Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2024 – 07:51 AM EDT

PDB ID	:	6BXF
Title	:	Crystal structure of an extended b3 integrin L33
Authors	:	Zhou, D.; Zhu, J.
Deposited on	:	2017-12-18
Resolution	:	3.20 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:

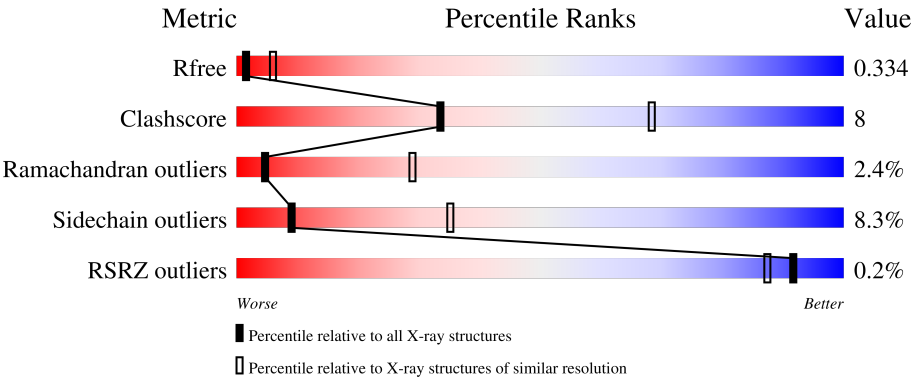
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.20 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	466	75% 21%
1	B	466	74% 23%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7328 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.

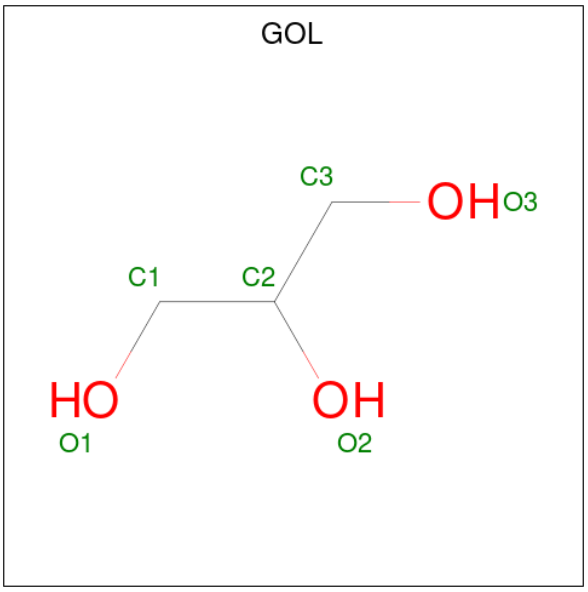
- Molecule 1 is a protein called Chimera protein of Integrin beta-3 and Integrin alpha-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	1	0
			3601	2243	613	713	32			
1	B	464	Total	C	N	O	S	0	0	0
			3607	2248	613	714	32			

There are 16 discrepancies between the modelled and reference sequences:

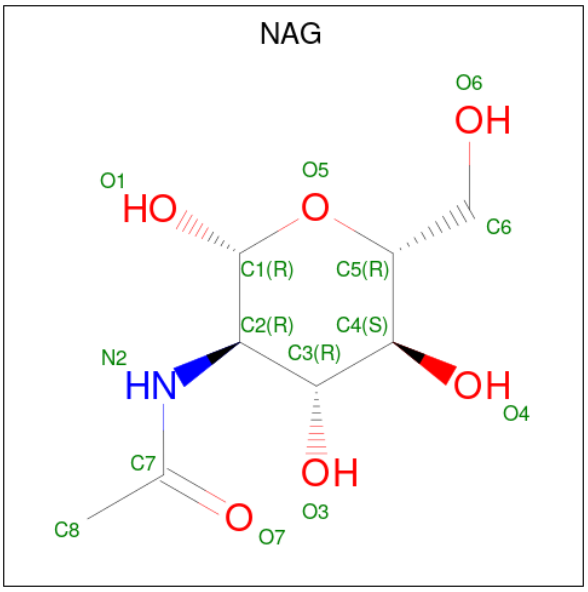
Chain	Residue	Modelled	Actual	Comment	Reference
A	171	TRP	ARG	conflict	UNP P20701
A	460	THR	-	expression tag	UNP P05106
A	461	ARG	-	expression tag	UNP P05106
A	462	GLU	-	expression tag	UNP P05106
A	463	LEU	-	expression tag	UNP P05106
A	464	TYR	-	expression tag	UNP P05106
A	465	PHE	-	expression tag	UNP P05106
A	466	GLN	-	expression tag	UNP P05106
B	171	TRP	ARG	conflict	UNP P20701
B	460	THR	-	expression tag	UNP P05106
B	461	ARG	-	expression tag	UNP P05106
B	462	GLU	-	expression tag	UNP P05106
B	463	LEU	-	expression tag	UNP P05106
B	464	TYR	-	expression tag	UNP P05106
B	465	PHE	-	expression tag	UNP P05106
B	466	GLN	-	expression tag	UNP P05106

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0

- Molecule 6 is water.

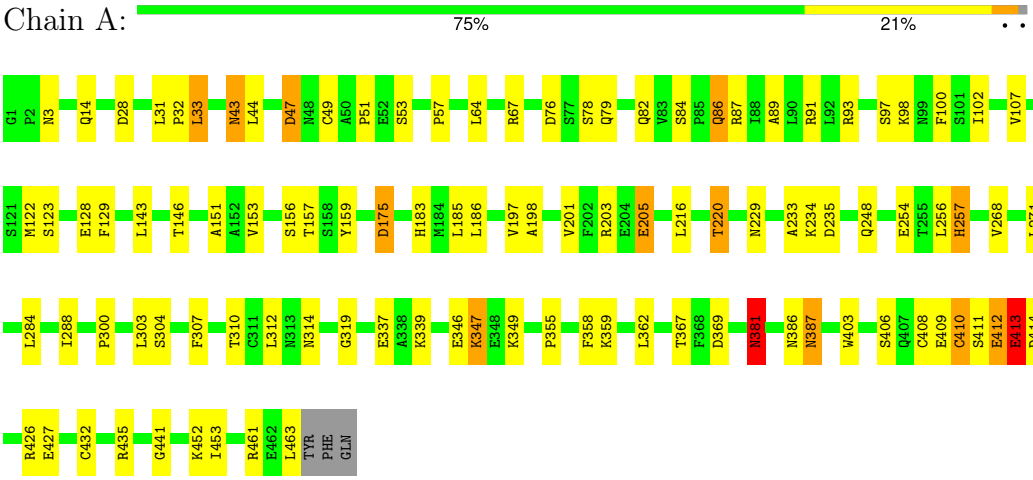
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	5	Total O 5 5	0	0
6	B	3	Total O 3 3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

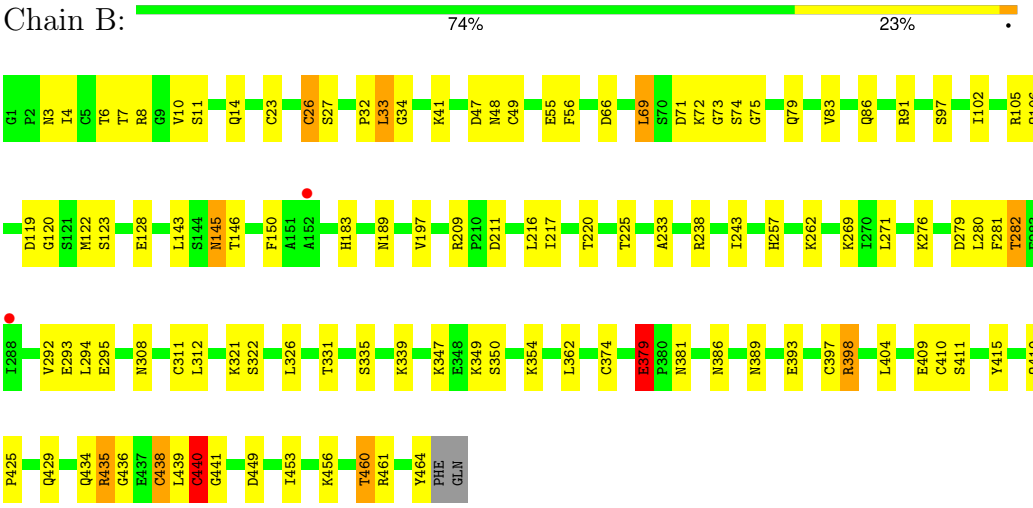
• Molecule 1: Chimera protein of Integrin beta-3 and Integrin alpha-L

Chain A:



• Molecule 1: Chimera protein of Integrin beta-3 and Integrin alpha-L

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.07Å 81.47Å 127.96Å 90.00° 97.07° 90.00°	Depositor
Resolution (Å)	63.49 – 3.20 63.49 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (63.49-3.20) 99.8 (63.49-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.265 , 0.335 0.268 , 0.334	Depositor DCC
R_{free} test set	1020 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	118.0	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 109.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7328	wwPDB-VP
Average B, all atoms (Å^2)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[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.

5 Model quality

5.1 Standard geometry

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

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	0/3668	0.46	0/4948
1	B	0.26	0/3672	0.47	0/4954
All	All	0.26	0/7340	0.47	0/9902

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	3601	0	3506	56	0
1	B	3607	0	3506	53	0
2	A	6	0	8	1	0
2	B	6	0	8	0	0
3	A	42	0	39	1	0
3	B	56	0	52	0	0
4	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	5	0	0	0	0
6	B	3	0	0	0	0
All	All	7328	0	7119	109	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (109) 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:413:GLU:HG2	1:A:415:TYR:H	1.50	0.76
1:B:281:PHE:O	1:B:285:GLN:NE2	2.24	0.70
1:B:386:ASN:HB3	1:B:389:ASN:HB2	1.74	0.68
1:B:282:THR:HA	1:B:285:GLN:HE21	1.60	0.67
1:B:32:PRO:O	1:B:34:GLY:N	2.30	0.64
1:B:4:ILE:HG13	1:B:464:TYR:HE2	1.63	0.64
1:A:43:ASN:OD1	1:A:43:ASN:N	2.31	0.64
1:B:3:ASN:H	1:B:6:THR:HG22	1.64	0.62
1:B:439:LEU:HB2	1:B:440:CYS:SG	2.39	0.62
1:A:271:LEU:HD11	1:A:280:LEU:HD22	1.81	0.62
1:B:119:ASP:HB2	1:B:220:THR:HA	1.80	0.62
1:A:102:ILE:HD13	1:A:362:LEU:HD22	1.82	0.60
1:B:439:LEU:O	1:B:441:GLY:N	2.36	0.58
1:A:426:ARG:HD3	1:A:427:GLU:H	1.69	0.58
1:B:69:LEU:HD22	1:B:105:ARG:HD2	1.86	0.57
1:A:31:LEU:HG	1:A:32:PRO:HD2	1.85	0.57
1:A:198:ALA:HB2	1:A:233:ALA:HB2	1.87	0.57
1:B:66:ASP:N	1:B:66:ASP:OD1	2.37	0.57
1:B:379:GLU:O	1:B:379:GLU:HG2	2.06	0.56
1:A:300:PRO:HD2	1:A:303:LEU:HD12	1.89	0.54
1:A:337:GLU:HB2	3:A:502:NAG:H83	1.90	0.54
1:A:411:SER:OG	1:A:412:GLU:N	2.39	0.54
1:B:308:ASN:HB2	1:B:335:SER:HB3	1.90	0.54
1:B:293:GLU:HG3	1:B:322:SER:HB3	1.90	0.53
1:A:203:ARG:NH1	1:A:205:GLU:OE2	2.41	0.53
1:A:346:GLU:HG2	1:A:349:LYS:HG2	1.89	0.53
1:A:28:ASP:HB3	1:A:31:LEU:HD13	1.90	0.53
1:A:387:ASN:OD1	1:A:387:ASN:N	2.42	0.53
1:B:8:ARG:NH2	1:B:449:ASP:OD1	2.42	0.53
1:B:271:LEU:HD22	1:B:276:LYS:HB2	1.90	0.52
1:B:197:VAL:HG11	1:B:216:LEU:HD13	1.90	0.52
1:B:410:CYS:SG	1:B:411:SER:N	2.83	0.52
1:B:143:LEU:O	1:B:146:THR:OG1	2.25	0.52
1:B:271:LEU:HD11	1:B:280:LEU:HD22	1.92	0.51
1:A:82:GLN:HG2	1:A:107:VAL:HG22	1.92	0.51
1:B:47:ASP:O	1:B:49:CYS:N	2.44	0.51
1:B:73:GLY:O	1:B:75:GLY:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASP:N	1:A:175:ASP:OD1	2.44	0.51
1:A:381:ASN:O	1:A:381:ASN:ND2	2.42	0.51
1:B:116:PHE:HE1	1:B:150:PHE:HB3	1.76	0.50
1:B:83:VAL:O	1:B:86:GLN:NE2	2.43	0.50
1:A:33:LEU:H	1:A:33:LEU:HD23	1.77	0.50
1:B:119:ASP:OD1	1:B:120:GLY:N	2.45	0.50
1:A:197:VAL:HG11	1:A:216:LEU:HD13	1.93	0.49
1:A:64:LEU:HD12	1:A:87:ARG:HG2	1.95	0.49
1:A:435:ARG:HD3	1:A:453:ILE:HD13	1.94	0.49
1:A:268:VAL:O	2:A:501:GOL:O2	2.31	0.49
1:B:435:ARG:HA	1:B:435:ARG:NH1	2.28	0.49
1:A:122:MET:HA	1:A:185:LEU:HD23	1.94	0.49
1:A:143:LEU:O	1:A:146:THR:OG1	2.22	0.48
1:B:4:ILE:HG13	1:B:464:TYR:CE2	2.46	0.48
1:B:97:SER:HB3	1:B:339:LYS:HG2	1.94	0.48
1:A:67:ARG:HG3	1:A:86:GLN:HE22	1.78	0.48
1:A:355:PRO:HG2	1:A:358:PHE:HB2	1.96	0.48
1:B:415:TYR:CZ	1:B:440:CYS:HA	2.48	0.47
1:B:243:ILE:HG12	1:B:271:LEU:HB2	1.97	0.47
1:B:436:GLY:C	1:B:438:CYS:H	2.16	0.47
1:B:189:ASN:OD1	1:B:225:THR:OG1	2.26	0.47
1:A:304:SER:HB2	1:A:339:LYS:HB2	1.96	0.47
1:A:307:PHE:O	1:A:319:GLY:N	2.32	0.47
1:B:145:ASN:OD1	1:B:146:THR:N	2.47	0.47
1:A:57:PRO:HG2	1:A:93:ARG:HD2	1.97	0.47
1:A:97:SER:O	1:A:98:LYS:HD2	2.16	0.46
1:B:114:LEU:HD21	1:B:217:ILE:HG12	1.98	0.46
1:A:47:ASP:N	1:A:47:ASP:OD1	2.47	0.46
1:B:393:GLU:OE1	1:B:398:ARG:NH1	2.49	0.46
1:A:414:ASP:OD1	1:A:414:ASP:N	2.47	0.46
1:A:67:ARG:O	1:A:84:SER:OG	2.28	0.46
1:B:41:LYS:HD3	1:B:56:PHE:CD2	2.51	0.46
1:A:347:LYS:H	1:A:347:LYS:HG3	1.58	0.45
1:B:284:LEU:HD22	1:B:287:LYS:HE2	1.98	0.45
1:A:254:GLU:HA	1:A:257:HIS:CE1	2.51	0.45
1:A:91:ARG:NH1	1:A:369:ASP:OD2	2.50	0.45
1:B:71:ASP:O	1:B:72:LYS:HE2	2.17	0.45
1:A:275:GLU:N	1:A:275:GLU:OE1	2.49	0.44
1:B:282:THR:HA	1:B:285:GLN:NE2	2.30	0.44
1:A:79:GLN:HG2	1:A:359:LYS:HE3	2.00	0.44
1:A:64:LEU:HD11	1:A:89:ALA:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:GLU:HG2	1:A:410:CYS:N	2.33	0.44
1:A:119:ASP:OD1	1:A:120:GLY:N	2.51	0.43
1:A:157:THR:HB	1:A:186:LEU:HD13	2.00	0.43
1:A:119:ASP:HB2	1:A:220:THR:HA	2.00	0.43
1:B:262:LYS:N	1:B:262:LYS:HD2	2.34	0.43
1:A:129:PHE:CG	1:A:183:HIS:HD2	2.36	0.43
1:A:91:ARG:HA	1:A:367:THR:O	2.19	0.43
1:A:310:THR:HG23	1:A:314:ASN:HA	2.01	0.42
1:B:349:LYS:HD3	1:B:350:SER:H	1.84	0.42
1:A:284:LEU:O	1:A:288:ILE:HG13	2.20	0.42
1:B:295:GLU:N	1:B:354:LYS:O	2.53	0.42
1:B:453:ILE:HA	1:B:460:THR:O	2.20	0.42
1:A:422:GLU:HB3	1:A:441:GLY:O	2.19	0.42
1:B:105:ARG:NE	1:B:331:THR:OG1	2.46	0.42
1:A:453:ILE:HG12	1:A:461:ARG:HG3	2.02	0.42
1:A:115:VAL:HG22	1:A:151:ALA:HB3	2.02	0.41
1:A:403:TRP:HA	1:A:410:CYS:O	2.20	0.41
1:A:49:CYS:O	1:A:53:SER:HB3	2.20	0.41
1:B:143:LEU:HD23	1:B:143:LEU:HA	1.94	0.41
1:B:128:GLU:H	1:B:128:GLU:HG2	1.69	0.41
1:B:26:CYS:SG	1:B:27:SER:N	2.93	0.41
1:A:234:LYS:HG3	1:A:235:ASP:OD1	2.21	0.41
1:B:233:ALA:O	1:B:238:ARG:NH1	2.54	0.41
1:A:153:VAL:HG21	1:A:201:VAL:HG21	2.03	0.41
1:A:49:CYS:O	1:A:49:CYS:SG	2.79	0.40
1:A:128:GLU:H	1:A:128:GLU:HG2	1.66	0.40
1:B:102:ILE:HD13	1:B:362:LEU:HD22	2.03	0.40
1:B:269:LYS:HA	1:B:269:LYS:HD3	1.95	0.40
1:B:294:LEU:HB2	1:B:321:LYS:HG2	2.03	0.40
1:B:420:GLN:N	1:B:420:GLN:OE1	2.54	0.40
1:B:145:ASN:OD1	1:B:145:ASN:C	2.60	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	462/466 (99%)	407 (88%)	45 (10%)	10 (2%)	5 30
1	B	462/466 (99%)	405 (88%)	45 (10%)	12 (3%)	4 27
All	All	924/932 (99%)	812 (88%)	90 (10%)	22 (2%)	5 29

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	GLU
1	B	33	LEU
1	B	48	ASN
1	B	74	SER
1	B	440	CYS
1	A	76	ASP
1	B	312	LEU
1	A	156	SER
1	A	312	LEU
1	A	406	SER
1	A	408	CYS
1	B	79	GLN
1	B	123	SER
1	B	425	PRO
1	A	386	ASN
1	B	311	CYS
1	A	51	PRO
1	A	381	ASN
1	A	416	ARG
1	B	379	GLU
1	B	424	SER
1	B	434	GLN

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	412/414 (100%)	382 (93%)	30 (7%)	11 41
1	B	412/414 (100%)	373 (90%)	39 (10%)	7 28
All	All	824/828 (100%)	755 (92%)	69 (8%)	9 34

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	14[A]	GLN
1	A	14[B]	GLN
1	A	33	LEU
1	A	43	ASN
1	A	44	LEU
1	A	47	ASP
1	A	78	SER
1	A	86	GLN
1	A	100	PHE
1	A	123	SER
1	A	159	TYR
1	A	175	ASP
1	A	205	GLU
1	A	220	THR
1	A	229	ASN
1	A	248	GLN
1	A	256	LEU
1	A	257	HIS
1	A	347	LYS
1	A	381	ASN
1	A	387	ASN
1	A	410	CYS
1	A	412	GLU
1	A	413	GLU
1	A	415	TYR
1	A	416	ARG
1	A	432	CYS
1	A	452	LYS
1	A	463	LEU
1	B	7	THR
1	B	10	VAL
1	B	11	SER
1	B	14	GLN
1	B	23	CYS

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Mol	Chain	Res	Type
1	B	26	CYS
1	B	33	LEU
1	B	55	GLU
1	B	69	LEU
1	B	91	ARG
1	B	106	GLN
1	B	122	MET
1	B	145	ASN
1	B	183	HIS
1	B	209	ARG
1	B	211	ASP
1	B	257	HIS
1	B	279	ASP
1	B	282	THR
1	B	285	GLN
1	B	292	VAL
1	B	326	LEU
1	B	347	LYS
1	B	374	CYS
1	B	379	GLU
1	B	381	ASN
1	B	397	CYS
1	B	398	ARG
1	B	404	LEU
1	B	409	GLU
1	B	419	GLN
1	B	423	CYS
1	B	429	GLN
1	B	435	ARG
1	B	438	CYS
1	B	440	CYS
1	B	456	LYS
1	B	460	THR
1	B	461	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	285	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 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
3	NAG	A	502	1	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	B	504	1	14,14,15	0.19	0	17,19,21	0.51	0
3	NAG	B	506	1	14,14,15	0.20	0	17,19,21	0.42	0
2	GOL	A	501	-	5,5,5	0.96	0	5,5,5	1.04	0
3	NAG	A	504	1	14,14,15	0.25	0	17,19,21	0.48	0
3	NAG	B	503	1	14,14,15	0.19	0	17,19,21	0.43	0
3	NAG	B	505	1	14,14,15	0.21	0	17,19,21	0.41	0
3	NAG	A	503	1	14,14,15	0.22	0	17,19,21	0.44	0
2	GOL	B	502	-	5,5,5	0.93	0	5,5,5	1.06	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
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	504	1	-	2/6/23/26	0/1/1/1
3	NAG	B	506	1	-	2/6/23/26	0/1/1/1
2	GOL	A	501	-	-	1/4/4/4	-
3	NAG	A	504	1	-	0/6/23/26	0/1/1/1
3	NAG	B	503	1	-	3/6/23/26	0/1/1/1
3	NAG	B	505	1	-	0/6/23/26	0/1/1/1
3	NAG	A	503	1	-	0/6/23/26	0/1/1/1
2	GOL	B	502	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	503	NAG	C4-C5-C6-O6
3	B	503	NAG	O5-C5-C6-O6
3	B	504	NAG	C4-C5-C6-O6
3	B	504	NAG	O5-C5-C6-O6
2	B	502	GOL	O1-C1-C2-C3
3	B	506	NAG	C4-C5-C6-O6
2	B	502	GOL	O1-C1-C2-O2
3	B	506	NAG	O5-C5-C6-O6
3	B	503	NAG	C1-C2-N2-C7
2	A	501	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	NAG	1	0
2	A	501	GOL	1	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, 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	463/466 (99%)	-0.74	0 100 100	65, 145, 221, 316	1 (0%)
1	B	464/466 (99%)	-0.58	2 (0%) 89 81	97, 164, 227, 303	0
All	All	927/932 (99%)	-0.66	2 (0%) 92 87	65, 157, 226, 316	1 (0%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	ILE	3.4
1	B	152	ALA	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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
3	NAG	B	506	14/15	0.17	0.08	266,268,272,272	0
3	NAG	A	504	14/15	0.43	0.07	229,235,247,250	0
3	NAG	A	503	14/15	0.53	0.10	227,234,253,255	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	B	502	6/6	0.60	0.08	151,157,162,165	0
3	NAG	B	504	14/15	0.81	0.11	141,160,166,166	0
3	NAG	B	505	14/15	0.84	0.07	151,164,178,185	0
2	GOL	A	501	6/6	0.86	0.07	157,161,163,165	0
3	NAG	B	503	14/15	0.89	0.09	108,137,147,148	0
3	NAG	A	502	14/15	0.89	0.04	127,144,150,150	0
5	MG	B	501	1/1	0.94	0.06	180,180,180,180	0
4	CA	A	505	1/1	0.99	0.04	125,125,125,125	0

6.5 Other polymers (i)

There are no such residues in this entry.