



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 01:05 AM GMT

PDB ID : 1LX5  
Title : Crystal Structure of the BMP7/ActRII Extracellular Domain Complex  
Authors : Greenwald, J.; Groppe, J.; Kwiatkowski, W.; Choe, S.  
Deposited on : 2002-06-04  
Resolution : 3.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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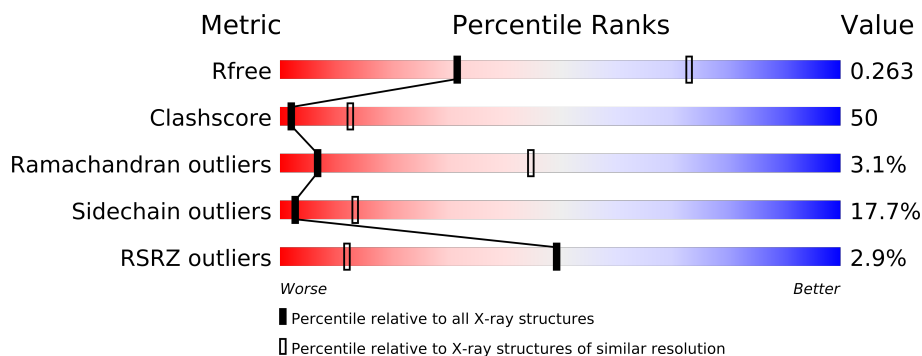
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 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))
$R_{free}$	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	139	
2	B	102	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 1695 atoms, of which 0 are hydrogen and 0 are deuterium.

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 bone morphogenetic protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	30	0	0
			827	530	139	149	9			

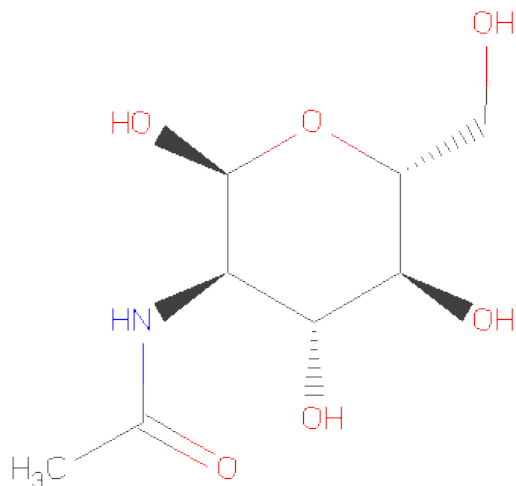
- Molecule 2 is a protein called Activin Type II Receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	94	Total	C	N	O	S	27	0	0
			768	477	131	149	11			

- Molecule 3 is a polymer of unknown type called SUGAR (NAG-NAG-MAN-MAN-MAN-MAN-MAN-MAN).

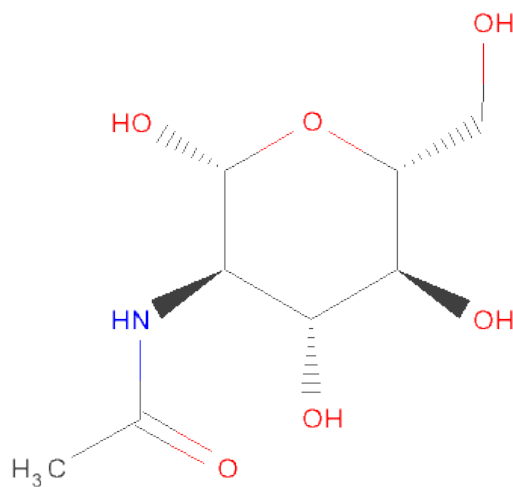
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NDG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.92Å 140.92Å 90.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.12 – 3.30 27.12 – 3.30	Depositor EDS
% Data completeness (in resolution range)	5.0 (27.12-3.30) 97.0 (27.12-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.65 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.238 , 0.279 0.266 , 0.263	Depositor DCC
$R_{free}$ test set	381 reflections (4.68%)	DCC
Wilson B-factor (Å <sup>2</sup> )	123.6	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 8150 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	1695	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, NDG, 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	2.98	16/851 (1.9%)	1.71	21/1160 (1.8%)
2	B	1.42	6/787 (0.8%)	1.35	11/1061 (1.0%)
All	All	2.36	22/1638 (1.3%)	1.55	32/2221 (1.4%)

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	0	1
2	B	1	0
All	All	1	1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	ASP	CB-CG	59.25	2.76	1.51
1	A	78	TYR	CB-CG	33.69	2.02	1.51
2	B	94	LYS	CB-CG	15.19	1.93	1.52
1	A	39	LYS	CB-CG	14.18	1.90	1.52
1	A	129	ARG	CB-CG	-11.66	1.21	1.52
2	B	35	LYS	CB-CG	-11.32	1.22	1.52
1	A	73	PHE	CB-CG	8.90	1.66	1.51
1	A	63	ALA	CA-CB	-7.68	1.36	1.52
1	A	60	GLU	CG-CD	7.11	1.62	1.51
1	A	112	ILE	CA-CB	-6.25	1.40	1.54
2	B	43	ALA	CA-CB	-5.94	1.40	1.52
1	A	78	TYR	CD2-CE2	5.90	1.48	1.39
1	A	114	VAL	CB-CG1	-5.88	1.40	1.52
1	A	128	TYR	CB-CG	-5.81	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	LYS	CB-CG	-5.81	1.36	1.52
1	A	97	GLU	CB-CG	-5.79	1.41	1.52
2	B	60	TRP	CB-CG	-5.49	1.40	1.50
1	A	104	CYS	CB-SG	-5.40	1.73	1.81
1	A	86	ILE	CB-CG2	-5.40	1.36	1.52
2	B	41	CYS	CB-SG	-5.39	1.73	1.81
1	A	37	ALA	CA-CB	-5.09	1.41	1.52
1	A	60	GLU	CD-OE1	5.06	1.31	1.25

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	129	ARG	CA-CB-CG	15.88	148.35	113.40
1	A	90	LEU	CA-CB-CG	10.81	140.16	115.30
1	A	54	ASP	CB-CG-OD1	-9.25	109.98	118.30
1	A	54	ASP	CA-CB-CG	-8.82	93.99	113.40
2	B	37	LYS	CA-CB-CG	7.77	130.49	113.40
2	B	73	ILE	CA-CB-CG1	7.33	124.94	111.00
1	A	78	TYR	CA-CB-CG	7.16	126.99	113.40
2	B	62	ASP	CB-CG-OD2	6.79	124.41	118.30
2	B	21	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	118	ASP	CB-CG-OD1	6.72	124.35	118.30
2	B	68	ASP	CB-CG-OD2	6.56	124.20	118.30
1	A	96	PRO	N-CD-CG	-6.46	93.50	103.20
1	A	39	LYS	CA-CB-CG	-6.39	99.34	113.40
1	A	74	PRO	N-CA-C	-6.12	96.19	112.10
2	B	36	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	138	CYS	CA-CB-SG	-5.99	103.22	114.00
1	A	75	LEU	CB-CG-CD2	-5.77	101.19	111.00
2	B	77	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	54	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	119	ASP	CB-CG-OD2	5.44	123.20	118.30
2	B	55	VAL	CB-CA-C	-5.44	101.06	111.40
1	A	41	HIS	CB-CA-C	-5.43	99.53	110.40
1	A	98	THR	CA-CB-CG2	-5.43	104.80	112.40
1	A	50	LEU	CB-CG-CD2	-5.37	101.87	111.00
2	B	71	ASP	CB-CG-OD2	5.27	123.04	118.30
2	B	36	ASP	N-CA-C	-5.23	96.87	111.00
1	A	71	CYS	CB-CA-C	-5.23	99.94	110.40
1	A	72	ALA	N-CA-C	5.22	125.11	111.00
2	B	73	ILE	CG1-CB-CG2	5.20	122.83	111.40
1	A	60	GLU	OE1-CD-OE2	-5.12	117.16	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ILE	N-CA-C	-5.11	97.20	111.00
1	A	125	LEU	CB-CG-CD1	-5.11	102.31	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	73	ILE	CB

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	78	TYR	Sidechain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	827	0	788	78	0
2	B	768	0	684	65	2
3	A	72	0	61	9	0
4	B	14	0	13	2	0
5	B	14	0	13	7	0
All	All	1695	0	1559	154	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 50.

All (154) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:97:TYR:CE2	2:B:99:PRO:HD3	1.65	1.30
3:A:182:BMA:H3	3:A:185:BMA:H2	1.13	1.10
1:A:126:LYS:HG2	1:A:128:TYR:HE2	1.20	1.07
2:B:97:TYR:CD2	2:B:99:PRO:HD3	1.95	1.00
1:A:126:LYS:HG2	1:A:128:TYR:CE2	2.00	0.95
2:B:97:TYR:CE2	2:B:99:PRO:CD	2.48	0.95

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:97:TYR:HE2	2:B:99:PRO:HD3	1.29	0.94
3:A:182:BMA:C3	3:A:185:BMA:H2	1.98	0.92
1:A:95:ASN:OD1	1:A:97:GLU:HB2	1.69	0.91
1:A:118:ASP:OD1	1:A:122:ASN:N	2.06	0.88
2:B:47:ASN:HD22	5:B:147:NAG:H82	1.42	0.85
1:A:116:TYR:CZ	1:A:124:ILE:HG21	2.12	0.85
1:A:74:PRO:HG2	1:A:74:PRO:O	1.76	0.83
2:B:29:GLU:OE1	2:B:59:CYS:HB2	1.80	0.81
1:A:64:ALA:O	1:A:65:TYR:HB2	1.81	0.80
2:B:97:TYR:HE2	2:B:99:PRO:CD	1.89	0.80
2:B:44:THR:HG23	2:B:55:VAL:HB	1.65	0.78
1:A:74:PRO:CG	1:A:74:PRO:O	2.31	0.78
1:A:62:TYR:OH	1:A:131:MET:HE3	1.84	0.75
2:B:40:HIS:HB3	2:B:86:CYS:O	1.88	0.74
2:B:45:TRP:CE2	2:B:82:TYR:HB2	2.24	0.73
2:B:31:CYS:O	2:B:39:ARG:NE	2.20	0.73
1:A:95:ASN:O	1:A:97:GLU:N	2.22	0.73
1:A:114:VAL:HG23	1:A:115:LEU:N	2.02	0.73
2:B:45:TRP:HE1	5:B:147:NAG:C8	2.02	0.72
3:A:182:BMA:H3	3:A:185:BMA:C2	2.06	0.71
1:A:38:CYS:HA	1:A:69:GLY:HA3	1.73	0.70
1:A:43:LEU:HD23	1:A:43:LEU:C	2.12	0.69
1:A:95:ASN:C	1:A:97:GLU:H	1.95	0.69
2:B:14:PHE:CE2	2:B:54:ILE:HD12	2.28	0.68
2:B:97:TYR:HE2	2:B:99:PRO:CG	2.06	0.68
1:A:48:ARG:HA	1:A:53:GLN:HB3	1.75	0.67
1:A:62:TYR:CZ	1:A:131:MET:HE3	2.31	0.65
2:B:38:ARG:NH1	2:B:87:GLU:OE1	2.29	0.65
2:B:97:TYR:HE2	2:B:99:PRO:HG3	1.62	0.65
2:B:73:ILE:HA	2:B:96:SER:O	1.97	0.65
4:B:124:NDG:O4	4:B:124:NDG:O6	2.10	0.65
3:A:180:NAG:H62	3:A:181:NAG:HN2	1.61	0.64
2:B:47:ASN:ND2	5:B:147:NAG:H82	2.11	0.64
1:A:95:ASN:C	1:A:97:GLU:N	2.48	0.63
1:A:53:GLN:H	1:A:53:GLN:CD	2.01	0.63
2:B:55:VAL:HG12	2:B:56:LYS:HG3	1.79	0.63
1:A:116:TYR:CE2	1:A:124:ILE:HG21	2.34	0.63
2:B:97:TYR:HD2	2:B:98:PHE:N	1.98	0.62
1:A:116:TYR:CZ	1:A:124:ILE:CG2	2.81	0.61
1:A:45:VAL:HG12	1:A:46:SER:N	2.15	0.61
2:B:97:TYR:CD2	2:B:97:TYR:C	2.73	0.61
1:A:94:ILE:HG22	1:A:95:ASN:N	2.16	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:29:GLU:OE1	2:B:59:CYS:CB	2.48	0.60
1:A:82:THR:O	1:A:85:ALA:HB3	2.02	0.60
2:B:13:PHE:HA	2:B:57:GLN:O	2.02	0.60
1:A:109:LEU:HA	1:A:132:VAL:O	2.02	0.59
2:B:47:ASN:O	2:B:49:SER:N	2.35	0.59
2:B:64:ILE:HG12	2:B:64:ILE:O	2.01	0.59
2:B:97:TYR:CE2	2:B:99:PRO:CG	2.85	0.58
1:A:79:MET:O	1:A:80:ASN:C	2.40	0.58
2:B:38:ARG:HD2	2:B:67:TYR:CE1	2.38	0.58
3:A:180:NAG:H62	3:A:181:NAG:N2	2.19	0.57
2:B:44:THR:HA	2:B:82:TYR:O	2.04	0.57
2:B:44:THR:HG22	2:B:56:LYS:H	1.68	0.57
1:A:90:LEU:O	1:A:91:VAL:C	2.39	0.56
2:B:45:TRP:NE1	5:B:147:NAG:C8	2.67	0.56
1:A:88:GLN:HG3	1:A:99:VAL:HG21	1.88	0.56
1:A:116:TYR:C	1:A:116:TYR:CD2	2.79	0.56
3:A:182:BMA:H4	3:A:184:MAN:H2	1.87	0.56
1:A:43:LEU:C	1:A:43:LEU:CD2	2.74	0.56
1:A:94:ILE:O	1:A:96:PRO:CD	2.55	0.54
2:B:45:TRP:NE1	5:B:147:NAG:H81	2.22	0.54
1:A:84:HIS:O	1:A:84:HIS:CG	2.62	0.53
2:B:12:LEU:O	2:B:92:ASN:ND2	2.34	0.53
1:A:115:LEU:HD12	1:A:124:ILE:O	2.08	0.53
1:A:99:VAL:HG23	1:A:100:PRO:HD2	1.90	0.53
2:B:48:ILE:O	2:B:51:SER:HB2	2.08	0.53
1:A:54:ASP:O	1:A:55:TRP:HE3	1.92	0.53
3:A:180:NAG:O3	3:A:180:NAG:O7	2.23	0.53
1:A:74:PRO:CD	1:A:74:PRO:O	2.56	0.53
2:B:97:TYR:HD2	2:B:97:TYR:C	2.12	0.52
1:A:43:LEU:HD23	1:A:44:TYR:N	2.24	0.52
2:B:60:TRP:O	2:B:61:LEU:C	2.48	0.52
2:B:24:ASN:OD1	2:B:24:ASN:N	2.43	0.51
1:A:116:TYR:CE2	1:A:124:ILE:CG2	2.94	0.51
1:A:82:THR:O	1:A:85:ALA:N	2.42	0.51
1:A:53:GLN:N	1:A:53:GLN:CD	2.64	0.51
2:B:41:CYS:HA	2:B:58:GLY:O	2.11	0.51
4:B:124:NDG:H6	4:B:124:NDG:HC	1.55	0.50
2:B:97:TYR:CE2	2:B:99:PRO:HG3	2.42	0.50
1:A:82:THR:O	1:A:83:ASN:C	2.47	0.49
1:A:53:GLN:OE1	1:A:53:GLN:N	2.41	0.49
2:B:12:LEU:HD12	2:B:93:GLU:HA	1.93	0.49
2:B:41:CYS:HB3	2:B:92:ASN:HB3	1.93	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:45:TRP:HE1	5:B:147:NAG:H81	1.72	0.49
1:A:94:ILE:HG22	1:A:95:ASN:H	1.77	0.49
1:A:128:TYR:CD2	1:A:128:TYR:N	2.80	0.48
1:A:128:TYR:N	1:A:128:TYR:HD2	2.10	0.48
2:B:47:ASN:ND2	5:B:147:NAG:C8	2.75	0.48
1:A:104:CYS:HA	1:A:137:GLY:O	2.12	0.48
1:A:94:ILE:O	1:A:96:PRO:HD2	2.13	0.48
2:B:39:ARG:O	2:B:40:HIS:HD2	1.97	0.47
2:B:76:LYS:O	2:B:79:PRO:HD3	2.13	0.47
1:A:64:ALA:O	1:A:65:TYR:CB	2.53	0.47
1:A:108:GLN:O	1:A:134:ARG:N	2.36	0.47
2:B:44:THR:CG2	2:B:55:VAL:HB	2.40	0.47
2:B:33:GLY:CA	2:B:39:ARG:HG3	2.45	0.47
1:A:67:CYS:HB3	1:A:104:CYS:SG	2.55	0.47
2:B:90:MET:O	2:B:93:GLU:HB2	2.15	0.47
1:A:72:ALA:HB1	1:A:73:PHE:CG	2.50	0.46
1:A:62:TYR:CZ	1:A:131:MET:CE	2.98	0.46
1:A:47:PHE:HA	1:A:50:LEU:HB2	1.98	0.46
1:A:118:ASP:OD2	1:A:122:ASN:ND2	2.49	0.46
1:A:45:VAL:CG1	1:A:46:SER:N	2.78	0.46
2:B:39:ARG:C	2:B:40:HIS:CD2	2.90	0.45
2:B:84:CYS:O	2:B:84:CYS:SG	2.74	0.45
1:A:88:GLN:CG	1:A:99:VAL:HG21	2.47	0.45
2:B:54:ILE:HG13	2:B:54:ILE:H	1.08	0.45
3:A:181:NAG:H62	3:A:182:BMA:C1	2.46	0.45
2:B:32:TYR:O	2:B:39:ARG:NH2	2.48	0.45
1:A:126:LYS:CG	1:A:128:TYR:HE2	2.09	0.45
1:A:115:LEU:HD13	1:A:125:LEU:CD1	2.47	0.45
2:B:68:ASP:N	2:B:87:GLU:OE2	2.50	0.45
2:B:44:THR:CG2	2:B:56:LYS:H	2.31	0.44
1:A:92:HIS:O	1:A:96:PRO:N	2.51	0.44
2:B:33:GLY:HA2	2:B:39:ARG:HG3	1.99	0.44
1:A:115:LEU:HA	1:A:115:LEU:HD12	1.34	0.44
1:A:109:LEU:HD23	1:A:133:VAL:HA	1.99	0.44
2:B:44:THR:O	2:B:44:THR:CG2	2.64	0.43
3:A:180:NAG:O3	3:A:180:NAG:C7	2.66	0.43
1:A:138:CYS:O	1:A:139:HIS:HD2	2.00	0.43
2:B:45:TRP:CD1	2:B:45:TRP:C	2.89	0.42
2:B:49:SER:C	2:B:51:SER:H	2.23	0.42
1:A:72:ALA:HB1	1:A:73:PHE:CD2	2.55	0.42
1:A:95:ASN:OD1	1:A:97:GLU:CB	2.54	0.42
1:A:86:ILE:HD13	1:A:86:ILE:HG21	1.78	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:131:MET:HE3	1:A:131:MET:HB3	1.47	0.42
1:A:115:LEU:HD13	1:A:125:LEU:HD12	2.02	0.42
1:A:76:ASN:HD22	1:A:76:ASN:H	1.66	0.41
2:B:82:TYR:CD1	2:B:82:TYR:N	2.88	0.41
1:A:57:ILE:HB	1:A:115:LEU:HB3	2.02	0.41
1:A:88:GLN:O	1:A:88:GLN:HG2	2.21	0.41
2:B:88:GLY:O	2:B:91:CYS:HB3	2.20	0.41
2:B:41:CYS:HB2	2:B:91:CYS:SG	2.60	0.41
2:B:14:PHE:CD2	2:B:54:ILE:HD12	2.53	0.41
1:A:83:ASN:C	1:A:85:ALA:N	2.74	0.41
2:B:11:CYS:SG	2:B:59:CYS:HA	2.60	0.41
1:A:118:ASP:OD1	1:A:121:SER:N	2.54	0.41
1:A:109:LEU:CD1	1:A:130:ASN:HB3	2.51	0.41
2:B:28:VAL:HG11	2:B:90:MET:HE2	2.03	0.41
2:B:82:TYR:HE2	2:B:97:TYR:CE1	2.38	0.41
2:B:44:THR:O	2:B:44:THR:HG23	2.21	0.40
1:A:57:ILE:HG22	1:A:57:ILE:O	2.17	0.40
1:A:98:THR:HB	1:A:99:VAL:H	1.77	0.40
1:A:52:TRP:N	1:A:52:TRP:CD1	2.87	0.40
1:A:76:ASN:HD22	1:A:76:ASN:N	2.19	0.40
1:A:89:THR:O	1:A:92:HIS:HB3	2.21	0.40
1:A:111:ALA:HA	1:A:128:TYR:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:93:GLU:OE2	2:B:93:GLU:OE2[4_765]	1.86	0.34
2:B:93:GLU:CD	2:B:93:GLU:OE2[4_765]	2.02	0.18

## 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	102/139 (73%)	85 (83%)	14 (14%)	3 (3%)	<b>7</b> 47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	92/102 (90%)	78 (85%)	11 (12%)	3 (3%)	6	43
All	All	194/241 (80%)	163 (84%)	25 (13%)	6 (3%)	7	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	35	LYS
2	B	61	LEU
2	B	99	PRO
1	A	48	ARG
1	A	94	ILE
1	A	80	ASN

### 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	90/121 (74%)	73 (81%)	17 (19%)	2	11
2	B	85/93 (91%)	71 (84%)	14 (16%)	3	16
All	All	175/214 (82%)	144 (82%)	31 (18%)	3	13

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	46	SER
1	A	54	ASP
1	A	55	TRP
1	A	59	PRO
1	A	73	PHE
1	A	74	PRO
1	A	76	ASN
1	A	90	LEU
1	A	98	THR
1	A	113	SER
1	A	115	LEU

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Mol	Chain	Res	Type
1	A	120	SER
1	A	121	SER
1	A	124	ILE
1	A	126	LYS
1	A	129	ARG
2	B	12	LEU
2	B	49	SER
2	B	54	ILE
2	B	61	LEU
2	B	64	ILE
2	B	66	CYS
2	B	67	TYR
2	B	69	ARG
2	B	70	THR
2	B	72	CYS
2	B	73	ILE
2	B	74	GLU
2	B	82	TYR
2	B	97	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	139	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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	180	1,3	12,14,15	1.25	1 (8%)	15,19,21	2.37	4 (26%)
3	NAG	A	181	3	12,14,15	0.68	0	15,19,21	1.89	3 (20%)
3	BMA	A	182	3	10,11,12	0.72	0	11,15,17	1.12	1 (9%)
3	MAN	A	183	3	10,11,12	0.74	0	11,15,17	1.21	2 (18%)
3	MAN	A	184	3	10,11,12	0.93	1 (10%)	11,15,17	1.55	3 (27%)
3	BMA	A	185	3	10,11,12	0.85	0	11,15,17	1.79	3 (27%)

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	180	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	181	3	-	0/6/23/26	0/1/1/1
3	BMA	A	182	3	-	0/2/19/22	0/1/1/1
3	MAN	A	183	3	-	0/2/19/22	0/1/1/1
3	MAN	A	184	3	-	0/2/19/22	0/1/1/1
3	BMA	A	185	3	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	180	NAG	O5-C5	-2.93	1.40	1.45
3	A	184	MAN	O5-C5	-2.44	1.40	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	180	NAG	C2-N2-C7	-5.28	114.23	123.09
3	A	181	NAG	O5-C5-C6	5.07	112.30	106.98
3	A	180	NAG	C3-C2-N2	-4.65	104.69	111.76
3	A	180	NAG	O4-C4-C3	-4.34	100.61	110.35
3	A	185	BMA	C3-C4-C5	3.91	117.19	110.20
3	A	181	NAG	C2-N2-C7	-3.38	117.41	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	184	MAN	C4-C3-C2	3.03	114.57	110.50
3	A	185	BMA	O5-C5-C4	2.94	114.38	110.65
3	A	180	NAG	C3-C4-C5	2.55	114.75	110.20
3	A	185	BMA	O5-C5-C6	2.48	109.59	106.98
3	A	181	NAG	O4-C4-C5	2.47	115.79	109.28
3	A	184	MAN	C3-C4-C5	2.44	114.56	110.20
3	A	182	BMA	O5-C5-C6	2.25	109.34	106.98
3	A	183	MAN	C4-C3-C2	-2.19	107.57	110.50
3	A	183	MAN	O5-C5-C6	2.08	109.16	106.98
3	A	184	MAN	O4-C4-C3	-2.07	105.70	110.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

2 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	$\# Z  > 2$
4	NDG	B	124	2	12,14,15	1.84	2 (16%)	15,19,21	3.33	7 (46%)
5	NAG	B	147	2	12,14,15	1.21	1 (8%)	15,19,21	2.00	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
4	NDG	B	124	2	-	0/6/23/26	1/1/1/1
5	NAG	B	147	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)
4	B	124	NDG	C2-N2	5.61	1.52	1.46
5	B	147	NAG	C2-N2	-2.92	1.42	1.46
4	B	124	NDG	O-C5	-2.32	1.41	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	124	NDG	C2-N2-C7	7.11	135.02	123.09
4	B	124	NDG	O-C5-C6	6.11	113.39	106.98
4	B	124	NDG	O7-C7-C8	-5.21	111.88	122.04
4	B	124	NDG	C3-C2-N2	4.35	118.38	111.76
5	B	147	NAG	C3-C4-C5	-3.95	103.15	110.20
5	B	147	NAG	O5-C5-C4	-3.83	105.79	110.65
4	B	124	NDG	O7-C7-N2	3.41	129.03	121.90
5	B	147	NAG	C2-N2-C7	-3.13	117.83	123.09
5	B	147	NAG	O4-C4-C5	2.68	116.34	109.28
4	B	124	NDG	O-C5-C4	-2.67	107.27	110.65
4	B	124	NDG	O3-C3-C2	2.18	113.67	109.09
5	B	147	NAG	C6-C5-C4	2.13	118.14	113.00

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	124	NDG	C1-C2-C3-C4-C5-O

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	104/139 (74%)	-0.08	0 100 100	45, 64, 79, 88	6 (5%)
2	B	94/102 (92%)	0.36	5 (5%) 25 6	54, 70, 96, 153	6 (6%)
All	All	198/241 (82%)	0.13	5 (2%) 49 14	45, 68, 88, 153	12 (6%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	33	GLY	3.5
2	B	100	GLU	3.0
2	B	34	ASP	2.8
2	B	7	GLU	2.7
2	B	75	LYS	2.3

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MAN	A	183	11/12	0.34	6.57	142,144,145,146	0
3	NAG	A	181	14/15	0.39	4.59	114,121,131,132	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	180	14/15	0.25	0.25	71,82,90,102	0
3	BMA	A	185	11/12	0.66	-	142,143,144,145	0
3	MAN	A	184	11/12	0.59	-	130,131,132,132	0
3	BMA	A	182	11/12	0.42	-	134,136,141,142	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	B	147	14/15	0.16	-0.68	64,68,71,72	0
4	NDG	B	124	14/15	0.20	-0.70	72,75,80,80	0

## 6.5 Other polymers

There are no such residues in this entry.