



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:26 PM GMT

PDB ID : 4BSR
Title : Structure of the ectodomain of LGR5 in complex with R-spondin-1 (Fu1Fu2) in P22121 crystal form
Authors : Peng, W.C.; de Lau, W.; Forneris, F.; Granneman, J.C.M.; Huch, M.; Clevers, H.; Gros, P.
Deposited on : 2013-06-11
Resolution : 3.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

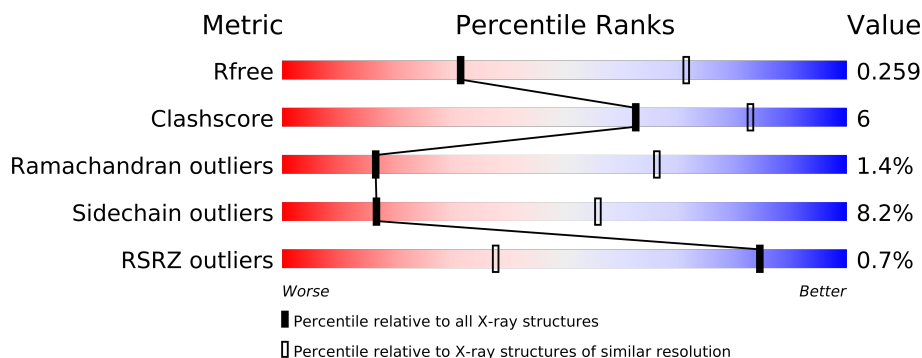
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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. 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	539	
1	B	539	
2	C	126	
2	D	126	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	1063	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9274 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 LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	483	Total	C	N	O	S	0	0	0
			3794	2420	648	709	17			
1	B	480	Total	C	N	O	S	0	0	0
			3781	2410	648	706	17			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	HIS	-	EXPRESSION TAG	UNP O75473
A	9	HIS	-	EXPRESSION TAG	UNP O75473
A	10	HIS	-	EXPRESSION TAG	UNP O75473
A	11	HIS	-	EXPRESSION TAG	UNP O75473
A	12	HIS	-	EXPRESSION TAG	UNP O75473
A	13	HIS	-	EXPRESSION TAG	UNP O75473
A	14	GLU	-	EXPRESSION TAG	UNP O75473
A	15	ASN	-	EXPRESSION TAG	UNP O75473
A	16	LEU	-	EXPRESSION TAG	UNP O75473
A	17	TYR	-	EXPRESSION TAG	UNP O75473
A	18	PHE	-	EXPRESSION TAG	UNP O75473
A	19	GLN	-	EXPRESSION TAG	UNP O75473
A	20	GLY	-	EXPRESSION TAG	UNP O75473
A	21	SER	-	EXPRESSION TAG	UNP O75473
A	544	ALA	-	EXPRESSION TAG	UNP O75473
A	545	ALA	-	EXPRESSION TAG	UNP O75473
A	546	ALA	-	EXPRESSION TAG	UNP O75473
B	8	HIS	-	EXPRESSION TAG	UNP O75473
B	9	HIS	-	EXPRESSION TAG	UNP O75473
B	10	HIS	-	EXPRESSION TAG	UNP O75473
B	11	HIS	-	EXPRESSION TAG	UNP O75473
B	12	HIS	-	EXPRESSION TAG	UNP O75473
B	13	HIS	-	EXPRESSION TAG	UNP O75473
B	14	GLU	-	EXPRESSION TAG	UNP O75473

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Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ASN	-	EXPRESSION TAG	UNP O75473
B	16	LEU	-	EXPRESSION TAG	UNP O75473
B	17	TYR	-	EXPRESSION TAG	UNP O75473
B	18	PHE	-	EXPRESSION TAG	UNP O75473
B	19	GLN	-	EXPRESSION TAG	UNP O75473
B	20	GLY	-	EXPRESSION TAG	UNP O75473
B	21	SER	-	EXPRESSION TAG	UNP O75473
B	544	ALA	-	EXPRESSION TAG	UNP O75473
B	545	ALA	-	EXPRESSION TAG	UNP O75473
B	546	ALA	-	EXPRESSION TAG	UNP O75473

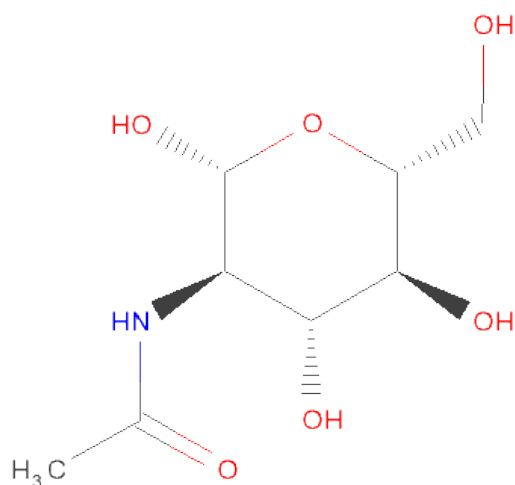
- Molecule 2 is a protein called R-SPONDIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	103	Total	C	N	O	S	0	0	0
			778	480	137	143	18			
2	D	104	Total	C	N	O	S	0	0	0
			784	483	138	145	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	GLY	-	EXPRESSION TAG	UNP Q2MKA7
C	30	SER	-	EXPRESSION TAG	UNP Q2MKA7
C	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7
C	148	ALA	-	EXPRESSION TAG	UNP Q2MKA7
C	149	HIS	-	EXPRESSION TAG	UNP Q2MKA7
C	150	HIS	-	EXPRESSION TAG	UNP Q2MKA7
C	151	HIS	-	EXPRESSION TAG	UNP Q2MKA7
C	152	HIS	-	EXPRESSION TAG	UNP Q2MKA7
C	153	HIS	-	EXPRESSION TAG	UNP Q2MKA7
C	154	HIS	-	EXPRESSION TAG	UNP Q2MKA7
D	29	GLY	-	EXPRESSION TAG	UNP Q2MKA7
D	30	SER	-	EXPRESSION TAG	UNP Q2MKA7
D	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7
D	148	ALA	-	EXPRESSION TAG	UNP Q2MKA7
D	149	HIS	-	EXPRESSION TAG	UNP Q2MKA7
D	150	HIS	-	EXPRESSION TAG	UNP Q2MKA7
D	151	HIS	-	EXPRESSION TAG	UNP Q2MKA7
D	152	HIS	-	EXPRESSION TAG	UNP Q2MKA7
D	153	HIS	-	EXPRESSION TAG	UNP Q2MKA7
D	154	HIS	-	EXPRESSION TAG	UNP Q2MKA7

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	HIS	-	EXPRESSION TAG	UNP O75473
A	9	HIS	-	EXPRESSION TAG	UNP O75473
A	10	HIS	-	EXPRESSION TAG	UNP O75473
A	11	HIS	-	EXPRESSION TAG	UNP O75473
A	12	HIS	-	EXPRESSION TAG	UNP O75473
A	13	HIS	-	EXPRESSION TAG	UNP O75473
A	14	GLU	-	EXPRESSION TAG	UNP O75473
A	15	ASN	-	EXPRESSION TAG	UNP O75473
A	16	LEU	-	EXPRESSION TAG	UNP O75473
A	17	TYR	-	EXPRESSION TAG	UNP O75473
A	18	PHE	-	EXPRESSION TAG	UNP O75473
A	19	GLN	-	EXPRESSION TAG	UNP O75473

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Chain	Residue	Modelled	Actual	Comment	Reference
A	20	GLY	-	EXPRESSION TAG	UNP O75473
A	21	SER	-	EXPRESSION TAG	UNP O75473
A	544	ALA	-	EXPRESSION TAG	UNP O75473
A	545	ALA	-	EXPRESSION TAG	UNP O75473
A	546	ALA	-	EXPRESSION TAG	UNP O75473

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

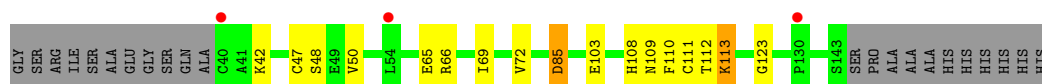
There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	HIS	-	EXPRESSION TAG	UNP O75473
A	9	HIS	-	EXPRESSION TAG	UNP O75473
A	10	HIS	-	EXPRESSION TAG	UNP O75473
A	11	HIS	-	EXPRESSION TAG	UNP O75473
A	12	HIS	-	EXPRESSION TAG	UNP O75473
A	13	HIS	-	EXPRESSION TAG	UNP O75473
A	14	GLU	-	EXPRESSION TAG	UNP O75473
A	15	ASN	-	EXPRESSION TAG	UNP O75473
A	16	LEU	-	EXPRESSION TAG	UNP O75473
A	17	TYR	-	EXPRESSION TAG	UNP O75473
A	18	PHE	-	EXPRESSION TAG	UNP O75473
A	19	GLN	-	EXPRESSION TAG	UNP O75473
A	20	GLY	-	EXPRESSION TAG	UNP O75473
A	21	SER	-	EXPRESSION TAG	UNP O75473
A	544	ALA	-	EXPRESSION TAG	UNP O75473
A	545	ALA	-	EXPRESSION TAG	UNP O75473
A	546	ALA	-	EXPRESSION TAG	UNP O75473
B	8	HIS	-	EXPRESSION TAG	UNP O75473
B	9	HIS	-	EXPRESSION TAG	UNP O75473
B	10	HIS	-	EXPRESSION TAG	UNP O75473
B	11	HIS	-	EXPRESSION TAG	UNP O75473
B	12	HIS	-	EXPRESSION TAG	UNP O75473
B	13	HIS	-	EXPRESSION TAG	UNP O75473

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Chain	Residue	Modelled	Actual	Comment	Reference
B	14	GLU	-	EXPRESSION TAG	UNP O75473
B	15	ASN	-	EXPRESSION TAG	UNP O75473
B	16	LEU	-	EXPRESSION TAG	UNP O75473
B	17	TYR	-	EXPRESSION TAG	UNP O75473
B	18	PHE	-	EXPRESSION TAG	UNP O75473
B	19	GLN	-	EXPRESSION TAG	UNP O75473
B	20	GLY	-	EXPRESSION TAG	UNP O75473
B	21	SER	-	EXPRESSION TAG	UNP O75473
B	544	ALA	-	EXPRESSION TAG	UNP O75473
B	545	ALA	-	EXPRESSION TAG	UNP O75473
B	546	ALA	-	EXPRESSION TAG	UNP O75473
B	8	HIS	-	EXPRESSION TAG	UNP O75473
B	9	HIS	-	EXPRESSION TAG	UNP O75473
B	10	HIS	-	EXPRESSION TAG	UNP O75473
B	11	HIS	-	EXPRESSION TAG	UNP O75473
B	12	HIS	-	EXPRESSION TAG	UNP O75473
B	13	HIS	-	EXPRESSION TAG	UNP O75473
B	14	GLU	-	EXPRESSION TAG	UNP O75473
B	15	ASN	-	EXPRESSION TAG	UNP O75473
B	16	LEU	-	EXPRESSION TAG	UNP O75473
B	17	TYR	-	EXPRESSION TAG	UNP O75473
B	18	PHE	-	EXPRESSION TAG	UNP O75473
B	19	GLN	-	EXPRESSION TAG	UNP O75473
B	20	GLY	-	EXPRESSION TAG	UNP O75473
B	21	SER	-	EXPRESSION TAG	UNP O75473
B	544	ALA	-	EXPRESSION TAG	UNP O75473
B	545	ALA	-	EXPRESSION TAG	UNP O75473
B	546	ALA	-	EXPRESSION TAG	UNP O75473



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	85.17Å 143.78Å 167.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.07 – 3.20 46.07 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.07-3.20) 99.6 (46.07-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.231 , 0.258 0.233 , 0.259	Depositor DCC
R_{free} test set	1737 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.688	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 17.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	1 of 34502 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9274	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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

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	0.23	0/3877	0.47	1/5277 (0.0%)
1	B	0.23	0/3864	0.46	0/5258
2	C	0.24	0/794	0.43	0/1066
2	D	0.26	0/800	0.55	0/1074
All	All	0.23	0/9335	0.47	1/12675 (0.0%)

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
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	LEU	CA-CB-CG	5.43	127.80	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	LEU	Peptide
1	B	81	LEU	Peptide

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	3794	0	9	24	0
1	B	3781	0	0	17	0
2	C	778	0	0	6	0
2	D	784	0	0	5	0
3	A	14	0	13	0	0
4	A	39	0	34	1	0
5	A	28	0	25	1	0
5	B	56	0	50	2	0
All	All	9274	0	131	53	0

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 6.

All (53) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:132:GLY:O	2:C:134:SER:N	2.30	0.65
5:A:1208:NAG:H83	5:A:1208:NAG:H3	1.78	0.64
1:A:79:SER:OG	4:A:1077:NAG:O6	2.17	0.62
2:D:103:GLU:OE1	2:D:113:LYS:NZ	2.33	0.62
1:A:521:ASP:N	1:A:521:ASP:OD1	2.33	0.61
1:B:327:THR:OG1	1:B:327:THR:O	2.19	0.61
1:B:57:LEU:N	1:B:76:ASN:OD1	2.34	0.60
1:A:327:THR:O	1:A:327:THR:OG1	2.18	0.58
2:C:111:CYS:N	2:C:123:GLY:O	2.37	0.57
1:B:170:ASP:OD1	1:B:170:ASP:N	2.37	0.57
1:B:51:ASP:OD1	1:B:53:SER:OG	2.23	0.57
1:A:170:ASP:OD1	1:A:170:ASP:N	2.38	0.56
5:B:1209:NAG:H3	5:B:1209:NAG:H83	1.88	0.55
1:B:144:ARG:NH2	1:B:146:ASP:OD2	2.39	0.55
1:A:135:GLN:NE2	1:A:156:SER:O	2.41	0.54
1:A:144:ARG:NH2	1:A:146:ASP:OD2	2.42	0.53
1:A:52:CYS:O	1:A:76:ASN:ND2	2.42	0.52
2:D:111:CYS:N	2:D:123:GLY:O	2.42	0.52
1:B:53:SER:O	1:B:55:LEU:N	2.43	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:43:ASP:OD2	1:A:49:ARG:NH1	2.43	0.51
1:B:395:GLN:OE1	1:B:420:THR:OG1	2.28	0.51
1:A:146:ASP:OD1	1:A:146:ASP:N	2.44	0.50
1:B:53:SER:O	1:B:76:ASN:ND2	2.45	0.49
1:A:146:ASP:OD2	2:C:87:ARG:NH1	2.45	0.49
1:B:117:LYS:O	1:B:141:GLN:N	2.45	0.49
2:D:47:CYS:SG	2:D:48:SER:N	2.86	0.49
1:A:274:GLU:OE1	1:A:299:SER:OG	2.31	0.49
1:B:454:HIS:O	1:B:475:TYR:OH	2.31	0.48
1:A:48:LEU:N	1:A:67:PHE:O	2.46	0.48
1:A:29:VAL:O	1:A:29:VAL:CG1	2.61	0.48
1:A:253:ILE:O	1:A:280:ASN:ND2	2.47	0.48
1:B:146:ASP:OD1	1:B:146:ASP:N	2.47	0.48
1:B:392:ASP:OD1	1:B:392:ASP:N	2.47	0.47
2:C:85:ASP:OD1	2:C:85:ASP:N	2.48	0.46
1:A:62:SER:O	1:A:64:LEU:N	2.49	0.46
1:A:408:ASN:N	1:A:432:ASN:OD1	2.49	0.46
1:A:392:ASP:OD1	1:A:392:ASP:N	2.48	0.46
2:D:108:HIS:O	2:D:110:PHE:N	2.50	0.45
1:A:87:PRO:O	1:A:88:SER:OG	2.35	0.44
1:B:441:GLY:O	1:B:443:HIS:N	2.51	0.44
2:D:85:ASP:N	2:D:85:ASP:OD1	2.51	0.44
1:A:146:ASP:O	1:A:148:ASN:ND2	2.51	0.44
1:A:355:GLN:O	1:A:377:GLN:N	2.51	0.43
1:B:180:GLN:OE1	1:B:180:GLN:N	2.51	0.43
1:B:48:LEU:O	1:B:69:SER:N	2.51	0.43
1:A:65:SER:OG	1:A:66:VAL:O	2.37	0.43
2:C:46:LEU:O	2:C:54:LEU:N	2.52	0.42
1:A:43:ASP:OD1	1:A:44:GLY:N	2.52	0.42
2:C:108:HIS:O	2:C:110:PHE:N	2.52	0.42
1:A:180:GLN:OE1	1:A:180:GLN:N	2.53	0.41
1:B:77:ASN:OD1	5:B:1077:NAG:O5	2.38	0.40
1:A:241:LEU:N	1:A:263:GLY:O	2.55	0.40
1:B:34:CYS:SG	1:B:40:CYS:N	2.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	479/539 (89%)	427 (89%)	47 (10%)	5 (1%)	22	74
1	B	476/539 (88%)	418 (88%)	53 (11%)	5 (1%)	21	72
2	C	101/126 (80%)	92 (91%)	5 (5%)	4 (4%)	5	32
2	D	102/126 (81%)	91 (89%)	9 (9%)	2 (2%)	11	56
All	All	1158/1330 (87%)	1028 (89%)	114 (10%)	16 (1%)	16	66

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	B	53	SER
2	C	109	ASN
2	C	133	SER
2	D	69	ILE
2	D	109	ASN
1	A	30	LEU
1	B	54	ASP
2	C	68	ASP
2	C	69	ILE
1	A	63	ASN
1	B	87	PRO
1	B	64	LEU
1	A	87	PRO
1	A	464	ASN
1	B	464	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	437/484 (90%)	398 (91%)	39 (9%)	14	49
1	B	436/484 (90%)	402 (92%)	34 (8%)	18	59
2	C	89/105 (85%)	84 (94%)	5 (6%)	30	75
2	D	90/105 (86%)	82 (91%)	8 (9%)	14	49
All	All	1052/1178 (89%)	966 (92%)	86 (8%)	17	56

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	46	MET
1	A	48	LEU
1	A	60	LEU
1	A	62	SER
1	A	71	LEU
1	A	80	GLN
1	A	82	LEU
1	A	90	ARG
1	A	92	LEU
1	A	93	GLU
1	A	95	LEU
1	A	97	LEU
1	A	111	THR
1	A	113	LEU
1	A	116	LEU
1	A	118	VAL
1	A	122	GLN
1	A	170	ASP
1	A	197	LYS
1	A	221	ARG
1	A	225	LEU
1	A	233	LEU
1	A	239	LEU
1	A	262	LEU
1	A	280	ASN
1	A	312	LEU
1	A	327	THR
1	A	334	THR
1	A	424	LEU
1	A	433	LEU
1	A	442	LEU
1	A	456	LEU

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Mol	Chain	Res	Type
1	A	465	PHE
1	A	473	MET
1	A	521	ASP
1	A	528	ASP
1	A	530	GLU
1	A	536	LEU
1	B	31	LEU
1	B	32	ARG
1	B	46	MET
1	B	48	LEU
1	B	53	SER
1	B	71	LEU
1	B	82	LEU
1	B	90	ARG
1	B	92	LEU
1	B	93	GLU
1	B	95	LEU
1	B	111	THR
1	B	113	LEU
1	B	116	LEU
1	B	118	VAL
1	B	122	GLN
1	B	125	GLN
1	B	170	ASP
1	B	192	THR
1	B	225	LEU
1	B	233	LEU
1	B	239	LEU
1	B	251	THR
1	B	262	LEU
1	B	280	ASN
1	B	312	LEU
1	B	327	THR
1	B	334	THR
1	B	420	THR
1	B	424	LEU
1	B	456	LEU
1	B	461	SER
1	B	465	PHE
1	B	473	MET
2	C	50	VAL
2	C	57	SER

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Mol	Chain	Res	Type
2	C	69	ILE
2	C	85	ASP
2	C	112	THR
2	D	42	LYS
2	D	50	VAL
2	D	65	GLU
2	D	66	ARG
2	D	72	VAL
2	D	85	ASP
2	D	112	THR
2	D	113	LYS

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

5.3.3 RNA ⓘ

There are no RNA 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 ⓘ

9 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	$\# Z > 2$
4	NAG	A	1077	1,4	12,14,15	0.26	0	15,19,21	0.42	0
4	NAG	A	1078	4	12,14,15	0.30	0	15,19,21	0.41	0
4	BMA	A	1079	4	10,11,12	0.64	0	11,15,17	1.18	1 (9%)
5	NAG	A	1208	1,5	12,14,15	0.42	0	15,19,21	1.03	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	1209	5	12,14,15	0.30	0	15,19,21	0.33	0
5	NAG	B	1077	1,5	12,14,15	0.37	0	15,19,21	0.59	0
5	NAG	B	1078	5	12,14,15	0.33	0	15,19,21	0.47	0
5	NAG	B	1208	1,5	12,14,15	0.29	0	15,19,21	0.38	0
5	NAG	B	1209	5	12,14,15	0.39	0	15,19,21	1.05	1 (6%)

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	NAG	A	1077	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1078	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1079	4	-	0/2/19/22	0/1/1/1
5	NAG	A	1208	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1209	5	-	0/6/23/26	0/1/1/1
5	NAG	B	1077	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1078	5	-	0/6/23/26	0/1/1/1
5	NAG	B	1208	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1209	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1209	NAG	C2-N2-C7	3.68	129.27	123.09
5	A	1208	NAG	C2-N2-C7	3.52	129.00	123.09
4	A	1079	BMA	O5-C5-C4	-2.78	107.13	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	$\# Z > 2$
3	NAG	A	1063	1	12,14,15	0.22	0	15,19,21	0.33	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	1063	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	483/539 (89%)	-0.10	2 (0%)	90 51	29, 57, 130, 182	0
1	B	480/539 (89%)	-0.16	1 (0%)	93 66	24, 53, 102, 172	0
2	C	103/126 (81%)	0.13	0	100 100	35, 67, 150, 222	0
2	D	104/126 (82%)	0.33	3 (2%)	49 10	43, 102, 157, 198	0
All	All	1170/1330 (87%)	-0.07	6 (0%)	84 46	24, 57, 138, 222	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	LEU	2.9
2	D	130	PRO	2.7
1	B	83	PRO	2.7
2	D	40	CYS	2.4
2	D	54	LEU	2.1
1	A	535	ALA	2.1

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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	B	1077	14/15	0.30	4.74	115,122,133,143	0
5	NAG	A	1208	14/15	0.38	4.71	88,93,100,104	0
5	NAG	B	1208	14/15	0.43	4.38	90,98,103,109	0
4	NAG	A	1077	14/15	0.25	1.49	97,105,115,124	0
4	BMA	A	1079	11/12	0.71	-	156,164,172,172	0
5	NAG	B	1078	14/15	0.66	-	152,159,161,162	0
5	NAG	B	1209	14/15	0.45	-	113,118,119,119	0
4	NAG	A	1078	14/15	0.42	-	134,138,144,151	0
5	NAG	A	1209	14/15	0.36	-	107,109,111,111	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, 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	1063	14/15	0.34	2.46	89,97,100,101	0

6.5 Other polymers

There are no such residues in this entry.