



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:00 PM GMT

PDB ID : 1IC1
Title : THE CRYSTAL STRUCTURE FOR THE N-TERMINAL TWO DOMAINS OF ICAM-1
Authors : Casasnovas, J.M.; Stehle, T.; Liu, J.-H.; Wang, J.-H.; Springer, T.A.
Deposited on : 1998-03-09
Resolution : 3.00 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

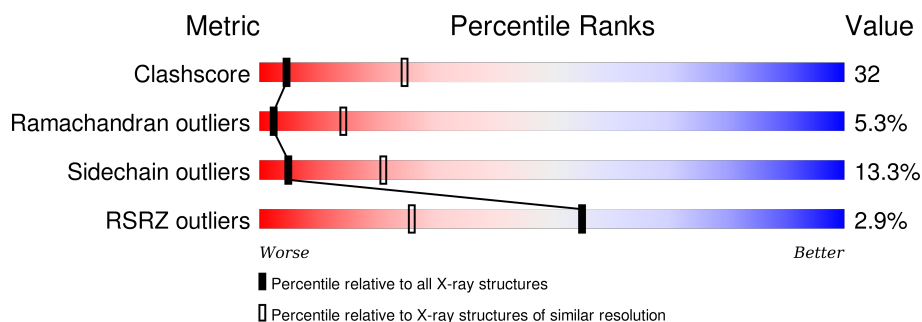
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	190	<div> <div>3%</div> <div>45% 39% 13%</div> </div>
1	B	190	<div> <div>3%</div> <div>42% 45% 10%</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
2	NAG	A	311	-	-	-	X
2	NAG	A	312	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	313	-	-	-	X
2	NAG	B	311	-	-	-	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3131 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 INTERCELLULAR ADHESION MOLECULE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	190	Total	C	N	O	S	0	0	0
			1467	921	256	283	7			
1	B	190	Total	C	N	O	S	0	0	0
			1467	921	256	283	7			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

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

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

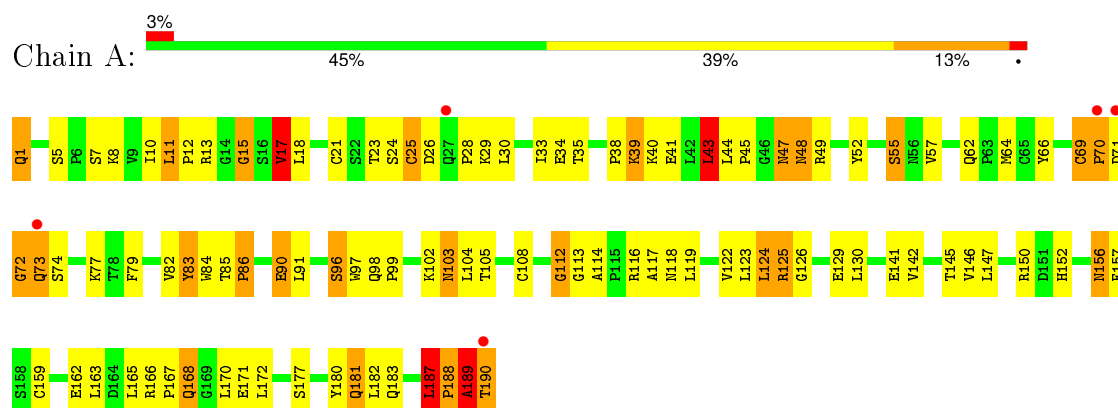
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	29	Total	O	0	0
			29	29		
5	B	14	Total	O	0	0
			14	14		

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 ($\text{RSRZ} > 2$). 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: INTERCELLULAR ADHESION MOLECULE-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	88.00Å 42.20Å 93.00Å 90.00° 109.30° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 20.03 – 2.91	Depositor EDS
% Data completeness (in resolution range)	91.3 (15.00-3.00) 90.5 (20.03-2.91)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 2.93Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.222 , 0.279 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 64.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 13177 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3131	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% 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: NAG, NDG

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	0.90	1/1498 (0.1%)	1.27	20/2043 (1.0%)
1	B	0.72	3/1498 (0.2%)	1.10	13/2043 (0.6%)
All	All	0.82	4/2996 (0.1%)	1.18	33/4086 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	B	0	2
All	All	1	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	ALA	N-CA	7.47	1.61	1.46
1	A	103	ASN	CB-CG	6.92	1.67	1.51
1	B	190	THR	CA-CB	6.20	1.69	1.53
1	B	189	ALA	CA-C	6.07	1.68	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	CYS	C-N-CD	-12.09	94.01	120.60
1	B	188	PRO	N-CA-C	11.57	142.19	112.10
1	A	189	ALA	N-CA-C	10.91	140.44	111.00
1	B	169	GLY	N-CA-C	9.76	137.51	113.10
1	A	187	LEU	C-N-CD	-8.34	102.26	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	SER	N-CA-C	8.15	133.00	111.00
1	A	72	GLY	N-CA-C	-7.58	94.14	113.10
1	A	43	LEU	CA-CB-CG	7.47	132.47	115.30
1	B	43	LEU	CA-CB-CG	-7.22	98.69	115.30
1	B	187	LEU	N-CA-C	6.95	129.75	111.00
1	A	71	ASP	N-CA-CB	6.66	122.59	110.60
1	B	43	LEU	N-CA-C	6.50	128.54	111.00
1	A	187	LEU	CA-CB-CG	6.45	130.13	115.30
1	B	168	GLN	N-CA-C	-5.96	94.90	111.00
1	A	47	ASN	O-C-N	5.80	131.97	122.70
1	A	69	CYS	CB-CA-C	5.71	121.82	110.40
1	A	190	THR	CB-CA-C	5.71	127.01	111.60
1	A	25	CYS	N-CA-C	-5.70	95.61	111.00
1	B	187	LEU	C-N-CD	-5.57	108.36	120.60
1	A	187	LEU	CB-CG-CD2	-5.54	101.57	111.00
1	A	125	ARG	N-CA-C	-5.53	96.08	111.00
1	A	71	ASP	CA-C-N	-5.53	105.15	116.20
1	B	189	ALA	N-CA-CB	-5.33	102.63	110.10
1	A	69	CYS	N-CA-C	-5.32	96.65	111.00
1	B	187	LEU	C-N-CA	5.27	144.12	122.00
1	A	17	VAL	CB-CA-C	-5.24	101.44	111.40
1	B	189	ALA	CA-C-O	-5.20	109.19	120.10
1	B	166	ARG	C-N-CD	-5.16	109.25	120.60
1	A	189	ALA	CA-C-N	-5.15	105.87	117.20
1	A	126	GLY	N-CA-C	-5.14	100.25	113.10
1	B	103	ASN	CB-CG-ND2	5.11	128.97	116.70
1	A	187	LEU	C-N-CA	5.08	143.31	122.00
1	B	169	GLY	CA-C-N	-5.05	106.09	117.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	190	THR	CA

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	TYR	Sidechain
1	B	188	PRO	Mainchain
1	B	189	ALA	Mainchain

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	1467	0	1475	93	0
1	B	1467	0	1475	104	0
2	A	42	0	39	9	0
2	B	28	0	26	6	0
3	A	28	0	25	1	0
3	B	28	0	25	1	0
4	B	28	0	25	1	0
5	A	29	0	0	0	0
5	B	14	0	0	0	0
All	All	3131	0	3090	198	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 32.

All (198) 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:B:103:ASN:HD21	1:B:145:THR:HG21	1.16	1.10
1:B:103:ASN:ND2	1:B:145:THR:HG21	1.78	0.98
1:A:1:GLN:HE21	1:A:1:GLN:HA	1.27	0.98
1:B:186:VAL:O	1:B:187:LEU:HB2	1.67	0.93
1:B:22:SER:HB3	1:B:49:ARG:HG2	1.52	0.92
1:A:187:LEU:HD12	1:A:189:ALA:HB3	1.57	0.85
1:B:161:THR:HG22	1:B:175:ASN:HB2	1.58	0.84
1:B:187:LEU:HB3	1:B:188:PRO:HD3	1.58	0.84
1:B:90:GLU:HG3	1:B:177:SER:HB2	1.60	0.81
1:A:156:ASN:HB3	1:A:181:GLN:HA	1.63	0.79
1:A:187:LEU:CD1	1:A:189:ALA:HB3	2.12	0.79
1:A:188:PRO:O	1:A:189:ALA:HB2	1.82	0.78
1:A:105:THR:HB	1:A:145:THR:HG22	1.65	0.78
1:A:44:LEU:HD12	1:A:45:PRO:HD2	1.65	0.76
1:A:64:MET:HB2	1:A:77:LYS:HG2	1.70	0.74
1:A:1:GLN:NE2	1:A:1:GLN:HA	2.02	0.74
1:A:25:CYS:HB2	1:A:28:PRO:HG3	1.68	0.74
1:B:116:ARG:HD3	1:B:135:ALA:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLN:HG2	1:A:74:SER:H	1.52	0.71
1:B:9:VAL:HB	1:B:80:LEU:HD22	1.73	0.71
1:A:156:ASN:CB	1:A:181:GLN:HA	2.20	0.71
1:A:66:TYR:HB2	1:A:73:GLN:NE2	2.06	0.71
1:B:165:LEU:HD23	1:B:168:GLN:HE21	1.57	0.70
1:A:86:PRO:HA	1:A:112:GLY:O	1.91	0.70
1:A:44:LEU:HD23	1:A:49:ARG:HB3	1.76	0.68
1:A:187:LEU:HD12	1:A:189:ALA:CB	2.24	0.67
1:B:64:MET:CE	1:B:77:LYS:HE2	2.25	0.67
1:B:187:LEU:CB	1:B:188:PRO:HD3	2.22	0.66
1:B:165:LEU:CD2	1:B:168:GLN:HE21	2.08	0.66
1:B:40:LYS:HB2	1:B:53:GLU:HB3	1.79	0.64
1:A:85:THR:HG21	3:A:314:NAG:H5	1.79	0.64
1:B:89:VAL:HG12	1:B:110:VAL:HG13	1.80	0.64
1:A:152:HIS:HB3	1:A:182:LEU:HD23	1.80	0.64
1:A:124:LEU:HD23	1:A:129:GLU:HG2	1.81	0.63
1:B:100:VAL:HG22	1:B:184:THR:HB	1.81	0.63
1:B:58:GLN:HG2	1:B:59:GLU:HG3	1.81	0.62
1:A:113:GLY:H	1:A:116:ARG:HH21	1.46	0.62
1:A:156:ASN:HB2	1:A:180:TYR:O	1.99	0.62
1:A:125:ARG:HB2	1:A:130:LEU:HD11	1.80	0.62
1:B:167:PRO:C	1:B:169:GLY:N	2.48	0.62
1:A:1:GLN:N	1:A:24:SER:OG	2.31	0.62
1:A:72:GLY:O	1:A:73:GLN:HB2	2.00	0.61
1:A:105:THR:HB	1:A:145:THR:CG2	2.30	0.61
1:B:165:LEU:HB2	1:B:171:GLU:O	2.01	0.61
1:A:1:GLN:HE21	1:A:1:GLN:CA	2.07	0.60
1:A:147:LEU:H	2:A:311:NAG:C7	2.14	0.60
1:B:64:MET:HE3	1:B:77:LYS:HE2	1.83	0.60
1:B:23:THR:O	1:B:48:ASN:ND2	2.34	0.60
1:B:66:TYR:HB2	1:B:73:GLN:NE2	2.17	0.60
1:B:103:ASN:ND2	1:B:145:THR:CG2	2.61	0.60
1:A:15:GLY:O	1:A:57:VAL:HG23	2.02	0.59
1:B:145:THR:HG23	2:B:311:NAG:C7	2.33	0.58
1:B:13:ARG:HA	1:B:82:VAL:CG1	2.33	0.58
1:B:145:THR:HG23	2:B:311:NAG:H82	1.85	0.58
1:B:88:ARG:HB3	1:B:111:GLU:HG2	1.85	0.58
1:B:100:VAL:HG23	1:B:185:PHE:O	2.04	0.57
1:B:11:LEU:HD21	1:B:57:VAL:HG21	1.85	0.57
1:B:108:CYS:HB3	1:B:142:VAL:CG1	2.34	0.57
1:B:124:LEU:HD23	1:B:129:GLU:HA	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:CD2	1:A:129:GLU:HG2	2.35	0.56
1:B:161:THR:CG2	1:B:175:ASN:HB2	2.34	0.56
1:B:84:TRP:HE1	1:B:114:ALA:HB3	1.69	0.56
1:B:122:VAL:HG12	1:B:160:ARG:O	2.06	0.56
1:B:90:GLU:HA	1:B:177:SER:HB2	1.87	0.56
1:B:131:LYS:HG3	1:B:132:ARG:H	1.71	0.56
1:A:99:PRO:HD2	1:A:102:LYS:HD2	1.87	0.55
1:B:131:LYS:O	1:B:132:ARG:HB2	2.07	0.55
1:A:98:GLN:HB2	1:A:182:LEU:HD11	1.88	0.55
1:A:146:VAL:HG13	2:A:311:NAG:H82	1.88	0.55
1:A:147:LEU:HB3	2:A:311:NAG:O7	2.08	0.54
1:A:113:GLY:N	1:A:116:ARG:HH21	2.04	0.54
1:A:90:GLU:HA	1:A:177:SER:HB2	1.88	0.54
1:B:186:VAL:O	1:B:187:LEU:CB	2.50	0.54
1:B:2:THR:OG1	1:B:74:SER:HB2	2.06	0.54
1:B:119:LEU:HD23	1:B:135:ALA:CB	2.37	0.54
1:B:44:LEU:HD13	1:B:51:VAL:HG21	1.90	0.54
1:B:124:LEU:HD11	1:B:160:ARG:NH1	2.24	0.53
1:A:41:GLU:HG3	1:A:52:TYR:CE1	2.43	0.53
1:A:157:PHE:CD1	1:A:157:PHE:N	2.76	0.53
1:A:62:GLN:HG2	1:A:79:PHE:CE1	2.43	0.52
1:B:64:MET:HE2	1:B:77:LYS:HE2	1.91	0.52
1:A:187:LEU:HA	1:A:188:PRO:O	2.10	0.52
1:A:167:PRO:HG3	2:A:312:NAG:H82	1.92	0.52
1:A:44:LEU:CD2	1:A:49:ARG:HB3	2.41	0.51
1:A:108:CYS:HB2	1:A:123:LEU:HD21	1.91	0.51
1:B:187:LEU:HB3	1:B:188:PRO:CD	2.35	0.51
1:A:66:TYR:HB2	1:A:73:GLN:HE21	1.76	0.51
1:A:13:ARG:HA	1:A:82:VAL:CG1	2.42	0.50
1:B:11:LEU:HD12	1:B:11:LEU:H	1.77	0.50
1:B:145:THR:HG23	2:B:311:NAG:N2	2.26	0.50
1:B:73:GLN:HG2	1:B:74:SER:N	2.26	0.50
1:B:145:THR:CG2	2:B:311:NAG:N2	2.75	0.50
1:B:8:LYS:HD3	1:B:9:VAL:N	2.26	0.50
1:B:1:GLN:NE2	1:B:25:CYS:HA	2.27	0.49
1:B:11:LEU:HD23	1:B:17:VAL:HB	1.93	0.49
1:B:20:THR:OG1	1:B:51:VAL:HG22	2.12	0.49
1:B:116:ARG:NH1	1:B:137:GLY:O	2.45	0.49
1:B:119:LEU:HD23	1:B:135:ALA:HB3	1.94	0.49
1:A:62:GLN:HG2	1:A:79:PHE:CD1	2.48	0.49
1:A:38:PRO:HB2	1:A:55:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:VAL:HG23	1:B:131:LYS:O	2.13	0.49
1:A:117:ALA:HB3	2:A:312:NAG:O6	2.13	0.49
1:A:96:SER:OG	1:A:183:GLN:HG3	2.13	0.49
1:B:11:LEU:CD2	1:B:17:VAL:HB	2.43	0.48
1:B:190:THR:O	1:B:190:THR:HG23	2.13	0.48
1:B:153:HIS:HB2	1:B:184:THR:OG1	2.12	0.48
1:B:84:TRP:NE1	1:B:114:ALA:HB3	2.27	0.48
1:A:104:LEU:O	1:A:146:VAL:N	2.47	0.48
1:B:124:LEU:O	1:B:157:PHE:HA	2.13	0.48
1:B:96:SER:OG	1:B:183:GLN:HG3	2.14	0.48
4:B:313:NDG:O3	4:B:323:NAG:O5	2.20	0.48
1:B:181:GLN:O	1:B:181:GLN:HG3	2.14	0.48
1:B:165:LEU:HB3	1:B:169:GLY:HA2	1.94	0.48
1:B:73:GLN:HG2	1:B:74:SER:H	1.78	0.48
1:B:125:ARG:HG2	1:B:125:ARG:HH11	1.79	0.48
1:A:165:LEU:HB2	1:A:170:LEU:HB2	1.96	0.48
1:A:150:ARG:HH11	1:A:150:ARG:HG3	1.79	0.48
1:B:63:PRO:O	1:B:77:LYS:HA	2.14	0.47
1:A:97:TRP:HA	1:A:183:GLN:O	2.14	0.47
1:B:15:GLY:O	1:B:57:VAL:HG23	2.14	0.47
1:A:118:ASN:OD1	2:A:312:NAG:O5	2.29	0.47
1:A:40:LYS:O	1:A:52:TYR:HA	2.14	0.47
1:B:123:LEU:HD13	1:B:144:THR:HG22	1.97	0.47
1:B:43:LEU:HD23	1:B:44:LEU:H	1.78	0.47
1:A:35:THR:HG22	1:A:39:LYS:HE2	1.95	0.47
1:B:30:LEU:HD13	1:B:66:TYR:HE1	1.80	0.47
1:B:5:SER:HA	1:B:6:PRO:C	2.35	0.47
1:A:165:LEU:CB	1:A:170:LEU:HB2	2.45	0.47
1:B:99:PRO:HD2	1:B:102:LYS:HD2	1.97	0.47
1:A:147:LEU:HB3	2:A:311:NAG:C7	2.45	0.46
1:B:44:LEU:HA	1:B:45:PRO:HD2	1.52	0.46
1:A:18:LEU:HA	1:A:18:LEU:HD23	1.65	0.46
1:B:9:VAL:HB	1:B:80:LEU:CD2	2.45	0.46
1:A:11:LEU:O	1:A:82:VAL:HA	2.16	0.46
1:A:57:VAL:HG12	1:A:82:VAL:CG2	2.44	0.46
1:B:182:LEU:HD22	1:B:184:THR:HG23	1.98	0.46
1:B:145:THR:HG23	2:B:311:NAG:C8	2.45	0.46
1:A:187:LEU:CG	1:A:189:ALA:HB3	2.45	0.46
1:B:125:ARG:HA	1:B:157:PHE:CD2	2.51	0.46
1:A:96:SER:O	1:A:182:LEU:HD12	2.15	0.46
1:B:19:VAL:HG22	1:B:20:THR:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:THR:HG21	3:B:314:NAG:H5	1.98	0.45
1:B:89:VAL:CG1	1:B:110:VAL:HG13	2.47	0.45
1:A:156:ASN:OD1	2:A:313:NAG:H2	2.16	0.45
1:A:166:ARG:N	1:A:167:PRO:HD2	2.31	0.45
1:B:8:LYS:HG2	1:B:79:PHE:HB2	1.98	0.45
1:B:165:LEU:HA	1:B:165:LEU:HD23	1.62	0.45
1:B:86:PRO:HA	1:B:113:GLY:N	2.32	0.45
1:A:165:LEU:HA	1:A:168:GLN:HG3	1.98	0.45
1:A:147:LEU:HB2	2:A:311:NAG:H2	1.98	0.44
1:B:69:CYS:HB3	1:B:70:PRO:HD2	1.98	0.44
1:A:108:CYS:CB	1:A:123:LEU:HD21	2.47	0.44
1:B:11:LEU:HD22	1:B:15:GLY:O	2.18	0.44
1:B:10:ILE:HG23	1:B:10:ILE:O	2.16	0.44
1:A:12:PRO:HG3	1:A:83:TYR:CZ	2.52	0.44
1:A:108:CYS:HB3	1:A:142:VAL:CG1	2.48	0.44
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.87	0.43
1:B:88:ARG:NH1	1:B:90:GLU:HB3	2.33	0.43
1:B:98:GLN:HA	1:B:99:PRO:HD3	1.76	0.43
1:B:83:TYR:CE2	1:B:170:LEU:HD13	2.53	0.43
1:B:17:VAL:HG22	1:B:18:LEU:N	2.34	0.43
1:A:43:LEU:HG	1:A:43:LEU:O	2.18	0.43
1:A:105:THR:CB	1:A:145:THR:HG22	2.43	0.43
1:B:39:LYS:HA	1:B:53:GLU:O	2.18	0.43
1:B:10:ILE:HA	1:B:81:THR:O	2.17	0.43
1:B:88:ARG:O	1:B:110:VAL:HA	2.18	0.43
1:B:188:PRO:HB3	1:B:189:ALA:H	1.61	0.42
1:B:166:ARG:HA	1:B:167:PRO:HD3	1.81	0.42
1:B:13:ARG:HA	1:B:82:VAL:HG13	2.01	0.42
1:B:43:LEU:HA	1:B:43:LEU:HD23	1.48	0.42
1:A:21:CYS:SG	1:A:33:ILE:HB	2.59	0.42
1:B:66:TYR:C	1:B:66:TYR:CD1	2.92	0.42
1:A:11:LEU:CD2	1:A:17:VAL:HG22	2.50	0.42
1:A:181:GLN:HE21	1:A:181:GLN:HB3	1.56	0.42
1:A:125:ARG:HG3	1:A:157:PHE:CE2	2.55	0.42
1:A:84:TRP:NE1	1:A:114:ALA:HB3	2.34	0.42
1:B:145:THR:HG21	2:B:311:NAG:C1	2.48	0.42
1:A:34:GLU:HG2	1:A:64:MET:CE	2.50	0.42
1:A:28:PRO:HB3	1:A:69:CYS:SG	2.60	0.42
1:A:119:LEU:HD13	1:A:163:LEU:HD13	2.02	0.42
1:A:113:GLY:H	1:A:116:ARG:NH2	2.15	0.42
1:A:124:LEU:HD23	1:A:129:GLU:CG	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:CYS:O	1:A:141:GLU:HA	2.20	0.41
1:A:91:LEU:CD2	1:A:159:CYS:HB2	2.50	0.41
1:A:104:LEU:O	1:A:145:THR:HA	2.20	0.41
1:A:98:GLN:HA	1:A:99:PRO:HD3	1.73	0.41
1:A:23:THR:HG21	1:A:28:PRO:HG2	2.01	0.41
1:A:29:LYS:HE2	1:A:70:PRO:HA	2.03	0.41
1:A:48:ASN:HA	1:A:48:ASN:HD22	1.60	0.41
1:B:11:LEU:N	1:B:11:LEU:HD12	2.36	0.41
1:A:118:ASN:OD1	1:A:168:GLN:NE2	2.54	0.41
1:A:165:LEU:N	1:A:171:GLU:O	2.49	0.41
1:B:4:VAL:HB	1:B:65:CYS:SG	2.60	0.41
1:A:181:GLN:H	1:A:181:GLN:HG2	1.62	0.40
1:A:11:LEU:O	1:A:11:LEU:HD12	2.22	0.40
1:B:86:PRO:HG3	1:B:113:GLY:HA3	2.03	0.40
1:A:162:GLU:HB3	1:A:172:LEU:HD11	2.03	0.40
1:B:116:ARG:NH1	1:B:140:ALA:HB2	2.36	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	188/190 (99%)	166 (88%)	14 (7%)	8 (4%)	3	19
1	B	188/190 (99%)	161 (86%)	15 (8%)	12 (6%)	2	9
All	All	376/380 (99%)	327 (87%)	29 (8%)	20 (5%)	2	14

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	70	PRO
1	A	73	GLN

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Mol	Chain	Res	Type
1	A	188	PRO
1	B	46	GLY
1	B	132	ARG
1	B	167	PRO
1	B	169	GLY
1	B	187	LEU
1	B	188	PRO
1	B	189	ALA
1	A	43	LEU
1	A	112	GLY
1	A	189	ALA
1	B	71	ASP
1	B	138	GLU
1	A	15	GLY
1	B	86	PRO
1	B	100	VAL
1	B	113	GLY
1	A	86	PRO

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	169/169 (100%)	146 (86%)	23 (14%)	5	20
1	B	169/169 (100%)	147 (87%)	22 (13%)	5	22
All	All	338/338 (100%)	293 (87%)	45 (13%)	5	21

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	5	SER
1	A	7	SER
1	A	8	LYS
1	A	10	ILE

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Mol	Chain	Res	Type
1	A	11	LEU
1	A	17	VAL
1	A	26	ASP
1	A	30	LEU
1	A	39	LYS
1	A	43	LEU
1	A	47	ASN
1	A	48	ASN
1	A	90	GLU
1	A	96	SER
1	A	103	ASN
1	A	122	VAL
1	A	124	LEU
1	A	156	ASN
1	A	168	GLN
1	A	181	GLN
1	A	187	LEU
1	A	190	THR
1	B	11	LEU
1	B	22	SER
1	B	30	LEU
1	B	37	LEU
1	B	42	LEU
1	B	44	LEU
1	B	53	GLU
1	B	88	ARG
1	B	90	GLU
1	B	94	LEU
1	B	107	ARG
1	B	118	ASN
1	B	125	ARG
1	B	132	ARG
1	B	143	THR
1	B	145	THR
1	B	164	ASP
1	B	167	PRO
1	B	170	LEU
1	B	171	GLU
1	B	187	LEU
1	B	188	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	48	ASN
1	A	73	GLN
1	A	153	HIS
1	A	181	GLN
1	A	183	GLN
1	B	1	GLN
1	B	48	ASN
1	B	73	GLN
1	B	168	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 ⓘ

6 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	314	1,3	14,14,15	0.51	0	15,19,21	1.01	1 (6%)
3	NAG	A	324	3	14,14,15	0.68	0	15,19,21	1.19	1 (6%)
4	NDG	B	313	1,4	14,14,15	0.76	1 (7%)	15,19,21	1.35	2 (13%)
3	NAG	B	314	1,3	14,14,15	1.08	1 (7%)	15,19,21	1.43	2 (13%)
4	NAG	B	323	4	14,14,15	0.46	0	15,19,21	1.22	2 (13%)
3	NAG	B	324	3	14,14,15	1.19	1 (7%)	15,19,21	0.78	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	314	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	324	3	-	0/6/23/26	0/1/1/1
4	NDG	B	313	1,4	-	0/6/23/26	0/1/1/1
3	NAG	B	314	1,3	-	0/6/23/26	0/1/1/1
4	NAG	B	323	4	-	0/6/23/26	0/1/1/1
3	NAG	B	324	3	-	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)
4	B	313	NDG	C4-C3	2.04	1.57	1.52
3	B	314	NAG	O4-C4	3.03	1.50	1.43
3	B	324	NAG	C1-C2	3.03	1.56	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	324	NAG	C2-N2-C7	-3.59	118.43	123.04
4	B	313	NDG	C2-N2-C7	-2.35	120.02	123.04
3	A	314	NAG	C2-N2-C7	-2.24	120.16	123.04
4	B	313	NDG	C4-C3-C2	-2.23	107.76	111.23
4	B	323	NAG	C4-C3-C2	-2.08	108.00	111.23
3	B	314	NAG	O4-C4-C5	2.57	116.05	109.24
3	B	314	NAG	O4-C4-C3	3.05	117.20	110.34
4	B	323	NAG	C1-O5-C5	3.39	116.55	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	314	NAG	1	0
4	B	313	NDG	1	0
3	B	314	NAG	1	0
4	B	323	NAG	1	0

5.6 Ligand geometry

5 ligands 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$
2	NAG	A	311	1	14,14,15	3.61	2 (14%)	15,19,21	2.22	4 (26%)
2	NAG	A	312	1	14,14,15	0.68	0	15,19,21	1.31	3 (20%)
2	NAG	A	313	1	14,14,15	0.68	0	15,19,21	0.94	0
2	NAG	B	311	1	14,14,15	2.98	3 (21%)	15,19,21	1.70	3 (20%)
2	NAG	B	312	1	14,14,15	1.29	2 (14%)	15,19,21	1.98	5 (33%)

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
2	NAG	A	311	1	-	0/6/23/26	0/1/1/1
2	NAG	A	312	1	-	0/6/23/26	0/1/1/1
2	NAG	A	313	1	-	0/6/23/26	0/1/1/1
2	NAG	B	311	1	-	0/6/23/26	0/1/1/1
2	NAG	B	312	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	312	NAG	O5-C5	-3.35	1.36	1.43
2	B	311	NAG	O5-C5	2.40	1.48	1.43
2	B	312	NAG	C1-C2	2.40	1.55	1.52
2	B	311	NAG	C3-C2	2.72	1.58	1.52
2	A	311	NAG	C3-C2	4.37	1.62	1.52
2	B	311	NAG	C1-C2	10.15	1.66	1.52
2	A	311	NAG	C1-C2	12.33	1.69	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	312	NAG	C2-N2-C7	-4.26	117.57	123.04
2	A	311	NAG	C3-C2-N2	-3.52	102.14	110.56
2	B	311	NAG	C3-C2-N2	-3.17	102.97	110.56
2	A	312	NAG	C3-C4-C5	-2.73	105.43	110.20
2	B	312	NAG	O7-C7-C8	-2.70	117.10	122.06
2	A	311	NAG	O5-C5-C6	-2.31	102.34	107.35
2	A	311	NAG	O7-C7-C8	-2.14	118.14	122.06
2	B	311	NAG	O5-C5-C6	-2.02	102.98	107.35
2	A	312	NAG	C2-N2-C7	-2.01	120.45	123.04
2	B	312	NAG	C4-C3-C2	2.20	114.66	111.23
2	B	312	NAG	C1-O5-C5	2.49	115.41	112.25
2	A	312	NAG	C6-C5-C4	2.69	119.64	113.02
2	B	312	NAG	C8-C7-N2	3.35	122.52	116.11
2	B	311	NAG	C1-O5-C5	4.61	118.10	112.25
2	A	311	NAG	C1-O5-C5	6.34	120.29	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	311	NAG	5	0
2	A	312	NAG	3	0
2	A	313	NAG	1	0
2	B	311	NAG	6	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	190/190 (100%)	-0.56	5 (2%) 59 29	7, 25, 69, 93	0
1	B	190/190 (100%)	-0.02	6 (3%) 51 23	33, 68, 95, 111	0
All	All	380/380 (100%)	-0.29	11 (2%) 55 26	7, 48, 91, 111	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	THR	5.4
1	A	71	ASP	3.8
1	B	58	GLN	3.5
1	A	70	PRO	2.7
1	A	190	THR	2.7
1	B	166	ARG	2.4
1	B	149	ARG	2.4
1	B	136	VAL	2.3
1	B	26	ASP	2.3
1	A	27	GLN	2.3
1	A	73	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, 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
3	NAG	B	314	14/15	0.90	0.20	-0.40	61,65,68,74	0
3	NAG	A	314	14/15	0.93	0.14	-0.94	29,34,40,42	0
4	NDG	B	313	14/15	0.88	0.33	-	73,77,79,83	0
3	NAG	B	324	14/15	0.67	0.70	-	76,79,83,84	0
3	NAG	A	324	14/15	0.89	0.23	-	33,38,44,50	0
4	NAG	B	323	14/15	0.79	0.37	-	85,86,87,89	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, 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
2	NAG	B	311	14/15	0.42	0.89	15.05	78,86,94,98	0
2	NAG	A	311	14/15	0.80	0.66	11.37	74,82,88,90	0
2	NAG	A	312	14/15	0.88	0.25	5.36	50,52,57,58	0
2	NAG	A	313	14/15	0.85	0.27	2.23	48,51,53,57	0
2	NAG	B	312	14/15	0.78	0.29	-	105,107,109,109	0

6.5 Other polymers [i](#)

There are no such residues in this entry.