



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:19 AM GMT

PDB ID : 4BSU  
Title : Structure of the ectodomain of LGR5 in complex with R-spondin-1 (Fu1Fu2) in C2 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 validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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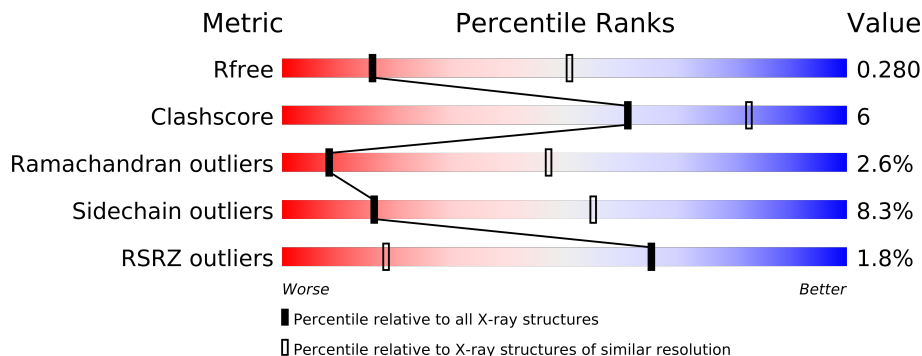
The following versions of software and data (see [references](#)) were used in the production of this report:

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  $\geq 3$ , 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	
1	E	539	
1	F	539	
2	C	126	
2	D	126	
2	G	126	
2	H	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
5	NAG	B	1077	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
5	NAG	F	1077	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17955 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	474	Total	C	N	O	S	118	0	0
			3725	2377	639	692	17			
1	B	471	Total	C	N	O	S	107	0	0
			3698	2359	633	689	17			
1	E	462	Total	C	N	O	S	0	0	0
			3616	2303	622	674	17			
1	F	463	Total	C	N	O	S	0	0	0
			3630	2313	627	673	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
			772	477	134	143	18			
2	H	104	Total	C	N	O	S	0	0	0
			779	480	137	144	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		

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 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		
4	E	3	Total	C	N	O	0	0
			39	22	2	15		
4	F	3	Total	C	N	O	0	0
			39	22	2	15		

There are 51 discrepancies between the modelled and reference sequences:

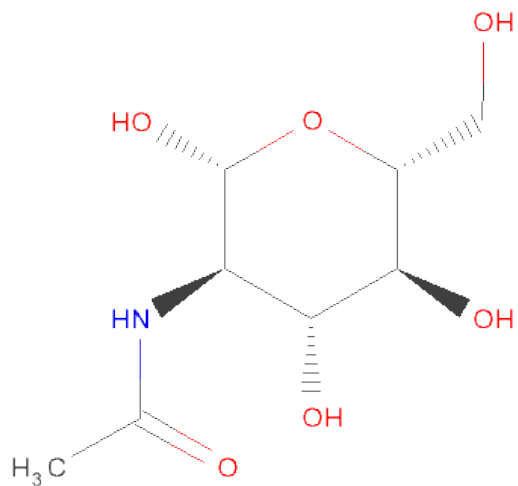
Chain	Residue	Modelled	Actual	Comment	Reference
A	8	HIS	-	EXPRESSION TAG	UNP O75473
A	9	HIS	-	EXPRESSION TAG	UNP O75473
A	10	HIS	-	EXPRESSION TAG	UNP O75473
A	11	HIS	-	EXPRESSION TAG	UNP O75473
A	12	HIS	-	EXPRESSION TAG	UNP O75473
A	13	HIS	-	EXPRESSION TAG	UNP O75473
A	14	GLU	-	EXPRESSION TAG	UNP O75473
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
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

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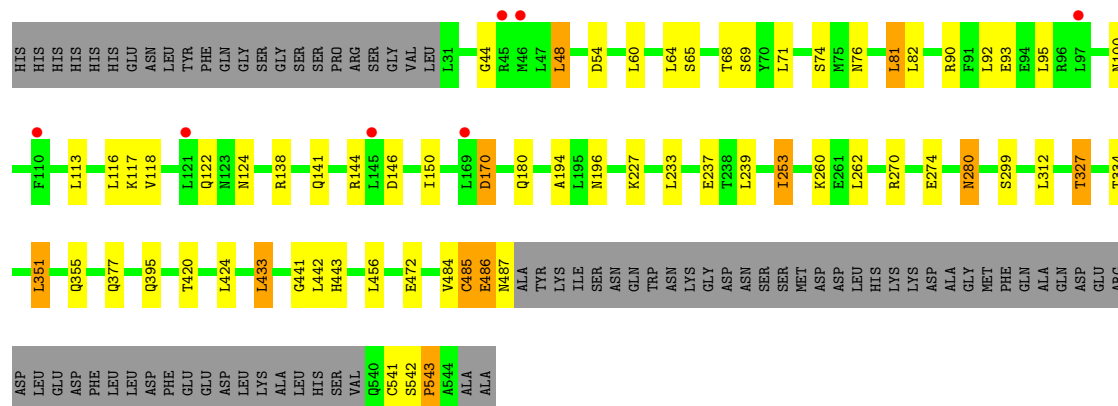
Chain	Residue	Modelled	Actual	Comment	Reference
E	14	GLU	-	EXPRESSION TAG	UNP O75473
E	15	ASN	-	EXPRESSION TAG	UNP O75473
E	16	LEU	-	EXPRESSION TAG	UNP O75473
E	17	TYR	-	EXPRESSION TAG	UNP O75473
E	18	PHE	-	EXPRESSION TAG	UNP O75473
E	19	GLN	-	EXPRESSION TAG	UNP O75473
E	20	GLY	-	EXPRESSION TAG	UNP O75473
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
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 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

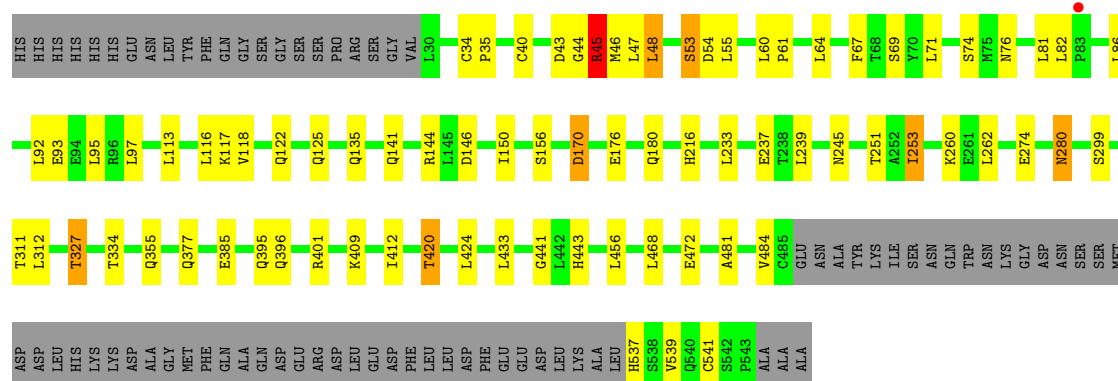




# Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR

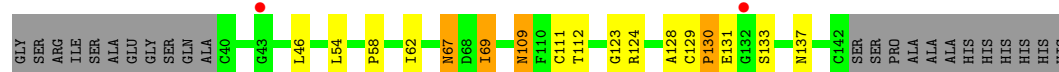
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Chain F:



# 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: 

GLY	SER	ARG	ILE	SER	ALA	GLU	GLY	SER	GLN	ALA	C40	C47	K55	F58	I62	R66	N67	D68	R87	E103	N109	F110	C111	T112	K113	G123	A128	C129	P130	E131	G132	S133	N137	C142	S143	SER	PRO	ALA	ALA	ALA	HIS	HIS	HIS	HIS	HIS
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## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	495.13Å 62.15Å 104.87Å 90.00° 91.19° 90.00°	Depositor
Resolution (Å)	65.50 – 3.20 97.27 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (65.50-3.20) 93.6 (97.27-3.20)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.2.1309)	Depositor
R, $R_{free}$	0.240 , 0.287 0.233 , 0.280	Depositor DCC
$R_{free}$ test set	2537 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	94.8	Xtriage
Anisotropy	0.938	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 75.2	EDS
Estimated twinning fraction	0.039 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 50116 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	17955	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	0.24	0/3808	0.54	3/5183 (0.1%)
1	B	0.24	0/3780	0.52	0/5146
1	E	0.24	0/3696	0.74	8/5033 (0.2%)
1	F	0.25	0/3710	0.53	0/5049
2	C	0.28	0/794	0.59	1/1066 (0.1%)
2	D	0.28	0/800	0.58	1/1074 (0.1%)
2	G	0.29	0/788	0.59	1/1059 (0.1%)
2	H	0.29	0/795	0.61	1/1067 (0.1%)
All	All	0.25	0/18171	0.59	15/24677 (0.1%)

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	E	0	1

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	543	PRO	CA-C-O	-29.91	48.41	120.20
1	E	543	PRO	CA-C-N	15.20	150.63	117.20
1	E	543	PRO	O-C-N	-12.79	102.23	122.70
1	E	44	GLY	N-CA-C	-5.90	98.36	113.10
1	E	351	LEU	CA-CB-CG	5.70	128.41	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	543	PRO	Mainchain

## 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	3725	0	0	23	0
1	B	3698	0	0	21	0
1	E	3616	0	0	23	0
1	F	3630	0	0	25	0
2	C	778	0	0	5	0
2	D	784	0	0	2	0
2	G	772	0	0	4	0
2	H	779	0	0	7	0
3	A	28	0	25	0	0
4	A	39	0	34	0	0
4	E	39	0	34	0	0
4	F	39	0	34	1	0
5	B	14	0	13	0	0
5	F	14	0	13	0	0
All	All	17955	0	153	104	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.

The worst 5 of 104 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:203:ASP:OD2	1:E:270:ARG:NH2	2.12	0.83
1:F:53:SER:O	1:F:55:LEU:N	2.23	0.70
1:F:170:ASP:N	1:F:170:ASP:OD1	2.26	0.68
1:B:53:SER:O	1:B:76:ASN:ND2	2.27	0.68
1:B:170:ASP:OD1	1:B:170:ASP:N	2.27	0.67

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	470/539 (87%)	424 (90%)	44 (9%)	2 (0%)	43	88
1	B	467/539 (87%)	406 (87%)	52 (11%)	9 (2%)	12	59
1	E	458/539 (85%)	415 (91%)	39 (8%)	4 (1%)	25	76
1	F	459/539 (85%)	407 (89%)	43 (9%)	9 (2%)	11	56
2	C	101/126 (80%)	86 (85%)	7 (7%)	8 (8%)	1	11
2	D	102/126 (81%)	86 (84%)	7 (7%)	9 (9%)	1	8
2	G	101/126 (80%)	85 (84%)	8 (8%)	8 (8%)	1	11
2	H	102/126 (81%)	84 (82%)	9 (9%)	9 (9%)	1	8
All	All	2260/2660 (85%)	1993 (88%)	209 (9%)	58 (3%)	8	47

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	35	PRO
1	B	36	THR
2	C	69	ILE
2	C	128	ALA
2	C	129	CYS

### 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	429/484 (89%)	392 (91%)	37 (9%)	15	52
1	B	427/484 (88%)	388 (91%)	39 (9%)	14	47
1	E	416/484 (86%)	383 (92%)	33 (8%)	18	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	418/484 (86%)	376 (90%)	42 (10%)	11	41
2	C	89/105 (85%)	84 (94%)	5 (6%)	30	75
2	D	90/105 (86%)	85 (94%)	5 (6%)	30	75
2	G	88/105 (84%)	84 (96%)	4 (4%)	38	81
2	H	88/105 (84%)	83 (94%)	5 (6%)	29	74
All	All	2045/2356 (87%)	1875 (92%)	170 (8%)	16	55

5 of 170 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	62	ILE
1	E	93	GLU
1	F	468	LEU
2	C	109	ASN
1	E	48	LEU

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 ⓘ

11 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	12,14,15	0.27	0	15,19,21	0.68	0
3	NAG	A	1078	3	12,14,15	0.27	0	15,19,21	0.38	0
4	NAG	A	1208	1,4	12,14,15	0.34	0	15,19,21	0.83	0
4	NAG	A	1209	4	12,14,15	0.41	0	15,19,21	0.84	0
4	BMA	A	1210	4	10,11,12	0.42	0	11,15,17	0.73	0
4	NAG	E	1208	1,4	12,14,15	0.37	0	15,19,21	0.64	0
4	NAG	E	1209	4	12,14,15	0.23	0	15,19,21	0.39	0
4	BMA	E	1210	4	10,11,12	0.80	0	11,15,17	0.80	0
4	NAG	F	1208	1,4	12,14,15	0.23	0	15,19,21	0.54	0
4	NAG	F	1209	4	12,14,15	0.33	0	15,19,21	0.88	1 (6%)
4	BMA	F	1210	4	10,11,12	0.64	0	11,15,17	0.74	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
4	NAG	A	1208	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1209	4	-	0/6/23/26	0/1/1/1
4	BMA	A	1210	4	-	0/2/19/22	0/1/1/1
4	NAG	E	1208	1,4	-	0/6/23/26	0/1/1/1
4	NAG	E	1209	4	-	0/6/23/26	0/1/1/1
4	BMA	E	1210	4	-	0/2/19/22	0/1/1/1
4	NAG	F	1208	1,4	-	0/6/23/26	0/1/1/1
4	NAG	F	1209	4	-	0/6/23/26	0/1/1/1
4	BMA	F	1210	4	-	0/2/19/22	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(°)
4	F	1209	NAG	O5-C5-C4	-2.11	107.98	110.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

2 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	$\# Z  > 2$
5	NAG	B	1077	1	12,14,15	0.27	0	15,19,21	0.26	0
5	NAG	F	1077	1	12,14,15	0.26	0	15,19,21	0.27	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
5	NAG	B	1077	1	-	0/6/23/26	0/1/1/1
5	NAG	F	1077	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	460/539 (85%)	0.09	5 (1%) 77 27	75, 111, 163, 220	0
1	B	458/539 (84%)	0.24	19 (4%) 35 7	81, 140, 212, 247	0
1	E	462/539 (85%)	0.13	7 (1%) 70 21	65, 118, 173, 212	0
1	F	463/539 (85%)	0.07	1 (0%) 93 66	67, 109, 158, 252	0
2	C	103/126 (81%)	0.08	2 (1%) 64 18	99, 146, 212, 291	0
2	D	104/126 (82%)	0.23	3 (2%) 49 10	110, 180, 237, 288	0
2	G	103/126 (81%)	0.28	3 (2%) 49 10	91, 165, 231, 258	0
2	H	104/126 (82%)	0.05	0 100 100	74, 135, 217, 247	0
All	All	2257/2660 (84%)	0.14	40 (1%) 65 18	65, 123, 204, 291	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	46	MET	4.6
1	B	121	LEU	4.1
1	A	81	LEU	3.5
2	D	132	GLY	3.3
1	B	110	PHE	3.2

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	NAG	A	1077	14/15	0.23	3.39	183,197,210,211	0
4	NAG	A	1208	14/15	0.35	2.20	124,157,182,183	0
4	NAG	F	1208	14/15	0.22	0.28	113,137,179,189	0
4	NAG	E	1208	14/15	0.11	-0.38	106,149,169,170	0
4	BMA	E	1210	11/12	0.20	-1.36	146,179,203,205	0
3	NAG	A	1078	14/15	0.51	-	209,218,221,223	0
4	BMA	F	1210	11/12	0.16	-	169,183,198,200	0
4	NAG	A	1209	14/15	0.35	-	196,208,220,222	0
4	NAG	E	1209	14/15	0.12	-	134,155,165,172	0
4	NAG	F	1209	14/15	0.26	-	182,194,202,205	0
4	BMA	A	1210	11/12	0.41	-	216,222,226,228	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	F	1077	14/15	0.30	10.59	169,175,193,196	0
5	NAG	B	1077	14/15	0.32	2.47	144,180,196,201	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.