



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 20, 2023 – 06:49 PM EDT

PDB ID : 5E6R
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 : 2.90 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

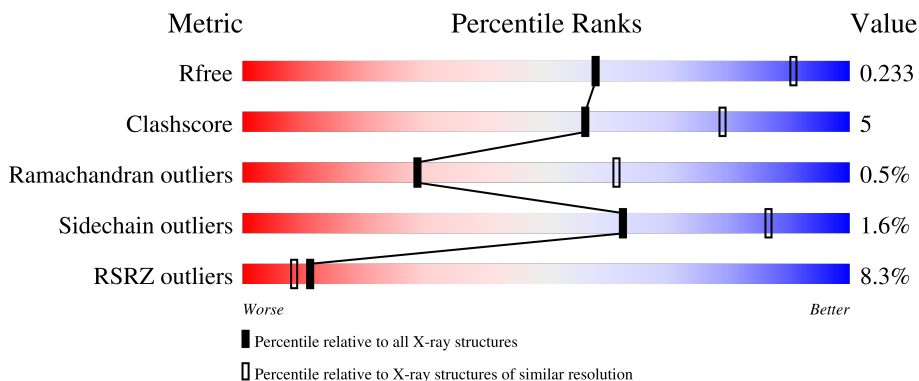
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	795	
2	B	510	

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
5	NAG	B	3028	-	-	-	X

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8264 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	581	4481	2834	768	863	16	0	4	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
			Total	C	N	O	S			
2	B	454	3516	2190	622	675	29	0	2	0

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

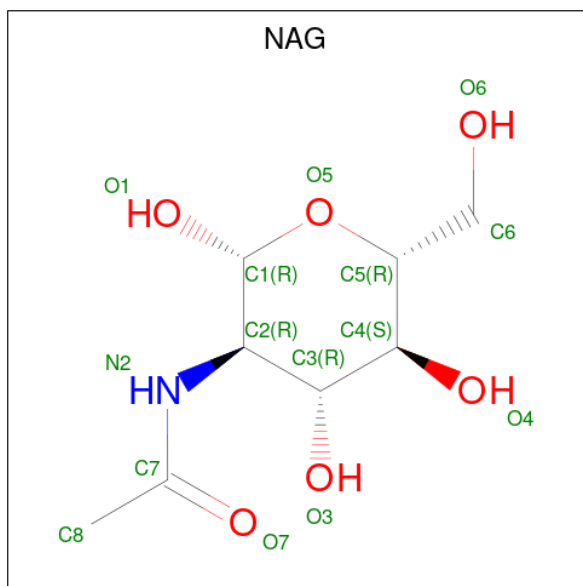
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

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

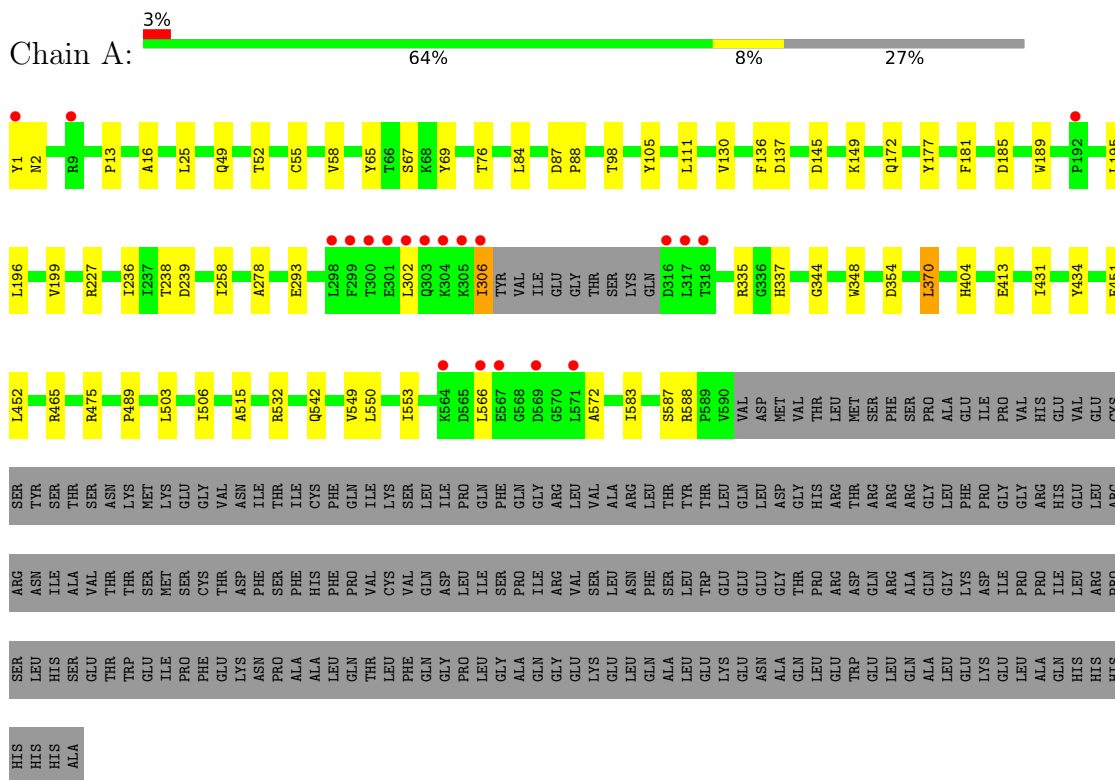
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	140	Total	O	0	0
			140	140		
6	B	66	Total	O	0	0
			66	66		

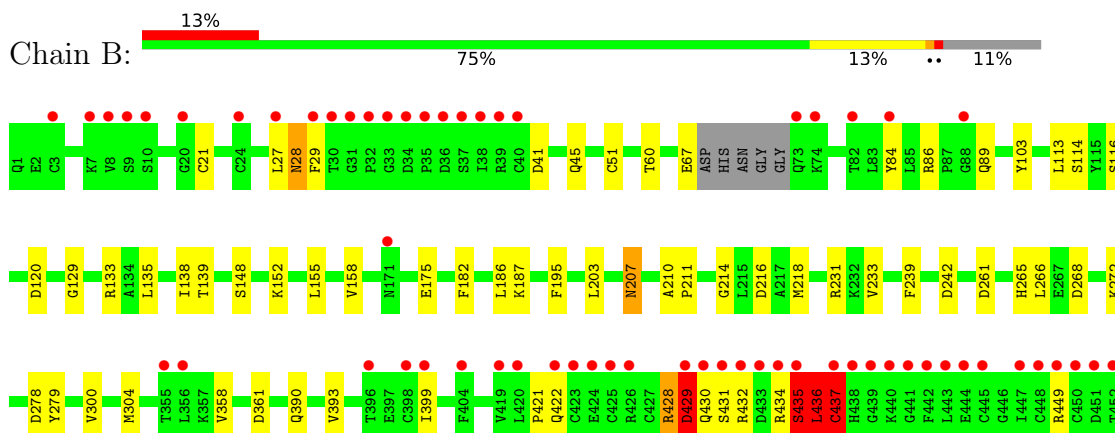
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Integrin alpha-L



• Molecule 2: Integrin beta-2



6453	GLU
7494	PRO
1455	ALA
6456	ALA
K457	LEU
M458	GLN
6459	THR
	LEU
	PHE
	GLN
	GLY
	PRO
	LEU
	GLY
	ALA
	GLN
	GLY
	LYS
	LYS
	LYS
	LEU
	GLN
	ALA
	LEU
	LYS
	LYS
	ASN
	ALA
	GLN
	LEU
	LYS
	TRP
	LYS
	LEU
	GLN
	ALA
	LEU
	LYS
	LYS
	LYS
	LEU
	ALA
	GLN
	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	153.93Å 153.93Å 116.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.24 – 2.90 46.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.24-2.90) 97.7 (46.24-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.91Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.193 , 0.229 0.196 , 0.233	Depositor DCC
R_{free} test set	2737 reflections (8.05%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtrriage
Anisotropy	0.019	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.043 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8264	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/4579	0.50	0/6195
2	B	0.29	0/3582	0.50	0/4851
All	All	0.29	0/8161	0.50	0/11046

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	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	429	ASP	Peptide
2	B	435	SER	Peptide
2	B	436	LEU	Peptide
2	B	437	CYS	Peptide
2	B	458	ASN	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	4481	0	4354	41	0
2	B	3516	0	3403	39	0
3	A	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	14	0	13	0	0
5	B	42	0	39	1	0
6	A	140	0	0	3	0
6	B	66	0	0	3	0
All	All	8264	0	7809	79	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 5.

All (79) 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:114:SER:OG	6:B:4001:HOH:O	2.08	0.70
2:B:138:ILE:HG22	2:B:139:THR:HG23	1.78	0.66
1:A:506:ILE:O	1:A:587:SER:OG	2.14	0.65
1:A:25:LEU:HD21	1:A:76:THR:HB	1.80	0.64
1:A:475:ARG:NH2	6:A:4004:HOH:O	2.30	0.64
2:B:27:LEU:O	2:B:28:ASN:HB2	2.00	0.61
2:B:84:TYR:HB3	2:B:422:GLN:HG3	1.84	0.60
2:B:268:ASP:OD2	2:B:272:LYS:NZ	2.26	0.59
2:B:428:ARG:HG2	2:B:429:ASP:N	2.17	0.59
2:B:361:ASP:HB2	2:B:390:GLN:HB3	1.85	0.58
1:A:67:SER:OG	1:A:87:ASP:OD1	2.21	0.58
1:A:149:LYS:NZ	1:A:293:GLU:OE2	2.37	0.57
1:A:572:ALA:H	1:A:587:SER:HB3	1.68	0.57
1:A:549:VAL:HG11	1:A:583:ILE:HD13	1.87	0.56
1:A:335:ARG:NH1	6:A:4003:HOH:O	2.26	0.56
2:B:152:LYS:NZ	2:B:216:ASP:OD2	2.34	0.56
1:A:58:VAL:HG21	1:A:111:LEU:HD13	1.88	0.56
1:A:550:LEU:HB2	1:A:553:ILE:HB	1.88	0.55
2:B:41:ASP:OD2	2:B:45:GLN:HG2	2.06	0.55
1:A:13:PRO:HD2	1:A:16:ALA:HB2	1.90	0.54
1:A:130:VAL:O	1:A:227:ARG:NH2	2.41	0.54
2:B:231:ARG:HB2	2:B:233:VAL:HG22	1.89	0.53
1:A:337[A]:HIS:NE2	1:A:354:ASP:OD1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:VAL:HG22	2:B:393:VAL:HG22	1.91	0.53
2:B:21:CYS:O	2:B:86:ARG:NH2	2.36	0.52
1:A:65:TYR:HE1	1:A:67:SER:HB3	1.75	0.51
1:A:69:TYR:HD2	1:A:88:PRO:HG2	1.77	0.49
2:B:300:VAL:HB	2:B:304:MET:HB2	1.94	0.49
2:B:214:GLY:HA3	2:B:239:PHE:HZ	1.78	0.49
2:B:431:SER:HA	2:B:434:ARG:CB	2.43	0.48
1:A:503:LEU:HD11	1:A:515:ALA:HB2	1.95	0.48
1:A:532[A]:ARG:NH2	6:A:4018:HOH:O	2.45	0.48
2:B:27:LEU:HD13	5:B:3028:NAG:H81	1.95	0.48
1:A:302:LEU:HD22	1:A:306:ILE:HD11	1.94	0.48
2:B:207:ASN:HD22	2:B:207:ASN:N	2.12	0.48
1:A:451:GLU:HG2	1:A:452:LEU:HG	1.96	0.47
1:A:69:TYR:CD2	1:A:88:PRO:HG2	2.49	0.47
1:A:137:ASP:HB2	1:A:238:THR:HA	1.97	0.47
2:B:103:TYR:HE2	6:B:4028:HOH:O	1.98	0.47
2:B:218:MET:HB3	2:B:218:MET:HE2	1.72	0.47
2:B:186:LEU:HD22	2:B:195:PHE:HA	1.98	0.46
2:B:113:LEU:HG	2:B:148:SER:HB2	1.96	0.46
1:A:344:GLY:HA2	1:A:348:TRP:CD1	2.51	0.46
1:A:185:ASP:O	1:A:189:TRP:HE3	1.98	0.46
1:A:335:ARG:NH2	1:A:413:GLU:OE1	2.49	0.46
1:A:2:ASN:ND2	1:A:588:ARG:O	2.48	0.46
2:B:116:SER:OG	2:B:242:ASP:OD2	2.26	0.46
2:B:210:ALA:HB3	2:B:211:PRO:HD3	1.99	0.45
2:B:449:ARG:HD2	2:B:449:ARG:HA	1.37	0.45
1:A:236:ILE:HB	1:A:258:ILE:HG13	1.99	0.45
1:A:404:HIS:HB3	1:A:431:ILE:HG13	1.98	0.45
2:B:152:LYS:O	2:B:158:VAL:HG13	2.17	0.45
2:B:175:GLU:HB3	2:B:203:LEU:HD22	1.99	0.45
1:A:49:GLN:HB3	1:A:52:THR:OG1	2.18	0.44
1:A:98[B]:THR:OG1	2:B:155:LEU:HD11	2.18	0.44
1:A:465:ARG:HB3	1:A:489:PRO:HA	1.99	0.44
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.88	0.43
1:A:181:PHE:CD1	1:A:195:LEU:HB3	2.54	0.43
2:B:399:ILE:HG22	2:B:421:PRO:HB3	2.01	0.43
1:A:196:LEU:O	1:A:199:VAL:HG12	2.19	0.43
2:B:60:THR:HB	2:B:89:GLN:HE22	1.84	0.43
2:B:135:LEU:HD23	2:B:135:LEU:HA	1.87	0.43
1:A:69:TYR:HB3	1:A:88:PRO:HD2	2.01	0.43
2:B:436:LEU:HD23	2:B:437:CYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:114:SER:HB2	6:B:4018:HOH:O	2.19	0.42
1:A:1:TYR:HA	1:A:542:GLN:HB2	2.02	0.42
1:A:145:ASP:OD2	1:A:149:LYS:HE3	2.20	0.42
2:B:278:ASP:OD1	2:B:279:TYR:N	2.53	0.42
1:A:84:LEU:HD12	1:A:105:TYR:O	2.20	0.41
2:B:29:PHE:CE1	2:B:51:CYS:HB2	2.54	0.41
1:A:13:PRO:HG3	1:A:55:CYS:HB2	2.02	0.41
1:A:136:PHE:CZ	1:A:172:GLN:HB2	2.56	0.41
1:A:258:ILE:HG22	1:A:278:ALA:HB2	2.02	0.41
2:B:129:GLY:O	2:B:133:ARG:HG2	2.21	0.41
2:B:435:SER:OG	2:B:436:LEU:HD12	2.21	0.41
1:A:65:TYR:CE1	1:A:67:SER:HB3	2.55	0.41
2:B:182:PHE:CE2	2:B:266:LEU:HD21	2.56	0.41
2:B:186:LEU:HG	2:B:187:LYS:O	2.20	0.41
2:B:261:ASP:CG	2:B:265:HIS:HE2	2.24	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	581/795 (73%)	558 (96%)	23 (4%)	0	100	100
2	B	452/510 (89%)	420 (93%)	27 (6%)	5 (1%)	14	42
All	All	1033/1305 (79%)	978 (95%)	50 (5%)	5 (0%)	29	61

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	455	ILE
2	B	457	LYS
2	B	432	ARG

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Mol	Chain	Res	Type
2	B	28	ASN
2	B	430	GLN

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	476/666 (72%)	470 (99%)	6 (1%)	69	90
2	B	389/440 (88%)	381 (98%)	8 (2%)	53	81
All	All	865/1106 (78%)	851 (98%)	14 (2%)	62	86

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	TYR
1	A	239	ASP
1	A	306	ILE
1	A	370	LEU
1	A	434	TYR
1	A	566	LEU
2	B	67	GLU
2	B	120	ASP
2	B	207	ASN
2	B	428	ARG
2	B	429	ASP
2	B	435	SER
2	B	436	LEU
2	B	437	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	89	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 5 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
5	NAG	B	3094	2	14,14,15	0.73	1 (7%)	17,19,21	0.54	0
5	NAG	B	3190	2	14,14,15	0.40	0	17,19,21	0.74	1 (5%)
5	NAG	A	3064	1	14,14,15	0.60	1 (7%)	17,19,21	0.47	0
5	NAG	B	3028	2	14,14,15	0.66	1 (7%)	17,19,21	0.48	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	NAG	B	3094	2	-	0/6/23/26	0/1/1/1
5	NAG	B	3190	2	-	4/6/23/26	0/1/1/1
5	NAG	A	3064	1	-	0/6/23/26	0/1/1/1
5	NAG	B	3028	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)
5	B	3094	NAG	O5-C1	-2.42	1.39	1.43
5	B	3028	NAG	O5-C1	-2.34	1.40	1.43
5	A	3064	NAG	O5-C1	-2.05	1.40	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3190	NAG	C1-O5-C5	2.73	115.90	112.19

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	3190	NAG	C8-C7-N2-C2
5	B	3190	NAG	O7-C7-N2-C2
5	B	3190	NAG	C4-C5-C6-O6
5	B	3190	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	3028	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, 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	581/795 (73%)	0.34	20 (3%) 45 40	48, 73, 115, 165	0
2	B	454/510 (89%)	0.77	66 (14%) 2 1	54, 85, 188, 224	0
All	All	1035/1305 (79%)	0.53	86 (8%) 11 8	48, 78, 134, 224	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	452	THR	9.6
2	B	423	CYS	8.1
2	B	433	ASP	7.8
2	B	34	ASP	7.6
2	B	431	SER	6.7
1	A	302	LEU	6.6
2	B	442	PHE	6.5
1	A	304	LYS	6.4
1	A	316	ASP	6.4
2	B	453	GLY	6.4
1	A	318	THR	6.1
2	B	443	LEU	5.6
2	B	451	ASP	5.4
2	B	35	PRO	5.4
2	B	441	GLY	5.1
1	A	303	GLN	5.1
1	A	1	TYR	5.1
1	A	301	GLU	5.0
2	B	448	CYS	5.0
2	B	29	PHE	4.9
1	A	306	ILE	4.9
2	B	33	GLY	4.6
2	B	454	TYR	4.5
2	B	430	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	444	GLU	4.3
2	B	445	CYS	4.2
1	A	298	LEU	4.2
2	B	450	CYS	4.2
1	A	566	LEU	4.0
2	B	447	ILE	3.9
2	B	10	SER	3.7
2	B	435	SER	3.6
2	B	8	VAL	3.6
2	B	31	GLY	3.6
1	A	317	LEU	3.5
2	B	440	LYS	3.5
2	B	399	ILE	3.5
1	A	569	ASP	3.4
2	B	73	GLN	3.4
2	B	74	LYS	3.4
1	A	571	LEU	3.3
2	B	32	PRO	3.2
2	B	27	LEU	3.2
1	A	192	PRO	3.2
2	B	434	ARG	3.1
2	B	36	ASP	3.1
2	B	425	CYS	3.1
1	A	567	GLU	3.0
2	B	419	VAL	3.0
2	B	355	THR	2.9
2	B	437	CYS	2.8
2	B	39	ARG	2.7
2	B	24	CYS	2.7
2	B	82	THR	2.6
2	B	38	ILE	2.6
2	B	9	SER	2.6
1	A	300	THR	2.6
2	B	459	CYS	2.5
2	B	456	GLY	2.5
2	B	30	THR	2.5
2	B	171	ASN	2.5
2	B	40	CYS	2.5
2	B	396	THR	2.5
2	B	449	ARG	2.4
1	A	299	PHE	2.4
2	B	439	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	3	CYS	2.4
2	B	432	ARG	2.4
2	B	20	GLY	2.4
2	B	356	LEU	2.4
1	A	305	LYS	2.3
2	B	398	CYS	2.3
2	B	422	GLN	2.3
2	B	455	ILE	2.3
2	B	438	HIS	2.3
1	A	564	LYS	2.3
2	B	84	TYR	2.2
2	B	420	LEU	2.2
2	B	37	SER	2.2
2	B	88	GLY	2.2
2	B	7	LYS	2.1
2	B	404	PHE	2.1
2	B	429	ASP	2.1
2	B	426	ARG	2.0
2	B	424	GLU	2.0
1	A	9	ARG	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](#)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	NAG	B	3190	14/15	0.73	0.29	135,147,157,163	0
5	NAG	B	3028	14/15	0.74	0.53	169,177,188,188	0
5	NAG	A	3064	14/15	0.78	0.32	128,141,148,149	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	A	2001	1/1	0.81	0.12	86,86,86,86	0
4	CA	A	2002	1/1	0.82	0.08	107,107,107,107	0
5	NAG	B	3094	14/15	0.91	0.20	91,103,115,118	0
4	CA	B	2003	1/1	0.97	0.24	91,91,91,91	0
4	CA	A	2003	1/1	0.98	0.06	95,95,95,95	0
4	CA	B	2002	1/1	0.99	0.07	78,78,78,78	0

6.5 Other polymers [i](#)

There are no such residues in this entry.