



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:21 PM GMT

PDB ID : 4BST
Title : Structure of the ectodomain of LGR5 in complex with R-spondin-1 (Fu1Fu2) in P6122 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 : 4.30 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

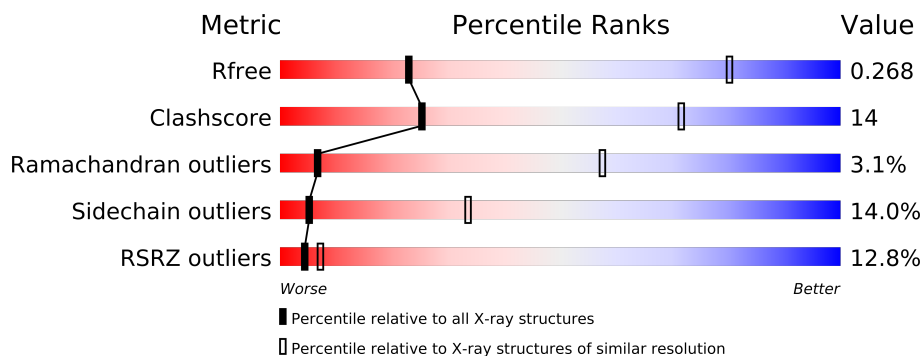
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.30 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	1016 (5.08-3.50)
Clashscore	79885	1280 (5.08-3.50)
Ramachandran outliers	78287	1210 (5.08-3.50)
Sidechain outliers	78261	1192 (5.08-3.50)
RSRZ outliers	66119	1016 (5.08-3.50)

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	1077	-	X
3	NAG	B	1077	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8833 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	457	Total	C	N	O	S	0	0	0
			3585	2287	616	666	16			
1	B	458	Total	C	N	O	S	0	0	0
			3591	2290	617	667	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

Continued on next page...

Continued from previous page...

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

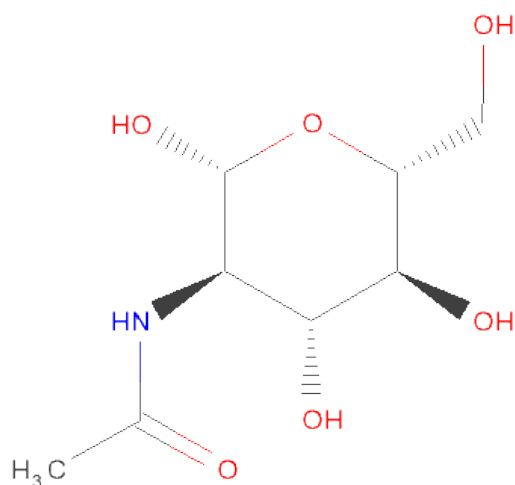
- Molecule 2 is a protein called R-SPONDIN-1.

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		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	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	B	3	Total	C	N	O	0	0
			39	22	2	15		

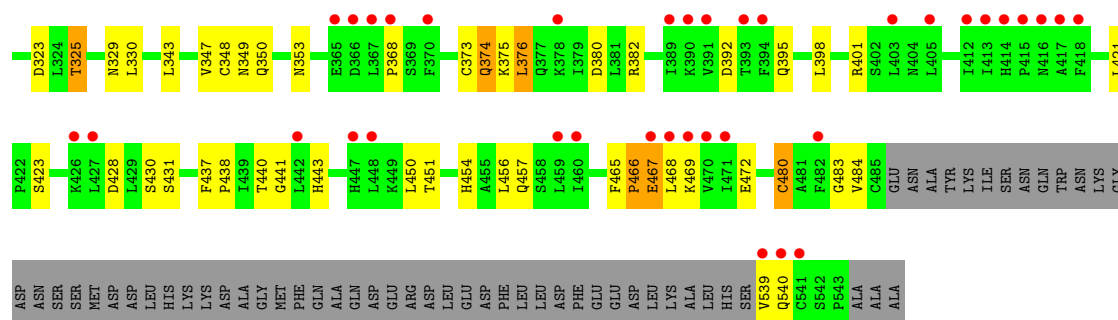
There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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

Continued on next page...

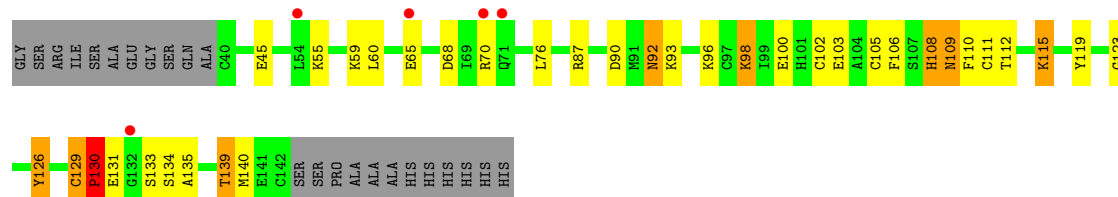
Continued from previous page...

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



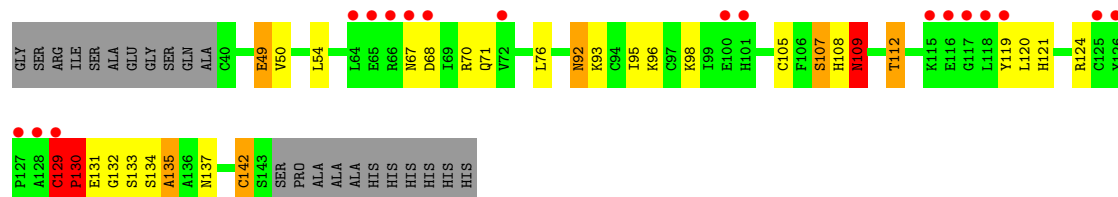
● Molecule 2: R-SPONDIN-1

Chain C:



● Molecule 2: R-SPONDIN-1

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	131.10Å 131.10Å 531.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.17 – 4.30 48.17 – 4.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.17-4.30) 99.6 (48.17-4.30)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 4.29Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.243 , 0.268 0.244 , 0.268	Depositor DCC
R_{free} test set	989 reflections (5.11%)	DCC
Wilson B-factor (Å ²)	180.2	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 199.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 19366 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8833	wwPDB-VP
Average B, all atoms (Å ²)	213.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% 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	0.37	0/3665	0.74	9/4991 (0.2%)
1	B	0.35	0/3671	0.65	3/4999 (0.1%)
2	C	0.45	0/794	0.83	1/1066 (0.1%)
2	D	0.50	0/800	0.82	4/1074 (0.4%)
All	All	0.38	0/8930	0.72	17/12130 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	TYR	CA-CB-CG	8.05	128.70	113.40
1	A	195	LEU	CA-CB-CG	7.31	132.12	115.30
1	A	198	ILE	CG1-CB-CG2	-6.96	96.08	111.40
1	A	81	LEU	CA-CB-CG	6.61	130.50	115.30
2	D	132	GLY	N-CA-C	-6.52	96.81	113.10
1	A	310	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	92	LEU	CA-CB-CG	6.28	129.74	115.30
2	D	142	CYS	CA-CB-SG	6.01	124.82	114.00
2	C	130	PRO	C-N-CA	5.83	136.26	121.70
2	D	129	CYS	CA-CB-SG	5.49	123.89	114.00
1	A	102	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	60	LEU	CA-CB-CG	5.41	127.73	115.30
1	A	312	LEU	CA-CB-CG	5.38	127.67	115.30
1	A	66	VAL	CB-CA-C	5.35	121.56	111.40
1	B	140	LEU	CA-CB-CG	5.33	127.57	115.30
1	A	113	LEU	CB-CG-CD1	-5.26	102.05	111.00
2	D	130	PRO	C-N-CA	5.25	134.82	121.70

There are no chirality outliers.

There are no planarity outliers.

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	3585	0	0	47	0
1	B	3591	0	0	48	0
2	C	778	0	0	15	0
2	D	784	0	0	15	0
3	A	42	0	0	0	0
3	B	14	0	0	0	0
4	B	39	0	0	2	0
All	All	8833	0	0	121	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 14.

All (121) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:104:TYR:OH	1:B:107:LYS:NZ	1.94	1.00
2:D:70:ARG:NH1	2:D:71:GLN:O	2.02	0.92
1:B:466:PRO:O	1:B:468:LEU:N	2.11	0.83
1:A:89:LEU:O	1:A:91:PHE:N	2.12	0.82
1:A:208:ASN:O	1:A:210:SER:N	2.14	0.80
1:B:480:CYS:O	2:C:70:ARG:NH2	2.15	0.80
2:C:96:LYS:O	2:C:98:LYS:NZ	2.17	0.78
2:C:139:THR:OG1	2:C:140:MET:N	2.18	0.76
2:C:108:HIS:O	2:C:110:PHE:N	2.21	0.73
1:A:100:ASN:O	1:A:124:ASN:ND2	2.21	0.73
2:C:119:TYR:N	2:C:126:TYR:O	2.21	0.72
1:B:170:ASP:OD1	1:B:170:ASP:N	2.23	0.72
1:B:208:ASN:O	1:B:210:SER:N	2.24	0.71
2:C:92:ASN:OD1	2:C:92:ASN:N	2.25	0.69
1:B:454:HIS:O	1:B:457:GLN:NE2	2.26	0.68
1:B:122:GLN:O	1:B:124:ASN:ND2	2.26	0.67
1:B:89:LEU:O	1:B:91:PHE:N	2.27	0.67
2:D:108:HIS:CG	2:D:109:ASN:N	2.61	0.67
2:D:67:ASN:N	2:D:70:ARG:O	2.28	0.66
1:A:420:THR:O	1:A:420:THR:OG1	2.13	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:84:ASN:N	1:A:84:ASN:OD1	2.31	0.63
1:B:69:SER:O	1:B:93:GLU:N	2.31	0.63
1:A:170:ASP:OD1	1:A:170:ASP:N	2.31	0.63
1:A:72:ASP:OD1	1:A:74:SER:OG	2.17	0.62
1:A:457:GLN:O	1:A:477:TYR:OH	2.17	0.62
1:B:299:SER:OG	1:B:302:GLN:OE1	2.19	0.61
1:B:298:ARG:NE	1:B:320:GLU:OE1	2.33	0.61
1:A:388:GLU:N	1:A:388:GLU:OE1	2.34	0.60
1:B:265:HIS:O	1:B:267:ASN:ND2	2.35	0.60
1:A:231:ASP:OD1	1:A:231:ASP:N	2.34	0.60
1:B:380:ASP:OD2	1:B:382:ARG:NH1	2.35	0.60
2:D:107:SER:OG	2:D:108:HIS:N	2.33	0.59
1:A:366:ASP:OD1	1:A:390:LYS:NZ	2.34	0.59
1:B:398:LEU:O	1:B:423:SER:OG	2.19	0.59
1:A:69:SER:O	1:A:93:GLU:N	2.35	0.59
1:A:117:LYS:O	1:A:141:GLN:N	2.36	0.58
1:B:329:ASN:OD1	1:B:353:ASN:ND2	2.37	0.58
1:A:74:SER:O	1:A:76:ASN:ND2	2.37	0.58
2:C:45:GLU:OE1	2:C:45:GLU:N	2.38	0.56
1:A:43:ASP:OD1	1:A:44:GLY:N	2.39	0.55
1:B:135:GLN:N	1:B:135:GLN:CD	2.60	0.55
1:A:65:SER:OG	1:A:66:VAL:O	2.24	0.55
1:A:433:LEU:N	1:A:453:ASN:OD1	2.38	0.55
1:A:147:ALA:N	1:A:171:ASP:OD1	2.40	0.54
2:C:100:GLU:N	2:C:100:GLU:OE1	2.40	0.54
1:B:428:ASP:OD1	1:B:430:SER:N	2.40	0.54
1:B:349:ASN:OD1	1:B:350:GLN:N	2.40	0.54
2:C:60:LEU:O	2:C:92:ASN:ND2	2.41	0.54
1:B:431:SER:N	1:B:451:THR:O	2.41	0.54
1:A:366:ASP:OD1	1:A:367:LEU:N	2.41	0.54
1:A:355:GLN:O	1:A:377:GLN:N	2.41	0.53
1:A:408:ASN:N	1:A:432:ASN:OD1	2.41	0.53
1:B:138:ARG:O	1:B:163:SER:OG	2.26	0.53
1:A:196:ASN:N	1:A:220:ASN:OD1	2.42	0.53
1:B:451:THR:N	1:B:472:GLU:OE1	2.43	0.52
2:D:71:GLN:N	2:D:71:GLN:OE1	2.43	0.52
1:B:253:ILE:O	1:B:280:ASN:ND2	2.43	0.52
1:B:43:ASP:OD1	1:B:44:GLY:N	2.42	0.52
1:B:208:ASN:ND2	4:B:1208:NAG:O7	2.42	0.51
1:B:156:SER:O	1:B:159:SER:OG	2.27	0.51
1:B:441:GLY:O	1:B:443:HIS:N	2.43	0.51
1:B:450:LEU:N	1:B:472:GLU:OE1	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:96:ARG:NE	1:B:120:MET:SD	2.85	0.50
1:B:480:CYS:O	1:B:483:GLY:N	2.45	0.50
2:C:134:SER:OG	2:C:135:ALA:N	2.44	0.50
1:B:99:GLY:N	1:B:123:ASN:OD1	2.45	0.49
2:D:119:TYR:CZ	2:D:120:LEU:O	2.65	0.49
1:A:141:GLN:O	1:A:165:ARG:N	2.45	0.49
1:B:374:GLN:O	1:B:376:LEU:N	2.46	0.49
1:A:208:ASN:N	1:A:208:ASN:OD1	2.46	0.48
1:B:166:HIS:NE2	2:D:112:THR:OG1	2.46	0.48
1:B:180:GLN:OE1	1:B:180:GLN:N	2.46	0.48
2:C:103:GLU:OE1	2:C:115:LYS:NZ	2.47	0.48
2:D:50:VAL:O	2:D:70:ARG:NH2	2.47	0.48
2:D:119:TYR:CG	2:D:120:LEU:N	2.82	0.48
2:D:119:TYR:CD1	2:D:120:LEU:N	2.83	0.47
1:B:94:GLU:OE2	1:B:96:ARG:NH2	2.47	0.47
1:A:131:THR:OG1	1:A:132:GLU:N	2.48	0.47
1:A:237:GLU:O	1:A:260:LYS:N	2.47	0.47
1:A:365:GLU:N	1:A:365:GLU:OE1	2.47	0.47
1:B:245:ASN:ND2	1:B:245:ASN:O	2.48	0.47
1:B:186:SER:OG	4:B:1208:NAG:O6	2.34	0.46
1:A:441:GLY:O	1:A:443:HIS:N	2.49	0.46
1:B:76:ASN:N	1:B:76:ASN:OD1	2.49	0.46
1:B:323:ASP:OD1	1:B:325:THR:OG1	2.34	0.46
1:B:53:SER:O	1:B:55:LEU:N	2.49	0.46
1:A:204:TYR:O	1:A:206:PHE:N	2.49	0.45
1:A:463:GLU:O	1:A:464:ASN:ND2	2.50	0.45
1:A:477:TYR:N	1:A:477:TYR:CD1	2.85	0.45
1:B:437:PHE:CD1	1:B:438:PRO:O	2.70	0.45
2:D:134:SER:OG	2:D:135:ALA:N	2.49	0.44
2:C:111:CYS:N	2:C:123:GLY:O	2.50	0.44
2:D:121:HIS:N	2:D:124:ARG:O	2.50	0.44
1:B:469:LYS:O	1:B:540:GLN:N	2.51	0.44
1:B:299:SER:OG	1:B:299:SER:O	2.35	0.43
1:A:469:LYS:O	1:A:540:GLN:N	2.51	0.43
1:A:381:LEU:O	1:A:384:ASN:ND2	2.52	0.43
1:B:93:GLU:O	1:B:117:LYS:N	2.51	0.43
1:A:156:SER:O	1:A:159:SER:OG	2.37	0.43
1:A:82:LEU:N	1:A:82:LEU:CD1	2.82	0.43
2:D:49:GLU:OE1	2:D:49:GLU:N	2.52	0.43
1:A:335:LEU:N	1:A:358:ASP:O	2.52	0.43
1:A:352:PRO:O	1:A:354:LEU:N	2.52	0.43
1:B:294:GLN:OE1	1:B:316:SER:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:291:ASN:O	1:A:293:ILE:N	2.52	0.42
2:D:92:ASN:OD1	2:D:92:ASN:N	2.51	0.42
1:A:345:GLN:CD	1:A:345:GLN:N	2.73	0.42
1:B:87:PRO:O	1:B:88:SER:OG	2.37	0.42
1:A:170:ASP:O	1:A:172:ASN:ND2	2.53	0.42
1:B:135:GLN:C	1:B:137:LEU:N	2.72	0.42
1:A:323:ASP:OD1	1:A:350:GLN:NE2	2.53	0.42
1:B:392:ASP:O	1:B:395:GLN:N	2.52	0.42
2:C:129:CYS:O	2:C:130:PRO:O	2.38	0.41
1:B:291:ASN:O	1:B:293:ILE:N	2.53	0.41
1:A:146:ASP:O	1:A:148:ASN:ND2	2.53	0.41
1:A:146:ASP:OD2	2:C:87:ARG:NE	2.53	0.41
1:A:192:THR:OG1	2:C:106:PHE:CZ	2.74	0.41
1:A:62:SER:OG	1:A:63:ASN:N	2.53	0.41
2:D:129:CYS:O	2:D:130:PRO:O	2.38	0.41
1:A:302:GLN:OE1	1:A:325:THR:N	2.55	0.40
1:A:65:SER:C	1:A:66:VAL:O	2.58	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	453/539 (84%)	388 (86%)	57 (13%)	8 (2%)	13	69
1	B	454/539 (84%)	378 (83%)	63 (14%)	13 (3%)	7	58
2	C	101/126 (80%)	82 (81%)	14 (14%)	5 (5%)	3	43
2	D	102/126 (81%)	82 (80%)	12 (12%)	8 (8%)	1	28
All	All	1110/1330 (84%)	930 (84%)	146 (13%)	34 (3%)	7	57

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	90	ARG
1	A	209	LEU
1	A	353	ASN
1	B	66	VAL
1	B	90	ARG
1	B	123	ASN
1	B	209	LEU
1	B	467	GLU
2	C	109	ASN
2	C	129	CYS
2	C	130	PRO
2	C	131	GLU
2	C	133	SER
2	D	129	CYS
2	D	130	PRO
2	D	133	SER
2	D	142	CYS
1	B	43	ASP
1	B	53	SER
1	B	54	ASP
2	D	109	ASN
1	B	466	PRO
2	D	131	GLU
1	A	82	LEU
1	B	64	LEU
2	D	137	ASN
1	A	66	VAL
1	B	374	GLN
2	D	135	ALA
1	A	87	PRO
1	A	368	PRO
1	B	347	VAL
1	B	368	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	414/484 (86%)	350 (84%)	64 (16%)	4	28
1	B	415/484 (86%)	368 (89%)	47 (11%)	9	44
2	C	89/105 (85%)	72 (81%)	17 (19%)	2	16
2	D	90/105 (86%)	77 (86%)	13 (14%)	5	31
All	All	1008/1178 (86%)	867 (86%)	141 (14%)	5	33

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	CYS
1	A	36	THR
1	A	47	LEU
1	A	55	LEU
1	A	60	LEU
1	A	64	LEU
1	A	66	VAL
1	A	76	ASN
1	A	81	LEU
1	A	82	LEU
1	A	84	ASN
1	A	89	LEU
1	A	90	ARG
1	A	92	LEU
1	A	93	GLU
1	A	102	LEU
1	A	103	THR
1	A	113	LEU
1	A	116	LEU
1	A	118	VAL
1	A	121	LEU
1	A	135	GLN
1	A	152	TYR
1	A	153	VAL
1	A	159	SER
1	A	170	ASP
1	A	174	LEU
1	A	175	THR
1	A	195	LEU
1	A	198	ILE
1	A	208	ASN
1	A	214	VAL
1	A	228	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	231	ASP
1	A	233	LEU
1	A	238	THR
1	A	302	GLN
1	A	304	LEU
1	A	310	LEU
1	A	312	LEU
1	A	318	ILE
1	A	325	THR
1	A	327	THR
1	A	336	THR
1	A	343	LEU
1	A	348	CYS
1	A	356	VAL
1	A	373	CYS
1	A	381	LEU
1	A	389	ILE
1	A	402	SER
1	A	420	THR
1	A	421	LEU
1	A	424	LEU
1	A	433	LEU
1	A	440	THR
1	A	445	LEU
1	A	447	HIS
1	A	450	LEU
1	A	458	SER
1	A	459	LEU
1	A	460	ILE
1	A	477	TYR
1	A	478	GLN
1	B	40	CYS
1	B	60	LEU
1	B	64	LEU
1	B	65	SER
1	B	70	TYR
1	B	77	ASN
1	B	82	LEU
1	B	89	LEU
1	B	92	LEU
1	B	102	LEU
1	B	103	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	113	LEU
1	B	116	LEU
1	B	118	VAL
1	B	131	THR
1	B	137	LEU
1	B	142	SER
1	B	150	ILE
1	B	159	SER
1	B	161	LEU
1	B	170	ASP
1	B	209	LEU
1	B	233	LEU
1	B	238	THR
1	B	245	ASN
1	B	246	LEU
1	B	256	LEU
1	B	280	ASN
1	B	299	SER
1	B	304	LEU
1	B	312	LEU
1	B	325	THR
1	B	330	LEU
1	B	343	LEU
1	B	348	CYS
1	B	373	CYS
1	B	375	LYS
1	B	376	LEU
1	B	401	ARG
1	B	421	LEU
1	B	440	THR
1	B	456	LEU
1	B	465	PHE
1	B	467	GLU
1	B	480	CYS
1	B	484	VAL
1	B	539	VAL
2	C	55	LYS
2	C	59	LYS
2	C	65	GLU
2	C	68	ASP
2	C	76	LEU
2	C	90	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	92	ASN
2	C	93	LYS
2	C	98	LYS
2	C	102	CYS
2	C	105	CYS
2	C	108	HIS
2	C	109	ASN
2	C	112	THR
2	C	115	LYS
2	C	126	TYR
2	C	139	THR
2	D	49	GLU
2	D	54	LEU
2	D	68	ASP
2	D	76	LEU
2	D	92	ASN
2	D	93	LYS
2	D	95	ILE
2	D	96	LYS
2	D	98	LYS
2	D	105	CYS
2	D	107	SER
2	D	109	ASN
2	D	112	THR

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 ⓘ

3 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	B	1208	1,4	12,14,15	0.58	0	15,19,21	1.49	3 (20%)
4	NAG	B	1209	4	12,14,15	0.50	0	15,19,21	0.99	1 (6%)
4	BMA	B	1210	4	10,11,12	0.86	0	11,15,17	1.18	1 (9%)

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	B	1208	1,4	-	1/6/23/26	0/1/1/1
4	NAG	B	1209	4	-	0/6/23/26	0/1/1/1
4	BMA	B	1210	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1208	NAG	O4-C4-C3	3.82	118.92	110.35
4	B	1208	NAG	C2-N2-C7	3.16	128.40	123.09
4	B	1209	NAG	C3-C4-C5	2.65	114.94	110.20
4	B	1210	BMA	O2-C2-C3	-2.39	105.02	110.18
4	B	1208	NAG	O5-C5-C4	-2.01	108.10	110.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1208	NAG	C1-C2-N2-C7

There are no ring outliers.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
3	NAG	A	1063	1	12,14,15	0.27	0	15,19,21	0.30	0
3	NAG	A	1077	1	12,14,15	0.31	0	15,19,21	0.50	0
3	NAG	A	1208	1	12,14,15	0.34	0	15,19,21	0.45	0
3	NAG	B	1077	1	12,14,15	0.43	0	15,19,21	0.63	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
3	NAG	A	1077	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1208	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	1077	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1208	NAG	C1

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	457/539 (84%)	0.76	50 (10%) 6 10	131, 205, 257, 372	0
1	B	458/539 (84%)	0.99	70 (15%) 3 6	135, 205, 259, 373	0
2	C	103/126 (81%)	0.49	5 (4%) 28 26	165, 243, 334, 392	0
2	D	104/126 (82%)	1.08	18 (17%) 2 4	176, 245, 333, 390	0
All	All	1122/1330 (84%)	0.86	143 (12%) 4 7	131, 210, 288, 392	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	65	GLU	7.1
1	B	540	GLN	6.6
1	A	83	PRO	6.0
1	B	539	VAL	6.0
1	B	82	LEU	5.5
2	D	67	ASN	5.5
2	D	68	ASP	4.9
1	A	82	LEU	4.7
1	A	81	LEU	4.5
1	B	427	LEU	4.5
1	B	469	LYS	4.4
1	A	61	PRO	4.4
1	B	59	GLU	4.3
2	D	127	PRO	4.3
1	B	60	LEU	4.3
1	B	83	PRO	4.3
1	B	448	LEU	4.2
1	A	60	LEU	4.2
1	B	81	LEU	4.0
1	B	470	VAL	3.9
1	B	390	LYS	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	471	ILE	3.9
2	D	118	LEU	3.9
1	B	403	LEU	3.9
2	D	66	ARG	3.8
1	B	414	HIS	3.8
1	A	57	LEU	3.8
1	B	417	ALA	3.7
1	B	447	HIS	3.7
2	D	126	TYR	3.7
1	B	78	ILE	3.6
1	B	365	GLU	3.6
1	A	59	GLU	3.5
1	B	460	ILE	3.5
1	A	331	GLU	3.5
1	B	276	ALA	3.5
1	B	249	PHE	3.5
2	D	116	GLU	3.5
2	D	101	HIS	3.5
1	A	54	ASP	3.4
1	A	204	TYR	3.3
1	B	389	ILE	3.3
1	B	80	GLN	3.3
1	A	205	ALA	3.3
1	A	64	LEU	3.3
1	A	228	LYS	3.3
1	B	413	ILE	3.2
1	A	355	GLN	3.2
1	B	61	PRO	3.2
1	B	541	CYS	3.2
1	B	52	CYS	3.2
1	B	415	PRO	3.2
1	B	57	LEU	3.1
1	B	227	LYS	3.1
1	A	227	LYS	3.1
2	D	117	GLY	3.0
1	B	64	LEU	3.0
1	B	468	LEU	3.0
1	B	250	PRO	3.0
2	C	132	GLY	2.9
1	B	391	VAL	2.9
1	B	79	SER	2.9
1	A	80	GLN	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	55	LEU	2.8
1	B	367	LEU	2.8
1	A	105	ILE	2.8
2	D	128	ALA	2.8
2	D	125	CYS	2.8
1	B	73	LEU	2.8
1	B	368	PRO	2.8
1	A	233	LEU	2.8
1	B	366	ASP	2.7
1	A	357	LEU	2.7
2	C	54	LEU	2.7
2	D	129	CYS	2.6
1	A	343	LEU	2.6
2	D	115	LYS	2.6
1	B	313	ASN	2.6
1	B	300	ALA	2.6
1	A	378	LYS	2.6
1	A	50	VAL	2.6
2	D	100	GLU	2.6
1	B	106	PRO	2.5
1	B	418	PHE	2.5
1	B	405	LEU	2.5
2	D	64	LEU	2.5
1	A	324	LEU	2.5
1	A	377	GLN	2.5
1	A	403	LEU	2.5
1	B	394	PHE	2.5
1	B	459	LEU	2.5
1	A	62	SER	2.4
1	B	393	THR	2.4
1	B	84	ASN	2.4
1	B	416	ASN	2.4
2	C	65	GLU	2.4
1	A	52	CYS	2.4
1	A	229	CYS	2.4
1	B	275	LYS	2.4
1	B	467	GLU	2.4
1	B	50	VAL	2.4
1	A	134	LEU	2.4
2	D	72	VAL	2.4
1	A	202	PRO	2.3
1	A	367	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	106	PRO	2.3
1	A	370	PHE	2.3
1	A	322	PRO	2.3
1	B	272	ILE	2.3
2	D	119	TYR	2.3
1	A	230	PHE	2.3
1	B	412	ILE	2.2
2	C	70	ARG	2.2
1	B	75	MET	2.2
1	B	105	ILE	2.2
1	A	133	ALA	2.2
1	B	104	TYR	2.2
1	A	78	ILE	2.2
2	C	71	GLN	2.2
1	B	33	GLY	2.2
1	A	75	MET	2.2
1	A	330	LEU	2.2
1	B	378	LYS	2.2
1	B	426	LYS	2.2
1	A	55	LEU	2.2
1	B	370	PHE	2.2
1	B	442	LEU	2.2
1	A	226	GLY	2.1
1	B	301	PHE	2.1
1	A	390	LYS	2.1
1	A	177	ILE	2.1
1	B	225	LEU	2.1
1	A	79	SER	2.1
1	A	379	ILE	2.1
1	A	209	LEU	2.1
1	B	133	ALA	2.1
1	A	375	LYS	2.0
1	B	138	ARG	2.0
1	B	482	PHE	2.0
1	A	277	PHE	2.0
1	A	161	LEU	2.0
1	A	185	LEU	2.0
1	B	102	LEU	2.0

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(Å ²)	Q<0.9
4	BMA	B	1210	11/12	0.86	27.70	206,247,350,359	0
4	NAG	B	1208	14/15	0.21	-0.83	120,232,277,284	0
4	NAG	B	1209	14/15	0.37	-	179,259,273,274	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(Å ²)	Q<0.9
3	NAG	A	1077	14/15	0.93	1.43	199,261,288,316	0
3	NAG	A	1208	14/15	0.38	-0.19	227,283,330,353	0
3	NAG	B	1077	14/15	0.54	-1.60	216,285,322,322	0
3	NAG	A	1063	14/15	0.42	-1.71	182,291,310,317	0

6.5 Other polymers ⓘ

There are no such residues in this entry.