



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:28 AM GMT

PDB ID : 3IJE  
Title : Crystal structure of the complete integrin  $\alpha$ V $\beta$ 3 ectodomain plus an Alpha/beta transmembrane fragment  
Authors : Xiong, J.-P.; Mahalingham, B.; Rui, X.; Hyman, B.T.; Goodman, S.L.; Arnaout, M.A.  
Deposited on : 2009-08-04  
Resolution : 2.90 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

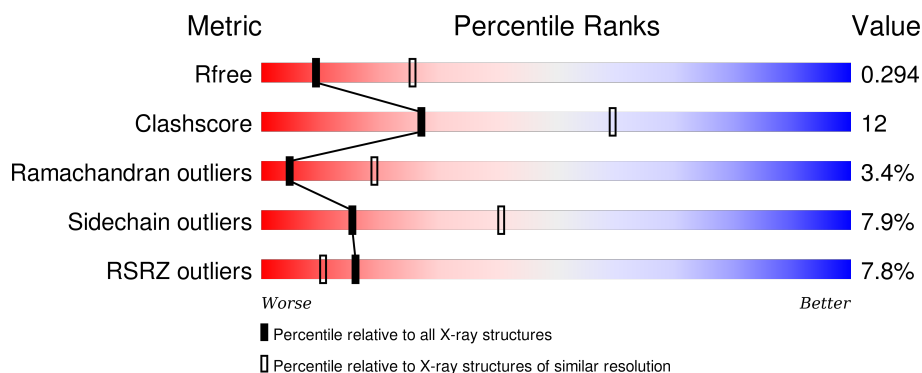
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	967	<div> <div>7%</div> <div>71%</div> <div>23%</div> <div>• •</div> </div>
2	B	695	<div> <div>9%</div> <div>70%</div> <div>26%</div> <div>•</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	2045	-	-	X	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 13087 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 Integrin alpha-V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	938	Total	C	N	O	S	0	0	0
			7300	4628	1236	1400	36			

- Molecule 2 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	695	Total	C	N	O	S	0	0	0
			5332	3276	909	1077	70			

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

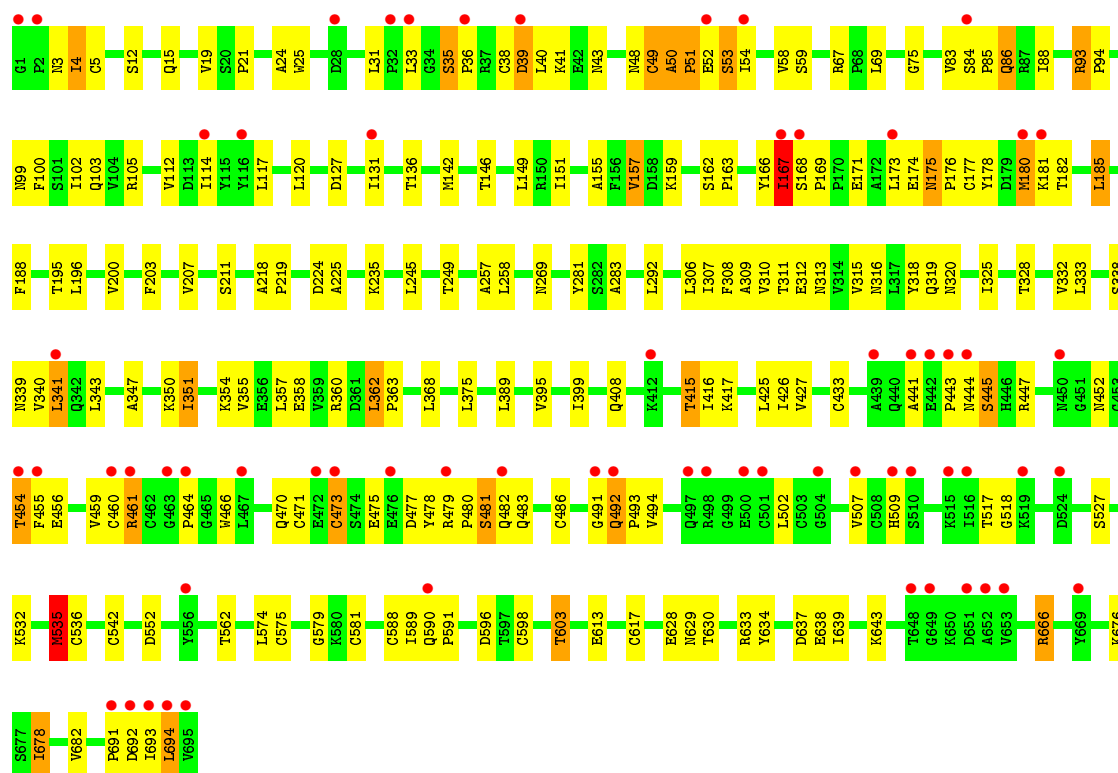
- Molecule 7 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	3	Total	C	N	O	0	0
			39	22	2	15		
7	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total 1	Ca 1	0	0
8	A	5	Total 5	Ca 5	0	0







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.87Å 129.87Å 305.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 64.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.90) 92.7 (64.94-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.244 , 0.285 0.242 , 0.294	Depositor DCC
$R_{free}$ test set	2917 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.4	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.9	EDS
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 62236 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	13087	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.33	0/7462	0.54	0/10123
2	B	0.35	0/5429	0.54	0/7344
All	All	0.34	0/12891	0.54	0/17467

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	546	SER	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	7300	0	7126	164	0
2	B	5332	0	5071	139	0
3	A	61	0	52	7	0
4	A	140	0	125	2	0
4	B	28	0	25	0	0
5	A	72	0	61	0	0
6	A	28	0	26	0	0
6	B	42	0	39	5	0
7	A	39	0	34	0	0
7	B	39	0	34	0	0
8	A	5	0	0	0	0
8	B	1	0	0	0	0
All	All	13087	0	12593	306	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 12.

All (306) 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:3:LEU:HD11	1:A:350:LEU:HD11	1.58	0.85
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.59	0.82
2:B:281:TYR:CE1	2:B:283:ALA:HB3	2.14	0.82
1:A:639:TYR:H	1:A:721:ASN:HD21	1.30	0.80
1:A:546:SER:O	1:A:547:GLU:HB2	1.82	0.77
1:A:958:ALA:HB1	1:A:959:PRO:HD2	1.65	0.77
2:B:169:PRO:HG2	2:B:173:LEU:HD23	1.65	0.77
1:A:821:ASN:HD21	4:A:2821:NAG:C1	1.98	0.76
1:A:3:LEU:CD1	1:A:350:LEU:HD11	2.15	0.76
1:A:772:VAL:HG21	1:A:833:ILE:HD13	1.70	0.74
2:B:579:GLY:HA2	2:B:589:ILE:HD13	1.71	0.73
2:B:375:LEU:HD13	2:B:633:ARG:HD2	1.70	0.73
1:A:443:VAL:HG21	1:A:561:TYR:CE1	2.23	0.72
1:A:596:CYS:HG	1:A:602:CYS:HG	0.80	0.72
2:B:454:THR:HG23	2:B:461:ARG:O	1.91	0.71
1:A:617:ILE:HD13	1:A:701:VAL:HG11	1.70	0.71
2:B:589:ILE:HG22	2:B:591:PRO:HD3	1.71	0.71
2:B:574:LEU:HD11	2:B:581:CYS:HB2	1.73	0.70
2:B:5:CYS:HB3	2:B:38:CYS:SG	2.33	0.69
2:B:292:LEU:HD22	2:B:325:ILE:HD11	1.75	0.68
1:A:499:LEU:HD23	1:A:557:ILE:HD12	1.77	0.67
2:B:333:LEU:HD11	2:B:340:VAL:HG22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:479:ARG:O	2:B:481:SER:N	2.28	0.66
1:A:116:THR:HG21	1:A:147:ILE:HD13	1.78	0.66
2:B:355:VAL:HG12	2:B:389:LEU:CD1	2.26	0.66
2:B:320:ASN:OD1	6:B:3320:NAG:H82	1.96	0.66
2:B:454:THR:O	2:B:460:CYS:HB2	1.96	0.65
2:B:362:LEU:HD23	2:B:363:PRO:HD2	1.79	0.65
1:A:885:GLN:N	1:A:885:GLN:HE21	1.95	0.65
2:B:589:ILE:HG23	2:B:590:GLN:H	1.62	0.64
1:A:527:ILE:HG22	1:A:534:GLN:HB3	1.79	0.63
1:A:368:ASP:O	1:A:370:LYS:N	2.31	0.63
1:A:617:ILE:HD11	1:A:625:LEU:HD22	1.81	0.63
1:A:147:ILE:O	1:A:147:ILE:HD12	1.97	0.63
1:A:314:GLN:HE21	1:A:332:ASN:HD21	1.45	0.63
1:A:443:VAL:HG21	1:A:561:TYR:HE1	1.63	0.62
1:A:116:THR:CG2	1:A:118:MET:SD	2.87	0.62
1:A:27:VAL:HG13	1:A:34:MET:HE2	1.81	0.62
2:B:588:CYS:HG	2:B:598:CYS:HG	0.70	0.62
3:A:2045:NAG:H82	3:A:2048:MAN:H62	1.82	0.62
1:A:807:THR:O	1:A:807:THR:HG22	2.00	0.61
1:A:236:ILE:HD12	1:A:237:ASP:H	1.65	0.61
2:B:149:LEU:HD21	2:B:151:ILE:HG23	1.83	0.61
2:B:50:ALA:O	2:B:54:ILE:HG23	2.00	0.61
1:A:768:THR:HB	1:A:835:ILE:HD12	1.82	0.61
2:B:613:GLU:O	2:B:617:CYS:HB2	2.00	0.61
1:A:769:GLU:HG2	1:A:812:LEU:HD11	1.82	0.60
2:B:281:TYR:CZ	2:B:283:ALA:HB3	2.36	0.60
1:A:248:ARG:HD2	6:B:3320:NAG:H81	1.83	0.60
2:B:589:ILE:CG2	2:B:590:GLN:H	2.14	0.60
2:B:180:MET:O	2:B:182:THR:HG22	2.00	0.60
2:B:332:VAL:O	2:B:343:LEU:HD21	2.02	0.60
2:B:316:ASN:HB3	6:B:3320:NAG:H83	1.84	0.60
2:B:589:ILE:CG2	2:B:590:GLN:N	2.65	0.60
2:B:218:ALA:HB3	2:B:219:PRO:HD3	1.84	0.59
1:A:610:VAL:HG11	1:A:715:LEU:HD21	1.85	0.59
1:A:546:SER:O	1:A:547:GLU:CB	2.51	0.59
1:A:508:ILE:HD11	2:B:475:GLU:O	2.02	0.59
2:B:502:LEU:HD13	2:B:507:VAL:CG2	2.33	0.59
1:A:745:ARG:HG3	2:B:603:THR:HG21	1.84	0.59
2:B:694:LEU:HD23	2:B:694:LEU:O	2.03	0.59
1:A:672:THR:HG23	1:A:676:THR:O	2.03	0.58
1:A:187:GLN:O	1:A:191:ILE:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:VAL:HG12	2:B:389:LEU:HD11	1.85	0.58
1:A:627:LEU:HD12	1:A:627:LEU:O	2.03	0.58
1:A:755:LEU:HD11	1:A:908:PHE:HB3	1.86	0.58
1:A:70:ILE:HD13	1:A:105:ILE:HD11	1.86	0.58
1:A:165:LYS:O	1:A:166:ALA:HB3	2.04	0.57
1:A:666:LEU:HD21	1:A:693:LEU:HD23	1.86	0.57
2:B:51:PRO:O	2:B:53:SER:N	2.37	0.57
1:A:721:ASN:HD22	1:A:721:ASN:N	2.02	0.57
1:A:936:LEU:HD22	1:A:937:PRO:HD2	1.85	0.57
2:B:169:PRO:CG	2:B:173:LEU:HD23	2.35	0.56
2:B:24:ALA:O	2:B:38:CYS:HA	2.05	0.56
1:A:567:THR:HG23	1:A:567:THR:O	2.05	0.56
1:A:685:ASN:HB3	1:A:686:PRO:CD	2.36	0.56
1:A:816:ILE:HG23	1:A:820:MET:HE3	1.87	0.56
2:B:441:ALA:HB1	2:B:456:GLU:CB	2.35	0.56
1:A:116:THR:HG22	1:A:118:MET:H	1.68	0.56
1:A:170:LEU:HD13	1:A:226:VAL:HG22	1.87	0.56
2:B:39:ASP:O	2:B:40:LEU:HD22	2.06	0.56
1:A:24:ASP:OD2	1:A:25:PHE:N	2.38	0.56
1:A:61:TRP:O	1:A:63:SER:N	2.39	0.56
2:B:159:LYS:NZ	2:B:224:ASP:OD1	2.39	0.56
1:A:502:LEU:HD12	2:B:509:HIS:CD2	2.41	0.56
1:A:3:LEU:H	1:A:389:GLN:HE22	1.53	0.55
1:A:757:ILE:O	1:A:757:ILE:HG23	2.04	0.55
1:A:936:LEU:HD13	1:A:937:PRO:HD2	1.89	0.55
1:A:3:LEU:HD13	1:A:350:LEU:HD21	1.88	0.55
2:B:149:LEU:HD23	2:B:149:LEU:C	2.27	0.55
1:A:332:ASN:N	1:A:332:ASN:HD22	2.02	0.55
2:B:112:VAL:HG11	2:B:142:MET:CE	2.38	0.54
2:B:173:LEU:O	2:B:173:LEU:HD12	2.06	0.54
2:B:50:ALA:HB3	2:B:51:PRO:HD3	1.89	0.54
1:A:946:LEU:HD23	1:A:946:LEU:H	1.73	0.54
2:B:83:VAL:O	2:B:86:GLN:NE2	2.36	0.54
1:A:816:ILE:HG23	1:A:820:MET:CE	2.37	0.54
2:B:15:GLN:O	2:B:19:VAL:HG23	2.07	0.54
1:A:936:LEU:HD13	1:A:937:PRO:CD	2.38	0.54
1:A:547:GLU:CD	2:B:477:ASP:HA	2.28	0.53
2:B:157:VAL:O	2:B:157:VAL:HG12	2.09	0.53
1:A:547:GLU:O	1:A:548:PHE:C	2.43	0.53
2:B:441:ALA:CB	2:B:456:GLU:HB2	2.39	0.53
1:A:792:LYS:HB2	1:A:930:GLU:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:491:GLY:O	2:B:492:GLN:HB2	2.09	0.53
1:A:795:LEU:HB3	1:A:884:CYS:HB2	1.90	0.53
1:A:648:PRO:HG3	1:A:711:VAL:HG22	1.90	0.53
1:A:154:PHE:O	1:A:175:GLY:HA3	2.08	0.53
1:A:414:ILE:HG21	1:A:434:LEU:HD21	1.91	0.53
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.44	0.53
1:A:617:ILE:HD11	1:A:625:LEU:CD2	2.39	0.52
2:B:131:ILE:HG22	2:B:207:VAL:HG21	1.91	0.52
1:A:314:GLN:HE21	1:A:332:ASN:ND2	2.06	0.52
1:A:755:LEU:O	1:A:757:ILE:N	2.43	0.52
2:B:637:ASP:O	2:B:639:ILE:HD12	2.09	0.52
1:A:347:LEU:CD1	1:A:375:ILE:HD13	2.37	0.52
1:A:510:ARG:O	1:A:542:LEU:HD12	2.10	0.52
1:A:347:LEU:HD13	1:A:350:LEU:HD22	1.91	0.52
2:B:375:LEU:HD21	2:B:630:THR:HG22	1.91	0.52
2:B:459:VAL:HG22	2:B:460:CYS:N	2.25	0.52
1:A:165:LYS:O	1:A:236:ILE:HD11	2.09	0.52
1:A:453:ILE:HD11	1:A:639:TYR:CE2	2.45	0.52
1:A:246:ALA:HB1	1:A:252:MET:HE3	1.92	0.52
1:A:400:MET:HE1	1:A:427:PHE:CE1	2.44	0.52
2:B:441:ALA:HB1	2:B:456:GLU:HB3	1.92	0.52
2:B:693:ILE:O	2:B:693:ILE:HG23	2.10	0.52
2:B:166:TYR:CD2	2:B:173:LEU:HD21	2.45	0.51
1:A:222:LEU:HA	1:A:243:VAL:HG22	1.92	0.51
1:A:100:SER:HB2	1:A:105:ILE:HG22	1.91	0.51
1:A:903:LEU:HD21	1:A:908:PHE:CD1	2.45	0.51
1:A:880:LEU:C	1:A:880:LEU:HD23	2.30	0.51
2:B:112:VAL:HG12	2:B:146:THR:HG21	1.93	0.51
1:A:246:ALA:HB1	1:A:252:MET:CE	2.41	0.51
1:A:769:GLU:HG2	1:A:902:LEU:HD21	1.92	0.51
1:A:903:LEU:HD23	1:A:903:LEU:C	2.31	0.51
2:B:112:VAL:CG1	2:B:146:THR:HG21	2.41	0.51
2:B:185:LEU:HD11	2:B:211:SER:O	2.11	0.51
1:A:43:ALA:HB3	1:A:55:GLN:HG2	1.92	0.51
2:B:3:ASN:O	2:B:5:CYS:N	2.43	0.50
1:A:116:THR:HG22	1:A:117:GLU:N	2.25	0.50
1:A:946:LEU:HD23	1:A:946:LEU:N	2.25	0.50
2:B:310:VAL:HG11	2:B:318:TYR:CD1	2.46	0.50
2:B:33:LEU:HD21	2:B:470:GLN:HE21	1.76	0.50
1:A:625:LEU:HD12	1:A:626:THR:N	2.28	0.49
2:B:333:LEU:CD1	2:B:340:VAL:HG22	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:ASN:HB3	2:B:4:ILE:HD12	1.94	0.49
1:A:243:VAL:HG12	1:A:246:ALA:HB2	1.94	0.49
1:A:253:VAL:HG21	1:A:295:ILE:HD13	1.93	0.49
2:B:40:LEU:HD23	2:B:43:ASN:HD22	1.78	0.49
2:B:39:ASP:OD1	2:B:40:LEU:N	2.43	0.49
2:B:99:ASN:HD22	6:B:3099:NAG:H61	1.78	0.49
1:A:514:LEU:HD23	1:A:539:ILE:HD13	1.95	0.49
2:B:535:MET:SD	2:B:536:CYS:N	2.78	0.48
1:A:472:CYS:HA	1:A:541:TYR:HA	1.94	0.48
2:B:177:CYS:HB3	2:B:182:THR:HG23	1.94	0.48
1:A:183:LEU:HD13	1:A:222:LEU:HG	1.95	0.48
1:A:809:LEU:HG	1:A:920:LEU:HD13	1.95	0.48
1:A:936:LEU:HD13	1:A:937:PRO:N	2.29	0.48
2:B:40:LEU:HD23	2:B:43:ASN:ND2	2.27	0.48
2:B:117:LEU:HD21	2:B:225:ALA:HB1	1.95	0.48
2:B:456:GLU:O	2:B:459:VAL:O	2.32	0.48
2:B:574:LEU:HD13	2:B:575:CYS:N	2.29	0.48
2:B:67:ARG:N	2:B:86:GLN:OE1	2.47	0.48
1:A:645:VAL:O	1:A:645:VAL:HG13	2.13	0.48
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.94	0.47
1:A:567:THR:O	1:A:568:ALA:HB2	2.14	0.47
1:A:70:ILE:HD13	1:A:105:ILE:CD1	2.45	0.47
2:B:21:PRO:HA	2:B:93:ARG:HD2	1.96	0.47
2:B:375:LEU:HD21	2:B:630:THR:CG2	2.43	0.47
2:B:455:PHE:O	2:B:456:GLU:HB3	2.13	0.47
1:A:499:LEU:CD2	1:A:557:ILE:HD12	2.45	0.47
1:A:514:LEU:CD2	1:A:539:ILE:HD13	2.44	0.47
2:B:175:ASN:OD1	2:B:175:ASN:N	2.47	0.47
2:B:307:ILE:HD13	2:B:347:ALA:CB	2.45	0.47
2:B:166:TYR:HD2	2:B:173:LEU:HD21	1.78	0.47
2:B:195:THR:HG22	2:B:235:LYS:O	2.15	0.47
2:B:88:ILE:CG2	2:B:427:VAL:HG22	2.44	0.47
3:A:2045:NAG:H82	3:A:2048:MAN:C6	2.46	0.47
1:A:400:MET:HE1	1:A:427:PHE:CZ	2.49	0.46
1:A:397:ALA:HB2	1:A:402:PRO:HD3	1.97	0.46
2:B:517:THR:HG22	2:B:518:GLY:H	1.79	0.46
1:A:596:CYS:CB	1:A:602:CYS:HG	2.28	0.46
1:A:27:VAL:HG13	1:A:34:MET:CE	2.45	0.46
2:B:332:VAL:HG13	2:B:332:VAL:O	2.15	0.46
2:B:362:LEU:HD11	2:B:368:LEU:HD13	1.97	0.46
2:B:93:ARG:HD3	2:B:94:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:927:ASN:HD21	1:A:940:ASP:HB3	1.81	0.46
1:A:962:VAL:N	1:A:963:PRO:CD	2.78	0.46
1:A:257:ASP:O	1:A:260:ASN:O	2.34	0.46
3:A:2045:NAG:O3	3:A:2046:BMA:C2	2.63	0.46
1:A:685:ASN:HD22	1:A:685:ASN:C	2.19	0.46
2:B:249:THR:HG22	2:B:309:ALA:CB	2.38	0.46
2:B:312:GLU:O	2:B:315:VAL:HG12	2.15	0.46
1:A:649:LEU:HD12	1:A:677:ARG:HB3	1.97	0.46
2:B:360:ARG:HB2	2:B:415:THR:HG23	1.98	0.46
1:A:738:VAL:HG23	1:A:936:LEU:HD12	1.98	0.46
2:B:389:LEU:HD23	2:B:633:ARG:HH12	1.81	0.45
2:B:426:ILE:HD12	2:B:426:ILE:N	2.31	0.45
2:B:114:ILE:HB	2:B:151:ILE:HG22	1.98	0.45
2:B:39:ASP:C	2:B:40:LEU:HD22	2.37	0.45
1:A:821:ASN:ND2	4:A:2821:NAG:C1	2.74	0.45
2:B:25:TRP:HZ2	2:B:459:VAL:HG11	1.80	0.45
1:A:170:LEU:HD13	1:A:226:VAL:CG2	2.47	0.45
2:B:84:SER:HB3	2:B:85:PRO:HD3	1.98	0.45
2:B:339:ASN:O	2:B:343:LEU:HD13	2.17	0.45
2:B:445:SER:OG	6:B:3452:NAG:H82	2.16	0.45
1:A:144:SER:OG	1:A:152:GLN:NE2	2.50	0.45
1:A:511:ALA:O	1:A:512:LEU:HD23	2.17	0.45
2:B:441:ALA:HB1	2:B:456:GLU:HB2	1.99	0.45
1:A:100:SER:CB	1:A:105:ILE:HG22	2.47	0.45
1:A:546:SER:O	1:A:546:SER:OG	2.28	0.45
1:A:253:VAL:HG21	1:A:295:ILE:CD1	2.47	0.44
2:B:355:VAL:HG11	2:B:395:VAL:HG21	1.98	0.44
1:A:610:VAL:HG12	1:A:629:VAL:HG22	2.00	0.44
2:B:103:GLN:OE1	2:B:103:GLN:N	2.51	0.44
1:A:797:LEU:HD23	1:A:882:ILE:HD12	1.99	0.44
2:B:306:LEU:O	2:B:328:THR:HG23	2.17	0.44
1:A:504:GLN:HE22	1:A:509:ARG:HB3	1.81	0.44
2:B:666:ARG:O	2:B:682:VAL:HG12	2.18	0.44
2:B:180:MET:O	2:B:182:THR:N	2.50	0.44
2:B:166:TYR:O	2:B:167:ILE:C	2.56	0.44
1:A:757:ILE:HG23	1:A:760:TRP:CB	2.48	0.44
1:A:740:ALA:O	1:A:742:VAL:HG23	2.17	0.44
1:A:477:PHE:HD2	1:A:497:LEU:HD21	1.82	0.44
1:A:250:LEU:HD22	1:A:269:GLY:O	2.18	0.44
1:A:559:MET:HE1	1:A:586:ILE:HG22	2.00	0.44
2:B:441:ALA:HB2	2:B:456:GLU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:THR:HG22	1:A:118:MET:SD	2.57	0.44
1:A:757:ILE:HG23	1:A:760:TRP:HB3	2.00	0.44
1:A:962:VAL:O	1:A:962:VAL:HG12	2.18	0.44
1:A:885:GLN:H	1:A:885:GLN:HE21	1.63	0.43
2:B:69:LEU:HB3	2:B:105:ARG:HE	1.83	0.43
1:A:183:LEU:HD21	1:A:241:SER:HB2	2.00	0.43
1:A:165:LYS:O	1:A:166:ALA:CB	2.66	0.43
1:A:243:VAL:CG1	1:A:246:ALA:HB2	2.49	0.43
1:A:253:VAL:CG2	1:A:295:ILE:HD13	2.48	0.43
1:A:640:GLU:N	1:A:685:ASN:O	2.52	0.43
1:A:660:ASN:ND2	1:A:663:LEU:HD13	2.32	0.43
2:B:638:GLU:HB2	2:B:678:ILE:HG22	2.00	0.43
1:A:375:ILE:HD12	1:A:376:PHE:N	2.33	0.43
1:A:477:PHE:CD2	1:A:497:LEU:HD21	2.54	0.43
2:B:88:ILE:HG23	2:B:427:VAL:HG22	2.00	0.43
1:A:50:ILE:HG23	1:A:90:SER:HA	2.01	0.43
2:B:100:PHE:CE1	2:B:399:ILE:HD12	2.54	0.43
1:A:502:LEU:HD21	1:A:556:THR:OG1	2.19	0.43
2:B:58:VAL:HG12	2:B:59:SER:O	2.18	0.43
2:B:83:VAL:HG13	2:B:102:ILE:HD11	2.00	0.42
1:A:647:ILE:HD12	1:A:647:ILE:C	2.39	0.42
1:A:945:THR:HG22	1:A:946:LEU:N	2.35	0.42
2:B:311:THR:OG1	2:B:313:ASN:ND2	2.52	0.42
2:B:136:THR:HA	2:B:200:VAL:HG11	1.99	0.42
3:A:2045:NAG:C3	3:A:2046:BMA:H2	2.50	0.42
1:A:236:ILE:HD12	1:A:237:ASP:N	2.32	0.42
1:A:27:VAL:HG22	1:A:34:MET:HE2	2.01	0.42
1:A:757:ILE:O	1:A:757:ILE:CG2	2.66	0.42
2:B:157:VAL:HG23	2:B:188:PHE:CZ	2.54	0.42
2:B:162:SER:HB3	2:B:167:ILE:HG23	2.02	0.42
1:A:648:PRO:O	1:A:650:GLN:N	2.52	0.42
1:A:50:ILE:HG23	1:A:90:SER:CA	2.49	0.42
1:A:336:VAL:HG12	1:A:337:PHE:CD2	2.55	0.42
3:A:2045:NAG:O3	3:A:2046:BMA:H2	2.20	0.42
1:A:801:TYR:CD2	1:A:802:LYS:HG3	2.55	0.42
1:A:702:HIS:O	1:A:703:GLN:C	2.58	0.42
1:A:344:ILE:HG22	1:A:358:ILE:HD11	2.00	0.42
2:B:358:GLU:N	2:B:417:LYS:O	2.45	0.42
1:A:114:TRP:CE3	1:A:143:ARG:HD2	2.55	0.42
2:B:48:ASN:O	2:B:49:CYS:C	2.58	0.42
1:A:240:VAL:HG22	1:A:255:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:ALA:O	2:B:258:LEU:HB2	2.19	0.42
1:A:835:ILE:HG22	1:A:836:SER:N	2.34	0.41
1:A:672:THR:O	1:A:672:THR:HG22	2.20	0.41
2:B:310:VAL:HG11	2:B:318:TYR:CG	2.55	0.41
1:A:905:THR:O	1:A:906:GLU:C	2.58	0.41
2:B:102:ILE:HD12	2:B:425:LEU:HB2	2.02	0.41
1:A:936:LEU:O	1:A:938:ILE:HG23	2.20	0.41
2:B:492:GLN:N	2:B:493:PRO:HD2	2.36	0.41
2:B:630:THR:HB	2:B:634:TYR:CD1	2.56	0.41
2:B:50:ALA:O	2:B:51:PRO:O	2.38	0.41
2:B:203:PHE:O	2:B:207:VAL:HG12	2.21	0.41
1:A:780:TYR:CZ	1:A:947:VAL:HG13	2.55	0.41
1:A:829:ASN:N	1:A:830:PRO:HD3	2.36	0.41
2:B:589:ILE:HG22	2:B:590:GLN:N	2.36	0.41
1:A:685:ASN:HB3	1:A:686:PRO:HD3	2.02	0.41
2:B:245:LEU:CD2	2:B:351:ILE:HD11	2.50	0.41
1:A:145:GLN:C	1:A:147:ILE:HG23	2.40	0.41
2:B:48:ASN:O	2:B:50:ALA:HB2	2.20	0.41
1:A:826:MET:HE2	1:A:880:LEU:HG	2.02	0.41
2:B:552:ASP:HA	2:B:562:THR:OG1	2.20	0.41
2:B:94:PRO:HD3	2:B:433:CYS:HB3	2.02	0.41
2:B:12:SER:HB3	2:B:461:ARG:HH21	1.86	0.41
2:B:682:VAL:HG13	2:B:682:VAL:O	2.20	0.41
2:B:399:ILE:HD13	2:B:416:ILE:HD13	2.02	0.41
1:A:349:ASP:O	1:A:352:GLN:NE2	2.47	0.41
2:B:340:VAL:O	2:B:341:LEU:C	2.59	0.41
1:A:373:VAL:HG23	1:A:404:PHE:CE2	2.56	0.41
1:A:440:VAL:HG22	1:A:577:ILE:CG2	2.50	0.41
1:A:63:SER:O	1:A:64:THR:C	2.60	0.40
1:A:332:ASN:N	1:A:332:ASN:ND2	2.69	0.40
2:B:502:LEU:HD13	2:B:507:VAL:HG23	2.03	0.40
2:B:35:SER:HB3	2:B:36:PRO:HD3	2.03	0.40
1:A:306:ASP:N	1:A:306:ASP:OD1	2.48	0.40
2:B:173:LEU:HD13	2:B:178:TYR:CE1	2.56	0.40
3:A:2045:NAG:HO3	3:A:2046:BMA:C2	2.33	0.40
3:A:2045:NAG:C3	3:A:2046:BMA:C2	3.00	0.40
1:A:801:TYR:CD2	1:A:826:MET:HE1	2.56	0.40
2:B:120:LEU:HG	2:B:155:ALA:HB1	2.03	0.40

There are no symmetry-related clashes.

## 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	934/967 (97%)	843 (90%)	68 (7%)	23 (2%)	7	27
2	B	693/695 (100%)	579 (84%)	82 (12%)	32 (5%)	3	11
All	All	1627/1662 (98%)	1422 (87%)	150 (9%)	55 (3%)	5	19

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	SER
1	A	505	LYS
1	A	547	GLU
1	A	568	ALA
1	A	703	GLN
1	A	741	ALA
1	A	961	PRO
2	B	39	ASP
2	B	51	PRO
2	B	52	GLU
2	B	167	ILE
2	B	168	SER
2	B	181	LYS
2	B	473	CYS
2	B	478	TYR
2	B	480	PRO
2	B	481	SER
2	B	492	GLN
1	A	64	THR
1	A	368	ASP
1	A	369	LYS
1	A	546	SER
1	A	707	MET
1	A	835	ILE
1	A	914	GLN

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Mol	Chain	Res	Type
2	B	35	SER
2	B	49	CYS
2	B	53	SER
2	B	196	LEU
2	B	444	ASN
2	B	535	MET
1	A	503	LYS
1	A	674	ASN
1	A	808	LEU
2	B	50	ALA
2	B	482	GLN
2	B	527	SER
1	A	399	SER
1	A	529	ARG
1	A	649	LEU
2	B	4	ILE
2	B	443	PRO
2	B	532	LYS
1	A	910	ASN
2	B	41	LYS
2	B	157	VAL
2	B	445	SER
1	A	756	PRO
2	B	464	PRO
2	B	691	PRO
2	B	163	PRO
2	B	176	PRO
1	A	962	VAL
2	B	75	GLY
2	B	494	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	797/821 (97%)	727 (91%)	70 (9%)	12 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	617/617 (100%)	575 (93%)	42 (7%)	20	49
All	All	1414/1438 (98%)	1302 (92%)	112 (8%)	15	41

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	SER
1	A	99	ARG
1	A	105	ILE
1	A	106	LEU
1	A	115	ARG
1	A	118	MET
1	A	120	GLN
1	A	145	GLN
1	A	162	ASP
1	A	170	LEU
1	A	216	ILE
1	A	226	VAL
1	A	275	TYR
1	A	327	GLN
1	A	331	LEU
1	A	339	ARG
1	A	367	GLU
1	A	368	ASP
1	A	375	ILE
1	A	379	ARG
1	A	392	GLU
1	A	399	SER
1	A	417	ASN
1	A	436	ARG
1	A	450	TYR
1	A	474	ASN
1	A	478	CYS
1	A	487	LEU
1	A	502	LEU
1	A	505	LYS
1	A	523	LYS
1	A	535	CYS
1	A	536	GLU
1	A	549	ARG
1	A	564	ASP
1	A	565	TYR

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Mol	Chain	Res	Type
1	A	598	GLU
1	A	602	CYS
1	A	605	LYS
1	A	606	LEU
1	A	633	ASN
1	A	646	SER
1	A	649	LEU
1	A	650	GLN
1	A	658	ARG
1	A	665	ARG
1	A	677	ARG
1	A	685	ASN
1	A	688	LYS
1	A	712	LYS
1	A	715	LEU
1	A	721	ASN
1	A	733	LYS
1	A	745	ARG
1	A	749	SER
1	A	764	GLU
1	A	783	ARG
1	A	817	ASP
1	A	832	ARG
1	A	835	ILE
1	A	868	ASP
1	A	878	GLN
1	A	885	GLN
1	A	894	SER
1	A	897	LEU
1	A	902	LEU
1	A	913	ASN
1	A	921	LYS
1	A	946	LEU
1	A	947	VAL
2	B	31	LEU
2	B	86	GLN
2	B	93	ARG
2	B	127	ASP
2	B	167	ILE
2	B	171	GLU
2	B	174	GLU
2	B	175	ASN

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Mol	Chain	Res	Type
2	B	180	MET
2	B	185	LEU
2	B	269	ASN
2	B	319	GLN
2	B	338	SER
2	B	341	LEU
2	B	350	LYS
2	B	351	ILE
2	B	354	LYS
2	B	357	LEU
2	B	362	LEU
2	B	408	GLN
2	B	415	THR
2	B	447	ARG
2	B	452	ASN
2	B	454	THR
2	B	461	ARG
2	B	466	TRP
2	B	471	CYS
2	B	473	CYS
2	B	483	GLN
2	B	486	CYS
2	B	535	MET
2	B	542	CYS
2	B	596	ASP
2	B	603	THR
2	B	628	GLU
2	B	629	ASN
2	B	643	LYS
2	B	666	ARG
2	B	676	LYS
2	B	678	ILE
2	B	692	ASP
2	B	694	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	152	GLN
1	A	187	GLN
1	A	205	ASN

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Mol	Chain	Res	Type
1	A	332	ASN
1	A	389	GLN
1	A	394	GLN
1	A	456	GLN
1	A	492	ASN
1	A	504	GLN
1	A	580	GLN
1	A	614	GLN
1	A	623	ASN
1	A	633	ASN
1	A	650	GLN
1	A	685	ASN
1	A	704	GLN
1	A	721	ASN
1	A	732	HIS
1	A	784	ASN
1	A	796	HIS
1	A	885	GLN
1	A	927	ASN
1	A	956	GLN
2	B	43	ASN
2	B	240	ASN
2	B	244	HIS
2	B	269	ASN
2	B	301	GLN
2	B	303	ASN
2	B	313	ASN
2	B	342	GLN
2	B	376	ASN
2	B	408	GLN
2	B	450	ASN
2	B	470	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 ⓘ

29 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	A	2044	1,3	14,14,15	0.60	0	15,19,21	1.27	1 (6%)
3	NAG	A	2045	3	14,14,15	0.40	0	15,19,21	1.59	3 (20%)
3	BMA	A	2046	3	11,11,12	0.49	0	14,15,17	2.75	3 (21%)
3	MAN	A	2047	3	11,11,12	0.58	0	14,15,17	1.09	1 (7%)
3	MAN	A	2048	3	11,11,12	0.54	0	14,15,17	1.10	2 (14%)
4	NAG	A	2260	1,4	14,14,15	0.49	0	15,19,21	0.75	0
4	NAG	A	2261	4	14,14,15	0.44	0	15,19,21	0.79	1 (6%)
5	NAG	A	2266	1,5	14,14,15	0.52	0	15,19,21	1.01	0
5	NAG	A	2267	5	14,14,15	0.52	0	15,19,21	0.70	0
5	BMA	A	2268	5	11,11,12	0.24	0	14,15,17	0.71	0
5	MAN	A	2269	5	11,11,12	0.61	0	14,15,17	0.76	1 (7%)
5	MAN	A	2270	5	11,11,12	0.60	0	14,15,17	1.27	1 (7%)
5	MAN	A	2271	5	11,11,12	0.63	0	14,15,17	0.89	1 (7%)
4	NAG	A	2458	1,4	14,14,15	0.56	0	15,19,21	1.22	1 (6%)
4	NAG	A	2459	4	14,14,15	0.48	0	15,19,21	0.74	0
4	NAG	A	2585	1,4	14,14,15	0.62	0	15,19,21	1.42	2 (13%)
4	NAG	A	2586	4	14,14,15	0.67	0	15,19,21	0.81	1 (6%)
4	NAG	A	2821	4	14,14,15	0.66	0	15,19,21	1.43	1 (6%)
4	NAG	A	2822	4	14,14,15	0.67	0	15,19,21	0.91	1 (6%)
4	NAG	A	2943	1,4	14,14,15	0.64	0	15,19,21	1.23	1 (6%)
4	NAG	A	2944	4	14,14,15	0.51	0	15,19,21	1.27	1 (6%)
7	NAG	A	2950	1,7	14,14,15	0.47	0	15,19,21	0.87	1 (6%)
7	NAG	A	2951	7	14,14,15	0.64	0	15,19,21	1.12	2 (13%)
7	BMA	A	2952	7	11,11,12	0.30	0	14,15,17	0.70	0
4	NAG	B	3371	2,4	14,14,15	0.45	0	15,19,21	2.03	2 (13%)
4	NAG	B	3372	4	14,14,15	0.49	0	15,19,21	1.29	1 (6%)
7	NAG	B	3559	2,7	14,14,15	0.49	0	15,19,21	0.80	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	B	3560	7	14,14,15	0.55	0	15,19,21	1.16	1 (6%)
7	BMA	B	3561	7	11,11,12	0.44	0	14,15,17	0.76	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	2044	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2045	3	-	0/6/23/26	0/1/1/1
3	BMA	A	2046	3	-	0/2/19/22	0/1/1/1
3	MAN	A	2047	3	-	0/2/19/22	0/1/1/1
3	MAN	A	2048	3	-	0/2/19/22	0/1/1/1
4	NAG	A	2260	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2261	4	-	0/6/23/26	0/1/1/1
5	NAG	A	2266	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	2267	5	-	0/6/23/26	0/1/1/1
5	BMA	A	2268	5	-	0/2/19/22	0/1/1/1
5	MAN	A	2269	5	-	0/2/19/22	0/1/1/1
5	MAN	A	2270	5	-	0/2/19/22	0/1/1/1
5	MAN	A	2271	5	-	0/2/19/22	0/1/1/1
4	NAG	A	2458	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2459	4	-	2/6/23/26	0/1/1/1
4	NAG	A	2585	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2586	4	-	0/6/23/26	0/1/1/1
4	NAG	A	2821	4	-	0/6/23/26	0/1/1/1
4	NAG	A	2822	4	-	0/6/23/26	0/1/1/1
4	NAG	A	2943	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2944	4	-	0/6/23/26	0/1/1/1
7	NAG	A	2950	1,7	-	0/6/23/26	0/1/1/1
7	NAG	A	2951	7	-	0/6/23/26	0/1/1/1
7	BMA	A	2952	7	-	0/2/19/22	0/1/1/1
4	NAG	B	3371	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	3372	4	-	1/6/23/26	0/1/1/1
7	NAG	B	3559	2,7	-	0/6/23/26	0/1/1/1
7	NAG	B	3560	7	-	0/6/23/26	0/1/1/1
7	BMA	B	3561	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2045	NAG	O3-C3-C2	-2.78	103.62	109.11
5	A	2270	MAN	O4-C4-C3	-2.77	104.09	110.34
3	A	2046	BMA	C2-C3-C4	-2.05	107.56	111.04
7	A	2950	NAG	C4-C3-C2	-2.03	108.08	111.23
7	A	2951	NAG	C3-C4-C5	2.04	113.75	110.20
5	A	2269	MAN	C1-C2-C3	2.17	112.11	109.54
4	A	2261	NAG	C1-O5-C5	2.21	115.05	112.25
3	A	2048	MAN	C1-C2-C3	2.26	112.21	109.54
4	A	2586	NAG	C4-C3-C2	2.30	114.81	111.23
7	B	3559	NAG	C1-O5-C5	2.38	115.27	112.25
4	A	2822	NAG	C4-C3-C2	2.46	115.05	111.23
4	A	2585	NAG	C3-C4-C5	2.61	114.74	110.20
5	A	2271	MAN	C1-C2-C3	2.70	112.73	109.54
3	A	2044	NAG	C1-O5-C5	2.97	116.02	112.25
7	B	3560	NAG	C4-C3-C2	2.99	115.87	111.23
3	A	2048	MAN	C1-O5-C5	3.04	116.11	112.25
4	A	2458	NAG	C4-C3-C2	3.12	116.07	111.23
3	A	2045	NAG	C1-O5-C5	3.16	116.26	112.25
3	A	2045	NAG	O4-C4-C3	3.23	117.61	110.34
3	A	2047	MAN	C1-C2-C3	3.32	113.46	109.54
7	A	2951	NAG	C4-C3-C2	3.43	116.57	111.23
4	A	2943	NAG	C4-C3-C2	3.71	117.00	111.23
4	B	3371	NAG	O4-C4-C5	4.00	119.85	109.24
4	B	3372	NAG	C1-O5-C5	4.06	117.40	112.25
4	A	2585	NAG	C4-C3-C2	4.09	117.59	111.23
4	A	2944	NAG	C1-O5-C5	4.38	117.81	112.25
4	A	2821	NAG	C3-C4-C5	4.52	118.07	110.20
3	A	2046	BMA	C1-C2-C3	5.13	115.61	109.54
4	B	3371	NAG	C1-O5-C5	5.92	119.76	112.25
3	A	2046	BMA	C1-O5-C5	8.25	122.72	112.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	3372	NAG	O7-C7-N2-C2
4	A	2459	NAG	O7-C7-N2-C2
4	A	2459	NAG	C8-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2045	NAG	7	0
3	A	2046	BMA	5	0
3	A	2048	MAN	2	0
4	A	2821	NAG	2	0

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	NAG	A	2524	1	14,14,15	0.42	0	15,19,21	1.05	2 (13%)
6	NAG	A	2805	1	14,14,15	0.56	0	15,19,21	0.77	0
6	NAG	B	3099	2	14,14,15	0.47	0	15,19,21	1.36	1 (6%)
6	NAG	B	3320	2	14,14,15	0.66	0	15,19,21	1.62	4 (26%)
6	NAG	B	3452	2	14,14,15	0.59	0	15,19,21	0.86	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
6	NAG	A	2524	1	-	0/6/23/26	0/1/1/1
6	NAG	A	2805	1	-	0/6/23/26	0/1/1/1
6	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
6	NAG	B	3320	2	-	0/6/23/26	0/1/1/1
6	NAG	B	3452	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2524	NAG	C3-C4-C5	2.12	113.88	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	3320	NAG	C1-O5-C5	2.45	115.36	112.25
6	B	3320	NAG	C3-C4-C5	2.48	114.52	110.20
6	B	3320	NAG	O5-C5-C6	2.66	113.11	107.35
6	B	3452	NAG	C1-O5-C5	2.67	115.64	112.25
6	A	2524	NAG	C1-O5-C5	2.89	115.91	112.25
6	B	3320	NAG	C4-C3-C2	3.88	117.25	111.23
6	B	3099	NAG	C1-O5-C5	3.95	117.26	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	3099	NAG	1	0
6	B	3320	NAG	3	0
6	B	3452	NAG	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	938/967 (97%)	0.62	63 (6%) 21 15	42, 51, 60, 123	0
2	B	695/695 (100%)	0.69	65 (9%) 11 6	44, 51, 61, 94	0
All	All	1633/1662 (98%)	0.65	128 (7%) 16 10	42, 51, 60, 123	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	868	ASP	14.8
1	A	965	TRP	9.4
1	A	967	ILE	8.0
1	A	963	PRO	7.9
2	B	693	ILE	7.7
2	B	509	HIS	7.4
1	A	565	TYR	7.4
2	B	695	VAL	7.2
2	B	694	LEU	6.7
1	A	960	MET	6.3
1	A	961	PRO	6.3
1	A	962	VAL	6.3
1	A	869	ILE	6.2
2	B	510	SER	6.1
1	A	964	VAL	6.0
1	A	966	VAL	5.9
2	B	649	GLY	5.7
2	B	450	ASN	5.5
1	A	957	PRO	4.9
2	B	492	GLN	4.8
2	B	515	LYS	4.8
1	A	838	LEU	4.7
2	B	467	LEU	4.6
1	A	959	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
2	B	507	VAL	4.4
2	B	39	ASP	4.3
2	B	691	PRO	4.2
2	B	52	GLU	4.1
2	B	28	ASP	4.1
2	B	516	ILE	4.0
2	B	444	ASN	3.9
2	B	648	THR	3.9
2	B	479	ARG	3.7
2	B	472	GLU	3.7
2	B	441	ALA	3.7
2	B	460	CYS	3.7
1	A	913	ASN	3.6
1	A	837	SER	3.5
1	A	836	SER	3.4
2	B	692	ASP	3.4
2	B	504	GLY	3.4
1	A	234	ASP	3.3
1	A	527	ILE	3.2
2	B	653	VAL	3.2
2	B	669	TYR	3.2
1	A	571	THR	3.2
2	B	652	ALA	3.2
2	B	464	PRO	3.2
2	B	84	SER	3.1
2	B	1	GLY	3.1
2	B	463	GLY	3.1
1	A	567	THR	3.1
2	B	556	TYR	3.0
2	B	173	LEU	3.0
2	B	500	GLU	3.0
2	B	482	GLN	2.9
1	A	566	ARG	2.9
2	B	167	ILE	2.9
1	A	713	PHE	2.8
1	A	647	ILE	2.8
1	A	617	ILE	2.8
1	A	955	ILE	2.8
2	B	116	TYR	2.8
2	B	33	LEU	2.8
2	B	54	ILE	2.8
2	B	461	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	542	LEU	2.7
1	A	493	PHE	2.7
1	A	649	LEU	2.7
2	B	519	LYS	2.7
1	A	470	VAL	2.7
1	A	509	ARG	2.6
1	A	933	TYR	2.6
1	A	481	ALA	2.6
1	A	663	LEU	2.6
2	B	473	CYS	2.5
2	B	651	ASP	2.5
1	A	956	GLN	2.5
1	A	569	ALA	2.5
2	B	168	SER	2.5
2	B	443	PRO	2.4
2	B	498	ARG	2.4
2	B	476	GLU	2.4
1	A	704	GLN	2.4
2	B	341	LEU	2.4
2	B	497	GLN	2.3
1	A	711	VAL	2.3
1	A	734	VAL	2.3
2	B	524	ASP	2.3
2	B	180	MET	2.3
2	B	2	PRO	2.3
1	A	715	LEU	2.3
1	A	618	TYR	2.3
2	B	491	GLY	2.3
2	B	590	GLN	2.3
2	B	455	PHE	2.3
1	A	490	LYS	2.3
2	B	439	ALA	2.2
1	A	670	PHE	2.2
2	B	454	THR	2.2
1	A	659	ASN	2.2
1	A	629	VAL	2.2
1	A	701	VAL	2.2
1	A	735	ASP	2.2
1	A	130	LEU	2.2
1	A	145	GLN	2.2
1	A	578	LEU	2.2
1	A	532	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	911	LYS	2.1
2	B	412	LYS	2.1
2	B	32	PRO	2.1
1	A	831	LEU	2.1
1	A	613	ASP	2.1
2	B	501	CYS	2.1
2	B	36	PRO	2.1
1	A	491	LEU	2.1
2	B	442	GLU	2.1
1	A	908	PHE	2.1
1	A	167	ASP	2.1
1	A	914	GLN	2.1
1	A	808	LEU	2.1
2	B	181	LYS	2.1
1	A	677	ARG	2.1
1	A	563	LEU	2.1
1	A	693	LEU	2.0
2	B	114	ILE	2.0
2	B	131	ILE	2.0
1	A	801	TYR	2.0

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

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

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
7	NAG	A	2950	14/15	0.91	0.21	0.42	85,89,91,95	0
4	NAG	B	3371	14/15	0.80	0.20	-0.34	71,76,78,80	0
4	NAG	A	2821	14/15	0.81	0.20	-0.34	106,107,108,110	0
4	NAG	A	2585	14/15	0.90	0.19	-0.47	79,84,86,89	0
7	NAG	B	3559	14/15	0.92	0.15	-0.98	69,73,75,78	0
5	NAG	A	2266	14/15	0.94	0.13	-1.89	58,59,62,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	2044	14/15	0.95	0.15	-2.38	61,64,69,75	0
4	NAG	A	2459	14/15	0.86	0.29	-	84,86,86,86	0
4	NAG	A	2261	14/15	0.81	0.28	-	85,87,88,88	0
3	MAN	A	2048	11/12	0.74	0.30	-	104,105,105,105	0
5	MAN	A	2271	11/12	0.80	0.28	-	97,98,98,98	0
7	NAG	B	3560	14/15	0.90	0.17	-	82,84,86,87	0
7	BMA	A	2952	11/12	0.76	0.40	-	105,106,106,107	0
5	BMA	A	2268	11/12	0.93	0.11	-	83,87,89,91	0
5	NAG	A	2267	14/15	0.95	0.13	-	65,69,74,79	0
4	NAG	B	3372	14/15	0.80	0.19	-	83,85,86,86	0
5	MAN	A	2269	11/12	0.82	0.26	-	91,92,93,93	0
4	NAG	A	2944	14/15	0.80	0.35	-	92,93,94,94	0
4	NAG	A	2458	14/15	0.82	0.23	-	72,77,79,81	0
3	BMA	A	2046	11/12	0.81	0.25	-	97,100,102,103	0
7	NAG	A	2951	14/15	0.81	0.36	-	98,101,102,104	0
4	NAG	A	2822	14/15	0.63	0.34	-	110,111,111,111	0
4	NAG	A	2260	14/15	0.86	0.17	-	74,78,80,82	0
3	NAG	A	2045	14/15	0.84	0.24	-	81,85,88,93	0
5	MAN	A	2270	11/12	0.85	0.15	-	93,95,95,97	0
3	MAN	A	2047	11/12	0.82	0.20	-	104,104,104,104	0
4	NAG	A	2586	14/15	0.79	0.35	-	91,93,93,94	0
4	NAG	A	2943	14/15	0.83	0.19	-	80,83,86,89	0
7	BMA	B	3561	11/12	0.90	0.10	-	88,90,90,90	0

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	CA	A	4006	1/1	0.96	0.28	1.56	59,59,59,59	0
8	CA	A	4007	1/1	0.93	0.26	0.74	34,34,34,34	0
8	CA	A	4008	1/1	0.94	0.22	0.37	32,32,32,32	0
8	CA	A	4005	1/1	0.92	0.21	0.31	46,46,46,46	0
8	CA	B	4002	1/1	0.91	0.17	0.10	55,55,55,55	0
6	NAG	B	3320	14/15	0.73	0.22	-0.19	68,71,72,73	0
8	CA	A	4004	1/1	0.92	0.16	-0.72	78,78,78,78	0
6	NAG	A	2805	14/15	0.71	0.34	-	74,79,79,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	B	3099	14/15	0.78	0.37	-	74,79,80,81	0
6	NAG	B	3452	14/15	0.58	0.35	-	86,90,91,91	0
6	NAG	A	2524	14/15	0.66	0.30	-	81,86,87,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.