



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 09:05 AM BST

PDB ID : 6BDZ
Title : ADAM10 Extracellular Domain Bound by the 11G2 Fab
Authors : Seegar, T.C.M.
Deposited on : 2017-10-24
Resolution : 3.10 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

<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

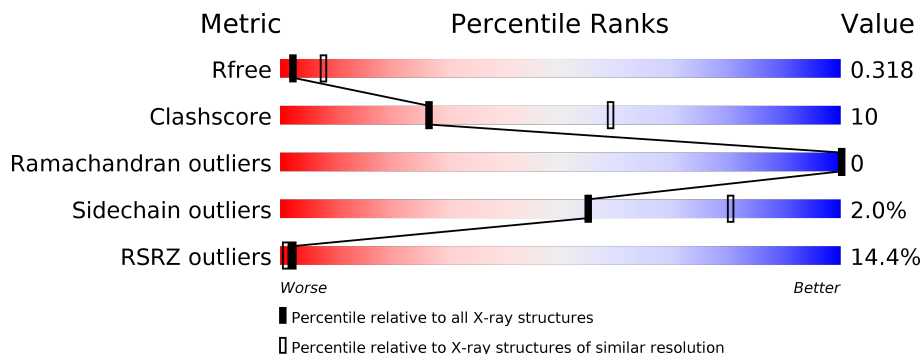
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 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	L	215	 81% 18%
2	H	226	 81% 16%
3	A	443	 27% 72% 22% 5%
4	B	4	 100%
5	C	3	 67% 33%

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
8	ZN	A	705	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6631 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 11G2 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	215	1645	1020	279	337	9	0	0	0

- Molecule 2 is a protein called 11G2 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	219	1643	1035	274	327	7	0	0	0

- Molecule 3 is a protein called Disintegrin and metalloproteinase domain-containing protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	421	3242	1991	574	637	40	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	267	GLN	ASN	conflict	UNP O14672
A	439	GLN	ASN	conflict	UNP O14672
A	551	GLN	ASN	conflict	UNP O14672
A	655	GLY	-	expression tag	UNP O14672
A	656	GLY	-	expression tag	UNP O14672
A	657	HIS	-	expression tag	UNP O14672
A	658	HIS	-	expression tag	UNP O14672
A	659	HIS	-	expression tag	UNP O14672
A	660	HIS	-	expression tag	UNP O14672
A	661	HIS	-	expression tag	UNP O14672
A	662	HIS	-	expression tag	UNP O14672

- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyran

ose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



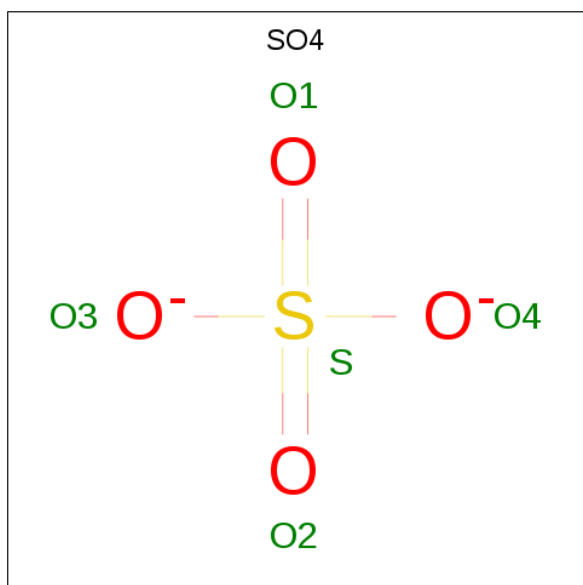
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
4	B	4	49	28	2	19	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
5	C	3	39	22	2	15	0	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Zn 1 1	0	0

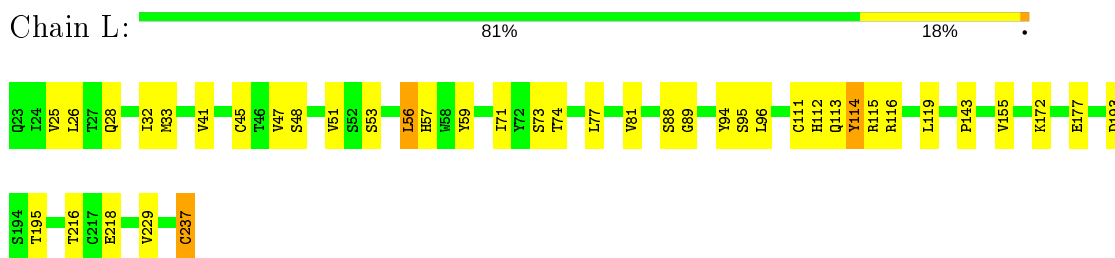
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	H	1	Total O 1 1	0	0

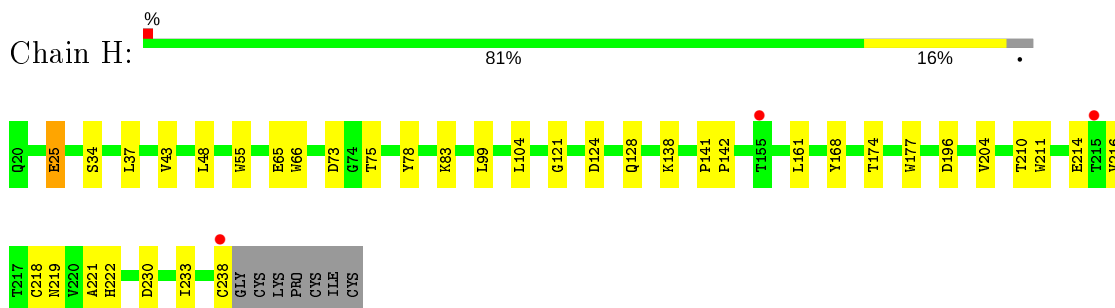
3 Residue-property plots

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.

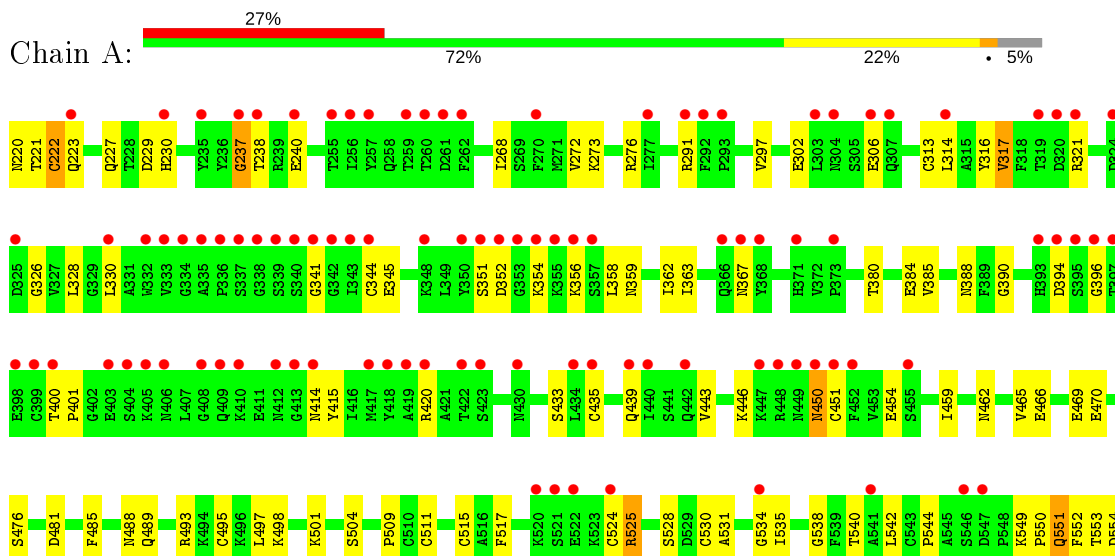
- Molecule 1: 11G2 Fab Light Chain

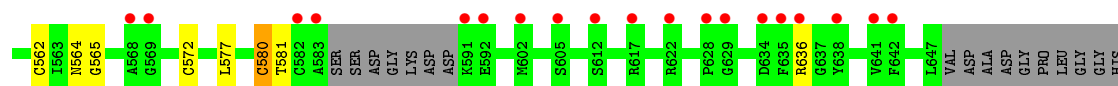


- Molecule 2: 11G2 Fab Heavy Chain



- Molecule 3: Disintegrin and metalloproteinase domain-containing protein 10





HIS
HIS
HIS
HIS
HIS

- Molecule 4: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%

MAG1
MAG2
MAN3
MAN4

- Molecule 5: alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 67% 33%

MAG1
MAG2
MAG3

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	79.23Å 97.58Å 262.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.79 – 3.10 48.79 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.79-3.10) 84.0 (48.79-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.56 (at 3.12Å)	Xtrriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.261 , 0.317 0.262 , 0.318	Depositor DCC
R_{free} test set	1895 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.8	Xtrriage
Anisotropy	0.768	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	6631	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MAN, CA, NAG, 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	L	0.30	0/1682	0.46	0/2282
2	H	0.24	0/1684	0.45	0/2305
3	A	0.26	0/3307	0.47	1/4454 (0.0%)
All	All	0.27	0/6673	0.46	1/9041 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	237	GLY	N-CA-C	7.25	131.23	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1645	0	1575	36	0
2	H	1643	0	1612	27	1
3	A	3242	0	3060	78	0
4	B	49	0	43	3	0
5	C	39	0	34	0	0
6	L	10	0	0	1	0
7	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	1	0	0	0	0
9	H	1	0	0	0	0
All	All	6631	0	6324	133	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 10.

All (133) 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)
3:A:344:CYS:CB	3:A:451:CYS:SG	2.32	1.17
3:A:344:CYS:SG	3:A:451:CYS:SG	1.35	1.17
1:L:28:GLN:HG2	1:L:45:CYS:SG	1.91	1.11
3:A:549:LYS:HB3	3:A:550:PRO:CD	1.84	1.06
3:A:551:GLN:OE1	3:A:564:ASN:ND2	2.01	0.94
3:A:549:LYS:HB3	3:A:550:PRO:HD3	1.50	0.93
3:A:549:LYS:CB	3:A:550:PRO:CD	2.54	0.85
3:A:341:GLY:H	3:A:345:GLU:HG3	1.39	0.85
3:A:306:GLU:OE2	3:A:354:LYS:HD3	1.81	0.81
3:A:237:GLY:O	3:A:238:THR:HG23	1.81	0.80
1:L:193:ASP:OD2	1:L:195:THR:OG1	1.99	0.80
3:A:549:LYS:HB3	3:A:550:PRO:HD2	1.65	0.77
1:L:25:VAL:HG22	1:L:48:SER:HB3	1.69	0.73
1:L:53:SER:O	1:L:74:THR:HG23	1.88	0.73
2:H:219:ASN:ND2	2:H:230:ASP:OD2	2.20	0.72
3:A:344:CYS:SG	3:A:451:CYS:CB	2.75	0.72
1:L:33:MET:CE	1:L:41:VAL:HB	2.21	0.71
3:A:540:THR:HG23	3:A:542:LEU:H	1.56	0.70
3:A:344:CYS:CA	3:A:451:CYS:SG	2.80	0.69
3:A:485:PHE:HB3	3:A:489:GLN:HG3	1.73	0.69
2:H:37:LEU:HB2	2:H:104:LEU:HD11	1.74	0.69
3:A:435:CYS:O	3:A:439:GLN:NE2	2.27	0.68
3:A:552:PHE:N	3:A:562:CYS:O	2.28	0.67
2:H:141:PRO:HA	2:H:222:HIS:HD2	1.60	0.66
2:H:73:ASP:OD2	3:A:498:LYS:NZ	2.27	0.66
1:L:28:GLN:CG	1:L:45:CYS:SG	2.78	0.65
3:A:328:LEU:HD21	3:A:367:ASN:HB2	1.80	0.63
3:A:390:GLY:HA3	3:A:443:VAL:HG21	1.81	0.63
1:L:33:MET:HE3	1:L:41:VAL:HB	1.81	0.62
2:H:78:TYR:HB2	2:H:83:LYS:HG2	1.81	0.62
2:H:73:ASP:OD1	2:H:75:THR:OG1	2.17	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:174:THR:HB	2:H:221:ALA:HB3	1.81	0.61
1:L:113:GLN:HE21	1:L:116:ARG:H	1.47	0.61
3:A:240:GLU:OE2	3:A:509:PRO:HB3	2.00	0.60
1:L:115:ARG:NH1	3:A:470:GLU:OE2	2.34	0.60
3:A:525:ARG:HB3	3:A:534:GLY:H	1.66	0.59
3:A:549:LYS:CB	3:A:550:PRO:HD2	2.28	0.59
3:A:580:CYS:SG	3:A:581:THR:N	2.76	0.58
1:L:33:MET:HE1	1:L:41:VAL:HB	1.85	0.58
3:A:344:CYS:HA	3:A:451:CYS:SG	2.43	0.58
1:L:116:ARG:NH1	6:L:301:SO4:O4	2.37	0.57
3:A:420:ARG:NH1	3:A:636:ARG:HG2	2.19	0.57
2:H:25:GLU:N	2:H:25:GLU:OE2	2.37	0.57
3:A:237:GLY:O	3:A:238:THR:CG2	2.51	0.56
3:A:345:GLU:O	3:A:359:ASN:ND2	2.38	0.56
2:H:65:GLU:OE2	4:B:1:NAG:H4	2.05	0.56
3:A:223:GLN:N	3:A:313:CYS:SG	2.79	0.56
1:L:114:TYR:HB3	3:A:493:ARG:HH12	1.70	0.56
1:L:114:TYR:HB3	3:A:493:ARG:NH1	2.20	0.56
3:A:227:GLN:HG2	3:A:276:ARG:HB3	1.87	0.56
3:A:351:SER:O	3:A:352:ASP:HB3	2.07	0.56
3:A:420:ARG:HH11	3:A:636:ARG:HG2	1.71	0.55
3:A:481:ASP:OD2	3:A:504:SER:OG	2.25	0.55
3:A:229:ASP:OD2	3:A:321:ARG:NH2	2.41	0.54
2:H:216:VAL:HG12	2:H:233:ILE:HD13	1.90	0.53
3:A:509:PRO:HG2	3:A:524:CYS:SG	2.48	0.53
3:A:302:GLU:HG3	3:A:356:LYS:NZ	2.25	0.52
3:A:396:GLY:O	3:A:400:THR:OG1	2.22	0.52
3:A:450:ASN:N	3:A:450:ASN:HD22	2.08	0.52
1:L:172:LYS:HB2	1:L:216:THR:HB	1.92	0.52
3:A:476:SER:N	3:A:488:ASN:OD1	2.43	0.51
3:A:314:LEU:HD23	3:A:359:ASN:HB2	1.92	0.51
3:A:553:THR:CG2	3:A:554:ASP:N	2.73	0.51
1:L:113:GLN:NE2	1:L:116:ARG:H	2.09	0.51
1:L:89:GLY:HA3	1:L:94:TYR:HA	1.93	0.51
3:A:222:CYS:C	3:A:313:CYS:SG	2.89	0.50
3:A:385:VAL:HA	3:A:388:ASN:HD22	1.76	0.50
3:A:363:ILE:HD11	3:A:380:THR:HG22	1.92	0.50
3:A:415:TYR:CG	3:A:433:SER:HB3	2.46	0.50
3:A:553:THR:HG22	3:A:554:ASP:N	2.26	0.49
2:H:210:THR:HG23	2:H:214:GLU:HG3	1.94	0.49
3:A:462:ASN:ND2	3:A:466:GLU:OE2	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:469:GLU:HB2	3:A:495:CYS:HB3	1.95	0.49
2:H:124:ASP:N	2:H:124:ASP:OD1	2.41	0.49
1:L:53:SER:O	1:L:74:THR:CG2	2.61	0.48
4:B:1:NAG:H62	4:B:2:NAG:N2	2.29	0.48
3:A:572:CYS:HB3	3:A:577:LEU:HB2	1.94	0.48
2:H:43:VAL:HG21	2:H:48:LEU:HD21	1.94	0.47
3:A:351:SER:O	3:A:352:ASP:CB	2.62	0.47
1:L:71:ILE:HD12	1:L:77:LEU:HD23	1.96	0.47
3:A:535:ILE:O	3:A:544:PRO:HG3	2.15	0.47
3:A:230:HIS:CE1	3:A:291:ARG:HA	2.50	0.47
3:A:221:THR:OG1	3:A:454:GLU:O	2.25	0.47
3:A:220:ASN:HA	3:A:268:ILE:HA	1.97	0.47
2:H:210:THR:O	2:H:214:GLU:N	2.40	0.47
1:L:218:GLU:HG3	1:L:229:VAL:HG22	1.97	0.46
3:A:297:VAL:HG22	3:A:330:LEU:HD22	1.98	0.46
1:L:59:TYR:HE1	1:L:112:HIS:HB3	1.79	0.46
1:L:114:TYR:CD1	1:L:119:LEU:HD12	2.51	0.46
2:H:55:TRP:CG	2:H:99:LEU:HD13	2.50	0.46
1:L:119:LEU:HD22	2:H:66:TRP:CD1	2.51	0.46
1:L:26:LEU:HG	1:L:47:VAL:HG12	1.98	0.46
3:A:317:VAL:HG13	3:A:362:ILE:HG22	1.98	0.46
2:H:142:PRO:HD3	2:H:222:HIS:CD2	2.51	0.46
2:H:75:THR:OG1	3:A:498:LYS:NZ	2.48	0.45
1:L:71:ILE:HG13	1:L:96:LEU:HD13	1.98	0.45
3:A:272:VAL:HG13	3:A:462:ASN:HD22	1.81	0.45
1:L:71:ILE:CD1	1:L:77:LEU:CD2	2.95	0.45
1:L:177:GLU:CD	1:L:177:GLU:H	2.19	0.45
3:A:273:LYS:HA	3:A:459:ILE:HD11	1.99	0.44
2:H:121:GLY:HA3	3:A:493:ARG:HH11	1.83	0.44
3:A:384:GLU:O	3:A:388:ASN:ND2	2.51	0.44
1:L:71:ILE:CD1	1:L:77:LEU:HD23	2.48	0.44
3:A:517:PHE:HB3	3:A:538:GLY:HA2	2.00	0.43
4:B:3:MAN:H62	4:B:4:MAN:H2	1.70	0.43
2:H:138:LYS:HD2	2:H:138:LYS:HA	1.84	0.43
2:H:161:LEU:O	2:H:204:VAL:N	2.40	0.43
2:H:142:PRO:HB3	2:H:168:TYR:HB3	2.00	0.43
1:L:71:ILE:HD12	1:L:77:LEU:CD2	2.48	0.43
3:A:341:GLY:HA2	3:A:358:LEU:HB3	2.00	0.43
3:A:401:PRO:HD2	3:A:414:ASN:HA	2.01	0.43
3:A:530:CYS:O	3:A:565:GLY:HA2	2.19	0.43
1:L:88:SER:O	1:L:95:SER:N	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:26:LEU:HD23	1:L:111:CYS:SG	2.59	0.43
2:H:177:TRP:CZ3	2:H:218:CYS:HB3	2.54	0.43
3:A:230:HIS:HE1	3:A:291:ARG:HA	1.84	0.42
3:A:454:GLU:CD	3:A:454:GLU:H	2.20	0.42
3:A:316:TYR:OH	3:A:388:ASN:ND2	2.53	0.42
1:L:51:VAL:HA	1:L:116:ARG:HH22	1.85	0.42
1:L:143:PRO:HD3	1:L:155:VAL:HG22	2.01	0.42
3:A:394:ASP:OD2	3:A:415:TYR:HB2	2.20	0.42
1:L:57:HIS:CD2	1:L:73:SER:H	2.38	0.42
3:A:501:LYS:HB3	3:A:515:CYS:HB3	2.01	0.42
3:A:528:SER:HB3	3:A:531:ALA:HB3	2.02	0.41
1:L:119:LEU:HB3	2:H:66:TRP:CD2	2.55	0.41
3:A:446:LYS:HE2	3:A:446:LYS:HA	2.02	0.41
3:A:326:GLY:HA2	3:A:367:ASN:OD1	2.21	0.41
2:H:161:LEU:HD11	2:H:211:TRP:CG	2.55	0.41
3:A:420:ARG:HD3	3:A:636:ARG:HA	2.03	0.40
1:L:237:CYS:HA	2:H:238:CYS:HB3	2.03	0.40
3:A:497:LEU:HD12	3:A:497:LEU:HA	1.96	0.40
1:L:56:LEU:HD22	1:L:94:TYR:CG	2.56	0.40
2:H:75:THR:CB	3:A:498:LYS:HZ2	2.34	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)
2:H:34:SER:OG	2:H:196:ASP:OD2[4_565]	2.19	0.01

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	L	213/215 (99%)	204 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	217/226 (96%)	208 (96%)	9 (4%)	0	100	100
3	A	417/443 (94%)	393 (94%)	24 (6%)	0	100	100
All	All	847/884 (96%)	805 (95%)	42 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	L	188/188 (100%)	183 (97%)	5 (3%)	44	74
2	H	190/196 (97%)	188 (99%)	2 (1%)	73	89
3	A	366/383 (96%)	358 (98%)	8 (2%)	52	78
All	All	744/767 (97%)	729 (98%)	15 (2%)	55	80

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	32	ILE
1	L	56	LEU
1	L	81	VAL
1	L	114	TYR
1	L	237	CYS
2	H	25	GLU
2	H	128	GLN
3	A	222	CYS
3	A	317	VAL
3	A	450	ASN
3	A	465	VAL
3	A	511	CYS
3	A	525	ARG
3	A	551	GLN
3	A	580	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	57	HIS
1	L	112	HIS
1	L	113	GLN
1	L	180	ASN
1	L	184	ASN
2	H	20	GLN
2	H	35	GLN
2	H	128	GLN
2	H	222	HIS
3	A	227	GLN
3	A	378	HIS
3	A	388	ASN
3	A	406	ASN
3	A	409	GLN
3	A	439	GLN
3	A	450	ASN
3	A	467	GLN
3	A	614	GLN
3	A	627	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

7 monosaccharides 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	1	2,4	13,13,15	0.63	0	16,17,21	1.58	1 (6%)
4	NAG	B	2	4	14,14,15	0.26	0	17,19,21	0.78	1 (5%)
4	MAN	B	3	4	11,11,12	1.20	2 (18%)	15,15,17	1.85	2 (13%)
4	MAN	B	4	4	11,11,12	0.72	1 (9%)	15,15,17	1.19	2 (13%)
5	NAG	C	1	3,5	14,14,15	0.26	0	17,19,21	0.41	0
5	NAG	C	2	5	14,14,15	0.30	0	17,19,21	0.64	0
5	MAN	C	3	5	11,11,12	0.70	0	15,15,17	0.97	1 (6%)

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	1	2,4	-	2/5/22/26	0/1/1/1
4	NAG	B	2	4	-	2/6/23/26	0/1/1/1
4	MAN	B	3	4	-	1/2/19/22	0/1/1/1
4	MAN	B	4	4	-	0/2/19/22	0/1/1/1
5	NAG	C	1	3,5	-	1/6/23/26	0/1/1/1
5	NAG	C	2	5	-	0/6/23/26	0/1/1/1
5	MAN	C	3	5	-	0/2/19/22	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3	MAN	C1-C2	2.86	1.58	1.52
4	B	4	MAN	C1-C2	2.19	1.57	1.52
4	B	3	MAN	O5-C1	2.06	1.47	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3	MAN	C1-O5-C5	5.96	120.27	112.19
4	B	1	NAG	C7-N2-C2	5.84	123.16	114.57
4	B	4	MAN	C1-O5-C5	3.38	116.77	112.19
4	B	2	NAG	C1-O5-C5	2.41	115.46	112.19
5	C	3	MAN	O2-C2-C3	-2.32	105.49	110.14
4	B	3	MAN	O2-C2-C3	-2.24	105.64	110.14
4	B	4	MAN	O2-C2-C3	-2.13	105.87	110.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2	NAG	O5-C5-C6-O6
4	B	2	NAG	C4-C5-C6-O6
5	C	1	NAG	C4-C5-C6-O6
4	B	1	NAG	C1-C2-N2-C7
4	B	3	MAN	C4-C5-C6-O6
4	B	1	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	4	MAN	1	0
4	B	1	NAG	2	0
4	B	3	MAN	1	0
4	B	2	NAG	1	0

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
6	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	0
6	SO4	L	302	-	4,4,4	0.14	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	L	301	SO4	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, 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	L	215/215 (100%)	0.15	0 100 100	22, 43, 83, 123	0
2	H	219/226 (96%)	0.15	3 (1%) 75 56	17, 38, 70, 124	0
3	A	421/443 (95%)	1.64	120 (28%) 0 0	33, 111, 159, 201	0
All	All	855/884 (96%)	0.88	123 (14%) 2 1	17, 67, 147, 201	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	395	SER	12.5
3	A	397	THR	11.8
3	A	569	GLY	11.6
3	A	259	THR	7.7
3	A	396	GLY	7.2
3	A	451	CYS	6.8
3	A	404	SER	6.6
3	A	356	LYS	6.6
3	A	352	ASP	6.4
3	A	398	GLU	6.4
3	A	400	THR	6.3
3	A	354	LYS	6.2
3	A	399	CYS	6.1
3	A	339	SER	6.0
3	A	357	SER	5.9
3	A	413	GLY	5.9
3	A	414	ASN	5.8
3	A	412	ASN	5.8
3	A	237	GLY	5.7
3	A	408	GLY	5.7
3	A	405	LYS	5.4
3	A	334	GLY	5.4
3	A	332	TRP	5.3

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Mol	Chain	Res	Type	RSRZ
3	A	292	PHE	5.2
3	A	419	ALA	5.2
3	A	342	GLY	5.0
3	A	409	GLN	4.8
3	A	335	ALA	4.8
3	A	337	SER	4.6
3	A	452	PHE	4.6
3	A	521	SER	4.5
3	A	546	SER	4.5
3	A	340	SER	4.5
3	A	591	LYS	4.5
3	A	338	GLY	4.4
3	A	450	ASN	4.3
3	A	256	ILE	4.2
3	A	235	TYR	4.1
3	A	336	PRO	4.1
3	A	321	ARG	4.1
3	A	353	GLY	4.0
3	A	430	ASN	3.9
3	A	366	GLN	3.9
3	A	393	HIS	3.8
3	A	368	TYR	3.8
3	A	406	ASN	3.8
3	A	434	LEU	3.8
3	A	351	SER	3.7
3	A	422	THR	3.7
3	A	355	LYS	3.6
3	A	582	CYS	3.5
3	A	636	ARG	3.5
3	A	448	ARG	3.5
3	A	394	ASP	3.4
3	A	330	LEU	3.4
3	A	304	ASN	3.3
3	A	371	HIS	3.2
3	A	403	GLU	3.2
3	A	320	ASP	3.2
3	A	439	GLN	3.2
3	A	628	PRO	3.2
3	A	629	GLY	3.1
3	A	635	PHE	3.1
3	A	602	MET	3.1
3	A	319	THR	3.1

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Mol	Chain	Res	Type	RSRZ
3	A	324	ASP	3.1
3	A	583	ALA	3.1
3	A	333	VAL	3.0
3	A	238	THR	3.0
3	A	223	GLN	3.0
2	H	238	CYS	3.0
3	A	230	HIS	2.9
3	A	423	SER	2.9
3	A	534	GLY	2.9
3	A	455	SER	2.9
3	A	350	TYR	2.9
3	A	440	ILE	2.9
3	A	240	GLU	2.8
3	A	341	GLY	2.8
3	A	293	PRO	2.8
3	A	638	TYR	2.8
2	H	155	THR	2.8
3	A	442	GLN	2.8
3	A	418	TYR	2.7
3	A	325	ASP	2.7
3	A	617	ARG	2.7
3	A	260	THR	2.7
3	A	592	GLU	2.6
3	A	547	ASP	2.6
3	A	420	ARG	2.6
3	A	634	ASP	2.6
3	A	435	CYS	2.6
3	A	306	GLU	2.5
3	A	410	LYS	2.5
3	A	622	ARG	2.5
3	A	261	ASP	2.5
3	A	541	ALA	2.4
3	A	447	LYS	2.4
3	A	344	CYS	2.4
3	A	449	ASN	2.4
3	A	277	ILE	2.4
2	H	215	THR	2.4
3	A	642	PHE	2.4
3	A	343	ILE	2.4
3	A	568	ALA	2.3
3	A	524	CYS	2.3
3	A	612	SER	2.3

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Mol	Chain	Res	Type	RSRZ
3	A	520	LYS	2.3
3	A	270	PHE	2.3
3	A	522	GLU	2.2
3	A	291	ARG	2.2
3	A	314	LEU	2.2
3	A	373	PRO	2.2
3	A	262	PHE	2.2
3	A	641	VAL	2.2
3	A	348	LYS	2.2
3	A	605	SER	2.2
3	A	307	GLN	2.2
3	A	257	TYR	2.1
3	A	367	ASN	2.1
3	A	303	LEU	2.1
3	A	417	MET	2.1
3	A	255	THR	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. 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
5	MAN	C	3	11/12	0.53	0.34	64,106,125,131	0
4	MAN	B	3	11/12	0.70	0.29	76,100,112,118	0
4	MAN	B	4	11/12	0.73	0.24	82,89,102,111	0
4	NAG	B	1	13/15	0.83	0.30	21,34,52,61	0
5	NAG	C	2	14/15	0.84	0.41	84,95,106,115	0
4	NAG	B	2	14/15	0.87	0.20	38,62,76,97	0
5	NAG	C	1	14/15	0.89	0.25	72,81,105,110	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. 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
8	ZN	A	705	1/1	0.30	0.68	749,749,749,749	0
7	CA	A	704	1/1	0.74	0.17	62,62,62,62	0
6	SO4	L	302	5/5	0.82	0.23	67,67,76,89	0
6	SO4	L	301	5/5	0.92	0.20	37,55,73,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.