



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:14 PM GMT

PDB ID : 1WMX
Title : Crystal Structure of Family 30 Carbohydrate Binding Module
Authors : Horiguchi, Y.; Kono, M.; Suzuki, A.; Yamane, T.; Arai, M.; Sakka, K.; Omiya, K.
Deposited on : 2004-07-21
Resolution : 2.00 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

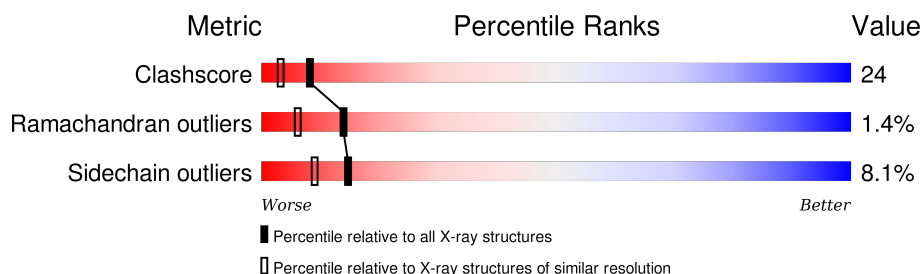
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	205	
1	B	205	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3148 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 COG3291: FOG: PKD repeat.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	7	0	0
			1384	892	221	268	3			
1	B	195	Total	C	N	O	S	9	0	0
			1556	1002	252	299	3			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	85	Total	O	0	0
			85	85		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	118	Total	O	0	0
			118	118		

Note EDS was not executed.

- Chain A:
-
- 54% 26% 16%
- ALA
PRO
GLU
GLY
TYR
ARG
LYS
L8
L9
D10
V11
W22
S23
G24
S25
G26
M27
G28
E29
L30
E31
M46
R52
V55
T58
V59
Q60
S61
M64
I65
S66
L67
L68
G72
W73
Q80
Y81
G85
Y86
D90
I91
K92
G96
F100
V101
I102
P105
- D106
K107
V108
Y109
E110
G114
L115
D118
T123
S124
M125
Y126
V127
W133
Q134
H135
V136
R144
T146
M147
M148
D151
P152
L158
V159
F160
S161
K162
R163
P167
F172
T175
K176
T177
T178
S179
E180
ASP
ASN
GLU
LYS
SER
ALA
PRO
ALA
ILE
LYS
VAL
ASN

- Chain B:
-
- Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows positions 1 to 100. A color scale at the top indicates conservation levels: 58% (green), 29% (yellow), 6% (red), and 5% (grey).

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.72Å 81.86Å 86.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.29 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (22.29-2.00)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.233	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3148	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.83	3/1418 (0.2%)	0.96	3/1935 (0.2%)
1	B	1.17	12/1594 (0.8%)	1.36	17/2172 (0.8%)
All	All	1.02	15/3012 (0.5%)	1.19	20/4107 (0.5%)

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	3
1	B	0	3
All	All	0	6

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	95	GLU	C-N	-15.24	1.05	1.33
1	B	139	PRO	C-N	-13.87	1.02	1.34
1	B	193	GLN	C-N	-12.18	1.06	1.34
1	A	96	GLY	C-N	11.93	1.54	1.33
1	B	6	ARG	CD-NE	-9.36	1.30	1.46
1	B	187	PRO	C-N	-9.16	1.12	1.34
1	B	183	GLU	C-N	-8.35	1.14	1.34
1	B	6	ARG	CZ-NH2	-7.63	1.23	1.33
1	A	86	TYR	C-N	-7.37	1.17	1.34
1	B	157	CYS	C-N	-7.09	1.17	1.34
1	B	138	ILE	C-N	-5.75	1.23	1.34
1	A	136	VAL	C-N	5.73	1.47	1.34
1	B	193	GLN	C-O	-5.45	1.12	1.23
1	B	110	GLU	CD-OE2	5.21	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	5	TYR	C-N	-5.07	1.22	1.34

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	ARG	NE-CZ-NH1	22.32	131.46	120.30
1	B	141	ARG	NE-CZ-NH1	16.33	128.46	120.30
1	B	141	ARG	CD-NE-CZ	13.46	142.45	123.60
1	B	6	ARG	NE-CZ-NH2	-13.26	113.67	120.30
1	B	141	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	B	138	ILE	C-N-CD	-9.00	100.81	120.60
1	B	6	ARG	CD-NE-CZ	8.85	135.99	123.60
1	B	139	PRO	O-C-N	8.69	136.60	122.70
1	B	138	ILE	O-C-N	-7.83	106.23	121.10
1	A	52	ARG	NE-CZ-NH2	7.21	123.90	120.30
1	B	183	GLU	O-C-N	-7.07	111.38	122.70
1	B	139	PRO	CA-C-N	-6.79	102.27	117.20
1	A	110	GLU	CA-CB-CG	6.51	127.72	113.40
1	B	144	MET	CG-SD-CE	6.34	110.35	100.20
1	B	110	GLU	CB-CG-CD	6.15	130.80	114.20
1	B	138	ILE	C-N-CA	5.81	146.39	122.00
1	B	138	ILE	CA-C-N	5.43	132.30	117.10
1	B	187	PRO	O-C-N	5.30	131.18	122.70
1	A	136	VAL	O-C-N	-5.24	114.32	122.70
1	B	110	GLU	CG-CD-OE1	-5.05	108.21	118.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	VAL	Mainchain
1	A	141	ARG	Sidechain
1	A	96	GLY	Mainchain
1	B	183	GLU	Mainchain
1	B	60	GLN	Mainchain
1	B	95	GLU	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	1384	0	1350	55	0
1	B	1556	0	1522	90	1
2	B	5	0	0	0	0
3	A	85	0	0	5	0
3	B	118	0	0	3	0
All	All	3148	0	2872	141	1

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 24.

All (141) 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:190:LYS:H	1:B:193:GLN:NE2	1.10	1.42
1:B:190:LYS:N	1:B:193:GLN:NE2	1.85	1.25
1:B:190:LYS:N	1:B:193:GLN:HE21	1.45	1.12
1:B:5:TYR:HA	1:B:8:LEU:HD22	1.14	1.11
1:B:5:TYR:HA	1:B:8:LEU:CD2	1.93	0.99
1:A:141:ARG:HH11	1:A:141:ARG:HB2	1.30	0.96
1:B:83:GLU:HA	1:B:83:GLU:OE2	1.62	0.96
1:B:189:ILE:CD1	1:B:193:GLN:HG2	1.96	0.95
1:B:189:ILE:HG13	1:B:193:GLN:HG2	1.49	0.94
1:B:189:ILE:CG1	1:B:193:GLN:HG2	1.98	0.94
1:A:141:ARG:HG2	3:A:225:HOH:O	1.69	0.91
1:A:141:ARG:HD2	3:A:286:HOH:O	1.70	0.90
1:A:110:GLU:OE2	3:A:257:HOH:O	1.88	0.89
1:B:193:GLN:O	1:B:194:LEU:HB2	1.74	0.88
1:B:183:GLU:O	1:B:184:LYS:O	1.93	0.86
1:B:182:ASN:N	1:B:182:ASN:OD1	2.06	0.85
1:B:84:ASN:HA	1:B:141:ARG:HH21	1.42	0.84
1:A:55:VAL:HG22	1:A:167:PRO:HA	1.59	0.84
1:A:100:PHE:H	1:A:123:ILE:HD11	1.42	0.84
1:B:5:TYR:CA	1:B:8:LEU:HD22	2.05	0.83
1:A:29:GLU:OE1	1:A:59:VAL:HG23	1.79	0.82
1:B:192:ASN:HD22	1:B:192:ASN:H	1.28	0.81
1:B:189:ILE:HD11	1:B:193:GLN:HG2	1.63	0.81
1:A:123:ILE:H	1:A:123:ILE:HD13	1.45	0.80
1:B:6:ARG:HG3	1:B:180:GLU:OE2	1.81	0.80
1:A:26:GLY:HA3	1:A:61:SER:HB2	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ARG:CG	1:B:180:GLU:OE2	2.29	0.80
1:B:193:GLN:O	1:B:194:LEU:CB	2.16	0.78
1:B:190:LYS:N	1:B:193:GLN:HE22	1.81	0.78
1:B:105:ARG:HG3	1:B:118:ASP:OD2	1.86	0.76
1:A:26:GLY:HA3	1:A:61:SER:CB	2.15	0.76
1:B:189:ILE:HG13	1:B:193:GLN:CG	2.16	0.75
1:A:146:ILE:HG22	1:A:147:ASN:N	2.02	0.74
1:B:190:LYS:HG3	1:B:193:GLN:HE22	1.52	0.73
1:B:146:ILE:CG1	1:B:147:ASN:N	2.50	0.73
1:B:83:GLU:CA	1:B:83:GLU:OE2	2.38	0.70
1:B:183:GLU:O	1:B:184:LYS:C	2.28	0.69
1:A:100:PHE:N	1:A:123:ILE:HD11	2.06	0.69
1:B:43:VAL:HG21	1:B:171:TRP:CD1	2.28	0.69
1:B:146:ILE:CG1	1:B:147:ASN:H	2.04	0.69
1:B:29:GLU:HG2	1:B:59:VAL:HA	1.74	0.68
1:B:189:ILE:HG23	1:B:190:LYS:N	2.10	0.67
1:B:181:ASP:C	1:B:181:ASP:OD2	2.33	0.66
1:A:100:PHE:O	1:A:123:ILE:HD13	1.96	0.65
1:B:121:THR:HG22	1:B:143:LEU:HD21	1.79	0.64
1:A:141:ARG:NH1	1:A:141:ARG:HB2	2.08	0.63
1:B:185:SER:OG	1:B:186:ALA:N	2.32	0.63
1:B:146:ILE:HG13	1:B:147:ASN:N	2.12	0.63
1:A:68:LEU:HD12	1:A:158:LEU:HD23	1.80	0.62
1:B:190:LYS:H	1:B:193:GLN:HE21	0.63	0.62
1:B:84:ASN:HA	1:B:141:ARG:NH2	2.12	0.62
1:B:189:ILE:CD1	1:B:193:GLN:CG	2.75	0.61
1:B:6:ARG:HG2	1:B:180:GLU:OE2	1.99	0.60
1:B:146:ILE:HD12	1:B:147:ASN:H	1.66	0.60
1:B:12:GLN:HA	1:B:176:LYS:HB3	1.84	0.60
1:B:6:ARG:HG3	1:B:180:GLU:CD	2.22	0.59
1:A:90:ASP:HA	1:A:134:GLN:O	2.04	0.58
1:B:187:PRO:HB2	1:B:189:ILE:HB	1.86	0.58
1:A:146:ILE:CG2	1:A:147:ASN:N	2.67	0.58
1:B:181:ASP:OD2	1:B:182:ASN:N	2.36	0.57
1:A:146:ILE:HD11	3:A:242:HOH:O	2.03	0.57
1:A:27:MET:N	1:A:29:GLU:OE2	2.36	0.57
1:B:190:LYS:HE2	3:B:324:HOH:O	2.04	0.56
1:B:83:GLU:OE1	1:B:145:LYS:NZ	2.31	0.55
1:B:72:GLY:O	1:B:73:TRP:HB2	2.06	0.55
1:B:146:ILE:CD1	1:B:147:ASN:H	2.18	0.55
1:B:190:LYS:CA	1:B:193:GLN:NE2	2.68	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:SER:HB3	1:A:160:PHE:HB2	1.87	0.55
1:B:190:LYS:CG	1:B:193:GLN:HE22	2.20	0.55
1:A:72:GLY:O	1:A:73:TRP:HB2	2.07	0.55
1:B:59:VAL:HG11	1:B:162:LYS:HD2	1.89	0.54
1:A:100:PHE:HA	1:A:163:ARG:HB2	1.90	0.53
1:B:94:LYS:HE3	1:B:169:THR:HB	1.91	0.52
1:B:141:ARG:O	1:B:145:LYS:HG3	2.10	0.52
1:A:64:TRP:CD1	1:A:162:LYS:HB2	2.45	0.52
1:B:189:ILE:HG23	1:B:190:LYS:O	2.10	0.51
1:B:100:PHE:HA	1:B:163:ARG:HB2	1.92	0.51
1:B:190:LYS:CB	1:B:193:GLN:NE2	2.74	0.50
1:A:146:ILE:HG22	1:A:147:ASN:H	1.75	0.50
1:A:27:MET:HG3	1:A:61:SER:HB3	1.94	0.50
1:B:11:VAL:HB	1:B:177:ILE:HB	1.94	0.49
1:B:43:VAL:CG2	1:B:43:VAL:O	2.59	0.49
1:B:131:THR:HG22	1:B:131:THR:O	2.12	0.49
1:A:100:PHE:O	1:A:123:ILE:CD1	2.60	0.49
1:B:66:SER:HB3	1:B:160:PHE:HB2	1.93	0.49
1:A:85:GLY:HA2	1:A:179:SER:HA	1.94	0.49
1:B:189:ILE:HG22	3:B:312:HOH:O	2.11	0.49
1:B:190:LYS:CE	3:B:324:HOH:O	2.61	0.49
1:B:100:PHE:HA	1:B:163:ARG:CB	2.44	0.48
1:A:125:ASN:ND2	3:A:228:HOH:O	2.47	0.48
1:A:102:ILE:HA	1:A:159:VAL:O	2.14	0.48
1:B:5:TYR:CE2	1:B:84:ASN:ND2	2.82	0.47
1:A:126:TYR:O	1:A:127:VAL:HG13	2.15	0.47
1:A:91:ILE:HG12	1:A:92:LYS:N	2.29	0.47
1:B:111:ARG:NH2	1:B:117:ILE:HG13	2.29	0.47
1:A:100:PHE:H	1:A:123:ILE:CD1	2.21	0.47
1:A:172:PHE:CB	1:A:175:ILE:HD11	2.45	0.47
1:A:107:LYS:HE2	1:A:109:TYR:OH	2.14	0.47
1:B:130:THR:HG23	1:B:134:GLN:NE2	2.30	0.46
1:A:58:THR:HA	1:A:167:PRO:HD3	1.97	0.46
1:B:106:ASP:C	1:B:106:ASP:OD2	2.54	0.46
1:A:59:VAL:O	1:A:59:VAL:HG22	2.16	0.46
1:B:26:GLY:O	1:B:27:MET:HE3	2.16	0.46
1:B:127:VAL:HG22	1:B:128:THR:N	2.30	0.46
1:B:91:ILE:HG12	1:B:92:LYS:N	2.30	0.46
1:A:22:TRP:CH2	1:A:24:GLY:HA3	2.51	0.45
1:B:9:LEU:N	1:B:9:LEU:HD22	2.32	0.45
1:A:58:THR:O	1:A:58:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:VAL:HG11	1:A:136:VAL:HB	1.98	0.45
1:B:102:ILE:HA	1:B:159:VAL:O	2.17	0.45
1:A:105:ARG:HB2	1:A:118:ASP:OD2	2.16	0.45
1:B:43:VAL:HG21	1:B:171:TRP:CG	2.51	0.45
1:B:43:VAL:CG2	1:B:171:TRP:CD1	2.97	0.44
1:A:80:GLN:NE2	1:A:80:GLN:HA	2.33	0.44
1:A:115:LEU:CD2	1:B:116:GLU:OE1	2.65	0.44
1:A:146:ILE:CG2	1:A:147:ASN:H	2.29	0.43
1:A:81:TYR:O	1:A:85:GLY:HA3	2.18	0.43
1:B:189:ILE:HD11	1:B:193:GLN:CG	2.40	0.43
1:A:9:LEU:N	1:A:9:LEU:HD12	2.33	0.43
1:B:121:THR:CG2	1:B:143:LEU:HD21	2.45	0.43
1:A:92:LYS:HD3	1:A:133:TRP:CE2	2.53	0.43
1:B:183:GLU:C	1:B:184:LYS:O	2.51	0.42
1:A:55:VAL:CG2	1:A:167:PRO:HA	2.39	0.42
1:A:22:TRP:CE3	1:B:113:TYR:HB3	2.55	0.42
1:B:22:TRP:CH2	1:B:24:GLY:HA3	2.54	0.42
1:B:186:ALA:HB1	1:B:187:PRO:HD2	2.01	0.42
1:A:115:LEU:HD23	1:B:116:GLU:CD	2.40	0.42
1:A:11:VAL:HB	1:A:177:ILE:HB	2.01	0.42
1:B:190:LYS:CB	1:B:193:GLN:HE22	2.33	0.41
1:B:103:GLY:O	1:B:158:LEU:HD12	2.20	0.41
1:B:6:ARG:CG	1:B:180:GLU:CD	2.84	0.41
1:B:146:ILE:O	1:B:147:ASN:HB2	2.20	0.41
1:A:115:LEU:CD2	1:B:116:GLU:CD	2.89	0.41
1:B:27:MET:HA	1:B:27:MET:HE2	2.01	0.41
1:B:141:ARG:HB2	1:B:145:LYS:HE2	2.03	0.41
1:B:192:ASN:ND2	1:B:192:ASN:H	2.06	0.41
1:A:31:GLU:OE1	1:A:52:ARG:HD2	2.21	0.41
1:A:151:ASP:HA	1:A:152:PRO:HD2	1.93	0.41
1:A:127:VAL:CG1	1:A:136:VAL:HB	2.51	0.40
1:A:176:LYS:HE2	1:A:178:THR:HG21	2.03	0.40
1:B:94:LYS:HE3	1:B:169:THR:CB	2.51	0.40

All (1) 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	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:GLU:O	1:B:190:LYS:NZ[3_656]	1.89	0.31

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	171/205 (83%)	155 (91%)	15 (9%)	1 (1%)	30	22
1	B	193/205 (94%)	175 (91%)	14 (7%)	4 (2%)	9	3
All	All	364/410 (89%)	330 (91%)	29 (8%)	5 (1%)	14	6

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	146	ILE
1	B	184	LYS
1	B	147	ASN
1	B	114	GLY
1	A	114	GLY

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	157/182 (86%)	146 (93%)	11 (7%)	19	12
1	B	175/182 (96%)	159 (91%)	16 (9%)	12	6
All	All	332/364 (91%)	305 (92%)	27 (8%)	15	9

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU

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Mol	Chain	Res	Type
1	A	46	ASN
1	A	55	VAL
1	A	59	VAL
1	A	110	GLU
1	A	123	ILE
1	A	136	VAL
1	A	141	ARG
1	A	148	ASN
1	A	179	SER
1	A	180	GLU
1	B	6	ARG
1	B	8	LEU
1	B	37	LEU
1	B	43	VAL
1	B	56	GLN
1	B	58	THR
1	B	80	GLN
1	B	83	GLU
1	B	95	GLU
1	B	136	VAL
1	B	176	LYS
1	B	182	ASN
1	B	184	LYS
1	B	189	ILE
1	B	192	ASN
1	B	193	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	80	GLN
1	A	125	ASN
1	A	135	HIS
1	A	148	ASN
1	B	46	ASN
1	B	54	ASN
1	B	56	GLN
1	B	74	ASN
1	B	84	ASN
1	B	125	ASN
1	B	148	ASN

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Mol	Chain	Res	Type
1	B	192	ASN
1	B	193	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	SO4	B	300	-	4,4,4	0.21	0	6,6,6	0.08	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
2	SO4	B	300	-	-	0/0/0/0	0/0/0/0

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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.