



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:12 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

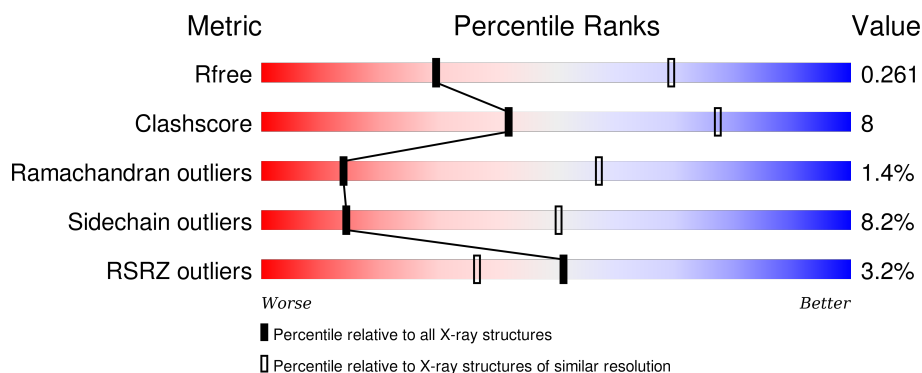
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	539	<div> <div>2%</div> <div>68%</div> <div>19%</div> <div>•</div> <div>10%</div> </div>
1	B	539	<div> <div>%</div> <div>66%</div> <div>20%</div> <div>•</div> <div>11%</div> </div>
2	C	126	<div> <div>9%</div> <div>63%</div> <div>14%</div> <div>• •</div> <div>18%</div> </div>
2	D	126	<div> <div>10%</div> <div>61%</div> <div>17%</div> <div>5%</div> <div>17%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9274 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 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

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: $C_8H_{15}NO_6$).



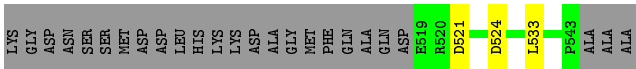
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- 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		

- 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		



● Molecule 2: R-SPONDIN-1



● Molecule 2: R-SPONDIN-1



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 0.238 , 0.261	Depositor DCC
R_{free} test set	1736 reflections (5.30%)	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 , 36.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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 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	3794	0	3791	57	0
1	B	3781	0	3780	68	0
2	C	778	0	744	11	0
2	D	784	0	749	19	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	9186	155	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (155) 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)
2:D:65:GLU:HA	2:D:66:ARG:HB3	1.51	0.92
1:A:82:LEU:HD13	1:A:85:PRO:HA	1.76	0.66
2:C:132:GLY:O	2:C:134:SER:N	2.30	0.65
2:C:50:VAL:HG23	2:C:70:ARG:HD2	1.80	0.64
5:A:1208:NAG:H83	5:A:1208:NAG:H3	1.78	0.64
1:A:29:VAL:O	1:A:29:VAL:HG12	1.98	0.63
1:A:81:LEU:HD11	1:A:106:PRO:HD2	1.80	0.62
1:A:79:SER:OG	4:A:1077:NAG:O6	2.17	0.61
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
2:D:101:HIS:HB3	2:D:118:LEU:HD13	1.83	0.59
2:D:112:THR:HG22	2:D:113:LYS:HG2	1.82	0.59
1:B:182:PHE:HB3	1:B:209:LEU:HD11	1.85	0.59
1:A:259:LEU:HD21	1:A:262:LEU:HG	1.85	0.59
2:C:101:HIS:HB3	2:C:118:LEU:HD13	1.84	0.59
1:A:327:THR:O	1:A:327:THR:OG1	2.18	0.58
1:A:230:PHE:HB3	1:A:256:LEU:HD21	1.85	0.58
2:D:45:GLU:HG3	2:D:55:LYS:HE3	1.85	0.58
1:A:28:GLY:HA2	1:A:32:ARG:HG3	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ARG:HD3	1:B:33:GLY:H	1.69	0.58
2:D:65:GLU:CA	2:D:66:ARG:HB3	2.29	0.58
1:A:238:THR:HG22	1:A:261:GLU:HB3	1.85	0.58
2:D:115:LYS:HE2	2:D:118:LEU:HD12	1.86	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:B:81:LEU:HD11	1:B:106:PRO:HD2	1.87	0.57
1:B:238:THR:HG22	1:B:261:GLU:HB3	1.86	0.57
1:B:521:ASP:HA	1:B:524:ASP:HB2	1.86	0.57
1:A:182:PHE:HB3	1:A:209:LEU:HD11	1.86	0.56
1:B:259:LEU:HD21	1:B:262:LEU:HG	1.88	0.56
1:A:170:ASP:OD1	1:A:170:ASP:N	2.38	0.56
1:B:425:ILE:HG13	1:B:426:LYS:HG3	1.87	0.56
2:D:68:ASP:HB3	2:D:70:ARG:H	1.71	0.56
1:B:144:ARG:HG2	1:B:168:TRP:CE3	2.40	0.56
5:B:1209:NAG:H83	5:B:1209:NAG:H3	1.88	0.55
1:A:236:LEU:HD23	1:A:256:LEU:HD13	1.88	0.55
1:B:144:ARG:NH2	1:B:146:ASP:OD2	2.39	0.55
1:A:425:ILE:HG13	1:A:426:LYS:HG3	1.89	0.55
1:A:135:GLN:NE2	1:A:156:SER:O	2.41	0.54
1:B:367:LEU:HD11	1:B:386:ILE:HD13	1.89	0.54
2:D:132:GLY:O	2:D:134:SER:HB3	2.08	0.53
1:B:231:ASP:HA	1:B:255:THR:HG21	1.90	0.53
1:B:230:PHE:HB3	1:B:256:LEU:HD21	1.89	0.53
2:D:103:GLU:OE1	2:D:113:LYS:NZ	2.33	0.53
1:A:144:ARG:NH2	1:A:146:ASP:OD2	2.42	0.53
1:B:57:LEU:N	1:B:76:ASN:OD1	2.34	0.53
1:B:284:ILE:HG22	1:B:285:THR:HG23	1.91	0.52
1:B:439:ILE:HD11	1:B:465:PHE:CZ	2.45	0.52
1:A:525:PHE:HE1	1:B:533:LEU:HD22	1.74	0.52
1:A:356:VAL:HG12	1:A:378:LYS:HB3	1.91	0.52
1:A:52:CYS:O	1:A:76:ASN:ND2	2.42	0.52
1:B:415:PRO:HA	1:B:438:PRO:HB3	1.92	0.52
1:A:144:ARG:HG2	1:A:168:TRP:CE3	2.45	0.51
1:A:158:PHE:HB3	1:A:185:LEU:HD21	1.92	0.51
1:A:43:ASP:OD2	1:A:49:ARG:NH1	2.43	0.51
1:B:130:PRO:HB3	1:B:133:ALA:HB3	1.93	0.51
1:B:236:LEU:HD23	1:B:256:LEU:HD13	1.92	0.51
1:B:53:SER:O	1:B:55:LEU:N	2.43	0.50
1:A:81:LEU:HD21	1:A:105:ILE:HD13	1.93	0.50
1:B:351:LEU:HD13	1:B:354:LEU:HD22	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:ASP:O	2:D:69:ILE:HB	2.12	0.50
1:B:250:PRO:HB2	1:B:253:ILE:HD13	1.94	0.50
1:A:374:GLN:HG3	1:A:375:LYS:HG3	1.93	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
2:C:68:ASP:O	2:C:69:ILE:HG12	2.12	0.49
2:D:124:ARG:HD2	2:D:126:TYR:OH	2.12	0.49
2:D:65:GLU:HA	2:D:66:ARG:CB	2.33	0.49
1:A:284:ILE:HG22	1:A:285:THR:HG23	1.93	0.49
2:D:47:CYS:SG	2:D:48:SER:N	2.86	0.49
1:B:82:LEU:HB3	1:B:84:ASN:H	1.76	0.49
2:D:65:GLU:HA	2:D:66:ARG:HD2	1.95	0.49
1:A:348:CYS:SG	1:A:370:PHE:HA	2.53	0.49
1:B:425:ILE:HB	1:B:446:THR:HG22	1.95	0.48
1:A:29:VAL:O	1:A:29:VAL:CG1	2.61	0.48
1:A:87:PRO:HB3	1:A:112:GLY:HA3	1.96	0.48
1:B:53:SER:HB2	1:B:54:ASP:H	1.45	0.48
1:B:373:CYS:HB3	1:B:376:LEU:HD22	1.95	0.47
1:A:418:PHE:HA	1:A:421:LEU:HD13	1.95	0.47
1:A:294:GLN:HB3	1:A:317:GLN:HG2	1.96	0.47
1:B:78:ILE:HB	1:B:100:ASN:HB3	1.96	0.47
2:D:132:GLY:C	2:D:134:SER:HB3	2.34	0.47
1:A:164:LEU:HD23	1:A:185:LEU:HD22	1.95	0.47
1:B:334:THR:HB	1:B:358:ASP:HB3	1.97	0.47
1:A:376:LEU:HD23	1:A:379:ILE:HD11	1.97	0.47
1:A:43:ASP:HB2	1:A:49:ARG:HG3	1.97	0.47
1:A:122:GLN:HE21	1:A:144:ARG:HD3	1.79	0.47
1:B:122:GLN:HE21	1:B:144:ARG:HD3	1.79	0.47
1:A:391:VAL:HG22	1:A:414:HIS:CG	2.50	0.47
1:B:146:ASP:OD1	1:B:146:ASP:N	2.47	0.46
1:B:391:VAL:HG22	1:B:414:HIS:CG	2.50	0.46
1:A:391:VAL:HG22	1:A:414:HIS:CD2	2.51	0.46
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:446:THR:HG22	1:A:447:HIS:ND1	2.31	0.45
1:A:130:PRO:HB3	1:A:133:ALA:HB3	1.99	0.45
1:B:144:ARG:HA	1:B:168:TRP:HB2	1.99	0.45
1:A:427:LEU:HD22	1:A:442:LEU:HD11	1.98	0.45
1:B:193:LEU:HB2	1:B:217:LEU:HD23	1.98	0.45
1:A:30:LEU:HD22	1:A:30:LEU:HA	1.82	0.45
2:D:108:HIS:O	2:D:110:PHE:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:69:ILE:HA	2:D:69:ILE:HD12	1.84	0.45
1:B:32:ARG:HD3	1:B:33:GLY:N	2.32	0.45
1:A:201:ILE:HG22	1:A:229:CYS:HB2	1.98	0.45
1:B:43:ASP:HB2	1:B:49:ARG:HG3	2.00	0.44
2:D:85:ASP:N	2:D:85:ASP:OD1	2.51	0.44
1:B:441:GLY:O	1:B:443:HIS:N	2.51	0.44
1:A:146:ASP:O	1:A:148:ASN:ND2	2.51	0.44
1:B:101:ALA:HB1	1:B:125:GLN:HE22	1.82	0.44
2:D:129:CYS:HB2	2:D:134:SER:OG	2.17	0.44
1:A:400:LEU:HD23	1:A:421:LEU:HD23	2.00	0.44
1:B:389:ILE:HD11	1:B:410:ILE:HD13	2.00	0.44
1:B:203:ASP:HA	1:B:229:CYS:HA	2.00	0.43
1:B:158:PHE:HB3	1:B:185:LEU:HD21	2.00	0.43
1:B:294:GLN:HB3	1:B:317:GLN:HG2	1.99	0.43
2:C:79:CYS:HA	2:C:80:PRO:HD3	1.85	0.43
1:B:233:LEU:H	1:B:233:LEU:HD13	1.83	0.43
1:B:391:VAL:HG22	1:B:414:HIS:CD2	2.54	0.43
1:B:49:ARG:HA	1:B:70:TYR:HB3	2.00	0.43
1:B:61:PRO:HB2	1:B:64:LEU:HD12	2.01	0.43
1:B:425:ILE:O	1:B:445:LEU:HB2	2.19	0.43
1:B:127:ARG:C	1:B:150:ILE:HA	2.39	0.42
1:B:66:VAL:O	1:B:67:PHE:HB2	2.19	0.42
1:B:82:LEU:HD12	1:B:82:LEU:HA	1.77	0.42
1:B:364:LEU:HB2	1:B:384:ASN:HD22	1.84	0.42
2:C:111:CYS:N	2:C:123:GLY:O	2.37	0.42
1:A:64:LEU:HD23	1:A:86:LEU:HD13	2.02	0.42
1:B:97:LEU:HA	1:B:97:LEU:HD12	1.88	0.42
1:B:83:PRO:C	1:B:85:PRO:HD3	2.40	0.42
1:A:471:ILE:O	1:A:541:CYS:HA	2.19	0.42
1:A:367:LEU:HD11	1:A:386:ILE:HD13	2.01	0.42
1:B:122:GLN:NE2	1:B:144:ARG:HD3	2.35	0.42
1:B:96:ARG:HA	1:B:120:MET:HB2	2.01	0.42
2:C:108:HIS:O	2:C:110:PHE:N	2.52	0.42
1:A:82:LEU:HG	1:A:82:LEU:H	1.35	0.41
1:A:376:LEU:HA	1:A:376:LEU:HD12	1.91	0.41
1:A:522:LEU:HA	1:A:522:LEU:HD23	1.72	0.41
1:B:376:LEU:HD23	1:B:379:ILE:HD11	2.01	0.41
2:C:105:CYS:HA	2:C:112:THR:H	1.83	0.41
1:B:35:PRO:HB2	1:B:38:CYS:SG	2.60	0.41
1:A:385:GLU:OE1	1:A:409:LYS:HE2	2.19	0.41
1:A:193:LEU:HB2	1:A:217:LEU:HD23	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASP:N	1:A:146:ASP:OD1	2.44	0.41
1:B:439:ILE:HD12	1:B:439:ILE:HA	1.82	0.41
1:B:389:ILE:HD12	1:B:413:ILE:HG12	2.03	0.41
1:A:387:TYR:HA	1:A:409:LYS:O	2.21	0.41
1:A:473:MET:O	1:A:543:PRO:HA	2.20	0.41
1:B:82:LEU:HB3	1:B:84:ASN:N	2.36	0.40
1:B:97:LEU:HB3	1:B:121:LEU:HD23	2.02	0.40
1:B:77:ASN:OD1	5:B:1077:NAG:O5	2.38	0.40
2:C:88:ASN:HB2	2:C:91:MET:O	2.21	0.40
1:B:53:SER:HA	1:B:74:SER:H	1.86	0.40
1:B:128:HIS:N	1:B:150:ILE:HG22	2.35	0.40
1:A:150:ILE:HG12	1:A:172:ASN:CG	2.42	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 [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	479/539 (89%)	427 (89%)	47 (10%)	5 (1%)	19	65
1	B	476/539 (88%)	418 (88%)	53 (11%)	5 (1%)	17	62
2	C	101/126 (80%)	92 (91%)	5 (5%)	4 (4%)	4	27
2	D	102/126 (81%)	91 (89%)	9 (9%)	2 (2%)	9	48
All	All	1158/1330 (87%)	1028 (89%)	114 (10%)	16 (1%)	14	57

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	B	53	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	12	44
1	B	436/484 (90%)	402 (92%)	34 (8%)	16	53
2	C	89/105 (85%)	84 (94%)	5 (6%)	26	68
2	D	90/105 (86%)	82 (91%)	8 (9%)	12	44
All	All	1052/1178 (89%)	966 (92%)	86 (8%)	14	50

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	245	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	383	HIS
1	B	302	GLN
1	B	383	HIS
2	D	88	ASN

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 ⓘ

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	14,14,15	0.23	0	15,19,21	0.62	1 (6%)
4	NAG	A	1078	4	14,14,15	0.37	0	15,19,21	0.35	0
4	BMA	A	1079	4	11,11,12	0.86	0	14,15,17	0.89	0
5	NAG	A	1208	1,5	14,14,15	0.75	1 (7%)	15,19,21	1.30	1 (6%)
5	NAG	A	1209	5	14,14,15	0.22	0	15,19,21	0.32	0
5	NAG	B	1077	1,5	14,14,15	0.43	0	15,19,21	0.56	0
5	NAG	B	1078	5	14,14,15	0.41	0	15,19,21	0.41	0
5	NAG	B	1208	1,5	14,14,15	0.34	0	15,19,21	0.30	0
5	NAG	B	1209	5	14,14,15	0.53	0	15,19,21	1.34	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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1208	NAG	O5-C1	-2.61	1.39	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1077	NAG	C1-O5-C5	2.05	114.85	112.25
5	A	1208	NAG	C2-N2-C7	4.64	129.00	123.04
5	B	1209	NAG	C2-N2-C7	4.85	129.27	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1077	NAG	1	0
5	A	1208	NAG	1	0
5	B	1077	NAG	1	0
5	B	1209	NAG	1	0

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	14,14,15	0.35	0	15,19,21	0.58	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
3	NAG	A	1063	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1063	NAG	C1-O5-C5	2.06	114.86	112.25

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.01	9 (1%) 70 55	29, 57, 130, 182	0
1	B	480/539 (89%)	-0.10	5 (1%) 84 75	24, 53, 102, 172	0
2	C	103/126 (81%)	0.41	11 (10%) 8 4	35, 67, 150, 222	0
2	D	104/126 (82%)	0.75	12 (11%) 6 4	43, 102, 157, 198	0
All	All	1170/1330 (87%)	0.06	37 (3%) 51 36	24, 57, 138, 222	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	536	LEU	5.8
2	C	139	THR	4.9
2	D	137	ASN	4.7
1	A	535	ALA	4.7
1	B	83	PRO	4.6
2	D	40	CYS	4.3
2	D	130	PRO	4.2
2	C	133	SER	3.6
2	D	67	ASN	3.4
2	C	118	LEU	3.4
2	D	119	TYR	3.4
2	D	54	LEU	3.3
1	B	84	ASN	3.3
2	C	134	SER	3.2
2	D	68	ASP	3.1
2	D	126	TYR	2.9
1	A	83	PRO	2.9
2	C	119	TYR	2.8
1	A	537	HIS	2.7
2	D	133	SER	2.7
2	D	136	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	467	GLU	2.6
2	C	126	TYR	2.6
1	A	440	THR	2.5
1	B	61	PRO	2.5
1	A	46	MET	2.5
2	C	117	GLY	2.4
2	D	139	THR	2.4
2	C	137	ASN	2.4
2	C	140	MET	2.4
1	B	31	LEU	2.4
1	A	528	ASP	2.3
2	C	116	GLU	2.2
1	B	43	ASP	2.2
2	D	117	GLY	2.2
2	C	136	ALA	2.1
1	A	532	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	NAG	B	1078	14/15	0.54	0.65	-	152,159,161,162	0
5	NAG	A	1208	14/15	0.85	0.38	-	88,93,100,104	0
5	NAG	B	1209	14/15	0.81	0.43	-	113,118,119,119	0
4	NAG	A	1078	14/15	0.74	0.48	-	134,138,144,151	0
4	BMA	A	1079	11/12	0.59	0.73	-	156,164,172,172	0
5	NAG	B	1077	14/15	0.76	0.31	-	115,122,133,143	0
4	NAG	A	1077	14/15	0.80	0.26	-	97,105,115,124	0
5	NAG	B	1208	14/15	0.87	0.41	-	90,98,103,109	0
5	NAG	A	1209	14/15	0.75	0.35	-	107,109,111,111	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	1063	14/15	0.79	0.30	-	89,97,100,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.