	C	800	14/15	0.90	0.26	71,74,77,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.