



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2016 – 04:28 PM EDT

PDB ID : 5L3S  
Title : Structure of the GTPase heterodimer of crenarchaeal SRP54 and FtsY  
Authors : Bange, G.; Wild, K.; Sinning, I.  
Deposited on : 2016-05-24  
Resolution : 1.90 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](mailto: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.

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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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
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) : rb-20027790

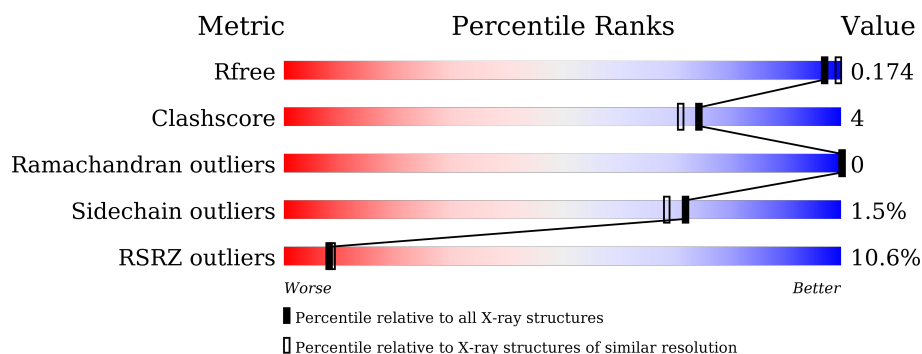
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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	298	<div> <div>7%</div> <div>83%</div> <div>9%</div> <div>8%</div> </div>
1	C	298	<div> <div>19%</div> <div>78%</div> <div>12%</div> <div>9%</div> </div>
1	E	298	<div> <div>11%</div> <div>83%</div> <div>7%</div> <div>9%</div> </div>
1	G	298	<div> <div>5%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
2	B	296	<div> <div>6%</div> <div>87%</div> <div>9%</div> <div>•</div> </div>
2	D	296	<div> <div>13%</div> <div>82%</div> <div>9%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	296	
2	H	296	

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
5	G	A	303	-	-	-	X
5	G	C	303	-	-	-	X
5	G	G	303	-	-	-	X
6	GOL	A	304	-	-	-	X
6	GOL	A	306	-	-	-	X
6	GOL	B	404	-	-	-	X
6	GOL	B	406	-	-	-	X
6	GOL	C	305	-	-	-	X
6	GOL	E	305	-	-	-	X
6	GOL	H	403	-	-	-	X
7	SO4	A	309	-	-	-	X
7	SO4	B	407	-	-	-	X
7	SO4	E	306	-	-	-	X
7	SO4	G	307	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 19033 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 Signal recognition particle 54 kDa protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	2	0
			2142	1380	353	404	5			
1	C	270	Total	C	N	O	S	0	2	0
			2110	1360	346	399	5			
1	E	271	Total	C	N	O	S	0	1	0
			2115	1362	349	399	5			
1	G	277	Total	C	N	O	S	0	0	0
			2150	1383	355	407	5			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q97ZE7
A	-4	HIS	-	expression tag	UNP Q97ZE7
A	-3	HIS	-	expression tag	UNP Q97ZE7
A	-2	HIS	-	expression tag	UNP Q97ZE7
A	-1	HIS	-	expression tag	UNP Q97ZE7
A	0	HIS	-	expression tag	UNP Q97ZE7
C	-5	HIS	-	expression tag	UNP Q97ZE7
C	-4	HIS	-	expression tag	UNP Q97ZE7
C	-3	HIS	-	expression tag	UNP Q97ZE7
C	-2	HIS	-	expression tag	UNP Q97ZE7
C	-1	HIS	-	expression tag	UNP Q97ZE7
C	0	HIS	-	expression tag	UNP Q97ZE7
E	-5	HIS	-	expression tag	UNP Q97ZE7
E	-4	HIS	-	expression tag	UNP Q97ZE7
E	-3	HIS	-	expression tag	UNP Q97ZE7
E	-2	HIS	-	expression tag	UNP Q97ZE7
E	-1	HIS	-	expression tag	UNP Q97ZE7
E	0	HIS	-	expression tag	UNP Q97ZE7
G	-5	HIS	-	expression tag	UNP Q97ZE7
G	-4	HIS	-	expression tag	UNP Q97ZE7
G	-3	HIS	-	expression tag	UNP Q97ZE7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-2	HIS	-	expression tag	UNP Q97ZE7
G	-1	HIS	-	expression tag	UNP Q97ZE7
G	0	HIS	-	expression tag	UNP Q97ZE7

- Molecule 2 is a protein called Signal recognition particle receptor FtsY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	283	Total	C	N	O	S	0	1	0
			2235	1429	374	429	3			
2	D	271	Total	C	N	O	S	0	1	0
			2128	1361	352	412	3			
2	F	283	Total	C	N	O	S	0	0	0
			2228	1426	371	428	3			
2	H	278	Total	C	N	O	S	0	2	0
			2198	1406	367	422	3			

There are 28 discrepancies between the modelled and reference sequences:

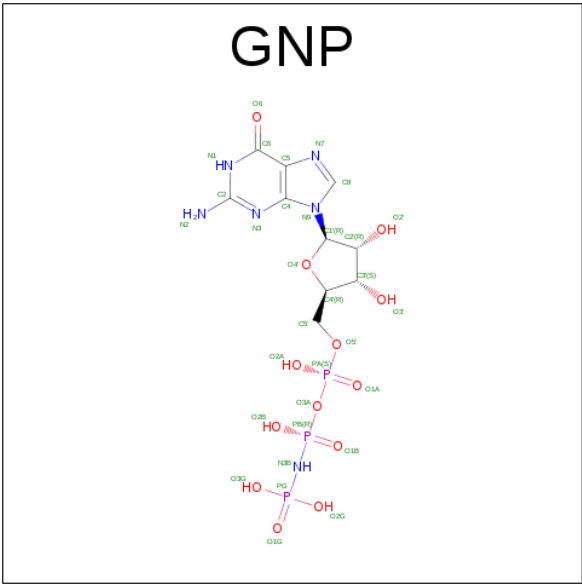
Chain	Residue	Modelled	Actual	Comment	Reference
B	73	HIS	-	expression tag	UNP P27414
B	74	HIS	-	expression tag	UNP P27414
B	75	HIS	-	expression tag	UNP P27414
B	76	HIS	-	expression tag	UNP P27414
B	77	HIS	-	expression tag	UNP P27414
B	78	HIS	-	expression tag	UNP P27414
B	279	LYS	ARG	conflict	UNP P27414
D	73	HIS	-	expression tag	UNP P27414
D	74	HIS	-	expression tag	UNP P27414
D	75	HIS	-	expression tag	UNP P27414
D	76	HIS	-	expression tag	UNP P27414
D	77	HIS	-	expression tag	UNP P27414
D	78	HIS	-	expression tag	UNP P27414
D	279	LYS	ARG	conflict	UNP P27414
F	73	HIS	-	expression tag	UNP P27414
F	74	HIS	-	expression tag	UNP P27414
F	75	HIS	-	expression tag	UNP P27414
F	76	HIS	-	expression tag	UNP P27414
F	77	HIS	-	expression tag	UNP P27414
F	78	HIS	-	expression tag	UNP P27414
F	279	LYS	ARG	conflict	UNP P27414
H	73	HIS	-	expression tag	UNP P27414
H	74	HIS	-	expression tag	UNP P27414

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Chain	Residue	Modelled	Actual	Comment	Reference
H	75	HIS	-	expression tag	UNP P27414
H	76	HIS	-	expression tag	UNP P27414
H	77	HIS	-	expression tag	UNP P27414
H	78	HIS	-	expression tag	UNP P27414
H	279	LYS	ARG	conflict	UNP P27414

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>13</sub>P<sub>3</sub>).

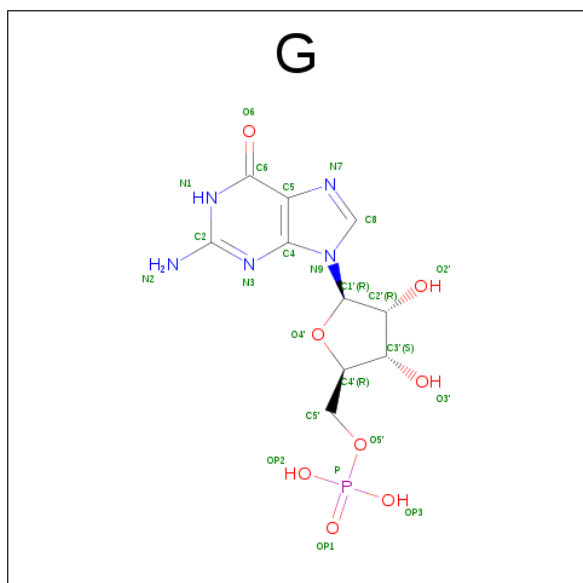


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	F	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	G	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
3	H	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		
4	H	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	A	1	Total	Mg	0	0
			1	1		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: G) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>5</sub>O<sub>8</sub>P).



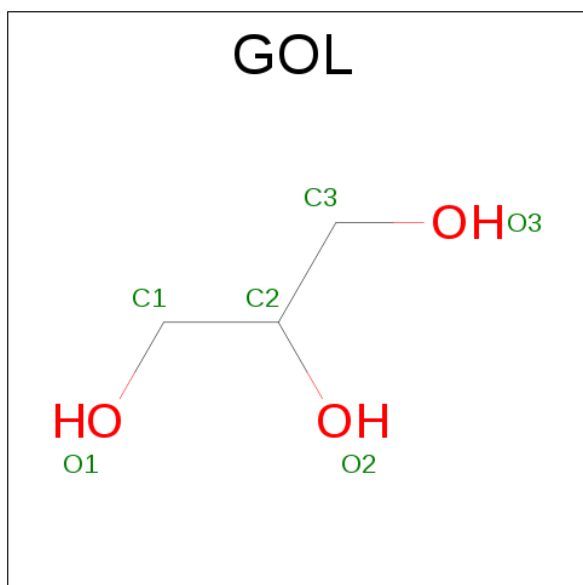
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
5	C	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			24	10	5	8	1		
5	G	1	Total	C	N	O	P	0	0
			24	10	5	8	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

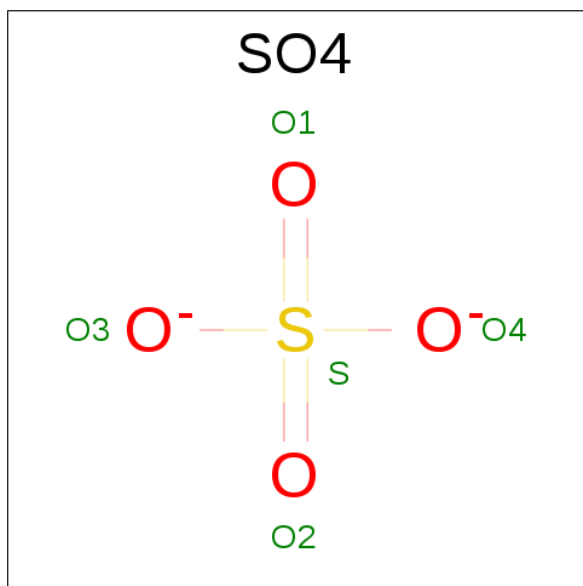
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	F	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	G	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		
6	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	C	1	Total	O	S	0	0
			5	4	1		
7	E	1	Total	O	S	0	0
			5	4	1		
7	G	1	Total	O	S	0	0
			5	4	1		
7	H	1	Total	O	S	0	0
			5	4	1		

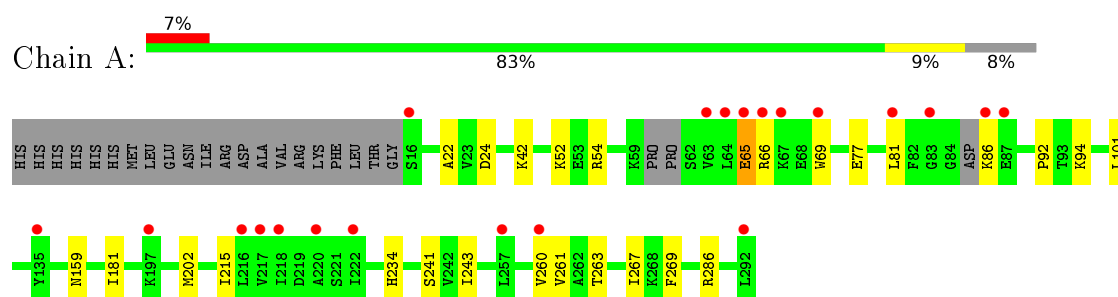
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	193	Total	O	0	0
			193	193		
8	B	190	Total	O	0	0
			190	190		
8	C	128	Total	O	0	0
			128	128		
8	D	135	Total	O	0	0
			135	135		
8	E	141	Total	O	0	0
			141	141		
8	F	106	Total	O	0	0
			106	106		
8	G	168	Total	O	0	0
			168	168		
8	H	153	Total	O	0	0
			153	153		

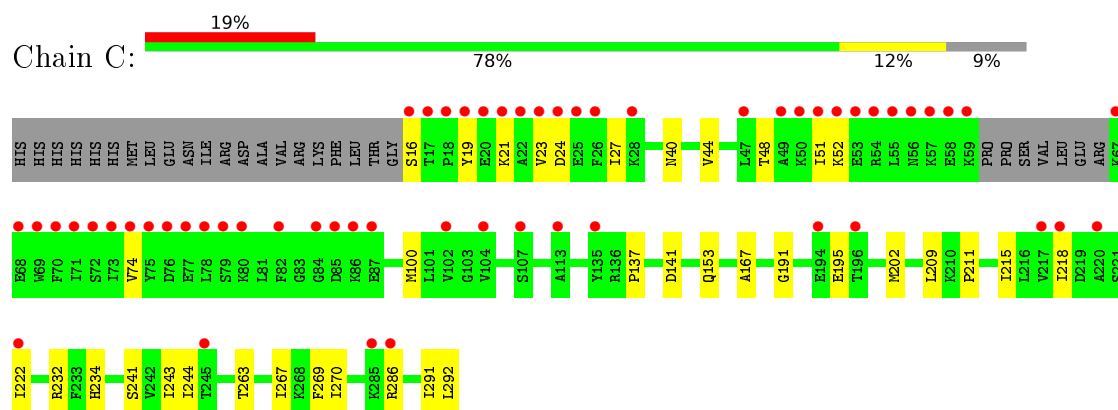
### 3 Residue-property plots [i](#)

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.

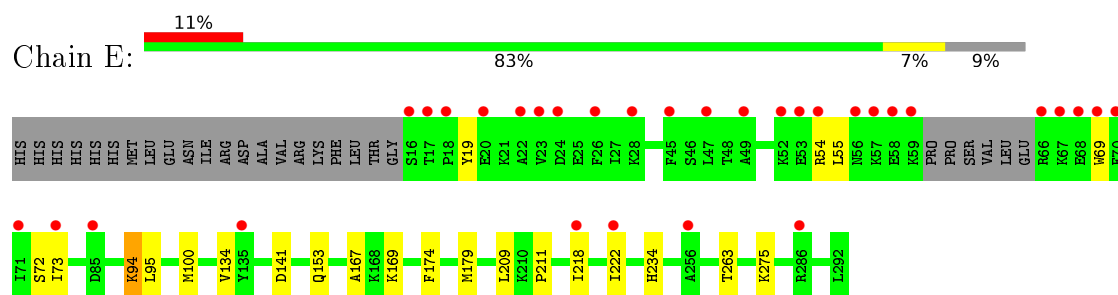
- Molecule 1: Signal recognition particle 54 kDa protein



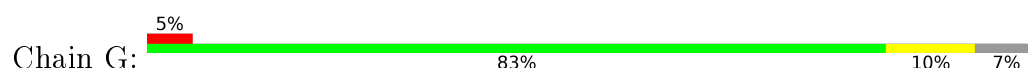
- Molecule 1: Signal recognition particle 54 kDa protein

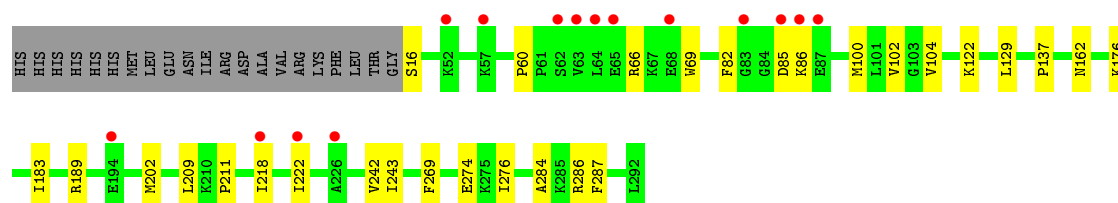


- Molecule 1: Signal recognition particle 54 kDa protein

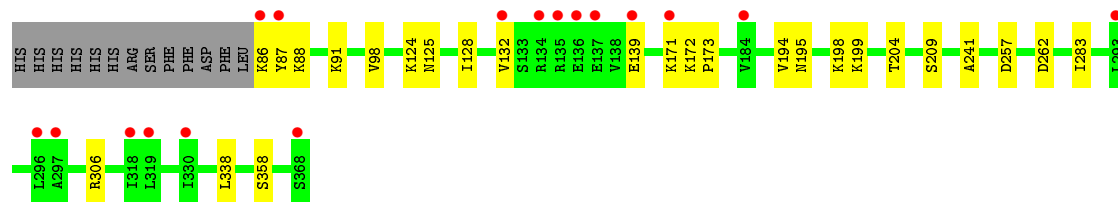
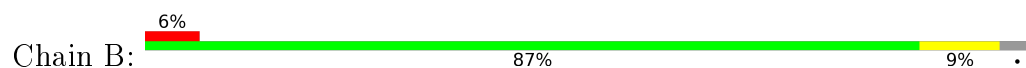


- Molecule 1: Signal recognition particle 54 kDa protein

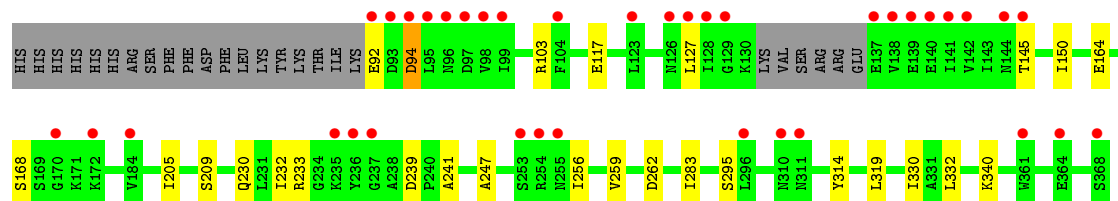
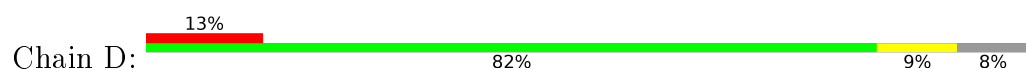




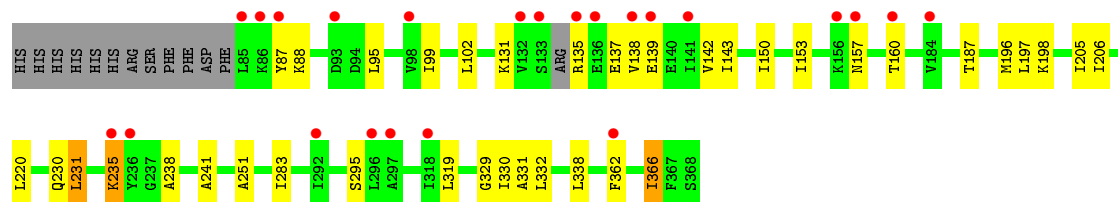
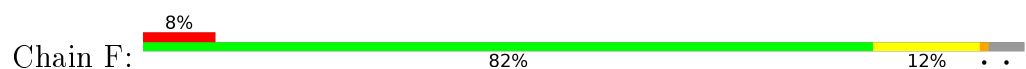
• Molecule 2: Signal recognition particle receptor FtsY



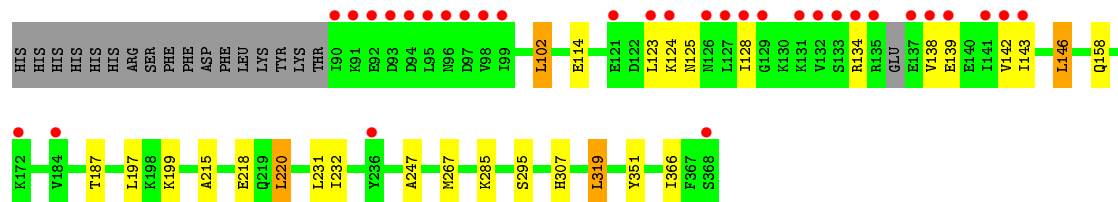
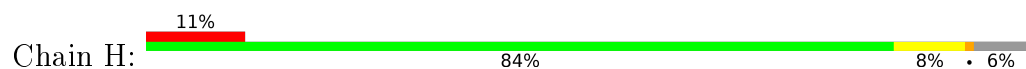
• Molecule 2: Signal recognition particle receptor FtsY



• Molecule 2: Signal recognition particle receptor FtsY



• Molecule 2: Signal recognition particle receptor FtsY



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.20 Å 199.67 Å 124.87 Å 90.00° 92.95° 90.00°	Depositor
Resolution (Å)	37.87 – 1.90 37.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (37.87-1.90) 89.8 (37.87-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 1.89 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.173 , 0.216 0.171 , 0.174	Depositor DCC
$R_{free}$ test set	3529 reflections (2.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.7	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 62.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	19033	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, GNP, SO4

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	0/2181	0.52	0/2934
1	C	0.33	0/2150	0.47	0/2894
1	E	0.34	0/2152	0.48	0/2896
1	G	0.35	0/2186	0.49	0/2946
2	B	0.37	0/2268	0.51	0/3059
2	D	0.33	0/2159	0.48	0/2915
2	F	0.32	0/2257	0.49	0/3043
2	H	0.37	0/2233	0.50	0/3010
All	All	0.35	0/17586	0.49	0/23697

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	2142	0	2217	17	0
1	C	2110	0	2180	22	0
1	E	2115	0	2185	14	0
1	G	2150	0	2222	20	0
2	B	2235	0	2310	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	2128	0	2184	15	0
2	F	2228	0	2300	21	0
2	H	2198	0	2268	18	0
3	A	32	0	13	0	0
3	B	32	0	13	0	0
3	C	32	0	13	0	0
3	D	32	0	13	0	0
3	E	32	0	13	0	0
3	F	32	0	13	0	0
3	G	32	0	13	0	0
3	H	32	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	24	0	12	0	0
5	C	24	0	12	1	0
5	E	24	0	12	0	0
5	G	24	0	12	1	0
6	A	18	0	24	3	0
6	B	24	0	32	1	0
6	C	12	0	16	3	0
6	D	6	0	8	0	0
6	E	12	0	16	0	0
6	F	6	0	8	0	0
6	G	18	0	24	2	0
6	H	12	0	16	1	0
7	A	15	0	0	0	0
7	B	10	0	0	0	0
7	C	5	0	0	1	0
7	E	5	0	0	0	0
7	G	5	0	0	0	0
7	H	5	0	0	0	0
8	A	193	0	0	4	0
8	B	190	0	0	5	3
8	C	128	0	0	3	0
8	D	135	0	0	2	0
8	E	141	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	106	0	0	2	3
8	G	168	0	0	6	0
8	H	153	0	0	6	0
All	All	19033	0	18162	145	3

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 4.

All (145) 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:A:202:MET:SD	8:A:567:HOH:O	2.33	0.86
1:C:153[B]:GLN:NE2	1:E:153:GLN:OE1	2.18	0.76
2:B:91:LYS:NZ	8:B:502:HOH:O	2.18	0.75
2:F:88:LYS:HG3	2:F:135:ARG:HB2	1.70	0.73
1:A:286:ARG:NH1	6:A:305:GOL:O2	2.23	0.72
2:H:114:GLU:OE2	8:H:501:HOH:O	2.09	0.69
1:G:162:ASN:OD1	8:G:401:HOH:O	2.11	0.68
1:G:102:VAL:HB	1:G:202:MET:HE2	1.74	0.68
1:A:159[A]:ASN:OD1	8:A:401:HOH:O	2.14	0.65
2:B:125:ASN:OD1	8:B:501:HOH:O	2.13	0.65
2:F:196:MET:SD	8:F:603:HOH:O	2.54	0.65
2:D:103:ARG:NH1	2:D:117:GLU:OE1	2.29	0.64
2:D:205:ILE:HG22	2:D:230:GLN:HB3	1.80	0.64
2:H:123:LEU:HD22	2:H:146:LEU:HG	1.80	0.63
1:G:176:LYS:NZ	8:G:406:HOH:O	2.33	0.61
6:C:304:GOL:O1	8:C:401:HOH:O	2.16	0.61
2:F:205:ILE:HG22	2:F:230:GLN:HB3	1.82	0.61
2:F:329:GLY:HA2	2:F:366:ILE:HD11	1.82	0.61
2:H:102:LEU:HG	2:H:146:LEU:HD12	1.83	0.61
2:F:153:ILE:O	2:F:157:ASN:ND2	2.32	0.61
2:F:187:THR:HG23	2:F:220:LEU:HD13	1.84	0.60
1:A:24:ASP:OD1	1:A:52:LYS:NZ	2.34	0.60
1:E:100:MET:HE3	1:E:211:PRO:HG3	1.84	0.60
2:H:187:THR:HG23	2:H:220:LEU:HD13	1.84	0.59
1:C:232:ARG:NH2	7:C:306:SO4:O4	2.35	0.59
1:G:286:ARG:NH1	6:G:306:GOL:O2	2.36	0.58
1:C:167:ALA:HB1	1:C:209:LEU:HD11	1.86	0.58
2:H:158:GLN:NE2	8:H:504:HOH:O	2.35	0.57
2:F:198:LYS:NZ	8:F:502:HOH:O	2.36	0.57
2:F:241:ALA:HB1	2:F:283:ILE:HD13	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ILE:HD11	1:C:222:ILE:HG21	1.87	0.56
2:B:306:ARG:NE	8:B:505:HOH:O	2.26	0.56
1:C:24:ASP:OD1	1:C:52:LYS:NZ	2.31	0.56
2:H:295:SER:HB3	2:H:319:LEU:HD12	1.87	0.56
2:D:319:LEU:HD21	2:D:330:ILE:HG21	1.87	0.55
1:C:51:ILE:HD13	1:C:74:VAL:HG22	1.89	0.55
2:B:124:LYS:O	2:B:128:ILE:HG12	2.07	0.55
2:D:314:TYR:CE2	2:D:340:LYS:HD3	2.42	0.54
1:C:16:SER:HB2	1:C:21:LYS:HE3	1.90	0.53
6:A:306:GOL:O1	8:A:402:HOH:O	2.19	0.53
2:H:139:GLU:O	2:H:143:ILE:HG12	2.09	0.53
2:H:124:LYS:O	2:H:128:ILE:HG12	2.10	0.52
2:H:267:MET:HE1	8:H:518:HOH:O	2.09	0.52
2:H:232:ILE:HG13	2:H:247:ALA:HA	1.91	0.52
1:C:291:ILE:O	1:C:292:LEU:HB2	2.10	0.52
2:D:241:ALA:HB1	2:D:283:ILE:HD12	1.90	0.52
1:A:54:ARG:NH1	1:A:77:GLU:OE2	2.41	0.52
1:C:286:ARG:NH2	8:C:412:HOH:O	2.43	0.52
1:A:260:VAL:HG21	1:A:267:ILE:HD11	1.91	0.51
1:E:54:ARG:HH11	1:E:73:ILE:HG23	1.75	0.51
1:A:243:ILE:HG12	1:A:269:PHE:HB2	1.92	0.51
2:D:164:GLU:O	2:D:168:SER:OG	2.22	0.51
1:C:270:ILE:HD13	6:C:304:GOL:H2	1.92	0.51
1:A:86:LYS:NZ	8:A:414:HOH:O	2.45	0.50
2:D:233:ARG:NH2	8:D:506:HOH:O	2.40	0.50
2:D:205:ILE:HD11	2:D:259:VAL:HG22	1.94	0.50
1:E:218:ILE:HD11	1:E:222:ILE:HG21	1.94	0.50
2:D:295:SER:HB3	2:D:319:LEU:HD22	1.94	0.50
2:H:285:LYS:NZ	8:H:507:HOH:O	2.39	0.50
1:G:243:ILE:HG12	1:G:269:PHE:HB2	1.94	0.50
1:A:22:ALA:HB1	1:A:65:GLU:HB3	1.92	0.50
2:F:235:LYS:HD2	2:F:238:ALA:HB2	1.93	0.50
2:D:150:ILE:HG23	2:D:332:LEU:HD13	1.93	0.50
2:F:205:ILE:HD11	2:F:251:ALA:HB2	1.93	0.49
1:A:215:ILE:HG12	1:A:241:SER:HB2	1.95	0.49
2:D:205:ILE:HG23	2:D:256:ILE:HG21	1.95	0.49
1:G:287:PHE:HB2	6:G:306:GOL:H11	1.94	0.49
1:A:92:PRO:HG3	1:A:181:ILE:HD11	1.95	0.49
1:C:234:HIS:HB2	1:C:263:THR:HG22	1.95	0.48
2:F:331:ALA:HB3	2:F:362:PHE:CE1	2.48	0.48
1:A:42:LYS:HB3	6:A:304:GOL:H32	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:LYS:N	2:B:132:VAL:O	2.42	0.48
2:D:92:GLU:HG2	2:D:94:ASP:HB2	1.96	0.48
1:G:82:PHE:HB2	8:G:452:HOH:O	2.13	0.48
2:F:138:VAL:O	2:F:142:VAL:HG23	2.14	0.48
1:A:234:HIS:HB2	1:A:263:THR:HG22	1.95	0.48
2:F:139:GLU:O	2:F:143:ILE:HG12	2.13	0.48
1:E:19:TYR:OH	1:E:55:LEU:O	2.23	0.47
2:F:295:SER:HB3	2:F:319:LEU:HD22	1.96	0.47
1:G:85:ASP:HA	1:G:284:ALA:HB3	1.95	0.47
1:C:100:MET:HE3	1:C:211:PRO:HG3	1.96	0.47
2:F:319:LEU:HD21	2:F:330:ILE:HG21	1.96	0.47
1:C:215:ILE:HG12	1:C:241:SER:HB2	1.95	0.47
2:H:199:LYS:NZ	8:H:505:HOH:O	2.36	0.46
1:C:243:ILE:HG12	1:C:269:PHE:HB2	1.98	0.46
1:G:122:LYS:NZ	8:G:415:HOH:O	2.49	0.46
2:B:257:ASP:OD1	6:B:405:GOL:O2	2.33	0.46
1:C:153[A]:GLN:NE2	8:C:407:HOH:O	2.38	0.46
1:G:100:MET:CE	1:G:209:LEU:HD12	2.46	0.46
1:G:100:MET:HE3	1:G:211:PRO:HG3	1.97	0.45
2:D:232:ILE:HG13	2:D:247:ALA:HA	1.98	0.45
1:G:16:SER:N	8:G:417:HOH:O	2.49	0.45
1:G:218:ILE:HD11	1:G:222:ILE:HG21	1.98	0.45
2:F:198:LYS:HE2	2:F:198:LYS:HB3	1.84	0.45
1:A:66:ARG:HG3	1:A:69:TRP:H	1.81	0.45
1:C:202:MET:HB2	1:C:202:MET:HE3	1.86	0.45
2:F:206:ILE:HB	2:F:231:LEU:HD23	1.99	0.45
2:B:241:ALA:HB1	2:B:283:ILE:HD13	1.99	0.44
1:E:169:LYS:NZ	8:E:412:HOH:O	2.48	0.44
2:B:204[A]:THR:HG22	8:B:520:HOH:O	2.17	0.44
1:C:244:ILE:HD11	1:C:267:ILE:HD13	2.00	0.44
1:G:137:PRO:HA	5:G:303:G:O3'	2.17	0.44
2:B:172:LYS:HA	2:B:173:PRO:HA	1.77	0.44
1:A:22:ALA:CB	1:A:65:GLU:HB3	2.48	0.43
2:B:194:VAL:HG13	2:B:204[A]:THR:HG21	1.99	0.43
2:F:87:TYR:CE1	2:F:131:LYS:HD2	2.54	0.43
2:H:102:LEU:HD21	2:H:143:ILE:HD13	2.00	0.43
2:B:195:ASN:O	2:B:199:LYS:HG2	2.19	0.43
1:C:137:PRO:HA	5:C:303:G:O3'	2.19	0.43
1:G:104:VAL:HA	1:G:189:ARG:O	2.19	0.43
1:G:274:GLU:OE1	8:G:402:HOH:O	2.22	0.43
2:D:127:LEU:HD21	2:D:145:THR:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:LYS:HE2	2:B:87:TYR:CZ	2.54	0.43
1:E:100:MET:HE3	1:E:211:PRO:CG	2.49	0.43
2:H:351:TYR:CD1	6:H:403:GOL:H32	2.54	0.43
2:F:150:ILE:HG23	2:F:332:LEU:HD13	2.01	0.42
2:B:306:ARG:HG2	2:B:338:LEU:HD21	2.02	0.42
1:A:101:LEU:HD23	1:A:215:ILE:HB	2.01	0.42
6:C:305:GOL:H31	8:D:607:HOH:O	2.19	0.42
2:D:209:SER:HB2	2:D:262:ASP:O	2.20	0.41
1:E:174:PHE:HB3	1:E:179:MET:HG2	2.01	0.41
2:B:98:VAL:HB	2:B:139:GLU:OE1	2.21	0.41
1:C:27:ILE:HG23	1:C:48:THR:HB	2.03	0.41
1:C:40:ASN:O	1:C:44:VAL:HG23	2.19	0.41
1:E:100:MET:HE2	1:E:209:LEU:HD12	2.02	0.41
1:E:94:LYS:O	1:E:95:LEU:HD23	2.20	0.41
2:B:171:LYS:HD3	2:B:171:LYS:HA	1.94	0.41
1:C:19:TYR:O	1:C:23:VAL:HG23	2.21	0.41
1:E:134:VAL:HG22	8:E:443:HOH:O	2.20	0.41
2:H:124:LYS:HE3	2:H:124:LYS:HB2	1.84	0.41
1:E:234:HIS:HB2	1:E:263:THR:HG22	2.03	0.41
2:F:95:LEU:O	2:F:99:ILE:HG12	2.21	0.41
2:B:209:SER:HB2	2:B:262:ASP:O	2.21	0.41
1:G:82:PHE:HE1	1:G:284:ALA:HB1	1.85	0.41
1:C:191:GLY:HA2	1:C:195:GLU:O	2.21	0.41
2:H:215:ALA:HA	2:H:218:GLU:OE1	2.21	0.41
2:B:198:LYS:HG2	8:B:520:HOH:O	2.21	0.41
2:H:125:ASN:O	8:H:503:HOH:O	2.22	0.40
1:A:81:LEU:HG	1:A:261:VAL:HG22	2.02	0.40
2:F:160:THR:OG1	1:G:86:LYS:NZ	2.55	0.40
1:G:60:PRO:HB3	1:G:69:TRP:CE3	2.56	0.40
1:G:129:LEU:HD23	1:G:183:ILE:HB	2.04	0.40
2:H:138:VAL:O	2:H:142:VAL:HG23	2.21	0.40
1:E:167:ALA:HB1	1:E:209:LEU:HD11	2.03	0.40
1:E:69:TRP:O	1:E:72:SER:OG	2.33	0.40

All (3) 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)
8:B:501:HOH:O	8:F:534:HOH:O[2_546]	2.13	0.07
8:B:502:HOH:O	8:F:599:HOH:O[2_546]	2.13	0.07
8:B:649:HOH:O	8:F:593:HOH:O[2_546]	2.19	0.01

## 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	270/298 (91%)	267 (99%)	3 (1%)	0	100	100
1	C	268/298 (90%)	267 (100%)	1 (0%)	0	100	100
1	E	268/298 (90%)	268 (100%)	0	0	100	100
1	G	275/298 (92%)	273 (99%)	2 (1%)	0	100	100
2	B	282/296 (95%)	276 (98%)	6 (2%)	0	100	100
2	D	268/296 (90%)	262 (98%)	6 (2%)	0	100	100
2	F	279/296 (94%)	273 (98%)	6 (2%)	0	100	100
2	H	276/296 (93%)	270 (98%)	6 (2%)	0	100	100
All	All	2186/2376 (92%)	2156 (99%)	30 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	232/252 (92%)	230 (99%)	2 (1%)	84	83
1	C	228/252 (90%)	227 (100%)	1 (0%)	93	94
1	E	228/252 (90%)	225 (99%)	3 (1%)	76	73
1	G	233/252 (92%)	230 (99%)	3 (1%)	76	73
2	B	247/259 (95%)	246 (100%)	1 (0%)	93	94
2	D	235/259 (91%)	233 (99%)	2 (1%)	84	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	246/259 (95%)	239 (97%)	7 (3%)	51	41
2	H	243/259 (94%)	234 (96%)	9 (4%)	41	29
All	All	1892/2044 (93%)	1864 (98%)	28 (2%)	72	69

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
1	A	94	LYS
2	B	358	SER
1	C	141	ASP
2	D	94	ASP
2	D	239	ASP
1	E	94	LYS
1	E	141	ASP
1	E	275	LYS
2	F	102	LEU
2	F	137	GLU
2	F	197	LEU
2	F	231	LEU
2	F	235	LYS
2	F	338	LEU
2	F	366	ILE
1	G	66	ARG
1	G	242	VAL
1	G	276	ILE
2	H	102	LEU
2	H	134	ARG
2	H	146	LEU
2	H	197	LEU
2	H	220	LEU
2	H	231	LEU
2	H	307	HIS
2	H	319	LEU
2	H	366	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	157	ASN

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Mol	Chain	Res	Type
1	E	177	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 47 ligands modelled in this entry, 8 are monoatomic - leaving 39 for Mogul analysis.

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	GNP	A	301	4	29,34,34	2.79	10 (34%)	28,54,54	1.89	7 (25%)
5	G	A	303	-	22,26,26	1.13	1 (4%)	25,40,40	2.63	5 (20%)
6	GOL	A	304	-	5,5,5	0.32	0	5,5,5	0.26	0
6	GOL	A	305	-	5,5,5	0.36	0	5,5,5	0.50	0
6	GOL	A	306	-	5,5,5	0.34	0	5,5,5	0.26	0
7	SO4	A	307	-	4,4,4	0.21	0	6,6,6	0.05	0
7	SO4	A	308	-	4,4,4	0.17	0	6,6,6	0.09	0
7	SO4	A	309	-	4,4,4	0.22	0	6,6,6	0.20	0
3	GNP	B	401	4	29,34,34	2.76	9 (31%)	28,54,54	1.44	2 (7%)
6	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.48	0
6	GOL	B	404	-	5,5,5	0.28	0	5,5,5	0.31	0
6	GOL	B	405	-	5,5,5	0.42	0	5,5,5	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	B	406	-	5,5,5	0.32	0	5,5,5	0.36	0
7	SO4	B	407	-	4,4,4	0.08	0	6,6,6	0.13	0
7	SO4	B	408	-	4,4,4	0.24	0	6,6,6	0.07	0
3	GNP	C	301	4	29,34,34	2.84	11 (37%)	28,54,54	2.01	6 (21%)
5	G	C	303	-	22,26,26	1.17	1 (4%)	25,40,40	2.69	3 (12%)
6	GOL	C	304	-	5,5,5	0.31	0	5,5,5	0.28	0
6	GOL	C	305	-	5,5,5	0.33	0	5,5,5	0.32	0
7	SO4	C	306	-	4,4,4	0.22	0	6,6,6	0.08	0
3	GNP	D	401	4	29,34,34	2.66	9 (31%)	28,54,54	1.71	4 (14%)
6	GOL	D	403	-	5,5,5	0.40	0	5,5,5	0.52	0
3	GNP	E	301	4	29,34,34	2.82	12 (41%)	28,54,54	1.97	7 (25%)
5	G	E	303	-	22,26,26	1.11	1 (4%)	25,40,40	2.58	4 (16%)
6	GOL	E	304	-	5,5,5	0.32	0	5,5,5	0.29	0
6	GOL	E	305	-	5,5,5	0.33	0	5,5,5	0.51	0
7	SO4	E	306	-	4,4,4	0.24	0	6,6,6	0.06	0
3	GNP	F	401	4	29,34,34	2.74	11 (37%)	28,54,54	1.66	3 (10%)
6	GOL	F	403	-	5,5,5	0.37	0	5,5,5	0.35	0
3	GNP	G	301	4	29,34,34	2.62	11 (37%)	28,54,54	1.88	7 (25%)
5	G	G	303	-	22,26,26	1.17	2 (9%)	25,40,40	2.66	4 (16%)
6	GOL	G	304	-	5,5,5	0.37	0	5,5,5	0.87	0
6	GOL	G	305	-	5,5,5	0.39	0	5,5,5	0.54	0
6	GOL	G	306	-	5,5,5	0.34	0	5,5,5	0.32	0
7	SO4	G	307	-	4,4,4	0.23	0	6,6,6	0.07	0
3	GNP	H	401	4	29,34,34	2.50	10 (34%)	28,54,54	1.60	4 (14%)
6	GOL	H	403	-	5,5,5	0.50	0	5,5,5	0.57	0
6	GOL	H	404	-	5,5,5	0.35	0	5,5,5	0.14	0
7	SO4	H	405	-	4,4,4	0.26	0	6,6,6	0.17	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	GNP	A	301	4	-	0/16/38/38	0/3/3/3
5	G	A	303	-	-	0/6/26/26	0/3/3/3
6	GOL	A	304	-	-	0/4/4/4	0/0/0/0
6	GOL	A	305	-	-	0/4/4/4	0/0/0/0
6	GOL	A	306	-	-	0/4/4/4	0/0/0/0
7	SO4	A	307	-	-	0/0/0/0	0/0/0/0
7	SO4	A	308	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	SO4	A	309	-	-	0/0/0/0	0/0/0/0
3	GNP	B	401	4	-	0/16/38/38	0/3/3/3
6	GOL	B	403	-	-	0/4/4/4	0/0/0/0
6	GOL	B	404	-	-	0/4/4/4	0/0/0/0
6	GOL	B	405	-	-	0/4/4/4	0/0/0/0
6	GOL	B	406	-	-	0/4/4/4	0/0/0/0
7	SO4	B	407	-	-	0/0/0/0	0/0/0/0
7	SO4	B	408	-	-	0/0/0/0	0/0/0/0
3	GNP	C	301	4	-	0/16/38/38	0/3/3/3
5	G	C	303	-	-	0/6/26/26	0/3/3/3
6	GOL	C	304	-	-	0/4/4/4	0/0/0/0
6	GOL	C	305	-	-	0/4/4/4	0/0/0/0
7	SO4	C	306	-	-	0/0/0/0	0/0/0/0
3	GNP	D	401	4	-	0/16/38/38	0/3/3/3
6	GOL	D	403	-	-	0/4/4/4	0/0/0/0
3	GNP	E	301	4	-	0/16/38/38	0/3/3/3
5	G	E	303	-	-	0/6/26/26	0/3/3/3
6	GOL	E	304	-	-	0/4/4/4	0/0/0/0
6	GOL	E	305	-	-	0/4/4/4	0/0/0/0
7	SO4	E	306	-	-	0/0/0/0	0/0/0/0
3	GNP	F	401	4	-	0/16/38/38	0/3/3/3
6	GOL	F	403	-	-	0/4/4/4	0/0/0/0
3	GNP	G	301	4	-	0/16/38/38	0/3/3/3
5	G	G	303	-	-	0/6/26/26	0/3/3/3
6	GOL	G	304	-	-	0/4/4/4	0/0/0/0
6	GOL	G	305	-	-	0/4/4/4	0/0/0/0
6	GOL	G	306	-	-	0/4/4/4	0/0/0/0
7	SO4	G	307	-	-	0/0/0/0	0/0/0/0
3	GNP	H	401	4	-	0/16/38/38	0/3/3/3
6	GOL	H	403	-	-	0/4/4/4	0/0/0/0
6	GOL	H	404	-	-	0/4/4/4	0/0/0/0
7	SO4	H	405	-	-	0/0/0/0	0/0/0/0

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	301	GNP	C4-N9	-7.80	1.37	1.47
3	A	301	GNP	C4-N9	-7.70	1.37	1.47
3	C	301	GNP	C4-N9	-7.60	1.37	1.47
3	D	401	GNP	C4-N9	-7.54	1.37	1.47
3	B	401	GNP	C4-N9	-7.51	1.37	1.47
3	F	401	GNP	C4-N9	-7.49	1.37	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	301	GNP	C4-N9	-6.91	1.38	1.47
3	H	401	GNP	C4-N9	-6.35	1.39	1.47
3	B	401	GNP	C5-C6	-6.30	1.41	1.53
3	F	401	GNP	C5-C6	-6.14	1.41	1.53
3	E	301	GNP	C5-C6	-6.12	1.41	1.53
3	B	401	GNP	PB-O3A	-5.92	1.51	1.59
3	C	301	GNP	C5-C6	-5.88	1.42	1.53
3	F	401	GNP	PB-O3A	-5.86	1.51	1.59
3	G	301	GNP	C5-C6	-5.84	1.42	1.53
3	D	401	GNP	C5-C6	-5.77	1.42	1.53
3	A	301	GNP	C5-C6	-5.74	1.42	1.53
3	H	401	GNP	C5-C6	-5.35	1.43	1.53
3	D	401	GNP	PB-O3A	-5.22	1.52	1.59
3	H	401	GNP	PB-O3A	-4.34	1.53	1.59
3	G	301	GNP	PB-O3A	-4.23	1.53	1.59
3	C	301	GNP	PB-O2B	-3.90	1.46	1.56
3	E	301	GNP	PB-O3A	-3.81	1.54	1.59
3	C	301	GNP	PB-O3A	-3.70	1.54	1.59
3	D	401	GNP	PB-O2B	-3.60	1.47	1.56
3	G	301	GNP	PB-O2B	-3.49	1.47	1.56
3	B	401	GNP	PB-O2B	-3.43	1.47	1.56
3	H	401	GNP	PB-O2B	-3.37	1.47	1.56
3	A	301	GNP	PB-O3A	-3.32	1.55	1.59
3	A	301	GNP	PB-O2B	-3.09	1.48	1.56
3	B	401	GNP	C8-N9	-3.06	1.37	1.47
3	G	301	GNP	C8-N9	-3.00	1.37	1.47
3	F	401	GNP	PB-O2B	-2.95	1.48	1.56
3	D	401	GNP	C8-N9	-2.91	1.37	1.47
3	F	401	GNP	C8-N9	-2.80	1.38	1.47
3	H	401	GNP	C8-N9	-2.79	1.38	1.47
3	A	301	GNP	C2-N3	-2.77	1.31	1.43
3	E	301	GNP	C8-N9	-2.73	1.38	1.47
3	C	301	GNP	C8-N9	-2.73	1.38	1.47
3	A	301	GNP	C8-N9	-2.71	1.38	1.47
3	E	301	GNP	C2-N3	-2.65	1.32	1.43
3	C	301	GNP	C2-N3	-2.65	1.32	1.43
3	G	301	GNP	C2-N3	-2.61	1.32	1.43
3	F	401	GNP	C2-N3	-2.61	1.32	1.43
3	E	301	GNP	PB-O2B	-2.60	1.49	1.56
3	C	301	GNP	PG-O2G	-2.57	1.49	1.56
3	B	401	GNP	C2-N3	-2.46	1.33	1.43
3	D	401	GNP	C2-N3	-2.43	1.33	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	301	GNP	PG-O2G	-2.35	1.50	1.56
3	E	301	GNP	PG-O2G	-2.31	1.50	1.56
3	F	401	GNP	PG-O3G	-2.30	1.50	1.56
5	G	303	G	P-OP3	-2.26	1.47	1.54
3	A	301	GNP	PG-O2G	-2.24	1.50	1.56
3	E	301	GNP	PG-O3G	-2.11	1.51	1.56
3	H	401	GNP	C2-N3	-2.10	1.34	1.43
3	F	401	GNP	PB-O1B	2.03	1.48	1.46
3	B	401	GNP	C1'-N9	2.35	1.46	1.42
3	G	301	GNP	C1'-N9	2.42	1.46	1.42
3	C	301	GNP	C1'-N9	2.69	1.47	1.42
3	D	401	GNP	C1'-N9	2.76	1.47	1.42
3	A	301	GNP	C1'-N9	2.80	1.47	1.42
3	F	401	GNP	C1'-N9	2.83	1.47	1.42
3	E	301	GNP	C1'-N9	2.95	1.47	1.42
3	H	401	GNP	C1'-N9	2.97	1.47	1.42
3	C	301	GNP	PB-O1B	3.20	1.49	1.46
3	H	401	GNP	PB-O1B	3.30	1.49	1.46
3	G	301	GNP	PB-O1B	3.44	1.49	1.46
5	E	303	G	C6-N1	3.64	1.39	1.33
3	E	301	GNP	PB-O1B	3.69	1.50	1.46
5	A	303	G	C6-N1	3.72	1.39	1.33
5	G	303	G	C6-N1	3.78	1.39	1.33
5	C	303	G	C6-N1	3.79	1.39	1.33
3	H	401	GNP	C6-N1	3.83	1.39	1.33
3	D	401	GNP	C6-N1	3.91	1.39	1.33
3	G	301	GNP	C6-N1	4.02	1.40	1.33
3	F	401	GNP	C6-N1	4.12	1.40	1.33
3	E	301	GNP	C6-N1	4.14	1.40	1.33
3	A	301	GNP	C6-N1	4.15	1.40	1.33
3	C	301	GNP	C6-N1	4.17	1.40	1.33
3	B	401	GNP	C6-N1	4.17	1.40	1.33
3	D	401	GNP	PG-O1G	4.50	1.51	1.46
3	H	401	GNP	PG-O1G	4.69	1.51	1.46
3	G	301	GNP	PG-O1G	4.78	1.51	1.46
3	F	401	GNP	PG-O1G	4.79	1.51	1.46
3	B	401	GNP	PG-O1G	5.04	1.51	1.46
3	E	301	GNP	PG-O1G	6.43	1.53	1.46
3	C	301	GNP	PG-O1G	6.70	1.53	1.46
3	A	301	GNP	PG-O1G	7.38	1.54	1.46

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	303	G	C5-C6-N1	-9.18	111.52	123.52
5	A	303	G	C5-C6-N1	-9.14	111.57	123.52
5	G	303	G	C5-C6-N1	-9.02	111.73	123.52
5	E	303	G	C5-C6-N1	-9.00	111.76	123.52
3	C	301	GNP	O3G-PG-O1G	-3.59	104.13	113.58
3	C	301	GNP	O6-C6-N1	-3.45	118.27	122.80
3	A	301	GNP	O3G-PG-O1G	-3.14	105.30	113.58
3	E	301	GNP	O3G-PG-O1G	-3.09	105.44	113.58
3	H	401	GNP	O6-C6-N1	-2.96	118.91	122.80
5	A	303	G	N3-C2-N1	-2.84	123.69	127.56
5	C	303	G	N3-C2-N1	-2.82	123.73	127.56
3	G	301	GNP	O6-C6-N1	-2.81	119.11	122.80
5	G	303	G	N3-C2-N1	-2.79	123.76	127.56
3	A	301	GNP	O6-C6-N1	-2.78	119.14	122.80
3	D	401	GNP	O6-C6-N1	-2.72	119.23	122.80
5	E	303	G	N3-C2-N1	-2.68	123.91	127.56
3	E	301	GNP	O6-C6-N1	-2.58	119.42	122.80
3	G	301	GNP	O3G-PG-O1G	-2.54	106.89	113.58
5	A	303	G	C6-C5-C4	-2.06	118.51	120.86
3	G	301	GNP	C8-N9-C4	2.03	107.09	104.78
3	A	301	GNP	C2'-C1'-N9	2.03	118.89	113.44
5	E	303	G	OP2-P-OP1	2.06	117.34	110.63
3	E	301	GNP	C2'-C1'-N9	2.20	119.34	113.44
3	E	301	GNP	O3G-PG-O2G	2.20	114.07	107.67
3	H	401	GNP	O2B-PB-O1B	2.22	114.39	110.02
5	A	303	G	OP2-P-OP1	2.39	118.44	110.63
3	A	301	GNP	O3G-PG-O2G	2.46	114.81	107.67
3	G	301	GNP	O3G-PG-O2G	2.56	115.09	107.67
5	G	303	G	OP2-P-OP1	2.72	119.52	110.63
3	C	301	GNP	O3G-PG-O2G	2.84	115.92	107.67
3	B	401	GNP	O6-C6-C5	3.37	126.14	119.69
3	F	401	GNP	O6-C6-C5	3.76	126.87	119.69
3	G	301	GNP	O2B-PB-O1B	3.83	117.57	110.02
3	C	301	GNP	O2B-PB-O1B	4.00	117.91	110.02
3	D	401	GNP	O2B-PB-O1B	4.04	117.97	110.02
3	A	301	GNP	C4-C5-N7	4.22	109.26	102.67
3	F	401	GNP	O2B-PB-O1B	4.37	118.63	110.02
3	G	301	GNP	O6-C6-C5	4.49	128.29	119.69
3	A	301	GNP	O2B-PB-O1B	4.52	118.93	110.02
3	G	301	GNP	C4-C5-N7	4.59	109.84	102.67
3	D	401	GNP	O6-C6-C5	4.63	128.54	119.69
3	E	301	GNP	O6-C6-C5	4.64	128.56	119.69
3	H	401	GNP	C4-C5-N7	4.68	109.97	102.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	GNP	O6-C6-C5	4.73	128.74	119.69
3	C	301	GNP	O6-C6-C5	4.76	128.79	119.69
3	C	301	GNP	C4-C5-N7	4.76	110.10	102.67
3	E	301	GNP	C4-C5-N7	4.79	110.15	102.67
3	D	401	GNP	C4-C5-N7	4.84	110.22	102.67
3	H	401	GNP	O6-C6-C5	4.90	129.07	119.69
3	E	301	GNP	O2B-PB-O1B	5.30	120.46	110.02
3	F	401	GNP	C4-C5-N7	5.36	111.03	102.67
3	B	401	GNP	C4-C5-N7	5.42	111.13	102.67
5	E	303	G	C6-N1-C2	7.81	125.04	115.88
5	G	303	G	C6-N1-C2	7.89	125.13	115.88
5	C	303	G	C6-N1-C2	8.01	125.26	115.88
5	A	303	G	C6-N1-C2	8.08	125.35	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	304	GOL	1	0
6	A	305	GOL	1	0
6	A	306	GOL	1	0
6	B	405	GOL	1	0
5	C	303	G	1	0
6	C	304	GOL	2	0
6	C	305	GOL	1	0
7	C	306	SO4	1	0
5	G	303	G	1	0
6	G	306	GOL	2	0
6	H	403	GOL	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<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	274/298 (91%)	0.41	21 (7%) 16 18	18, 34, 73, 113	0
1	C	270/298 (90%)	1.17	57 (21%) 1 1	22, 44, 106, 135	0
1	E	271/298 (90%)	0.48	32 (11%) 6 6	22, 39, 97, 126	0
1	G	277/298 (92%)	0.28	15 (5%) 29 33	18, 38, 70, 112	0
2	B	283/296 (95%)	0.29	17 (6%) 25 28	19, 33, 64, 107	0
2	D	271/296 (91%)	0.73	37 (13%) 4 4	23, 44, 100, 120	0
2	F	283/296 (95%)	0.60	23 (8%) 15 16	23, 46, 79, 123	0
2	H	278/296 (93%)	0.50	32 (11%) 6 7	19, 36, 90, 117	0
All	All	2207/2376 (92%)	0.56	234 (10%) 8 8	18, 39, 89, 135	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	236	TYR	9.8
1	G	63	VAL	9.4
1	C	19	TYR	9.0
2	H	368	SER	8.7
2	H	132	VAL	8.2
2	D	236	TYR	8.1
1	C	67	LYS	8.0
1	C	73	ILE	8.0
2	D	95	LEU	7.8
1	C	17	THR	7.7
1	C	23	VAL	7.4
2	D	138	VAL	7.2
2	H	90	ILE	7.1
1	C	58	GLU	7.0
2	H	95	LEU	6.9
1	E	70	PHE	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	56	ASN	6.5
1	A	63	VAL	6.2
1	C	49	ALA	6.2
2	D	94	ASP	6.0
2	F	87	TYR	6.0
2	D	128	ILE	6.0
1	C	55	LEU	6.0
1	C	57	LYS	5.9
2	B	87	TYR	5.9
1	A	65	GLU	5.9
1	C	71	ILE	5.8
1	C	70	PHE	5.6
1	C	74	VAL	5.5
1	C	285	LYS	5.3
1	C	69	TRP	5.2
2	D	97	ASP	5.2
2	H	127	LEU	5.2
2	D	139	GLU	5.2
2	H	138	VAL	5.2
2	H	128	ILE	5.1
1	C	59	LYS	5.1
2	F	132	VAL	5.1
1	C	76	ASP	5.0
1	E	66	ARG	5.0
1	C	53	GLU	5.0
2	H	91	LYS	5.0
2	D	141	ILE	4.9
1	C	20	GLU	4.9
1	G	64	LEU	4.9
2	H	93	ASP	4.7
2	H	97	ASP	4.7
1	C	50	LYS	4.7
1	E	16	SER	4.6
1	E	23	VAL	4.6
1	C	222	ILE	4.5
2	F	86	LYS	4.5
2	H	137	GLU	4.5
2	B	134	ARG	4.5
1	C	84	GLY	4.4
2	D	368	SER	4.4
2	H	94	ASP	4.4
2	H	236[A]	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	22	ALA	4.2
1	C	72	SER	4.2
1	C	18	PRO	4.1
1	C	51	ILE	4.1
2	F	138	VAL	4.1
1	C	54	ARG	4.1
1	C	28	LYS	4.1
1	C	75	TYR	4.0
2	H	92	GLU	3.9
1	C	218	ILE	3.9
1	A	222	ILE	3.9
2	D	361	TRP	3.8
2	H	141	ILE	3.8
2	D	235	LYS	3.8
1	G	62	SER	3.8
2	B	132	VAL	3.8
1	E	68	GLU	3.8
2	H	129	GLY	3.7
1	E	69	TRP	3.7
2	D	142	VAL	3.7
2	B	296	LEU	3.7
1	C	47	LEU	3.7
2	D	184	VAL	3.7
2	H	131	LYS	3.6
2	B	135	ARG	3.6
2	D	364	GLU	3.6
1	C	24	ASP	3.5
2	F	296	LEU	3.5
1	G	86	LYS	3.5
2	B	184	VAL	3.5
1	C	21	LYS	3.4
2	D	98	VAL	3.4
1	C	217	VAL	3.4
2	H	98	VAL	3.4
1	E	67	LYS	3.4
2	D	104	PHE	3.4
2	D	170	GLY	3.3
1	A	64	LEU	3.3
2	D	99	ILE	3.3
1	C	104	VAL	3.3
2	D	127	LEU	3.3
1	E	45	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
2	B	297	ALA	3.2
1	G	85	ASP	3.2
2	D	140	GLU	3.2
2	H	135	ARG	3.1
2	F	235	LYS	3.1
2	H	139	GLU	3.1
1	E	28	LYS	3.1
1	E	24	ASP	3.0
1	C	79	SER	3.0
2	D	92	GLU	3.0
1	E	85	ASP	3.0
2	B	319	LEU	3.0
1	C	80	LYS	3.0
1	C	194	GLU	3.0
2	H	121	GLU	3.0
2	D	311	ASN	3.0
1	G	83	GLY	3.0
2	H	133	SER	2.9
2	F	85	LEU	2.9
1	E	53	GLU	2.9
1	E	18	PRO	2.9
2	B	293	LEU	2.9
2	F	135	ARG	2.8
2	H	126	ASN	2.8
1	A	218	ILE	2.8
1	A	83	GLY	2.8
1	C	68	GLU	2.8
2	D	237	GLY	2.8
2	F	362	PHE	2.8
1	C	52	LYS	2.7
1	E	17	THR	2.7
1	E	54	ARG	2.7
1	G	68	GLU	2.7
1	C	286	ARG	2.7
2	D	255	ASN	2.7
1	A	87	GLU	2.7
1	E	135[A]	TYR	2.7
2	F	184	VAL	2.7
2	B	137	GLU	2.7
2	F	160	THR	2.7
2	F	93	ASP	2.6
2	F	141	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	184	VAL	2.6
1	C	86	LYS	2.6
1	E	56	ASN	2.6
1	A	81	LEU	2.6
2	F	136	GLU	2.6
1	G	218	ILE	2.6
1	E	49	ALA	2.5
1	A	16	SER	2.5
1	C	107	SER	2.5
2	B	136	GLU	2.5
2	H	96	ASN	2.5
1	C	196	THR	2.5
1	C	25	GLU	2.5
1	E	22	ALA	2.5
2	F	139	GLU	2.5
1	A	67	LYS	2.5
1	E	52	LYS	2.5
2	B	86	LYS	2.5
1	G	65	GLU	2.5
2	H	124	LYS	2.5
2	D	96	ASN	2.5
2	F	133	SER	2.5
2	H	99	ILE	2.4
2	B	330	ILE	2.4
2	D	253	SER	2.4
1	C	77	GLU	2.4
2	D	172	LYS	2.4
1	C	220	ALA	2.4
1	E	286	ARG	2.4
2	B	318	ILE	2.4
1	E	57	LYS	2.4
1	G	87	GLU	2.4
1	A	69	TRP	2.3
1	C	102	VAL	2.3
1	E	47	LEU	2.3
2	D	296	LEU	2.3
1	C	16	SER	2.3
1	E	71	ILE	2.3
1	G	222	ILE	2.3
1	C	85	ASP	2.3
1	C	87	GLU	2.3
1	C	78	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	82	PHE	2.3
1	E	26	PHE	2.3
1	A	86	LYS	2.3
2	H	142	VAL	2.3
1	G	226	ALA	2.3
2	B	368	SER	2.3
1	G	57	LYS	2.3
2	D	137	GLU	2.3
2	H	123	LEU	2.3
1	A	135[A]	TYR	2.2
1	C	26	PHE	2.2
1	E	59	LYS	2.2
2	F	297	ALA	2.2
1	A	216	LEU	2.2
1	C	135[A]	TYR	2.2
1	A	220	ALA	2.2
1	E	256	ALA	2.2
1	A	260	VAL	2.2
1	E	20	GLU	2.2
1	A	292	LEU	2.2
1	A	217	VAL	2.2
1	E	222	ILE	2.2
2	B	171	LYS	2.2
2	D	129	GLY	2.2
2	F	157	ASN	2.2
2	H	134	ARG	2.2
2	B	139	GLU	2.2
1	G	52	LYS	2.2
1	E	73	ILE	2.1
1	E	218	ILE	2.1
2	H	172	LYS	2.1
2	D	93	ASP	2.1
2	F	318	ILE	2.1
2	H	143	ILE	2.1
2	D	254	ARG	2.1
2	D	310	ASN	2.1
1	A	257	LEU	2.1
1	E	58	GLU	2.1
1	A	66	ARG	2.1
2	F	98	VAL	2.1
1	C	113	ALA	2.1
2	D	145	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	194	GLU	2.0
2	D	126	ASN	2.0
2	F	156	LYS	2.0
2	D	123	LEU	2.0
2	F	292	ILE	2.0
2	D	144	ASN	2.0
1	A	197	LYS	2.0
1	C	245	THR	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](#)

There are no carbohydrates in this entry.

## 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, 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	G	G	303	24/24	0.85	0.29	10.53	35,80,100,105	24
6	GOL	E	305	6/6	0.91	0.25	8.59	41,55,59,63	0
7	SO4	A	309	5/5	0.94	0.23	7.77	52,66,81,84	0
6	GOL	B	406	6/6	0.80	0.27	7.73	65,72,74,77	0
7	SO4	G	307	5/5	0.81	0.35	7.58	103,104,104,107	0
5	G	A	303	24/24	0.55	0.43	6.82	84,97,107,109	24
6	GOL	C	305	6/6	0.62	0.30	6.03	67,76,78,79	0
7	SO4	E	306	5/5	0.83	0.27	4.78	134,135,136,137	0
5	G	C	303	24/24	0.82	0.30	3.97	53,83,110,112	0
6	GOL	A	304	6/6	0.60	0.24	3.64	54,63,71,73	0
6	GOL	H	403	6/6	0.92	0.13	2.92	35,40,43,45	0
6	GOL	A	306	6/6	0.86	0.20	2.87	56,59,63,64	0
6	GOL	B	404	6/6	0.84	0.17	2.25	46,58,60,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SO4	B	407	5/5	0.95	0.15	2.12	38,44,60,65	0
6	GOL	F	403	6/6	0.80	0.20	1.80	50,55,58,58	0
5	G	E	303	24/24	0.70	0.36	1.79	58,83,95,99	24
6	GOL	B	405	6/6	0.86	0.17	1.78	40,45,52,54	0
6	GOL	B	403	6/6	0.78	0.22	1.72	45,47,52,52	0
6	GOL	G	304	6/6	0.90	0.14	1.49	30,37,51,61	0
6	GOL	D	403	6/6	0.89	0.16	1.41	40,43,47,48	0
6	GOL	G	306	6/6	0.83	0.14	1.10	39,52,53,56	0
6	GOL	A	305	6/6	0.88	0.15	1.04	29,35,43,45	0
6	GOL	G	305	6/6	0.88	0.18	0.80	45,54,60,60	0
6	GOL	C	304	6/6	0.82	0.16	0.40	46,51,56,59	0
6	GOL	E	304	6/6	0.88	0.13	0.22	45,46,55,63	0
3	GNP	C	301	32/32	0.99	0.15	0.09	17,24,28,28	0
3	GNP	H	401	32/32	0.99	0.12	0.08	16,22,25,26	0
7	SO4	A	308	5/5	0.95	0.16	0.03	56,58,62,71	0
3	GNP	A	301	32/32	0.98	0.14	-0.04	13,20,23,24	0
3	GNP	B	401	32/32	0.98	0.14	-0.13	12,18,23,24	0
4	MG	B	402	1/1	0.97	0.12	-0.21	19,19,19,19	0
3	GNP	D	401	32/32	0.98	0.12	-0.40	17,23,29,31	0
3	GNP	F	401	32/32	0.98	0.12	-0.42	18,22,27,30	0
3	GNP	G	301	32/32	0.99	0.10	-0.45	14,20,24,27	0
4	MG	A	302	1/1	0.99	0.12	-0.47	20,20,20,20	0
3	GNP	E	301	32/32	0.98	0.10	-0.70	16,23,30,31	0
4	MG	F	402	1/1	0.99	0.08	-1.09	24,24,24,24	0
4	MG	C	302	1/1	0.98	0.09	-1.13	25,25,25,25	0
4	MG	G	302	1/1	0.98	0.09	-1.27	22,22,22,22	0
4	MG	H	402	1/1	0.97	0.06	-1.56	21,21,21,21	0
4	MG	D	402	1/1	0.98	0.08	-1.71	22,22,22,22	0
4	MG	E	302	1/1	0.99	0.04	-2.49	25,25,25,25	0
7	SO4	A	307	5/5	0.95	0.26	-	59,67,71,72	0
7	SO4	H	405	5/5	0.98	0.16	-	58,60,68,70	0
6	GOL	H	404	6/6	0.48	0.45	-	74,84,86,87	0
7	SO4	C	306	5/5	0.81	0.29	-	108,109,110,111	0
7	SO4	B	408	5/5	0.85	0.25	-	119,121,122,122	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.