



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:01 am GMT

PDB ID : 4I2X  
Title : Crystal structure of Signal Regulatory Protein gamma (SIRP-gamma) in complex with FabOX117  
Authors : Nettleship, J.E.; Ren, J.; Stuart, D.I.; Owens, R.J.; Oxford Protein Production Facility (OPPF)  
Deposited on : 2012-11-23  
Resolution : 2.48 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

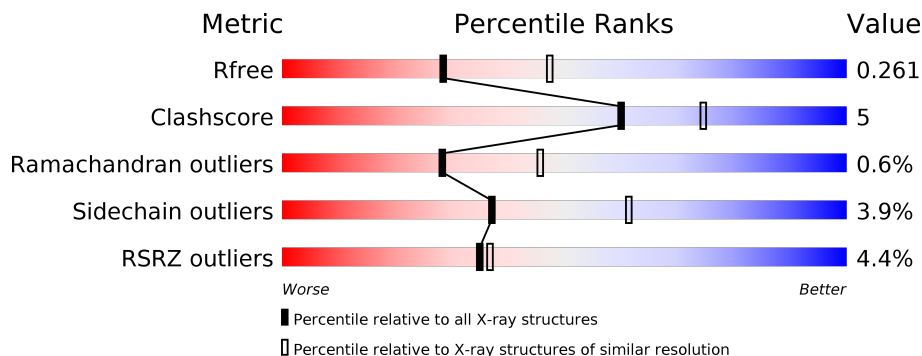
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.48 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))
$R_{free}$	100719	4719 (2.50-2.46)
Clashscore	112137	5483 (2.50-2.46)
Ramachandran outliers	110173	5388 (2.50-2.46)
Sidechain outliers	110143	5390 (2.50-2.46)
RSRZ outliers	101464	4754 (2.50-2.46)

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	214	<div> <div>83%</div> <div>17%</div> </div>
1	C	214	<div> <div>83%</div> <div>16%</div> <div>.</div> </div>
2	B	229	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
2	D	229	<div> <div>83%</div> <div>11%</div> <div>..</div> </div>
3	E	328	<div> <div>6%</div> <div>82%</div> <div>13%</div> <div>.</div> </div>
3	F	328	<div> <div>12%</div> <div>77%</div> <div>13%</div> <div>10%</div> </div>

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11813 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 FabOX117 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1663	1041	277	338	7			
1	C	214	Total	C	N	O	S	0	0	0
			1663	1041	277	338	7			

- Molecule 2 is a protein called FabOX117 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1746	1111	295	333	7			
2	D	219	Total	C	N	O	S	0	0	0
			1659	1060	272	321	6			

- Molecule 3 is a protein called Signal-regulatory protein gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	314	Total	C	N	O	S	0	0	0
			2442	1536	429	466	11			
3	F	296	Total	C	N	O	S	0	0	0
			2307	1454	404	439	10			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	320	SER	-	EXPRESSION TAG	UNP Q9P1W8
E	321	THR	-	EXPRESSION TAG	UNP Q9P1W8
E	322	ARG	-	EXPRESSION TAG	UNP Q9P1W8
E	323	HIS	-	EXPRESSION TAG	UNP Q9P1W8
E	324	HIS	-	EXPRESSION TAG	UNP Q9P1W8
E	325	HIS	-	EXPRESSION TAG	UNP Q9P1W8
E	326	HIS	-	EXPRESSION TAG	UNP Q9P1W8
E	327	HIS	-	EXPRESSION TAG	UNP Q9P1W8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	328	HIS	-	EXPRESSION TAG	UNP Q9P1W8
F	320	SER	-	EXPRESSION TAG	UNP Q9P1W8
F	321	THR	-	EXPRESSION TAG	UNP Q9P1W8
F	322	ARG	-	EXPRESSION TAG	UNP Q9P1W8
F	323	HIS	-	EXPRESSION TAG	UNP Q9P1W8
F	324	HIS	-	EXPRESSION TAG	UNP Q9P1W8
F	325	HIS	-	EXPRESSION TAG	UNP Q9P1W8
F	326	HIS	-	EXPRESSION TAG	UNP Q9P1W8
F	327	HIS	-	EXPRESSION TAG	UNP Q9P1W8
F	328	HIS	-	EXPRESSION TAG	UNP Q9P1W8

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Zn 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

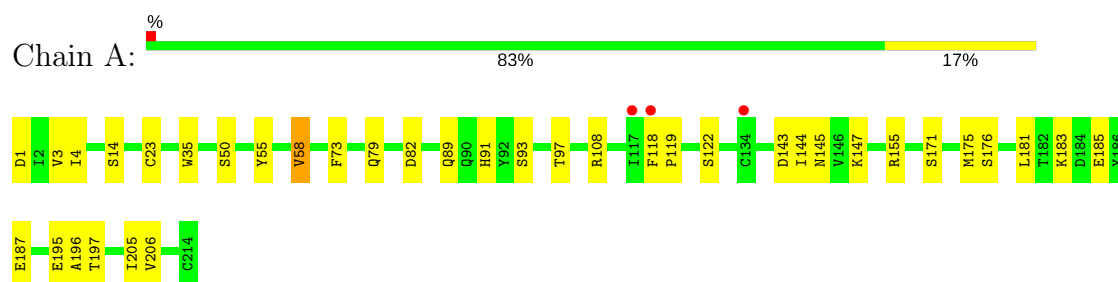
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	38	Total	O	0	0
			38	38		
7	B	64	Total	O	0	0
			64	64		
7	C	31	Total	O	0	0
			31	31		
7	D	52	Total	O	0	0
			52	52		
7	E	66	Total	O	0	0
			66	66		
7	F	51	Total	O	0	0
			51	51		

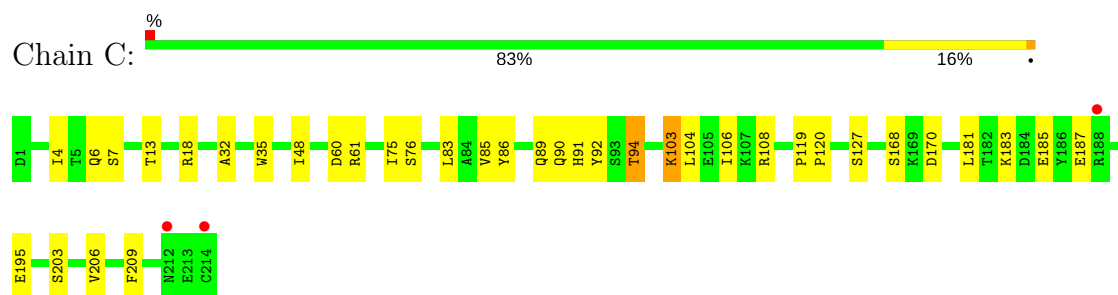
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

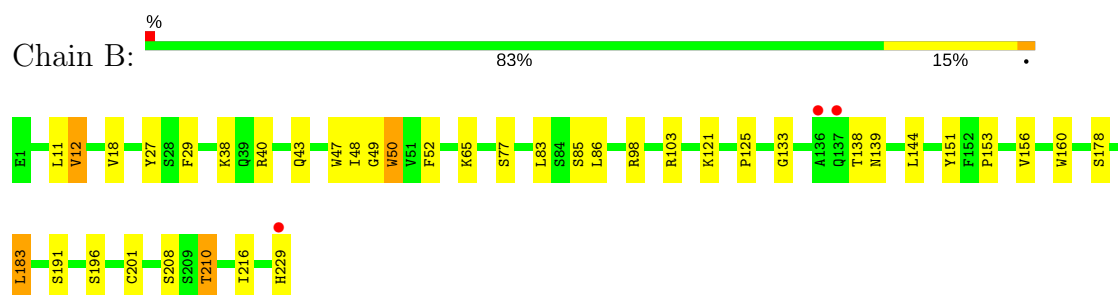
#### • Molecule 1: FabOX117 light chain



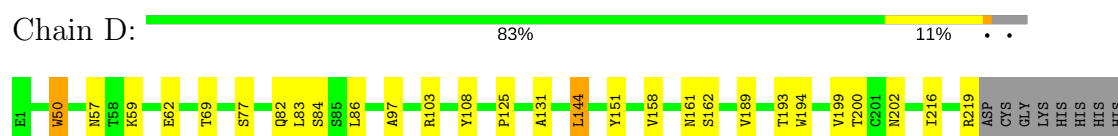
#### • Molecule 1: FabOX117 light chain



#### • Molecule 2: FabOX117 heavy chain

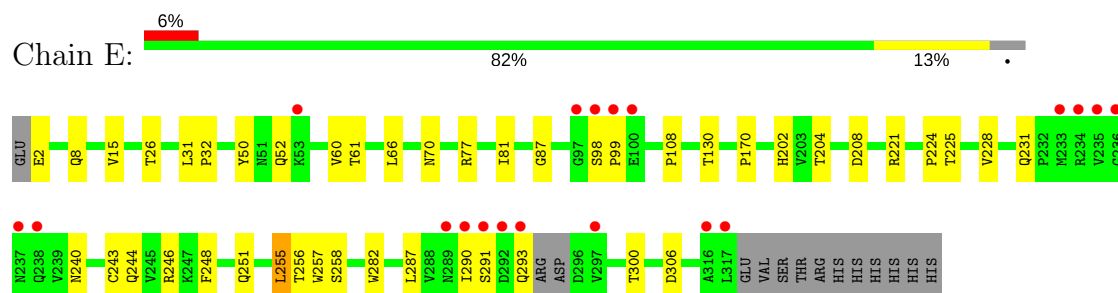


#### • Molecule 2: FabOX117 heavy chain

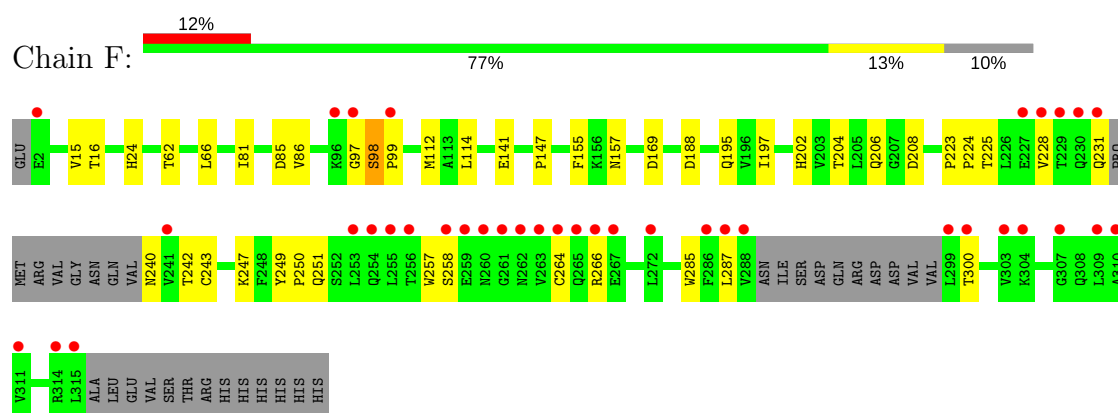


HIS  
HIS

- Molecule 3: Signal-regulatory protein gamma



- Molecule 3: Signal-regulatory protein gamma



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.36Å 174.19Å 81.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 2.48 29.80 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.82-2.48) 99.1 (29.80-2.48)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.196 , 0.260 0.195 , 0.261	Depositor DCC
$R_{free}$ test set	3594 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11813	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: ZN, NAG, CL

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	0/1703	0.57	0/2315
1	C	0.39	0/1703	0.58	0/2315
2	B	0.39	0/1801	0.58	0/2461
2	D	0.40	0/1708	0.59	0/2336
3	E	0.37	0/2495	0.56	0/3401
3	F	0.35	0/2358	0.57	0/3212
All	All	0.38	0/11768	0.57	0/16040

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	1663	0	1587	19	0
1	C	1663	0	1588	22	0
2	B	1746	0	1688	19	0
2	D	1659	0	1622	20	0
3	E	2442	0	2423	22	0
3	F	2307	0	2286	31	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	E	14	0	13	0	0
6	F	14	0	13	1	0
7	A	38	0	0	0	0
7	B	64	0	0	0	0
7	C	31	0	0	0	0
7	D	52	0	0	1	0
7	E	66	0	0	0	0
7	F	51	0	0	1	0
All	All	11813	0	11220	120	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (120) 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:C:94:THR:HG21	2:D:59:LYS:HE3	1.55	0.86
3:E:224:PRO:HB3	3:E:248:PHE:HB3	1.60	0.84
3:E:87:GLY:HA2	3:F:169:ASP:HB3	1.66	0.77
1:C:183:LYS:O	1:C:187:GLU:HG2	1.88	0.74
3:F:242:THR:HG22	3:F:285:TRP:HB3	1.76	0.68
3:F:242:THR:HG22	3:F:285:TRP:CB	2.23	0.68
3:E:2:GLU:HG2	3:E:2:GLU:O	1.93	0.68
3:F:157:ASN:HD21	3:F:195:GLN:H	1.42	0.68
1:A:145:ASN:HB2	1:A:197:THR:HB	1.79	0.65
3:F:188:ASP:HB3	7:F:546:HOH:O	1.97	0.65
1:C:89:GLN:HE22	1:C:91:HIS:HD2	1.45	0.63
3:F:98:SER:HB3	3:F:99:PRO:HD3	1.80	0.63
2:B:12:VAL:HG21	2:B:86:LEU:HD12	1.81	0.62
3:F:81:ILE:HD12	3:F:112:MET:HE1	1.82	0.61
1:C:91:HIS:HE1	2:D:103:ARG:O	1.83	0.61
3:E:202:HIS:HD2	3:E:204:THR:OG1	1.82	0.61
1:C:89:GLN:HE22	1:C:91:HIS:CD2	2.20	0.60
1:C:4:ILE:HD11	1:C:90:GLN:HG2	1.84	0.59
3:F:202:HIS:HD2	3:F:204:THR:OG1	1.85	0.59
1:C:6:GLN:NE2	1:C:86:TYR:O	2.33	0.58
1:A:55:TYR:O	1:A:58:VAL:HG13	2.03	0.58
3:E:8:GLN:HB2	3:E:108:PRO:HD2	1.86	0.58
3:F:231:GLN:HB3	3:F:240:ASN:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLN:HE22	1:A:91:HIS:HD2	1.51	0.56
3:F:157:ASN:ND2	3:F:195:GLN:H	2.03	0.56
3:E:221:ARG:NH1	3:E:306:ASP:OD2	2.39	0.56
2:B:144:LEU:HD23	2:B:216:ILE:HG21	1.88	0.55
1:A:183:LYS:O	1:A:187:GLU:HG2	2.06	0.55
3:E:244:GLN:HG2	3:E:246:ARG:CZ	2.36	0.55
2:D:83:LEU:HB3	2:D:86:LEU:HD21	1.89	0.54
1:A:89:GLN:HE22	1:A:91:HIS:CD2	2.25	0.54
2:B:83:LEU:HB3	2:B:86:LEU:HD21	1.90	0.53
1:A:147:LYS:HB2	1:A:195:GLU:HB2	1.91	0.53
2:D:97:ALA:HA	2:D:108:TYR:O	2.09	0.53
1:A:91:HIS:HE1	2:B:103:ARG:O	1.93	0.52
1:C:94:THR:HG23	7:D:438:HOH:O	2.09	0.52
2:B:50:TRP:CD1	2:B:50:TRP:C	2.83	0.52
3:F:62:THR:HG21	3:F:66:LEU:HD22	1.92	0.51
3:F:242:THR:HG22	3:F:285:TRP:HB2	1.92	0.51
1:A:79:GLN:O	1:A:82:ASP:HB2	2.10	0.51
3:E:170:PRO:HD3	3:F:86:VAL:HB	1.93	0.51
2:D:144:LEU:HD21	2:D:194:TRP:CG	2.46	0.51
3:F:202:HIS:CD2	3:F:204:THR:OG1	2.64	0.50
1:A:4:ILE:CG2	1:A:23:CYS:SG	3.00	0.50
2:B:125:PRO:HB3	2:B:151:TYR:HB3	1.93	0.50
3:E:61:THR:HG23	3:E:77:ARG:HB2	1.92	0.50
1:C:85:VAL:HG22	1:C:103:LYS:HG2	1.93	0.50
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.46	0.50
2:D:62:GLU:HG3	3:F:206:GLN:HA	1.95	0.49
3:E:31:LEU:HA	3:E:32:PRO:C	2.32	0.49
1:C:195:GLU:HG2	1:C:206:VAL:HG22	1.94	0.49
3:E:258:SER:HB2	3:E:300:THR:HB	1.93	0.49
1:C:18:ARG:HG3	1:C:76:SER:HA	1.95	0.49
2:B:12:VAL:HG11	2:B:18:VAL:HB	1.94	0.48
2:B:208:SER:OG	2:B:210:THR:HB	2.13	0.48
2:D:125:PRO:HB3	2:D:151:TYR:HB3	1.94	0.48
1:C:83:LEU:HB2	1:C:106:ILE:HG12	1.95	0.48
1:C:13:THR:CG2	1:C:104:LEU:HD11	2.44	0.47
1:A:196:ALA:HB3	1:A:205:ILE:HB	1.95	0.47
2:D:144:LEU:HG	2:D:216:ILE:HG21	1.96	0.47
2:B:12:VAL:CG2	2:B:86:LEU:HD12	2.43	0.47
3:F:249:TYR:CD1	3:F:250:PRO:HA	2.50	0.47
2:B:38:LYS:HB2	2:B:48:ILE:HD11	1.97	0.46
3:F:287:LEU:HD21	6:F:401:NAG:H82	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HG23	1:A:175:MET:HE3	1.98	0.46
1:C:35:TRP:HB2	1:C:48:ILE:HB	1.98	0.46
2:D:50:TRP:CD1	2:D:50:TRP:C	2.88	0.46
1:A:195:GLU:HG2	1:A:206:VAL:HG22	1.98	0.46
3:F:147:PRO:O	3:F:202:HIS:HE1	1.99	0.45
1:A:155:ARG:NH2	1:A:185:GLU:OE1	2.49	0.45
1:A:35:TRP:CD2	1:A:73:PHE:HB2	2.51	0.45
3:E:243:CYS:HB2	3:E:257:TRP:CH2	2.52	0.45
3:E:15:VAL:HG13	3:E:81:ILE:HG21	1.99	0.45
3:F:223:PRO:HA	3:F:224:PRO:HD3	1.82	0.45
3:F:249:TYR:CG	3:F:250:PRO:HA	2.52	0.45
1:C:32:ALA:HB3	1:C:92:TYR:HB2	1.98	0.45
3:F:264:CYS:HB3	3:F:266:ARG:HD2	1.99	0.44
2:B:40:ARG:O	2:B:43:GLN:HB2	2.17	0.44
3:E:52:GLN:HG3	3:E:66:LEU:HD23	2.00	0.44
2:B:29:PHE:CD2	2:B:77:SER:HA	2.52	0.44
2:D:161:ASN:ND2	2:D:200:THR:H	2.16	0.44
3:F:81:ILE:HD12	3:F:112:MET:CE	2.46	0.44
1:A:144:ILE:HG23	1:A:175:MET:CE	2.49	0.43
1:A:108:ARG:HD2	1:A:171:SER:HB2	2.00	0.43
1:C:61:ARG:O	1:C:75:ILE:HA	2.19	0.43
3:F:85:ASP:HB3	3:F:112:MET:HE1	1.99	0.43
3:E:231:GLN:HB3	3:E:240:ASN:HB3	1.99	0.43
1:C:91:HIS:CE1	2:D:103:ARG:O	2.69	0.43
2:D:57:ASN:HD21	3:F:24:HIS:CD2	2.37	0.43
2:D:161:ASN:HD21	2:D:199:VAL:HA	1.84	0.42
1:C:120:PRO:O	2:D:219:ARG:NH1	2.51	0.42
2:D:69:THR:HB	2:D:82:GLN:HB3	2.01	0.42
3:F:15:VAL:HG22	3:F:16:THR:N	2.34	0.42
2:B:27:TYR:CZ	2:B:98:ARG:HD2	2.55	0.42
2:B:160:TRP:CH2	2:B:201:CYS:HB3	2.55	0.42
3:F:155:PHE:HB2	3:F:197:ILE:HB	2.01	0.42
2:B:52:PHE:CD1	3:E:26:THR:HG21	2.54	0.42
3:F:114:LEU:HD12	3:F:114:LEU:HA	1.89	0.42
3:E:255:LEU:HD12	3:E:256:THR:N	2.35	0.41
3:F:157:ASN:HD21	3:F:195:GLN:N	2.13	0.41
3:F:258:SER:HB2	3:F:300:THR:HB	2.01	0.41
2:B:183:LEU:HD12	2:B:183:LEU:C	2.40	0.41
2:D:189:VAL:HB	2:D:193:THR:OG1	2.19	0.41
1:A:91:HIS:CE1	2:B:103:ARG:O	2.73	0.41
1:C:108:ARG:HD2	1:C:170:ASP:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:244:GLN:HG2	3:E:246:ARG:NH2	2.36	0.41
3:E:255:LEU:HD23	3:E:282:TRP:CD1	2.55	0.41
1:C:119:PRO:HG2	2:D:219:ARG:CZ	2.51	0.41
3:E:50:TYR:CD1	3:E:60:VAL:HG11	2.56	0.41
1:A:118:PHE:HA	1:A:119:PRO:HD3	1.85	0.41
2:B:11:LEU:HB2	2:B:153:PRO:HG3	2.01	0.41
3:E:81:ILE:HA	3:E:81:ILE:HD13	1.92	0.41
2:D:50:TRP:HZ2	3:F:24:HIS:CD2	2.38	0.41
1:C:119:PRO:HB3	1:C:209:PHE:CE1	2.56	0.40
2:D:131:ALA:O	2:D:219:ARG:NH2	2.54	0.40
1:A:175:MET:HG2	1:A:176:SER:N	2.36	0.40
3:F:243:CYS:HB2	3:F:257:TRP:CH2	2.56	0.40
1:C:4:ILE:HD11	1:C:90:GLN:CG	2.50	0.40
2:D:158:VAL:HA	2:D:202:ASN:O	2.22	0.40
3:E:15:VAL:CG1	3:E:81:ILE:HG21	2.52	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	212/214 (99%)	203 (96%)	9 (4%)	0	100	100
1	C	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
2	B	227/229 (99%)	205 (90%)	18 (8%)	4 (2%)	10	15
2	D	217/229 (95%)	207 (95%)	10 (5%)	0	100	100
3	E	310/328 (94%)	295 (95%)	13 (4%)	2 (1%)	28	46
3	F	290/328 (88%)	279 (96%)	8 (3%)	3 (1%)	18	30
All	All	1468/1542 (95%)	1393 (95%)	66 (4%)	9 (1%)	28	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	99	PRO
2	B	138	THR
3	E	291	SER
3	F	98	SER
2	B	133	GLY
2	B	178	SER
2	B	65	LYS
3	F	247	LYS
3	F	97	GLY

### 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	190/190 (100%)	180 (95%)	10 (5%)	26	46
1	C	190/190 (100%)	181 (95%)	9 (5%)	30	52
2	B	194/194 (100%)	183 (94%)	11 (6%)	24	42
2	D	185/194 (95%)	180 (97%)	5 (3%)	50	75
3	E	278/292 (95%)	267 (96%)	11 (4%)	36	60
3	F	262/292 (90%)	257 (98%)	5 (2%)	62	83
All	All	1299/1352 (96%)	1248 (96%)	51 (4%)	37	61

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	3	VAL
1	A	14	SER
1	A	50	SER
1	A	58	VAL
1	A	93	SER
1	A	97	THR
1	A	122	SER
1	A	143	ASP
1	A	181	LEU

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Mol	Chain	Res	Type
2	B	12	VAL
2	B	50	TRP
2	B	85	SER
2	B	121	LYS
2	B	139	ASN
2	B	156	VAL
2	B	183	LEU
2	B	191	SER
2	B	196	SER
2	B	210	THR
2	B	229	HIS
1	C	7	SER
1	C	60	ASP
1	C	94	THR
1	C	103	LYS
1	C	127	SER
1	C	168	SER
1	C	181	LEU
1	C	185	GLU
1	C	203	SER
2	D	50	TRP
2	D	77	SER
2	D	84	SER
2	D	144	LEU
2	D	162	SER
3	E	70	ASN
3	E	98	SER
3	E	130	THR
3	E	208	ASP
3	E	225	THR
3	E	228	VAL
3	E	251	GLN
3	E	255	LEU
3	E	287	LEU
3	E	290	ILE
3	E	293	GLN
3	F	141	GLU
3	F	208	ASP
3	F	225	THR
3	F	228	VAL
3	F	251	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	156	GLN
2	B	161	ASN
1	C	91	HIS
1	C	189	HIS
1	C	190	ASN
2	D	161	ASN
3	E	202	HIS
3	E	244	GLN
3	E	254	GLN
3	F	24	HIS
3	F	157	ASN
3	F	202	HIS
3	F	244	GLN
3	F	254	GLN

### 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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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
6	NAG	E	401	3	14,14,15	0.49	0	15,19,21	1.27	2 (13%)
6	NAG	F	401	3	14,14,15	0.48	0	15,19,21	0.86	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
6	NAG	E	401	3	-	0/6/23/26	0/1/1/1
6	NAG	F	401	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	401	NAG	O5-C1-C2	-2.91	107.42	111.47
6	E	401	NAG	C1-O5-C5	2.42	115.50	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	F	401	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<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	214/214 (100%)	-0.31	3 (1%) 75 76	25, 56, 92, 115	0
1	C	214/214 (100%)	-0.23	3 (1%) 75 76	29, 54, 94, 132	0
2	B	229/229 (100%)	-0.29	3 (1%) 77 78	29, 49, 92, 153	0
2	D	219/229 (95%)	-0.29	0 100 100	27, 49, 74, 119	0
3	E	314/328 (95%)	-0.07	19 (6%) 22 22	30, 51, 124, 204	0
3	F	296/328 (90%)	0.40	38 (12%) 4 3	27, 59, 178, 219	0
All	All	1486/1542 (96%)	-0.10	66 (4%) 35 37	25, 52, 120, 219	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	288	VAL	10.7
3	F	299	LEU	10.5
3	F	230	GLN	8.0
3	E	234	ARG	7.8
3	F	267	GLU	6.2
3	F	287	LEU	6.1
3	E	235	VAL	5.8
3	F	315	LEU	5.8
3	F	263	VAL	5.7
3	F	259	GLU	5.6
3	F	255	LEU	5.4
3	F	260	ASN	4.9
2	B	137	GLN	4.7
3	E	98	SER	4.7
3	E	97	GLY	4.7
3	F	300	THR	4.6
3	E	292	ASP	4.5
3	F	314	ARG	4.5
3	E	289	ASN	4.4

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Mol	Chain	Res	Type	RSRZ
3	F	228	VAL	4.4
3	F	231	GLN	4.4
3	F	286	PHE	4.4
3	F	2	GLU	4.3
3	F	97	GLY	4.2
3	E	99	PRO	4.2
3	F	266	ARG	4.1
3	F	241	VAL	4.0
3	F	256	THR	3.9
3	F	258	SER	3.8
3	E	291	SER	3.8
3	F	309	LEU	3.6
2	B	136	ALA	3.5
2	B	229	HIS	3.5
3	F	264	CYS	3.5
3	F	311	VAL	3.4
3	E	233	MET	3.3
3	F	307	GLY	3.3
3	F	261	GLY	3.3
3	F	254	GLN	3.2
3	F	96	LYS	3.1
3	F	229	THR	3.1
3	F	272	LEU	3.1
3	E	290	ILE	3.0
3	E	297	VAL	3.0
3	E	237	ASN	2.9
3	F	265	GLN	2.9
1	C	188	ARG	2.9
1	A	118	PHE	2.9
3	E	293	GLN	2.8
1	C	212	ASN	2.8
3	F	227	GLU	2.8
3	E	100	GLU	2.7
3	F	99	PRO	2.6
3	E	316	ALA	2.5
3	F	303	VAL	2.5
3	E	317	LEU	2.4
3	F	262	ASN	2.4
1	C	214	CYS	2.4
3	F	310	ALA	2.4
1	A	134	CYS	2.3
3	F	304	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	236	GLY	2.2
3	E	53	LYS	2.1
3	E	238	GLN	2.1
1	A	117	ILE	2.0
3	F	253	LEU	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
6	NAG	E	401	14/15	0.93	0.15	-0.42	63,86,128,134	0
5	CL	E	402	1/1	0.96	0.07	-1.30	68,68,68,68	0
4	ZN	B	301	1/1	1.00	0.06	-	68,68,68,68	0
5	CL	D	301	1/1	0.91	0.10	-	67,67,67,67	0
6	NAG	F	401	14/15	0.71	0.36	-	98,166,213,219	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.