



Full wwPDB X-ray Structure Validation Report ⓘ

May 2, 2016 – 05:17 PM EDT

PDB ID : 5E6U
Title : Structures of leukocyte integrin α Lb2: The α I domain, the headpiece, and the pocket for the internal ligand
Authors : Sen, M.; Springer, T.A.
Deposited on : 2015-10-10
Resolution : 2.50 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
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) : rb-20027457

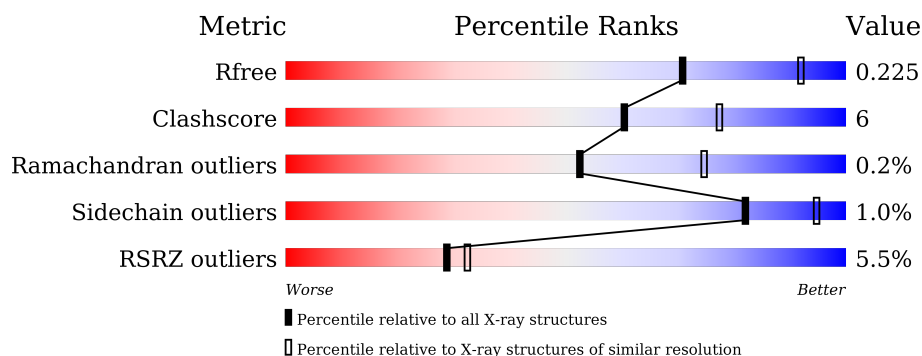
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	795	
2	B	510	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8784 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-L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	583	4525	2862	779	868	16	0	6	0

There are 53 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	189	TRP	ARG	variant	UNP P20701
A	645	ARG	ASN	engineered mutation	UNP P20701
A	701	ARG	ASN	engineered mutation	UNP P20701
A	746	PRO	-	expression tag	UNP P20701
A	747	ALA	-	expression tag	UNP P20701
A	748	ALA	-	expression tag	UNP P20701
A	749	LEU	-	expression tag	UNP P20701
A	750	GLN	-	expression tag	UNP P20701
A	751	THR	-	expression tag	UNP P20701
A	752	LEU	-	expression tag	UNP P20701
A	753	PHE	-	expression tag	UNP P20701
A	754	GLN	-	expression tag	UNP P20701
A	755	GLY	-	expression tag	UNP P20701
A	756	PRO	-	expression tag	UNP P20701
A	757	LEU	-	expression tag	UNP P20701
A	758	GLY	-	expression tag	UNP P20701
A	759	ALA	-	expression tag	UNP P20701
A	760	GLN	-	expression tag	UNP P20701
A	761	GLY	-	expression tag	UNP P20701
A	762	GLU	-	expression tag	UNP P20701
A	763	LYS	-	expression tag	UNP P20701
A	764	GLU	-	expression tag	UNP P20701
A	765	LEU	-	expression tag	UNP P20701
A	766	GLN	-	expression tag	UNP P20701
A	767	ALA	-	expression tag	UNP P20701
A	768	LEU	-	expression tag	UNP P20701
A	769	GLU	-	expression tag	UNP P20701

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Chain	Residue	Modelled	Actual	Comment	Reference
A	770	LYS	-	expression tag	UNP P20701
A	771	GLU	-	expression tag	UNP P20701
A	772	ASN	-	expression tag	UNP P20701
A	773	ALA	-	expression tag	UNP P20701
A	774	GLN	-	expression tag	UNP P20701
A	775	LEU	-	expression tag	UNP P20701
A	776	GLU	-	expression tag	UNP P20701
A	777	TRP	-	expression tag	UNP P20701
A	778	GLU	-	expression tag	UNP P20701
A	779	LEU	-	expression tag	UNP P20701
A	780	GLN	-	expression tag	UNP P20701
A	781	ALA	-	expression tag	UNP P20701
A	782	LEU	-	expression tag	UNP P20701
A	783	GLU	-	expression tag	UNP P20701
A	784	LYS	-	expression tag	UNP P20701
A	785	GLU	-	expression tag	UNP P20701
A	786	LEU	-	expression tag	UNP P20701
A	787	ALA	-	expression tag	UNP P20701
A	788	GLN	-	expression tag	UNP P20701
A	789	HIS	-	expression tag	UNP P20701
A	790	HIS	-	expression tag	UNP P20701
A	791	HIS	-	expression tag	UNP P20701
A	792	HIS	-	expression tag	UNP P20701
A	793	HIS	-	expression tag	UNP P20701
A	794	HIS	-	expression tag	UNP P20701
A	795	ALA	-	expression tag	UNP P20701

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	453	Total	C	N	O	S	0	6	0
			3556	2217	633	677	29			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	232	LYS	ASN	engineered mutation	UNP P05107
B	461	PRO	-	expression tag	UNP P05107
B	462	ALA	-	expression tag	UNP P05107
B	463	ALA	-	expression tag	UNP P05107
B	464	LEU	-	expression tag	UNP P05107
B	465	GLN	-	expression tag	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
B	466	THR	-	expression tag	UNP P05107
B	467	LEU	-	expression tag	UNP P05107
B	468	PHE	-	expression tag	UNP P05107
B	469	GLN	-	expression tag	UNP P05107
B	470	GLY	-	expression tag	UNP P05107
B	471	PRO	-	expression tag	UNP P05107
B	472	LEU	-	expression tag	UNP P05107
B	473	GLY	-	expression tag	UNP P05107
B	474	ALA	-	expression tag	UNP P05107
B	475	GLN	-	expression tag	UNP P05107
B	476	GLY	-	expression tag	UNP P05107
B	477	LYS	-	expression tag	UNP P05107
B	478	LYS	-	expression tag	UNP P05107
B	479	LYS	-	expression tag	UNP P05107
B	480	LEU	-	expression tag	UNP P05107
B	481	GLN	-	expression tag	UNP P05107
B	482	ALA	-	expression tag	UNP P05107
B	483	LEU	-	expression tag	UNP P05107
B	484	LYS	-	expression tag	UNP P05107
B	485	LYS	-	expression tag	UNP P05107
B	486	LYS	-	expression tag	UNP P05107
B	487	ASN	-	expression tag	UNP P05107
B	488	ALA	-	expression tag	UNP P05107
B	489	GLN	-	expression tag	UNP P05107
B	490	LEU	-	expression tag	UNP P05107
B	491	LYS	-	expression tag	UNP P05107
B	492	TRP	-	expression tag	UNP P05107
B	493	LYS	-	expression tag	UNP P05107
B	494	LEU	-	expression tag	UNP P05107
B	495	GLN	-	expression tag	UNP P05107
B	496	ALA	-	expression tag	UNP P05107
B	497	LEU	-	expression tag	UNP P05107
B	498	LYS	-	expression tag	UNP P05107
B	499	LYS	-	expression tag	UNP P05107
B	500	LYS	-	expression tag	UNP P05107
B	501	LEU	-	expression tag	UNP P05107
B	502	ALA	-	expression tag	UNP P05107
B	503	GLN	-	expression tag	UNP P05107
B	504	HIS	-	expression tag	UNP P05107
B	505	HIS	-	expression tag	UNP P05107
B	506	HIS	-	expression tag	UNP P05107
B	507	HIS	-	expression tag	UNP P05107

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Chain	Residue	Modelled	Actual	Comment	Reference
B	508	HIS	-	expression tag	UNP P05107
B	509	HIS	-	expression tag	UNP P05107
B	510	ALA	-	expression tag	UNP P05107

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

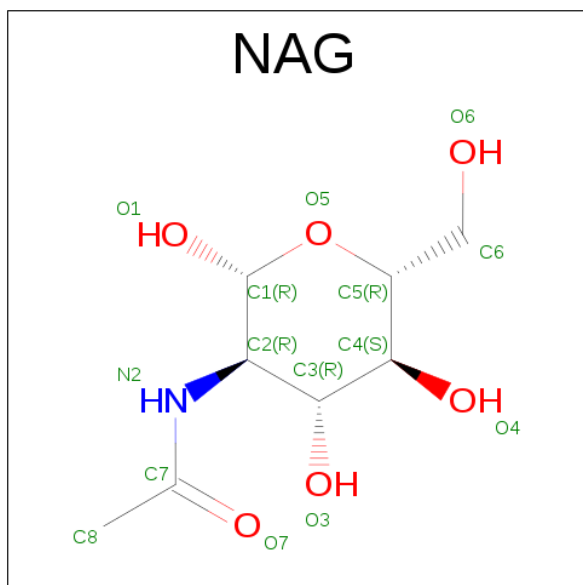
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	403	Total	O	0	0
			403	403		
7	B	251	Total	O	0	0
			251	251		

LEU
LYS
LYS
LYS
LEU
ALA
GLN
HIS
HIS
HIS
HIS
HIS
HIS
ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	154.98Å 154.98Å 115.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.44 – 2.50 46.44 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.44-2.50) 99.5 (46.44-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.179 , 0.226 0.177 , 0.225	Depositor DCC
R_{free} test set	1643 reflections (3.03%)	DCC
Wilson B-factor (Å ²)	40.1	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8784	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.30	0/4630	0.52	0/6264
2	B	0.29	0/3637	0.51	0/4919
All	All	0.30	0/8267	0.52	0/11183

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
2	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	242	ASP	Peptide
2	B	453	GLY	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	4525	0	4414	51	0
2	B	3556	0	3488	40	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	1	0	0	1	0
6	A	14	0	13	0	0
6	B	28	0	26	0	0
7	A	403	0	0	13	0
7	B	251	0	0	11	0
All	All	8784	0	7941	90	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 6.

All (90) 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:173:GLU:OE2	7:B:4001:HOH:O	2.02	0.76
1:A:337[A]:HIS:NE2	1:A:354:ASP:OD1	2.21	0.70
2:B:3:CYS:SG	7:B:4186:HOH:O	2.49	0.69
2:B:361:ASP:HB2	2:B:390:GLN:HB3	1.73	0.69
1:A:4:ASP:OD2	1:A:588:ARG:NH1	2.27	0.68
1:A:123:GLN:NE2	7:A:4005:HOH:O	2.27	0.67
1:A:427:HIS:ND1	7:A:4008:HOH:O	2.28	0.67
1:A:13:PRO:HD2	1:A:16:ALA:HB2	1.78	0.65
1:A:137:ASP:HB2	1:A:238:THR:HA	1.79	0.65
2:B:133[B]:ARG:NH1	7:B:4005:HOH:O	2.29	0.65
1:A:532[A]:ARG:NH2	7:A:4010:HOH:O	2.31	0.62
1:A:27:VAL:HG11	1:A:83:ILE:HD11	1.81	0.62
2:B:293[A]:ASN:OD1	2:B:407:ARG:NH2	2.32	0.62
1:A:25:LEU:HD21	1:A:76:THR:HB	1.82	0.62
2:B:303:ARG:NH1	7:B:4007:HOH:O	2.34	0.60
2:B:243:ASP:HA	2:B:304:MET:HG3	1.83	0.60
1:A:161:LEU:HG	1:A:303:GLN:OE1	2.02	0.59
2:B:194[B]:GLN:NE2	7:B:4003:HOH:O	2.26	0.59
1:A:548:GLN:OE1	7:A:4001:HOH:O	2.17	0.58
2:B:130:ASP:OD1	2:B:133[A]:ARG:NH2	2.35	0.57
2:B:36:ASP:OD2	2:B:447:ILE:HD13	2.03	0.57
2:B:183[B]:ARG:NH2	7:B:4006:HOH:O	2.29	0.56
1:A:554[B]:GLN:NE2	7:A:4019:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:GLN:NE2	2:B:434:ARG:HH21	2.05	0.55
1:A:280:LYS:O	7:A:4002:HOH:O	2.18	0.55
1:A:503:LEU:HD11	1:A:515:ALA:HB2	1.90	0.53
2:B:243:ASP:HB3	2:B:303:ARG:NH2	2.23	0.53
2:B:133[B]:ARG:NH1	2:B:137:GLU:OE2	2.41	0.52
1:A:97:ASN:ND2	1:A:315:GLN:O	2.35	0.52
1:A:410:LEU:HD12	1:A:424:GLN:HB3	1.91	0.52
2:B:76:LEU:HD13	2:B:415:VAL:HG23	1.93	0.51
1:A:390[B]:GLN:OE1	7:A:4003:HOH:O	2.19	0.51
1:A:184:SER:HB2	7:A:4083:HOH:O	2.10	0.50
2:B:74:LYS:O	7:B:4002:HOH:O	2.20	0.49
2:B:430:GLN:HE21	2:B:434:ARG:HH21	1.60	0.48
2:B:231:ARG:HB2	2:B:233:VAL:HG22	1.95	0.48
1:A:182:ASP:HB2	7:A:4083:HOH:O	2.14	0.47
2:B:243:ASP:HA	2:B:304:MET:SD	2.54	0.47
1:A:221:ARG:HD3	1:A:223:GLU:OE2	2.15	0.47
1:A:95:ASP:OD2	1:A:315:GLN:HG2	2.14	0.47
1:A:335[A]:ARG:NH2	1:A:413:GLU:OE1	2.46	0.47
2:B:132:LEU:HD12	2:B:192:SER:HB3	1.96	0.47
2:B:430:GLN:HB2	2:B:443:LEU:HB3	1.97	0.47
1:A:88:PRO:HA	1:A:102:GLY:HA2	1.97	0.47
1:A:344:GLY:HA2	1:A:348:TRP:CD1	2.50	0.47
1:A:128:GLY:O	1:A:165:SER:HB2	2.15	0.47
1:A:430:GLN:HG3	2:B:314:ILE:HD11	1.97	0.47
1:A:371:THR:O	1:A:374:VAL:HG22	2.14	0.46
1:A:506:ILE:HG12	1:A:513:ASP:OD2	2.14	0.46
2:B:194[B]:GLN:NE2	7:B:4017:HOH:O	2.48	0.46
2:B:27:LEU:HD21	2:B:443:LEU:HD21	1.98	0.46
1:A:136:PHE:CZ	1:A:172:GLN:HB2	2.51	0.46
1:A:321:ASN:HB3	7:A:4005:HOH:O	2.15	0.46
2:B:428:ARG:HG2	2:B:429:ASP:H	1.81	0.46
2:B:243:ASP:HA	2:B:304:MET:CG	2.46	0.46
1:A:135:LEU:HD11	1:A:211:ALA:HB1	1.97	0.45
2:B:41:ASP:OD2	2:B:49:ARG:NH1	2.49	0.45
1:A:139:SER:HB2	5:A:2004:CL:CL	2.53	0.45
1:A:156:ASP:HB2	1:A:299:PHE:CZ	2.51	0.45
1:A:506:ILE:O	1:A:587:SER:OG	2.34	0.45
1:A:565:ASP:HB3	7:A:4286:HOH:O	2.17	0.45
1:A:368:GLU:HA	1:A:369:PRO:HA	1.76	0.45
1:A:399:ALA:O	1:A:406:GLY:HA2	2.16	0.45
1:A:258:ILE:HG22	1:A:278:ALA:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:PRO:O	1:A:495:ARG:HA	2.18	0.44
2:B:23:TRP:CZ2	2:B:39:ARG:HD2	2.52	0.44
1:A:572:ALA:H	1:A:587:SER:HB3	1.82	0.44
1:A:296:LYS:HA	1:A:299:PHE:CE2	2.53	0.44
2:B:85:LEU:HB3	7:B:4041:HOH:O	2.17	0.44
1:A:58:VAL:HG21	1:A:111:LEU:HD13	2.00	0.43
1:A:324:LEU:O	1:A:344:GLY:HA3	2.17	0.43
2:B:353:PRO:HG3	2:B:402:GLN:NE2	2.34	0.43
1:A:465:ARG:HA	7:A:4210:HOH:O	2.19	0.43
2:B:84:TYR:HB3	2:B:422:GLN:HB2	2.01	0.42
1:A:185:ASP:O	1:A:195:LEU:HD21	2.20	0.41
1:A:11:PHE:HB2	1:A:582:MET:HE3	2.01	0.41
2:B:407:ARG:NH2	7:B:4024:HOH:O	2.52	0.41
1:A:445:ASP:N	1:A:445:ASP:OD1	2.52	0.41
2:B:111:MET:HG2	2:B:112:ASP:O	2.21	0.41
2:B:204:ILE:HD12	2:B:204:ILE:HA	1.90	0.41
1:A:335[A]:ARG:NH2	7:A:4009:HOH:O	2.30	0.41
2:B:23:TRP:CE3	2:B:40:CYS:HB2	2.55	0.41
1:A:346:LYS:HG3	1:A:370:LEU:HD11	2.02	0.41
1:A:69:TYR:CD1	1:A:89:GLY:HA3	2.57	0.41
2:B:302:SER:HB2	2:B:322:GLU:OE2	2.21	0.41
2:B:431:SER:O	2:B:432:ARG:HB2	2.21	0.40
2:B:434:ARG:C	2:B:436:LEU:H	2.24	0.40
1:A:483:SER:OG	1:A:484:GLU:N	2.55	0.40
2:B:196:GLN:NE2	7:B:4023:HOH:O	2.52	0.40
2:B:354:ASP:OD1	2:B:354:ASP:N	2.36	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	585/795 (74%)	564 (96%)	19 (3%)	2 (0%)	46	68
2	B	455/510 (89%)	436 (96%)	19 (4%)	0	100	100
All	All	1040/1305 (80%)	1000 (96%)	38 (4%)	2 (0%)	52	75

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLY
1	A	316	ASP

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	482/666 (72%)	479 (99%)	3 (1%)	90	97
2	B	398/440 (90%)	392 (98%)	6 (2%)	72	91
All	All	880/1106 (80%)	871 (99%)	9 (1%)	82	95

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	TYR
1	A	434	TYR
1	A	580	SER
2	B	65	THR
2	B	76	LEU
2	B	175	GLU
2	B	207	ASN
2	B	403	SER
2	B	459	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 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	3064	1	14,14,15	0.33	0	15,19,21	0.41	0
6	NAG	B	3094	2	14,14,15	0.50	0	15,19,21	0.40	0
6	NAG	B	3190	2	14,14,15	0.28	0	15,19,21	0.50	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
6	NAG	A	3064	1	-	0/6/23/26	0/1/1/1
6	NAG	B	3094	2	-	0/6/23/26	0/1/1/1
6	NAG	B	3190	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 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	583/795 (73%)	-0.19	14 (2%) 62 66	27, 39, 82, 222	0
2	B	453/510 (88%)	0.17	43 (9%) 10 11	26, 49, 148, 350	0
All	All	1036/1305 (79%)	-0.03	57 (5%) 29 32	26, 44, 114, 350	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	431	SER	10.2
2	B	432	ARG	9.2
2	B	455	ILE	7.2
2	B	454	TYR	7.2
2	B	457	LYS	6.9
1	A	303	GLN	6.5
1	A	302	LEU	6.4
2	B	442	PHE	6.1
2	B	438	HIS	6.0
1	A	306	ILE	5.8
2	B	433	ASP	5.7
1	A	301	GLU	5.3
1	A	315	GLN	5.3
2	B	434	ARG	5.1
1	A	299	PHE	4.9
2	B	450	CYS	4.8
2	B	456	GLY	4.6
1	A	1	TYR	4.5
2	B	451	ASP	4.4
2	B	452	THR	4.3
1	A	304	LYS	4.0
2	B	453	GLY	3.8
2	B	8	VAL	3.7
2	B	440	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	73	GLN	3.5
2	B	430	GLN	3.5
2	B	33	GLY	3.2
2	B	437	CYS	3.1
1	A	305	LYS	3.1
2	B	400	GLN	2.9
2	B	420	LEU	2.9
2	B	35	PRO	2.9
2	B	447	ILE	2.8
1	A	300	THR	2.8
2	B	448	CYS	2.7
2	B	38	ILE	2.7
2	B	423	CYS	2.7
2	B	441	GLY	2.7
2	B	458	ASN	2.6
2	B	399	ILE	2.6
2	B	66	GLN	2.6
2	B	34	ASP	2.5
2	B	449	ARG	2.5
2	B	32	PRO	2.5
2	B	426	ARG	2.4
2	B	421	PRO	2.4
1	A	567	GLU	2.3
2	B	446	GLY	2.3
2	B	396	THR	2.2
1	A	590	VAL	2.2
1	A	72	MET	2.1
2	B	4	THR	2.1
2	B	81	VAL	2.1
1	A	533[A]	HIS	2.1
2	B	36	ASP	2.1
2	B	84	TYR	2.0
2	B	398	CYS	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 ⓘ

There are no carbohydrates in this entry.

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, 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
4	CA	B	2003	1/1	1.00	0.16	1.72	34,34,34,34	0
6	NAG	B	3094	14/15	0.95	0.14	0.53	49,63,71,79	0
4	CA	B	2002	1/1	0.97	0.09	-0.51	56,56,56,56	0
3	MG	B	2001	1/1	0.97	0.06	-1.84	27,27,27,27	1
4	CA	A	2002	1/1	0.93	0.07	-1.95	57,57,57,57	0
5	CL	A	2004	1/1	0.98	0.07	-2.12	61,61,61,61	0
4	CA	A	2003	1/1	0.96	0.06	-2.32	49,49,49,49	0
3	MG	A	2001	1/1	0.96	0.03	-6.01	25,25,25,25	1
6	NAG	B	3190	14/15	0.87	0.23	-	93,101,104,105	0
6	NAG	A	3064	14/15	0.83	0.34	-	114,126,130,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.