wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 03:20 PM GMT

PDB ID	:	4BSS
Title	:	Structure of the ectodomain of LGR5 in complex with R-spondin-1 (Fu1Fu2) in P21 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 wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

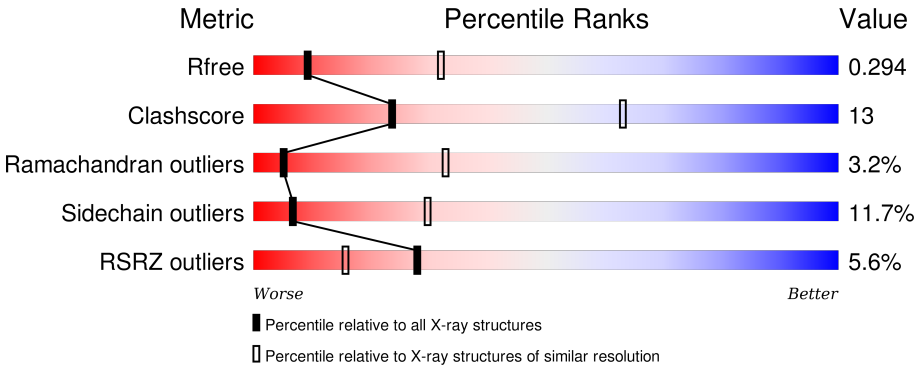
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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 <=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	% 59% 24% • • 14%
1	B	539	% 57% 25% • 13%
1	E	539	5% 48% 32% 7% 13%
1	F	539	3% 56% 26% • 14%
2	C	126	13% 54% 22% 6% 18%

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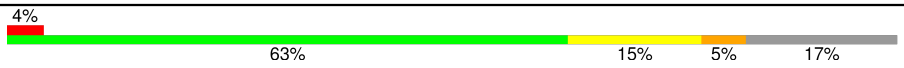
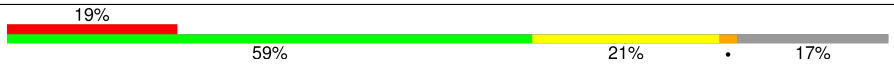
Mol	Chain	Length	Quality of chain
2	D	126	
2	G	126	
2	H	126	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1208	X	-	-	-
3	NAG	E	1063	-	-	-	X
3	NAG	E	1064	-	-	-	X
4	NAG	F	1077	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17925 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	466	Total	C	N	O	S	68	0	0
			3653	2328	627	682	16			
1	B	469	Total	C	N	O	S	42	0	0
			3671	2342	633	679	17			
1	E	468	Total	C	N	O	S	53	0	0
			3672	2339	630	686	17			
1	F	464	Total	C	N	O	S	46	0	0
			3637	2320	626	674	17			

There are 68 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

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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	19	GLN	-	EXPRESSION TAG	UNP O75473
F	20	GLY	-	EXPRESSION TAG	UNP O75473
F	21	SER	-	EXPRESSION TAG	UNP O75473
F	544	ALA	-	EXPRESSION TAG	UNP O75473
F	545	ALA	-	EXPRESSION TAG	UNP O75473
F	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			
2	G	103	Total	C	N	O	S	0	0	0
			778	480	137	143	18			
2	H	104	Total	C	N	O	S	0	0	0
			784	483	138	145	18			

There are 40 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

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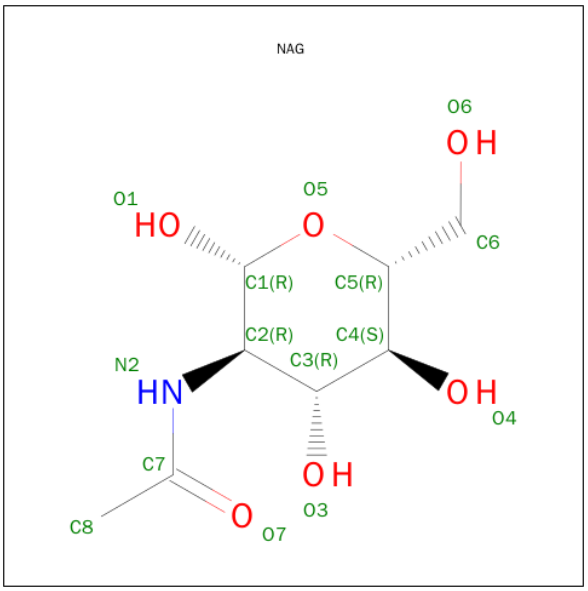
Chain	Residue	Modelled	Actual	Comment	Reference
G	29	GLY	-	EXPRESSION TAG	UNP Q2MKA7
G	30	SER	-	EXPRESSION TAG	UNP Q2MKA7
G	147	ALA	-	EXPRESSION TAG	UNP Q2MKA7
G	148	ALA	-	EXPRESSION TAG	UNP Q2MKA7
G	149	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	150	HIS	-	EXPRESSION TAG	UNP Q2MKA7
G	151	HIS	-	EXPRESSION TAG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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

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



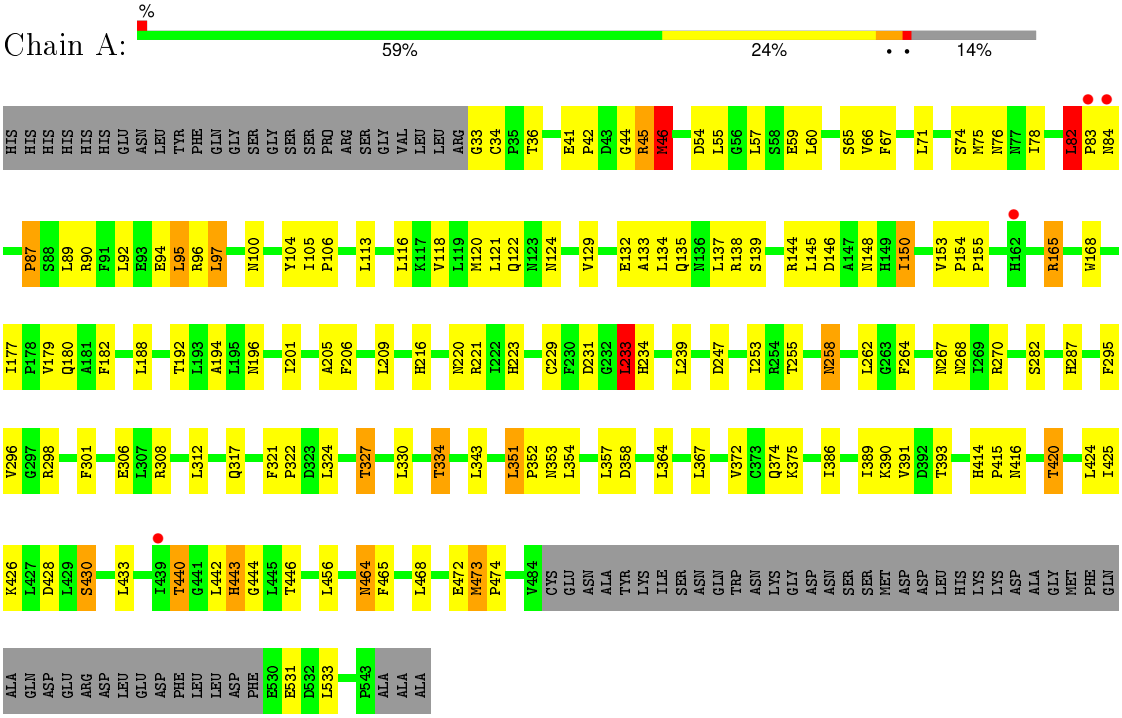
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	F	1	Total C N O 14 8 1 5	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

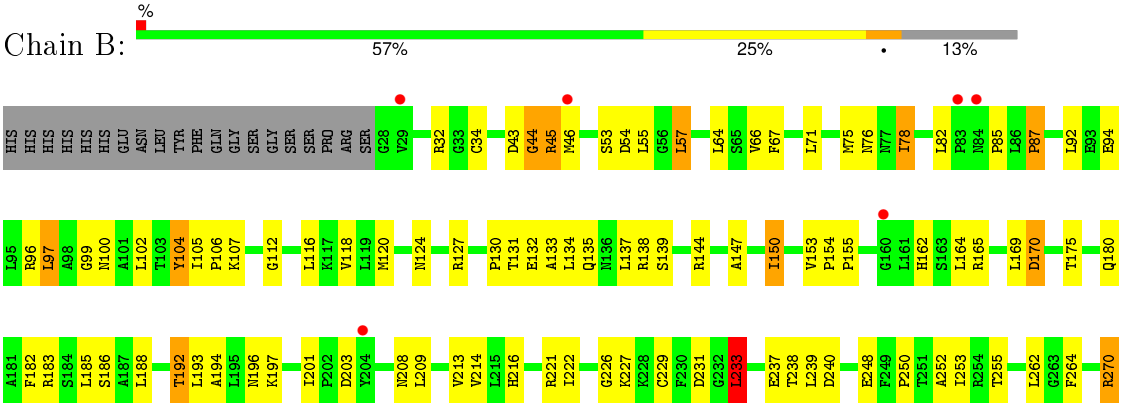
• Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5

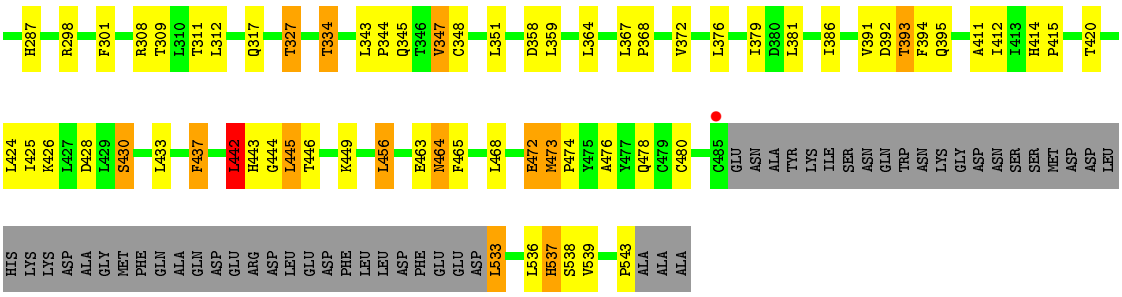
Chain A:



• Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5

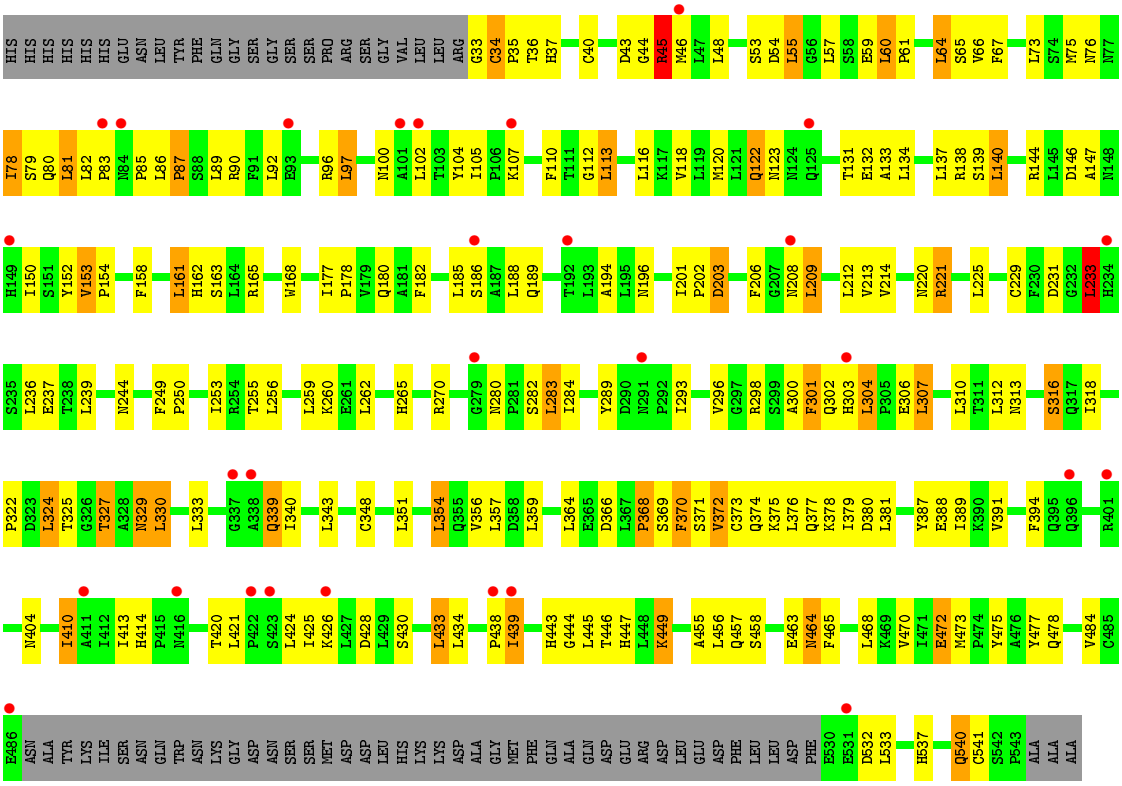
Chain B:





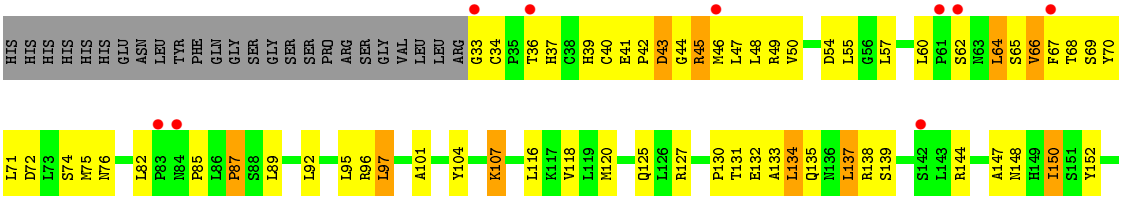
• Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5

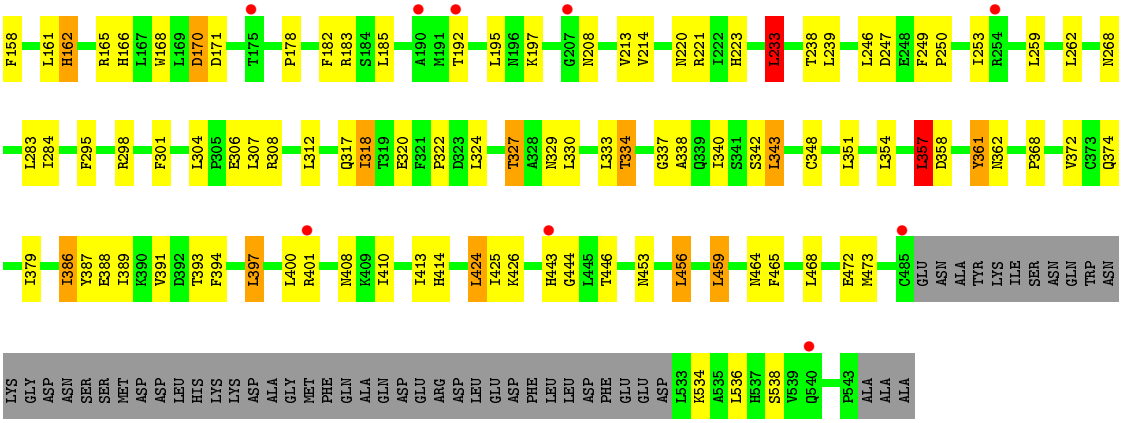
Chain E:



• Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5

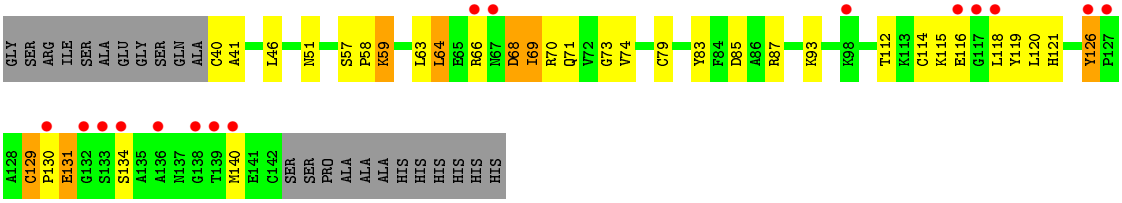
Chain F:





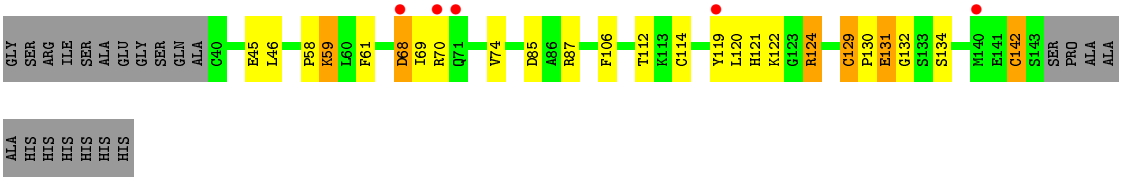
• Molecule 2: R-SPONDIN-1

Chain C:



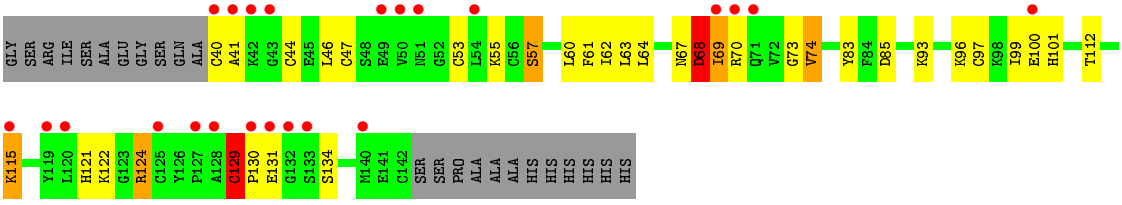
• Molecule 2: R-SPONDIN-1

Chain D:



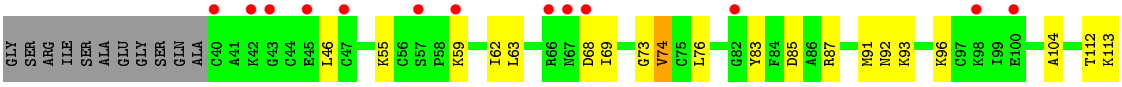
• Molecule 2: R-SPONDIN-1

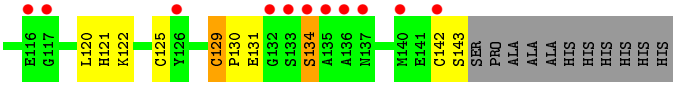
Chain G:



• Molecule 2: R-SPONDIN-1

Chain H:




E116
G117
L120
H121
K122
C125
Y126
C129
P130
E131
G132
S133
S134
A135
A136
N137
M140
E141
C142
S143
SER
PRO
ALA
ALA
ALA
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.36Å 111.30Å 130.61Å 90.00° 109.19° 90.00°	Depositor
Resolution (Å)	28.90 – 3.20 28.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (28.90-3.20) 97.1 (28.90-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 3.18Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.246 , 0.290 0.249 , 0.294	Depositor DCC
R_{free} test set	2660 reflections (5.09%)	DCC
Wilson B-factor (Å^2)	87.3	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 80.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 52320 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	17925	wwPDB-VP
Average B, all atoms (Å^2)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.27	0/3734	0.58	3/5085 (0.1%)
1	B	0.27	0/3752	0.55	2/5109 (0.0%)
1	E	0.27	0/3753	0.61	1/5109 (0.0%)
1	F	0.27	0/3718	0.57	1/5062 (0.0%)
2	C	0.29	0/794	0.59	0/1066
2	D	0.27	0/800	0.54	0/1074
2	G	0.27	0/794	0.55	0/1066
2	H	0.29	0/800	0.56	0/1074
All	All	0.27	0/18145	0.57	7/24645 (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
3	A	1	0

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	533	LEU	CA-CB-CG	6.58	130.44	115.30
1	A	82	LEU	CA-CB-CG	6.57	130.40	115.30
1	B	442	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	433	LEU	CA-CB-CG	5.76	128.56	115.30
1	E	354	LEU	CA-CB-CG	5.58	128.14	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1208	NAG	C1

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3653	0	3652	74	9
1	B	3671	0	3685	94	0
1	E	3672	0	3674	142	1
1	F	3637	0	3652	96	8
2	C	778	0	744	22	0
2	D	784	0	749	16	0
2	G	778	0	744	21	0
2	H	784	0	749	20	0
3	A	56	0	50	0	0
3	B	28	0	25	0	0
3	E	28	0	25	0	0
4	B	28	0	26	2	0
4	E	14	0	13	1	0
4	F	14	0	13	0	0
All	All	17925	0	17801	467	9

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 13.

The worst 5 of 467 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:F:408:ASN:HD21	1:F:410:ILE:HG13	1.23	1.01
1:E:343:LEU:HD11	1:E:368:PRO:HG3	1.53	0.87
1:A:282:SER:HA	1:A:306:GLU:HG3	1.58	0.86
1:E:259:LEU:HD13	1:E:262:LEU:HD11	1.57	0.85
1:B:107:LYS:HD2	1:B:132:GLU:HB2	1.57	0.85

The worst 5 of 9 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:A:531:GLU:OE2	1:F:67:PHE:CE2[1_454]	0.65	1.55
1:A:531:GLU:OE2	1:F:67:PHE:CZ[1_454]	0.80	1.40
1:A:531:GLU:CD	1:F:67:PHE:CE2[1_454]	1.47	0.73
1:A:531:GLU:CD	1:F:67:PHE:CZ[1_454]	1.67	0.53
1:A:531:GLU:OE2	1:F:67:PHE:CD2[1_454]	1.91	0.29

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	462/539 (86%)	383 (83%)	69 (15%)	10 (2%)	8	45
1	B	465/539 (86%)	385 (83%)	67 (14%)	13 (3%)	6	37
1	E	464/539 (86%)	386 (83%)	61 (13%)	17 (4%)	4	29
1	F	460/539 (85%)	377 (82%)	69 (15%)	14 (3%)	5	35
2	C	101/126 (80%)	81 (80%)	16 (16%)	4 (4%)	4	27
2	D	102/126 (81%)	81 (79%)	16 (16%)	5 (5%)	3	22
2	G	101/126 (80%)	79 (78%)	18 (18%)	4 (4%)	4	27
2	H	102/126 (81%)	82 (80%)	15 (15%)	5 (5%)	3	22
All	All	2257/2660 (85%)	1854 (82%)	331 (15%)	72 (3%)	5	33

5 of 72 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	133	ALA
1	A	138	ARG
1	B	45	ARG
1	B	54	ASP

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	421/484 (87%)	378 (90%)	43 (10%)	9 36
1	B	423/484 (87%)	374 (88%)	49 (12%)	7 30
1	E	424/484 (88%)	362 (85%)	62 (15%)	4 19
1	F	420/484 (87%)	374 (89%)	46 (11%)	8 33
2	C	89/105 (85%)	77 (86%)	12 (14%)	5 22
2	D	90/105 (86%)	83 (92%)	7 (8%)	16 53
2	G	89/105 (85%)	77 (86%)	12 (14%)	5 22
2	H	90/105 (86%)	82 (91%)	8 (9%)	12 44
All	All	2046/2356 (87%)	1807 (88%)	239 (12%)	7 30

5 of 239 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	124	ARG
1	E	209	LEU
2	G	46	LEU
1	E	34	CYS
1	E	107	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	135	GLN
1	F	135	GLN
1	E	302	GLN
1	A	355	GLN
1	E	339	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

8 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	A	1077	1,3	14,14,15	0.80	1 (7%)	15,19,21	0.57	0
3	NAG	A	1078	3	14,14,15	0.59	0	15,19,21	0.72	1 (6%)
3	NAG	A	1208	1,3	14,14,15	0.41	0	15,19,21	0.60	0
3	NAG	A	1209	3	14,14,15	0.63	0	15,19,21	0.56	0
3	NAG	B	1063	1,3	14,14,15	0.35	0	15,19,21	0.86	0
3	NAG	B	1064	3	14,14,15	0.60	0	15,19,21	0.30	0
3	NAG	E	1063	1,3	14,14,15	0.49	0	15,19,21	0.52	0
3	NAG	E	1064	3	14,14,15	0.33	0	15,19,21	0.53	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	1077	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1078	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1208	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	1209	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1063	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1064	3	-	0/6/23/26	0/1/1/1
3	NAG	E	1063	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	1064	3	-	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)
3	A	1077	NAG	C1-C2	2.77	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1078	NAG	C1-O5-C5	2.22	115.06	112.25

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.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	NAG	B	1077	1	14,14,15	0.43	0	15,19,21	1.05	1 (6%)
4	NAG	B	1208	1	14,14,15	0.53	0	15,19,21	0.36	0
4	NAG	E	1077	1	14,14,15	0.69	0	15,19,21	0.35	0
4	NAG	F	1077	1	14,14,15	0.74	1 (7%)	15,19,21	1.24	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	B	1077	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1208	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1077	1	-	0/6/23/26	0/1/1/1
4	NAG	F	1077	1	1/1/5/7	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)
4	F	1077	NAG	O5-C1	-2.44	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1077	NAG	C2-N2-C7	-2.92	119.28	123.04
4	F	1077	NAG	C3-C4-C5	3.67	116.59	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	1077	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1077	NAG	1	0
4	B	1208	NAG	1	0
4	E	1077	NAG	1	0

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, 95^{th} 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%)	-0.23	4 (0%) 85 78	36, 85, 149, 296	0
1	B	463/539 (85%)	-0.29	7 (1%) 76 63	42, 86, 161, 250	0
1	E	462/539 (85%)	0.26	29 (6%) 23 13	72, 152, 223, 276	1 (0%)
1	F	458/539 (84%)	0.07	18 (3%) 43 28	89, 143, 196, 310	0
2	C	103/126 (81%)	0.49	16 (15%) 3 2	64, 120, 210, 233	0
2	D	104/126 (82%)	0.12	5 (4%) 34 21	64, 113, 205, 350	0
2	G	103/126 (81%)	1.28	23 (22%) 1 1	112, 173, 257, 293	0
2	H	104/126 (82%)	1.10	24 (23%) 1 1	97, 160, 240, 267	0
All	All	2254/2660 (84%)	0.10	126 (5%) 28 16	36, 125, 210, 350	1 (0%)

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	83	PRO	9.1
1	A	83	PRO	9.1
2	G	70	ARG	7.9
2	G	71	GLN	7.1
2	G	127	PRO	7.1

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, 95^{th} 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(Å^2)	Q<0.9
3	NAG	E	1063	14/15	0.71	0.49	4.22	191,204,213,213	0
3	NAG	E	1064	14/15	0.66	0.98	2.59	202,216,225,228	0
3	NAG	A	1077	14/15	0.80	0.49	-	141,178,197,205	0
3	NAG	B	1064	14/15	0.62	0.74	-	219,230,233,235	0
3	NAG	A	1209	14/15	0.57	0.68	-	173,191,200,201	0
3	NAG	B	1063	14/15	0.60	0.58	-	174,189,216,220	0
3	NAG	A	1078	14/15	0.71	0.65	-	188,200,224,227	0
3	NAG	A	1208	14/15	0.44	0.53	-	167,181,192,200	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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(Å^2)	Q<0.9
4	NAG	F	1077	14/15	0.50	0.55	-	148,163,167,172	0
4	NAG	E	1077	14/15	0.80	0.35	-	169,181,184,186	0
4	NAG	B	1077	14/15	0.81	0.35	-	109,149,161,170	0
4	NAG	B	1208	14/15	0.55	0.54	-	144,191,199,206	0

6.5 Other polymers

There are no such residues in this entry.