



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:45 PM GMT

PDB ID : 4G1M  
Title : Re-refinement of alpha V beta 3 structure  
Authors : Springer, T.A.; Mi, L.; Zhu, J.  
Deposited on : 2012-07-10  
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.

---

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

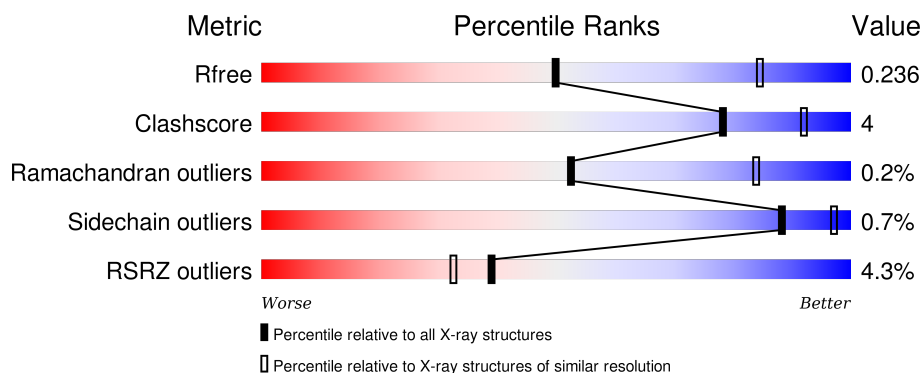
# 1 Overall quality at a glance

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	959	<div> <div>3%</div> <div>86%</div> <div>11%</div> <div>.</div> </div>
2	B	692	<div> <div>6%</div> <div>91%</div> <div>9%</div> </div>

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13132 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	929	Total	C	N	O	S	0	0	2
			7215	4568	1226	1386	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	692	Total	C	N	O	S	0	1	1
			5312	3261	907	1074	70			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		
3	A	5	Total	Ca	0	0
			5	5		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

*Continued on next page...*

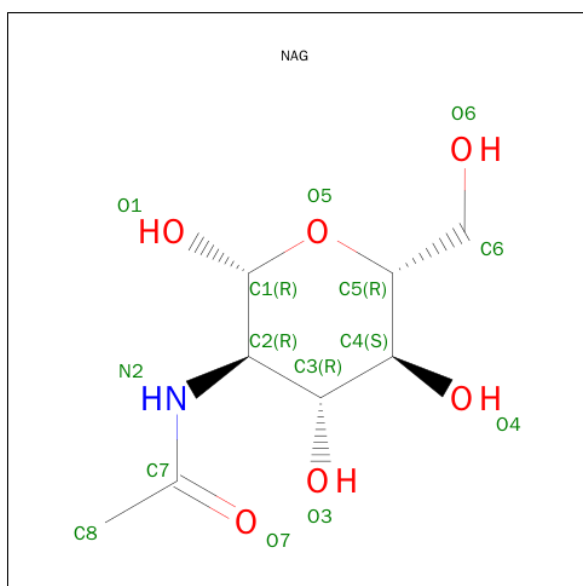
Continued from previous page...

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

- Molecule 6 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

Continued on next page...

*Continued from previous page...*

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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

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

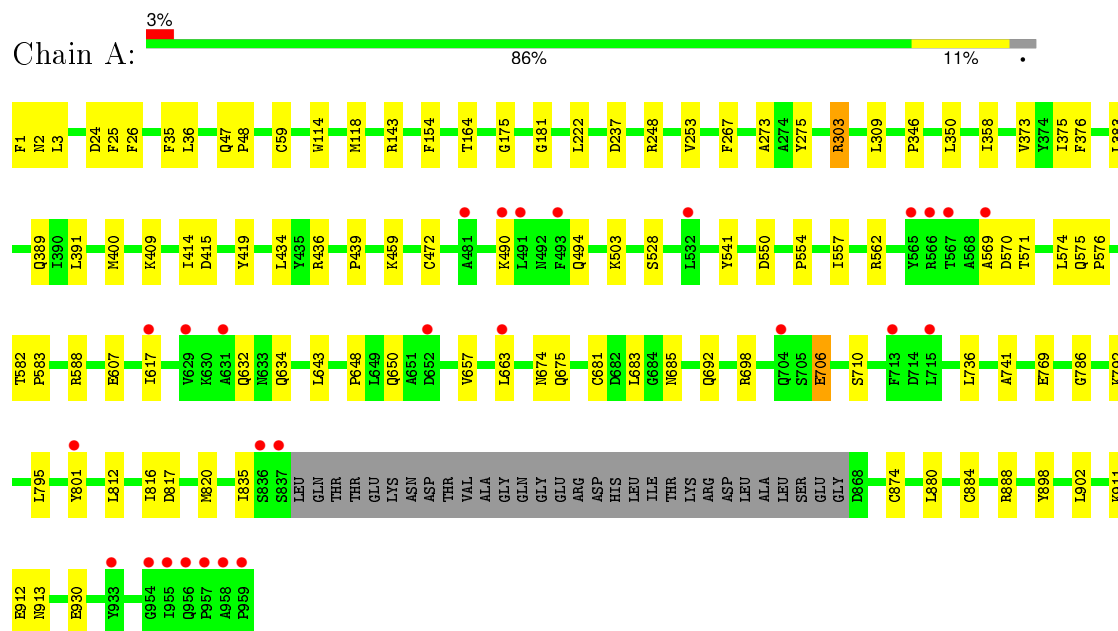
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	66	Total	O	0	0
			66	66		
10	B	40	Total	O	0	0
			40	40		

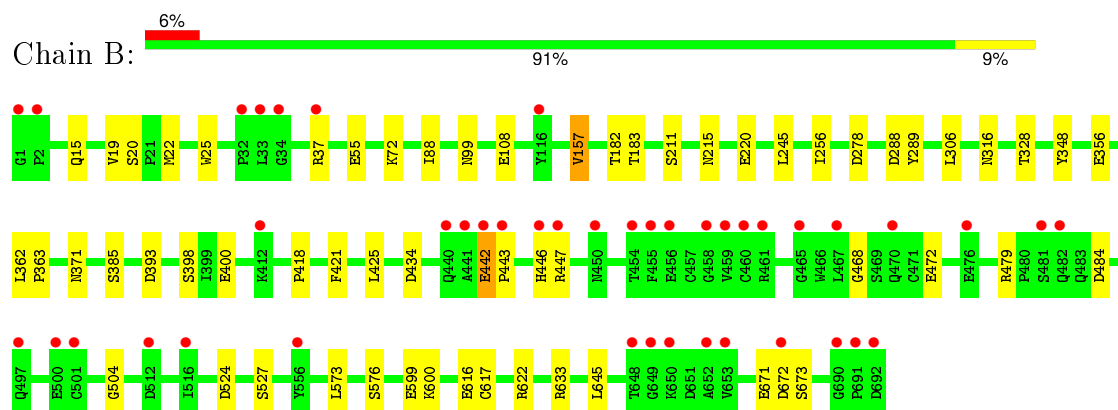
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Integrin alpha-V



#### • Molecule 2: Integrin beta-3



## 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)	65.00 – 2.90 64.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	92.7 (65.00-2.90) 92.7 (64.94-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.16 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.179 , 0.233 0.180 , 0.236	Depositor DCC
$R_{free}$ test set	2924 reflections (4.70%)	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> )	0.30 , 67.2	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	0.95	EDS
Total number of atoms	13132	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	97.0	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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.24	0/7372	0.42	0/9996
2	B	0.23	0/5409	0.41	0/7316
All	All	0.23	0/12781	0.41	0/17312

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	7215	0	7028	60	0
2	B	5312	0	5036	33	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0
4	A	61	0	52	0	0
5	A	196	0	175	0	0
5	B	56	0	50	2	0
6	A	83	0	70	0	0
7	A	28	0	26	0	0
7	B	28	0	26	0	0
8	A	1	0	0	0	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	39	0	34	0	0
10	A	66	0	0	0	0
10	B	40	0	0	0	0
All	All	13132	0	12497	92	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 4.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:484:ASP:HB2	2:B:504:GLY:HA2	1.80	0.64
2:B:616[A]:GLU:HG3	2:B:622:ARG:HG3	1.80	0.63
1:A:741:ALA:H	1:A:786:GLY:HA3	1.66	0.59
1:A:490:LYS:NZ	1:A:528:SER:HB2	2.18	0.58
1:A:1:PHE:HA	1:A:389:GLN:HB2	1.85	0.58
2:B:362:LEU:HD12	2:B:363:PRO:HD2	1.88	0.56
1:A:24:ASP:OD2	1:A:25:PHE:N	2.37	0.56
2:B:15:GLN:O	2:B:19:VAL:HG23	2.08	0.54
1:A:607:GLU:HG3	1:A:632:GLN:HG3	1.91	0.53
2:B:72:LYS:NZ	2:B:108:GLU:HG2	2.24	0.52
1:A:26:PHE:HB3	1:A:35:PHE:HB2	1.90	0.52
1:A:24:ASP:HA	1:A:409:LYS:HG2	1.93	0.51
1:A:181:GLY:HA3	1:A:222:LEU:HB3	1.93	0.51
1:A:494:GLN:HB3	1:A:562:ARG:HB3	1.92	0.51
2:B:88:ILE:HG13	2:B:425:LEU:HD11	1.92	0.50
1:A:472:CYS:HA	1:A:541:TYR:HA	1.93	0.50
1:A:817:ASP:HB2	1:A:898:TYR:HE1	1.76	0.50
2:B:288:ASP:OD1	2:B:289:TYR:N	2.44	0.49
1:A:118:MET:SD	1:A:118:MET:N	2.85	0.49
1:A:648:PRO:HB2	1:A:650:GLN:OE1	2.12	0.49
2:B:316:ASN:HB2	5:B:3320:NAG:H82	1.94	0.49
1:A:911:LYS:O	1:A:913:ASN:N	2.47	0.48
1:A:769:GLU:HG2	1:A:812:LEU:HD11	1.95	0.48
1:A:632:GLN:OE1	1:A:634:GLN:NE2	2.47	0.47
1:A:570:ASP:OD1	1:A:574:LEU:N	2.29	0.47
2:B:182:THR:OG1	2:B:183:THR:N	2.47	0.47
2:B:356:GLU:HG3	2:B:385:SER:HB3	1.97	0.47
1:A:503:LYS:HE3	1:A:550:ASP:OD2	2.14	0.47
1:A:248:ARG:HD2	5:B:3320:NAG:C7	2.45	0.47
1:A:36:LEU:HB2	1:A:59:CYS:HB2	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:569:ALA:HB2	1:A:575:GLN:HG2	1.97	0.47
1:A:801:TYR:HB2	1:A:880:LEU:HB2	1.96	0.46
1:A:795:LEU:HB3	1:A:884:CYS:HB2	1.98	0.46
1:A:414:ILE:HG21	1:A:434:LEU:HD21	1.98	0.46
2:B:157:VAL:O	2:B:220:GLU:HB3	2.17	0.45
2:B:215:ASN:OD1	2:B:215:ASN:N	2.49	0.45
1:A:554:PRO:HG3	1:A:685:ASN:ND2	2.31	0.45
1:A:490:LYS:HZ3	1:A:528:SER:HB2	1.81	0.45
1:A:273:ALA:HA	2:B:256:ILE:HD12	1.98	0.45
2:B:468:GLY:HA3	2:B:472:GLU:HB2	1.98	0.45
1:A:154:PHE:O	1:A:175:GLY:HA3	2.17	0.45
2:B:446:HIS:ND1	2:B:447:ARG:HG3	2.32	0.44
1:A:114:TRP:CE3	1:A:143:ARG:HD2	2.53	0.44
2:B:371:ASN:HB2	2:B:398:SER:HB3	2.00	0.44
1:A:582:THR:HA	1:A:583:PRO:HD3	1.83	0.44
1:A:253:VAL:HB	1:A:267:PHE:HB2	2.00	0.43
1:A:164:THR:HB	1:A:237:ASP:HB2	1.99	0.43
1:A:3:LEU:HD21	1:A:350:LEU:HD11	2.00	0.43
1:A:47:GLN:HA	1:A:48:PRO:HD3	1.83	0.43
2:B:393:ASP:OD1	2:B:633:ARG:NH2	2.52	0.43
1:A:792:LYS:HB2	1:A:930:GLU:HB2	2.01	0.43
1:A:643:LEU:HB2	1:A:683:LEU:HD11	2.01	0.43
1:A:373:VAL:HB	1:A:391:LEU:HB2	2.01	0.43
1:A:816:ILE:HG21	1:A:820:MET:O	2.19	0.43
2:B:306:LEU:HB3	2:B:328:THR:HG23	2.01	0.43
1:A:617:ILE:HB	1:A:736:LEU:HD23	2.01	0.43
1:A:2:ASN:OD1	1:A:2:ASN:N	2.52	0.43
1:A:643:LEU:HB3	1:A:681:CYS:HB2	2.01	0.42
2:B:599:GLU:HG2	2:B:600:LYS:HG3	1.99	0.42
2:B:573:LEU:HB3	2:B:576:SER:O	2.19	0.42
1:A:376:PHE:HB3	1:A:383:LEU:HD11	2.01	0.42
2:B:20:SER:OG	2:B:22:MET:HG2	2.19	0.42
1:A:657:VAL:HG12	1:A:698:ARG:HG3	2.01	0.42
1:A:490:LYS:HZ2	1:A:528:SER:HB2	1.83	0.42
2:B:37:ARG:HD2	2:B:37:ARG:HA	1.92	0.42
1:A:632:GLN:HB3	1:A:692:GLN:HG2	2.02	0.42
2:B:72:LYS:HZ2	2:B:108:GLU:HG2	1.84	0.42
1:A:769:GLU:HG2	1:A:902:LEU:HD11	2.01	0.42
1:A:706:GLU:OE1	1:A:888:ARG:NH2	2.50	0.42
2:B:418:PRO:HG2	2:B:421:PHE:HB2	2.01	0.42
1:A:303:ARG:NH1	1:A:309:LEU:HD21	2.35	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:ASN:HA	2:B:400:GLU:HA	2.03	0.41
2:B:245:LEU:HD11	2:B:348:TYR:HD1	1.84	0.41
1:A:459:LYS:HG2	1:A:459:LYS:H	1.62	0.41
1:A:663:LEU:HA	1:A:663:LEU:HD12	1.86	0.41
2:B:25:TRP:HB3	2:B:55:GLU:HB2	2.01	0.41
1:A:575:GLN:HA	1:A:576:PRO:HD3	1.92	0.41
1:A:346:PRO:HA	1:A:358:ILE:HG13	2.01	0.41
2:B:524:ASP:CG	2:B:527:SER:HB3	2.42	0.41
1:A:674:ASN:HB3	1:A:675:GLN:H	1.76	0.41
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.56	0.41
2:B:671:GLU:O	2:B:673:SER:N	2.49	0.41
2:B:645:LEU:HD23	2:B:645:LEU:HA	1.81	0.41
1:A:375:ILE:HD13	1:A:391:LEU:HD13	2.01	0.41
1:A:557:ILE:N	1:A:588:ARG:O	2.53	0.41
1:A:835:ILE:HD12	1:A:835:ILE:HA	1.99	0.41
2:B:278:ASP:OD1	2:B:278:ASP:N	2.55	0.40
1:A:415:ASP:OD2	1:A:436:ARG:HD2	2.21	0.40
2:B:468:GLY:HA3	2:B:472:GLU:H	1.86	0.40
1:A:911:LYS:HA	1:A:911:LYS:HD2	1.83	0.40
1:A:710:SER:HA	1:A:736:LEU:HG	2.02	0.40
2:B:442:GLU:HA	2:B:443:PRO:HD3	1.93	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	925/959 (96%)	862 (93%)	62 (7%)	1 (0%)	56	87
2	B	691/692 (100%)	630 (91%)	58 (8%)	3 (0%)	39	74
All	All	1616/1651 (98%)	1492 (92%)	120 (7%)	4 (0%)	52	84

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	912	GLU
2	B	672	ASP
2	B	479	ARG
2	B	157	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	785/813 (97%)	779 (99%)	6 (1%)	86	96
2	B	614/614 (100%)	610 (99%)	4 (1%)	88	97
All	All	1399/1427 (98%)	1389 (99%)	10 (1%)	88	97

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

Mol	Chain	Res	Type
1	A	275	TYR
1	A	303	ARG
1	A	400	MET
1	A	571	THR
1	A	706	GLU
1	A	874	CYS
2	B	211	SER
2	B	434	ASP
2	B	442	GLU
2	B	617	CYS

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

Mol	Chain	Res	Type
1	A	632	GLN
1	A	634	GLN
1	A	692	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 ⓘ

33 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	$\# Z  > 2$
4	NAG	A	3044	1,4	14,14,15	0.48	0	15,19,21	1.15	1 (6%)
4	NAG	A	3045	4	14,14,15	0.53	0	15,19,21	0.87	0
4	BMA	A	3046	4	11,11,12	0.61	0	14,15,17	1.15	1 (7%)
4	MAN	A	3047	4	11,11,12	0.59	0	14,15,17	0.77	0
4	MAN	A	3048	4	11,11,12	0.49	0	14,15,17	1.66	2 (14%)
5	NAG	A	3260	1,5	14,14,15	0.57	0	15,19,21	0.60	0
5	NAG	A	3261	5	14,14,15	0.59	0	15,19,21	0.70	0
6	NAG	A	3266	1,6	14,14,15	0.57	0	15,19,21	0.72	0
6	NAG	A	3267	6	14,14,15	0.53	0	15,19,21	0.78	0
6	BMA	A	3268	6	11,11,12	0.70	0	14,15,17	0.61	0
6	MAN	A	3269	6	11,11,12	0.50	0	14,15,17	1.58	3 (21%)
6	MAN	A	3270	6	11,11,12	0.68	0	14,15,17	1.18	1 (7%)
6	MAN	A	3271	6	11,11,12	0.63	0	14,15,17	0.56	0
6	MAN	A	3272	6	11,11,12	0.64	0	14,15,17	1.04	1 (7%)
5	NAG	A	3458	1,5	14,14,15	0.53	0	15,19,21	0.75	0
5	NAG	A	3459	5	14,14,15	0.48	0	15,19,21	0.75	0
5	NAG	A	3524	1,5	14,14,15	0.58	0	15,19,21	0.84	1 (6%)
5	NAG	A	3525	5	14,14,15	0.53	0	15,19,21	1.82	1 (6%)
5	NAG	A	3585	1,5	14,14,15	0.47	0	15,19,21	0.70	0
5	NAG	A	3586	5	14,14,15	0.54	0	15,19,21	0.70	0
5	NAG	A	3821	1,5	14,14,15	0.51	0	15,19,21	0.85	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	3822	5	14,14,15	0.51	0	15,19,21	0.72	0
5	NAG	A	3943	1,5	14,14,15	0.52	0	15,19,21	0.64	0
5	NAG	A	3944	5	14,14,15	0.52	0	15,19,21	0.62	0
5	NAG	A	3950	1,5	14,14,15	0.49	0	15,19,21	0.81	1 (6%)
5	NAG	A	3951	5	14,14,15	0.58	0	15,19,21	0.69	0
5	NAG	B	3320	2,5	14,14,15	0.55	0	15,19,21	0.63	0
5	NAG	B	3321	5	14,14,15	0.50	0	15,19,21	0.57	0
5	NAG	B	3371	2,5	14,14,15	0.51	0	15,19,21	0.88	1 (6%)
5	NAG	B	3372	5	14,14,15	0.55	0	15,19,21	0.94	0
9	NAG	B	3559	9,2	14,14,15	0.48	0	15,19,21	0.75	0
9	NAG	B	3560	9	14,14,15	0.55	0	15,19,21	0.95	0
9	BMA	B	3561	9	11,11,12	0.63	0	14,15,17	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	3044	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	3045	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3046	4	-	0/2/19/22	0/1/1/1
4	MAN	A	3047	4	-	0/2/19/22	0/1/1/1
4	MAN	A	3048	4	-	0/2/19/22	0/1/1/1
5	NAG	A	3260	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	3261	5	-	0/6/23/26	0/1/1/1
6	NAG	A	3266	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	3267	6	-	0/6/23/26	0/1/1/1
6	BMA	A	3268	6	-	0/2/19/22	0/1/1/1
6	MAN	A	3269	6	-	0/2/19/22	0/1/1/1
6	MAN	A	3270	6	-	0/2/19/22	0/1/1/1
6	MAN	A	3271	6	-	0/2/19/22	0/1/1/1
6	MAN	A	3272	6	-	0/2/19/22	0/1/1/1
5	NAG	A	3458	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	3459	5	-	0/6/23/26	0/1/1/1
5	NAG	A	3524	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	3525	5	-	0/6/23/26	0/1/1/1
5	NAG	A	3585	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	3586	5	-	0/6/23/26	0/1/1/1
5	NAG	A	3821	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	3822	5	-	0/6/23/26	0/1/1/1
5	NAG	A	3943	1,5	-	0/6/23/26	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	3944	5	-	0/6/23/26	0/1/1/1
5	NAG	A	3950	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	3951	5	-	0/6/23/26	0/1/1/1
5	NAG	B	3320	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	3321	5	-	0/6/23/26	0/1/1/1
5	NAG	B	3371	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	3372	5	-	0/6/23/26	0/1/1/1
9	NAG	B	3559	9,2	-	0/6/23/26	0/1/1/1
9	NAG	B	3560	9	-	0/6/23/26	0/1/1/1
9	BMA	B	3561	9	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	3269	MAN	C1-C2-C3	-3.67	105.19	109.54
5	A	3950	NAG	C2-N2-C7	-2.26	120.13	123.04
6	A	3270	MAN	O3-C3-C2	-2.24	105.96	110.00
5	B	3371	NAG	C2-N2-C7	-2.10	120.34	123.04
4	A	3048	MAN	C2-C3-C4	-2.06	107.54	111.04
5	A	3524	NAG	C4-C3-C2	2.08	114.46	111.23
6	A	3269	MAN	C1-O5-C5	2.16	114.98	112.25
6	A	3269	MAN	O2-C2-C3	2.23	114.60	110.12
4	A	3046	BMA	C3-C4-C5	2.43	114.43	110.20
4	A	3044	NAG	C1-O5-C5	2.68	115.65	112.25
6	A	3272	MAN	C1-C2-C3	2.72	112.75	109.54
4	A	3048	MAN	C1-O5-C5	5.20	118.85	112.25
5	A	3525	NAG	C1-O5-C5	6.43	120.41	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3320	NAG	2	0

## 5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\# Z  > 2$
7	NAG	A	3674	1	14,14,15	0.50	0	15,19,21	0.81	0
7	NAG	A	3805	1	14,14,15	0.54	0	15,19,21	0.74	0
7	NAG	B	3099	2	14,14,15	0.60	0	15,19,21	0.95	1 (6%)
7	NAG	B	3452	2	14,14,15	0.49	0	15,19,21	1.00	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
7	NAG	A	3674	1	-	0/6/23/26	0/1/1/1
7	NAG	A	3805	1	-	0/6/23/26	0/1/1/1
7	NAG	B	3099	2	-	0/6/23/26	0/1/1/1
7	NAG	B	3452	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3099	NAG	C2-N2-C7	-2.69	119.58	123.04
7	B	3452	NAG	C1-O5-C5	2.30	115.16	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

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	929/959 (96%)	0.28	27 (2%) 55 49	47, 81, 146, 235	0
2	B	692/692 (100%)	0.32	43 (6%) 24 17	50, 93, 187, 244	0
All	All	1621/1651 (98%)	0.30	70 (4%) 39 32	47, 86, 169, 244	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	837	SER	18.7
2	B	649	GLY	8.6
2	B	692	ASP	7.4
2	B	648	THR	7.0
1	A	569	ALA	6.0
1	A	565	TYR	5.9
1	A	704	GLN	5.6
2	B	1	GLY	5.3
2	B	460	CYS	5.2
2	B	447	ARG	5.2
1	A	959	PRO	4.9
2	B	441	ALA	4.8
2	B	467	LEU	4.7
2	B	481	SER	4.7
2	B	461	ARG	4.6
1	A	567	THR	4.6
1	A	836	SER	4.1
2	B	691	PRO	4.1
2	B	446	HIS	4.0
2	B	650	LYS	3.9
2	B	440	GLN	3.7
1	A	957	PRO	3.6
2	B	652	ALA	3.6
1	A	566	ARG	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	958	ALA	3.4
1	A	491	LEU	3.3
2	B	34	GLY	3.2
2	B	455	PHE	3.2
2	B	501	CYS	3.1
1	A	617	ILE	3.0
2	B	33	LEU	3.0
2	B	459	VAL	2.9
2	B	37	ARG	2.9
1	A	490	LYS	2.9
2	B	470	GLN	2.8
2	B	672	ASP	2.8
2	B	2	PRO	2.8
1	A	955	ILE	2.7
2	B	454	THR	2.7
2	B	556	TYR	2.7
2	B	443	PRO	2.7
1	A	532	LEU	2.7
2	B	450	ASN	2.6
1	A	801	TYR	2.6
2	B	32	PRO	2.6
1	A	933	TYR	2.5
1	A	956	GLN	2.5
2	B	442	GLU	2.5
1	A	631	ALA	2.5
2	B	465	GLY	2.5
2	B	456	GLU	2.5
1	A	715	LEU	2.4
2	B	482	GLN	2.4
2	B	476	GLU	2.4
1	A	713	PHE	2.4
2	B	458	GLY	2.4
1	A	663	LEU	2.4
1	A	629	VAL	2.4
2	B	412	LYS	2.3
1	A	652	ASP	2.3
1	A	954	GLY	2.3
2	B	653	VAL	2.2
2	B	500	GLU	2.2
2	B	690	GLY	2.2
2	B	116	TYR	2.1
2	B	516	ILE	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	512	ASP	2.1
1	A	481	ALA	2.1
1	A	493	PHE	2.0
2	B	497	GLN	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
5	NAG	A	3458	14/15	0.87	0.18	1.07	92,109,143,146	0
5	NAG	B	3320	14/15	0.88	0.22	0.56	93,124,141,164	0
5	NAG	B	3371	14/15	0.92	0.20	0.16	101,135,148,152	0
5	NAG	A	3821	14/15	0.88	0.18	-0.32	92,108,114,142	0
4	NAG	A	3044	14/15	0.97	0.18	-0.42	56,68,92,99	0
5	NAG	A	3950	14/15	0.96	0.16	-1.02	80,101,119,123	0
6	NAG	A	3266	14/15	0.97	0.15	-1.13	56,64,79,86	0
5	NAG	A	3585	14/15	0.91	0.11	-1.64	132,146,157,161	0
5	NAG	B	3321	14/15	0.76	0.29	-	140,161,168,170	0
4	MAN	A	3047	11/12	0.77	0.34	-	200,205,209,212	0
6	MAN	A	3271	11/12	0.86	0.23	-	98,126,134,136	0
4	NAG	A	3045	14/15	0.95	0.18	-	97,125,132,151	0
6	MAN	A	3272	11/12	0.87	0.25	-	139,156,169,170	0
5	NAG	A	3261	14/15	0.76	0.18	-	152,165,185,193	0
9	NAG	B	3560	14/15	0.94	0.14	-	103,117,142,151	0
5	NAG	A	3525	14/15	0.69	0.44	-	178,200,206,207	0
5	NAG	A	3951	14/15	0.90	0.30	-	141,156,164,168	0
6	MAN	A	3270	11/12	0.91	0.13	-	134,144,168,172	0
5	NAG	A	3943	14/15	0.89	0.19	-	99,126,141,168	0
9	BMA	B	3561	11/12	0.91	0.10	-	134,139,142,142	0
5	NAG	A	3524	14/15	0.82	0.21	-	158,176,190,201	0
6	NAG	A	3267	14/15	0.97	0.12	-	52,76,96,103	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	B	3372	14/15	0.86	0.15	-	90,151,161,163	0
5	NAG	A	3260	14/15	0.93	0.14	-	97,119,152,155	0
4	MAN	A	3048	11/12	0.84	0.17	-	174,188,196,197	0
5	NAG	A	3822	14/15	0.81	0.34	-	146,159,168,169	0
5	NAG	A	3944	14/15	0.78	0.33	-	149,179,195,197	0
5	NAG	A	3459	14/15	0.90	0.26	-	133,148,154,160	0
9	NAG	B	3559	14/15	0.94	0.15	-	84,99,109,109	0
6	BMA	A	3268	11/12	0.92	0.10	-	111,116,127,141	0
6	MAN	A	3269	11/12	0.93	0.17	-	116,132,152,164	0
5	NAG	A	3586	14/15	0.79	0.24	-	147,170,190,195	0
4	BMA	A	3046	11/12	0.85	0.18	-	170,180,188,189	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
3	CA	A	2005	1/1	0.91	0.20	0.75	80,80,80,80	0
3	CA	A	2007	1/1	0.98	0.21	0.41	78,78,78,78	0
3	CA	A	2008	1/1	0.98	0.16	-0.02	90,90,90,90	0
3	CA	A	2004	1/1	0.93	0.14	-0.54	82,82,82,82	0
3	CA	A	2006	1/1	0.99	0.16	-0.55	80,80,80,80	0
3	CA	B	2001	1/1	0.88	0.16	-0.55	121,121,121,121	0
3	CA	B	2002	1/1	0.96	0.12	-0.87	86,86,86,86	0
7	NAG	B	3099	14/15	0.88	0.21	-	138,164,185,190	0
7	NAG	A	3805	14/15	0.67	0.29	-	158,176,182,183	0
7	NAG	A	3674	14/15	0.63	0.37	-	181,199,203,206	0
8	NA	A	3000	1/1	0.78	0.19	-	127,127,127,127	0
7	NAG	B	3452	14/15	0.68	0.25	-	162,188,190,191	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.