



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:57 AM GMT

PDB ID : 2VDM
Title : RE-REFINEMENT OF INTEGRIN ALPHAIIIBBETA3 HEADPIECE
BOUND TO ANTAGONIST TIROFIBAN
Authors : Springer, T.A.; Zhu, J.; Xiao, T.
Deposited on : 2007-10-10
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
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

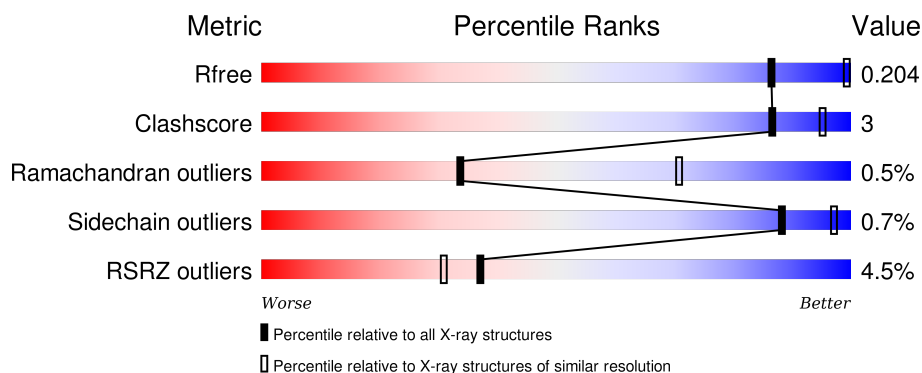
1 Overall quality at a glance

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 ≥ 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	452	<div> <div></div> <div>93% 6%</div> </div>
2	B	461	<div> <div>11%</div> <div>91% 8%</div> </div>
3	H	221	<div> <div></div> <div>90% 8%</div> </div>
4	L	214	<div> <div></div> <div>92% 8%</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
10	MAN	B	3322	X	-	-	-
11	MAN	B	3373	X	-	-	-
5	GOL	B	1463	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 10953 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-IIB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	4	0
			3504	2224	610	662	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	282	GLY	ALA	CONFLICT SEE REMARK 9	UNP P08514

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	456	Total	C	N	O	S	0	2	0
			3545	2209	606	698	32			

- Molecule 3 is a protein called MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	219	Total	C	N	O	S	0	2	0
			1672	1060	269	337	6			

- Molecule 4 is a protein called MONOCLONAL ANTIBODY 10E5 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	214	Total	C	N	O	S	0	1	0
			1642	1022	269	342	9			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

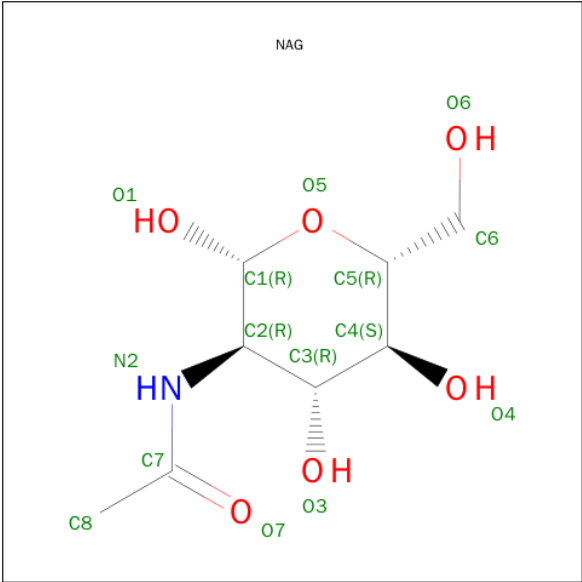


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

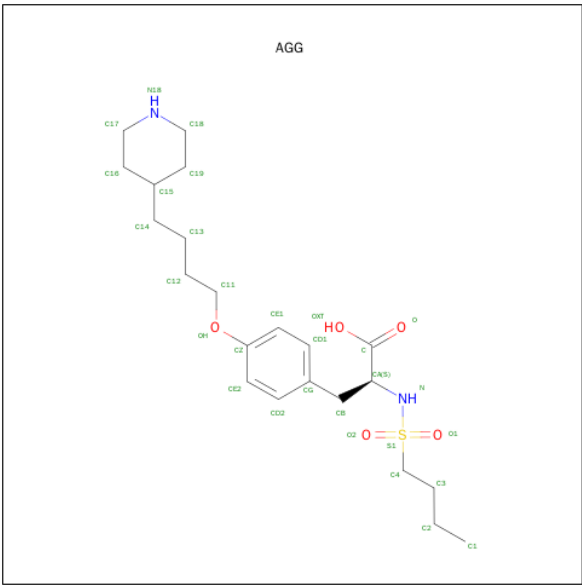
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Ca	0	0
			2	2		
6	A	4	Total	Ca	0	0
			4	4		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is TIROFIBAN (three-letter code: AGG) (formula: C₂₂H₃₆N₂O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			30	22	2	5	1		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 10 is a polymer of unknown type called SUGAR (5-MER).

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

- Molecule 11 is a polymer of unknown type called SUGAR (7-MER).

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

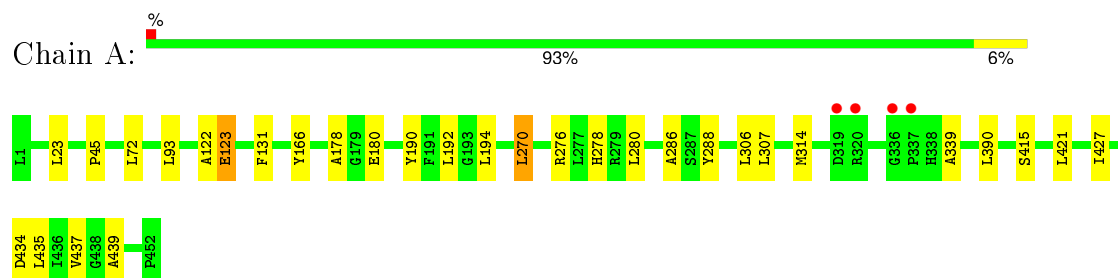
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	139	Total	O	0	0
			139	139		
12	B	75	Total	O	0	0
			75	75		
12	H	73	Total	O	0	0
			73	73		
12	L	68	Total	O	0	0
			68	68		

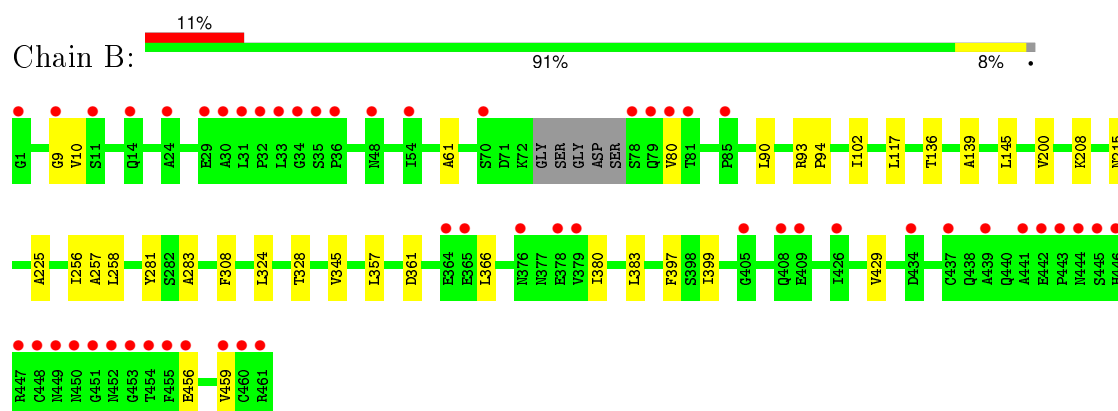
3 Residue-property plots

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.

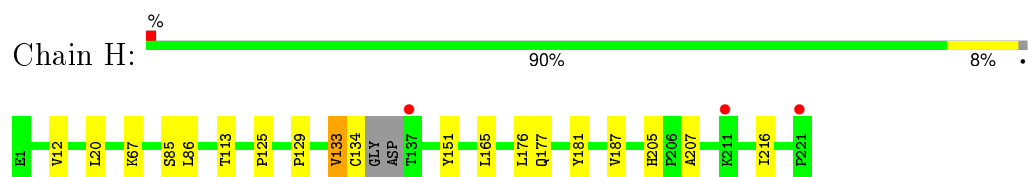
• Molecule 1: INTEGRIN ALPHA-IIB



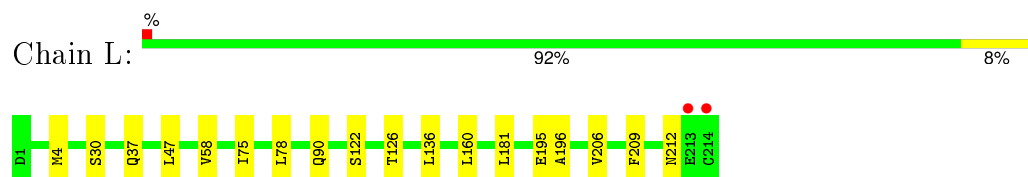
• Molecule 2: INTEGRIN BETA-3



• Molecule 3: MONOCLONAL ANTIBODY 10E5 HEAVY CHAIN



• Molecule 4: MONOCLONAL ANTIBODY 10E5 LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	148.58Å 148.58Å 177.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.23 – 2.90 43.52 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.23-2.90) 91.7 (43.52-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.167 , 0.206 0.174 , 0.204	Depositor DCC
R_{free} test set	2339 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 61.7	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 46595 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10953	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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, 0.375 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: GOL, MG, NAG, AGG, CA, 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	0.31	0/3607	0.50	0/4913
2	B	0.30	0/3608	0.47	0/4890
3	H	0.30	0/1721	0.48	0/2357
4	L	0.30	0/1681	0.49	0/2280
All	All	0.30	0/10617	0.49	0/14440

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
10	B	1	0
11	B	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	B	3322	MAN	C1
11	B	3373	MAN	C1

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	3504	0	3342	18	0
2	B	3545	0	3474	17	0
3	H	1672	0	1629	14	0
4	L	1642	0	1559	12	0
5	A	6	0	8	0	0
5	B	6	0	7	0	0
6	A	4	0	0	0	0
6	B	2	0	0	0	0
7	A	28	0	26	0	0
7	B	14	0	13	0	0
8	B	30	0	35	1	0
9	B	1	0	0	0	0
10	B	61	0	52	0	0
11	B	83	0	70	0	0
12	A	139	0	0	0	0
12	B	75	0	0	0	0
12	H	73	0	0	0	0
12	L	68	0	0	0	0
All	All	10953	0	10215	57	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 3.

All (57) 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:421:LEU:CD2	1:A:437:VAL:HG22	2.28	0.64
1:A:280:LEU:HD11	1:A:306:LEU:HD23	1.84	0.60
2:B:139:ALA:HB1	2:B:200:VAL:HG13	1.82	0.59
2:B:61:ALA:HB2	2:B:90:LEU:HD23	1.85	0.59
1:A:192:LEU:HD13	8:B:1462:AGG:H171	1.85	0.58
1:A:278[A]:HIS:CD2	1:A:339:ALA:HB1	2.42	0.55
2:B:117:LEU:HD22	2:B:225:ALA:HB1	1.89	0.53
3:H:177:GLN:HB3	4:L:160:LEU:HD21	1.91	0.53
3:H:12:VAL:CG2	3:H:86:LEU:HD13	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:136:LEU:N	4:L:136:LEU:HD12	2.26	0.51
3:H:20:LEU:HD22	3:H:113:THR:HG21	1.92	0.51
2:B:145:LEU:HD22	2:B:345:VAL:HG22	1.93	0.50
1:A:270:LEU:HD23	1:A:276[A]:ARG:HA	1.94	0.50
3:H:205:HIS:CE1	3:H:207:ALA:HB3	2.46	0.49
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.95	0.49
4:L:122:SER:O	4:L:126:THR:HG23	2.12	0.49
3:H:165:LEU:HD21	3:H:187:VAL:HG21	1.93	0.49
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.95	0.49
2:B:308:PHE:CE2	2:B:328:THR:HG21	2.47	0.49
1:A:427:ILE:HG22	1:A:434:ASP:OD1	2.13	0.48
4:L:136:LEU:HD23	4:L:196:ALA:CB	2.44	0.48
3:H:165:LEU:CD2	3:H:187:VAL:HG21	2.43	0.47
1:A:306:LEU:HD12	1:A:307:LEU:N	2.28	0.47
4:L:75:ILE:HG21	4:L:78:LEU:HD23	1.95	0.47
1:A:194:LEU:C	1:A:194:LEU:HD12	2.34	0.47
1:A:178:ALA:HB3	1:A:180:GLU:OE1	2.14	0.47
1:A:286:ALA:HA	2:B:256:ILE:HD12	1.97	0.47
1:A:270:LEU:HD23	1:A:276[B]:ARG:HA	1.95	0.47
3:H:176:LEU:HD13	3:H:181:TYR:CE1	2.51	0.46
1:A:421:LEU:HD22	1:A:435:LEU:HD11	1.97	0.46
2:B:456:GLU:O	2:B:459:VAL:HG12	2.16	0.46
4:L:195:GLU:HG2	4:L:206:VAL:HG22	1.97	0.46
4:L:181:LEU:N	4:L:181:LEU:HD23	2.31	0.45
4:L:136:LEU:HD23	4:L:196:ALA:HB2	1.98	0.45
2:B:102:ILE:HG21	2:B:399:ILE:HD11	1.99	0.45
1:A:122:ALA:O	1:A:123:GLU:HB2	2.17	0.44
2:B:281:TYR:CE1	2:B:283:ALA:HB3	2.52	0.44
1:A:314:MET:HE1	2:B:324:LEU:HB3	2.00	0.44
4:L:4:MET:HE2	4:L:90:GLN:HB3	1.99	0.44
2:B:93:ARG:HB2	2:B:94:PRO:HD2	2.00	0.44
3:H:133:VAL:HG11	4:L:209:PHE:HB2	1.99	0.43
3:H:67:LYS:NZ	3:H:85:SER:O	2.51	0.43
2:B:366:LEU:HD11	2:B:429:VAL:HG21	2.00	0.43
4:L:47:LEU:HA	4:L:58:VAL:HG21	2.01	0.42
3:H:176:LEU:HD13	3:H:181:TYR:CZ	2.54	0.42
1:A:390:LEU:HD12	1:A:390:LEU:N	2.34	0.42
3:H:125:PRO:HB3	3:H:151:TYR:HB3	2.02	0.41
1:A:93:LEU:HD13	1:A:131:PHE:CD1	2.55	0.41
2:B:380:ILE:HG21	2:B:383:LEU:HD22	2.03	0.41
2:B:136:THR:HG21	2:B:208:LYS:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:102:ILE:CG2	2:B:399:ILE:HD11	2.51	0.40
3:H:133:VAL:HG12	3:H:134:CYS:H	1.87	0.40
1:A:415:SER:HB2	1:A:439:ALA:HB1	2.03	0.40
2:B:257:ALA:O	2:B:258:LEU:HB2	2.22	0.40
2:B:357:LEU:HD11	2:B:397:PHE:CD2	2.56	0.40
3:H:129:PRO:CB	3:H:216:ILE:HD13	2.51	0.40
1:A:45:PRO:HD3	1:A:72:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	454/452 (100%)	443 (98%)	10 (2%)	1 (0%)	52 84
2	B	454/461 (98%)	423 (93%)	28 (6%)	3 (1%)	26 63
3	H	217/221 (98%)	209 (96%)	8 (4%)	0	100 100
4	L	213/214 (100%)	204 (96%)	7 (3%)	2 (1%)	21 57
All	All	1338/1348 (99%)	1279 (96%)	53 (4%)	6 (0%)	34 74

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
2	B	9	GLY
4	L	212	ASN
2	B	80	VAL
4	L	30	SER
2	B	10	VAL

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	364/360 (101%)	359 (99%)	5 (1%)	74	93
2	B	408/409 (100%)	406 (100%)	2 (0%)	92	98
3	H	191/190 (100%)	190 (100%)	1 (0%)	92	98
4	L	189/188 (100%)	189 (100%)	0	100	100
All	All	1152/1147 (100%)	1144 (99%)	8 (1%)	88	97

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	166	TYR
1	A	190	TYR
1	A	270	LEU
1	A	288	TYR
2	B	215	ASN
2	B	361	ASP
3	H	133	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	444	GLN
2	B	133	ASN
2	B	342	GLN
2	B	428	GLN
3	H	3	GLN

5.3.3 RNA [i](#)

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 ⓘ

12 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
10	NAG	B	3320	10,2	14,14,15	0.62	0	15,19,21	0.87	0
10	NAG	B	3321	10	14,14,15	0.55	0	15,19,21	0.62	0
10	MAN	B	3322	10	11,11,12	0.54	0	14,15,17	0.89	0
10	MAN	B	3323	10	11,11,12	0.52	0	14,15,17	0.70	0
10	MAN	B	3324	10	11,11,12	0.58	0	14,15,17	0.85	1 (7%)
11	NAG	B	3371	11,2	14,14,15	0.53	0	15,19,21	0.55	0
11	NAG	B	3372	11	14,14,15	0.47	0	15,19,21	0.84	0
11	MAN	B	3373	11	11,11,12	0.56	0	14,15,17	0.88	1 (7%)
11	MAN	B	3374	11	11,11,12	0.56	0	14,15,17	0.81	0
11	MAN	B	3375	11	11,11,12	0.57	0	14,15,17	0.95	1 (7%)
11	MAN	B	3376	11	11,11,12	0.56	0	14,15,17	1.23	2 (14%)
11	MAN	B	3377	11	11,11,12	0.55	0	14,15,17	1.02	1 (7%)

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
10	NAG	B	3320	10,2	-	0/6/23/26	0/1/1/1
10	NAG	B	3321	10	-	0/6/23/26	0/1/1/1
10	MAN	B	3322	10	1/1/4/5	0/2/19/22	0/1/1/1
10	MAN	B	3323	10	-	0/2/19/22	0/1/1/1
10	MAN	B	3324	10	-	0/2/19/22	0/1/1/1
11	NAG	B	3371	11,2	-	0/6/23/26	0/1/1/1
11	NAG	B	3372	11	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	MAN	B	3373	11	1/1/4/5	0/2/19/22	0/1/1/1
11	MAN	B	3374	11	-	0/2/19/22	0/1/1/1
11	MAN	B	3375	11	-	0/2/19/22	0/1/1/1
11	MAN	B	3376	11	-	0/2/19/22	0/1/1/1
11	MAN	B	3377	11	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	3373	MAN	O5-C1-C2	-2.04	107.54	110.86
10	B	3324	MAN	C1-C2-C3	2.42	112.40	109.54
11	B	3377	MAN	C1-O5-C5	2.43	115.34	112.25
11	B	3376	MAN	C1-O5-C5	2.72	115.69	112.25
11	B	3375	MAN	C1-O5-C5	2.80	115.80	112.25
11	B	3376	MAN	C1-C2-C3	3.05	113.15	109.54

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	B	3373	MAN	C1
10	B	3322	MAN	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 7 are monoatomic - leaving 6 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
5	GOL	A	1453	-	5,5,5	0.38	0	5,5,5	0.11	0
7	NAG	A	3015	1	14,14,15	0.69	0	15,19,21	1.38	2 (13%)
7	NAG	A	3249	1	14,14,15	0.62	0	15,19,21	0.89	0
8	AGG	B	1462	9	28,31,31	1.26	3 (10%)	30,40,40	1.59	2 (6%)
5	GOL	B	1463	6	5,5,5	0.35	0	5,5,5	0.11	0
7	NAG	B	3099	2	14,14,15	0.44	0	15,19,21	0.61	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
5	GOL	A	1453	-	-	0/4/4/4	0/0/0/0
7	NAG	A	3015	1	-	0/6/23/26	0/1/1/1
7	NAG	A	3249	1	-	0/6/23/26	0/1/1/1
8	AGG	B	1462	9	-	0/22/34/34	0/2/2/2
5	GOL	B	1463	6	-	0/4/4/4	0/0/0/0
7	NAG	B	3099	2	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1462	AGG	C4-S1	2.06	1.83	1.78
8	B	1462	AGG	O1-S1	3.88	1.49	1.43
8	B	1462	AGG	O2-S1	4.21	1.50	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	1462	AGG	O2-S1-O1	-6.31	108.45	119.34
7	A	3015	NAG	C3-C4-C5	2.20	114.02	110.20
8	B	1462	AGG	O2-S1-N	2.68	110.66	107.03
7	A	3015	NAG	C4-C3-C2	4.05	117.53	111.23

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
8	B	1462	AGG	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	A	452/452 (100%)	-0.01	4 (0%) 85 84	39, 51, 59, 67	1 (0%)
2	B	456/461 (98%)	0.56	52 (11%) 7 4	38, 50, 60, 70	1 (0%)
3	H	219/221 (99%)	0.01	3 (1%) 78 76	43, 51, 58, 72	0
4	L	214/214 (100%)	-0.06	2 (0%) 85 84	40, 50, 57, 71	0
All	All	1341/1348 (99%)	0.18	61 (4%) 37 31	38, 51, 59, 72	2 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	444	ASN	7.2
2	B	453	GLY	7.1
2	B	443	PRO	6.1
2	B	454	THR	6.0
2	B	451	GLY	5.7
1	A	337	PRO	5.5
2	B	11	SER	4.9
2	B	452	ASN	4.9
2	B	448	CYS	4.9
3	H	221	PRO	4.7
2	B	460	CYS	4.4
4	L	214	CYS	4.4
3	H	137	THR	3.8
2	B	459	VAL	3.7
2	B	79	GLN	3.6
2	B	449	ASN	3.6
2	B	450	ASN	3.6
2	B	31	LEU	3.4
2	B	33	LEU	3.4
2	B	35	SER	3.4
2	B	441	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	B	1	GLY	3.3
2	B	376	ASN	3.2
2	B	32	PRO	3.2
2	B	9	GLY	3.1
2	B	437	CYS	3.1
2	B	461	ARG	3.1
2	B	455	PHE	3.1
2	B	81	THR	3.0
1	A	320	ARG	3.0
2	B	445	SER	3.0
1	A	319	ASP	2.9
2	B	78	SER	2.9
2	B	34	GLY	2.9
2	B	446	HIS	2.9
2	B	447	ARG	2.8
2	B	408	GLN	2.8
2	B	378	GLU	2.8
2	B	29	GLU	2.8
2	B	456	GLU	2.8
2	B	364	GLU	2.7
2	B	36	PRO	2.7
2	B	48	ASN	2.5
2	B	442	GLU	2.5
2	B	30	ALA	2.4
2	B	85	PRO	2.3
2	B	70	SER	2.3
2	B	14	GLN	2.3
2	B	379	VAL	2.3
2	B	434	ASP	2.3
2	B	439	ALA	2.2
2	B	365	GLU	2.1
2	B	409	GLU	2.1
2	B	24	ALA	2.1
2	B	405	GLY	2.1
2	B	426	ILE	2.1
3	H	211	LYS	2.1
2	B	80	VAL	2.1
1	A	336	GLY	2.0
4	L	213	GLU	2.0
2	B	54	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

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, 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	LLDF	B-factors(Å ²)	Q<0.9
11	NAG	B	3371	14/15	0.89	0.24	0.26	72,75,79,82	0
11	MAN	B	3376	11/12	0.91	0.15	-	68,70,72,72	0
11	MAN	B	3373	11/12	0.87	0.23	-	83,89,90,90	0
11	NAG	B	3372	14/15	0.88	0.26	-	78,86,88,89	0
11	MAN	B	3377	11/12	0.90	0.32	-	87,88,90,92	0
10	MAN	B	3323	11/12	0.88	0.33	-	92,94,97,97	0
10	MAN	B	3322	11/12	0.79	0.39	-	93,98,104,108	0
10	NAG	B	3321	14/15	0.87	0.33	-	73,77,83,89	0
10	NAG	B	3320	14/15	0.97	0.14	-	46,54,61,68	0
11	MAN	B	3374	11/12	0.88	0.23	-	85,86,88,88	11
11	MAN	B	3375	11/12	0.94	0.23	-	74,78,81,85	0
10	MAN	B	3324	11/12	0.82	0.41	-	109,110,111,111	0

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	B	1463	6/6	0.93	0.20	2.64	53,57,59,59	0
5	GOL	A	1453	6/6	0.91	0.22	-0.36	61,62,63,64	0
8	AGG	B	1462	30/30	0.97	0.13	-1.68	39,44,49,51	0
6	CA	A	2005	1/1	0.97	0.05	-3.41	58,58,58,58	0
6	CA	A	2007	1/1	0.98	0.07	-3.72	59,59,59,59	0
6	CA	A	2006	1/1	0.97	0.03	-3.86	68,68,68,68	0
9	MG	B	2001	1/1	0.96	0.04	-4.72	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	CA	A	2004	1/1	0.96	0.05	-4.98	60,60,60,60	0
6	CA	B	2003	1/1	0.98	0.04	-6.33	38,38,38,38	0
7	NAG	B	3099	14/15	0.82	0.40	-	88,93,95,95	0
7	NAG	A	3015	14/15	0.76	0.54	-	90,94,96,96	0
6	CA	B	2002	1/1	0.99	0.04	-	38,38,38,38	0
7	NAG	A	3249	14/15	0.73	0.45	-	82,84,85,85	14

6.5 Other polymers [i](#)

There are no such residues in this entry.