



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:21 PM UTC

PDB ID : 4I2X / pdb_00004i2x
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

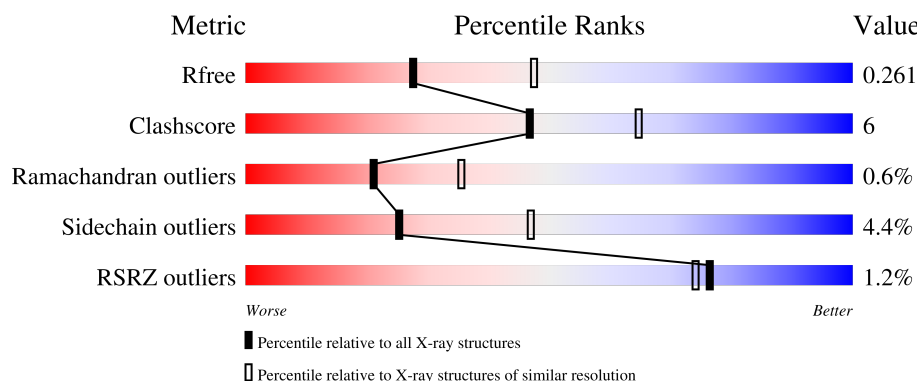
1 Overall quality at a glance

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}	180053	7589 (2.50-2.46)
Clashscore	190562	8295 (2.50-2.46)
Ramachandran outliers	187476	8164 (2.50-2.46)
Sidechain outliers	187428	8166 (2.50-2.46)
RSRZ outliers	180081	7593 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	
1	C	214	
2	B	229	
2	D	229	
3	E	328	

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Mol	Chain	Length	Quality of chain
3	F	328	3% 76% 14% 10%

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 (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is CHLORIDE ION (CCD ID: 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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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		

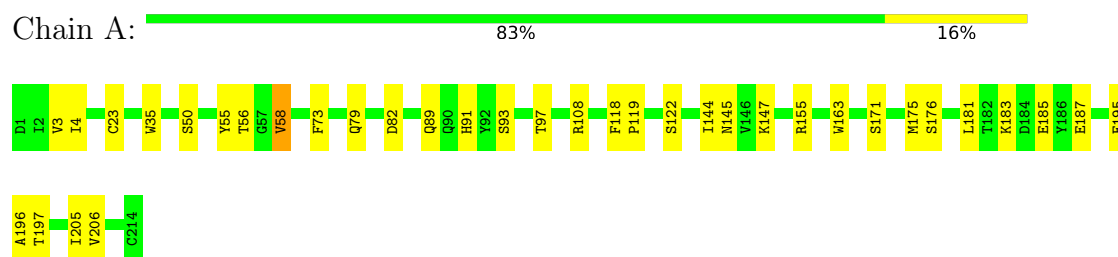
- Molecule 7 is water.

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		

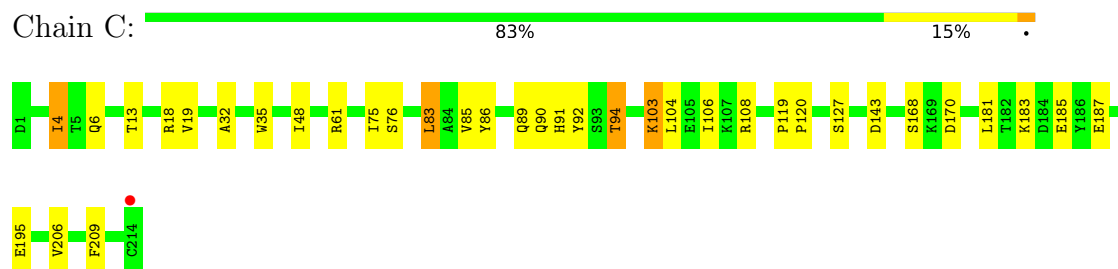
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

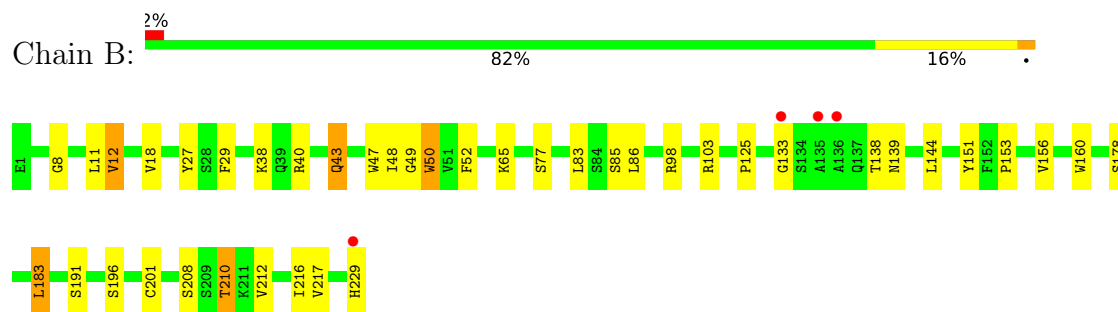
• Molecule 1: FabOX117 light chain



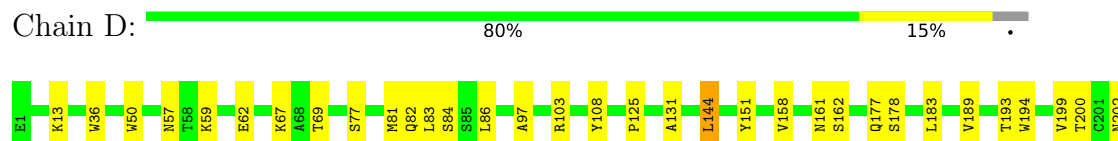
• Molecule 1: FabOX117 light chain

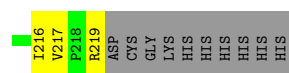


• Molecule 2: FabOX117 heavy chain

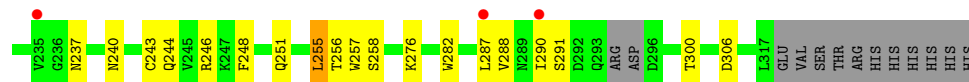
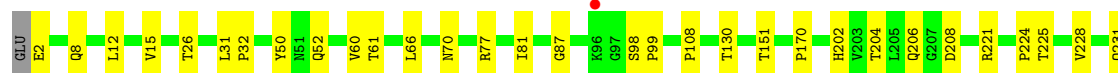
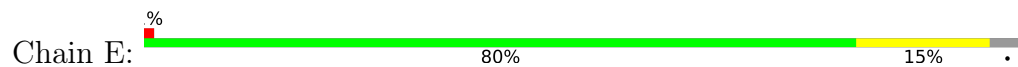


• Molecule 2: FabOX117 heavy chain

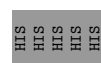
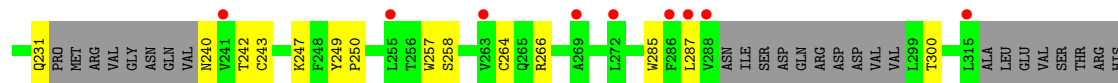
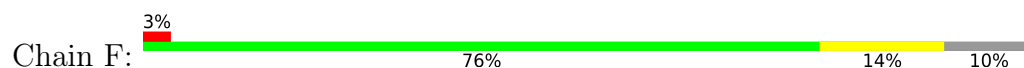




• Molecule 3: Signal-regulatory protein gamma



• 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, α , β , γ	140.36Å 174.19Å 81.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 2.48 29.82 – 2.48	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.82-2.48) 99.1 (29.82-2.48)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	42.6	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAG, ZN, 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	0.46	0/1703	0.80	0/2315
1	C	0.47	0/1703	0.80	1/2315 (0.0%)
2	B	0.51	0/1801	0.83	2/2461 (0.1%)
2	D	0.49	0/1708	0.80	0/2336
3	E	0.48	0/2495	0.77	0/3401
3	F	0.46	0/2358	0.78	1/3212 (0.0%)
All	All	0.48	0/11768	0.80	4/16040 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	GLY	CA-C-N	5.82	125.82	119.89
2	B	8	GLY	C-N-CA	5.82	125.82	119.89
1	C	19	VAL	N-CA-C	5.03	115.95	108.46
3	F	92	VAL	N-CA-C	5.01	115.33	108.12

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	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1663	0	1588	23	0
2	B	1746	0	1688	19	0
2	D	1659	0	1622	23	0
3	E	2442	0	2423	24	0
3	F	2307	0	2286	30	0
4	B	1	0	0	0	0
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	129	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 6.

All (129) 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:F:81:ILE:HD12	3:F:112:MET:HE1	1.60	0.82
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
2:D:36:TRP:CE3	2:D:81:MET:HE2	2.30	0.66
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:GLN:HE22	1:C:91:HIS:CD2	2.20	0.60
1:A:163:TRP:HE1	1:A:175:MET:HE2	1.65	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
1:A:89:GLN:HE22	1:A:91:HIS:HD2	1.51	0.56
2:B:50:TRP:C	2:B:50:TRP:CD1	2.83	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
3:E:31:LEU:HA	3:E:32:PRO:C	2.32	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
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
2:D:50:TRP:CD1	2:D:50:TRP:C	2.88	0.50
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:183:LEU:HD12	2:B:183:LEU:C	2.40	0.46
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
1:C:35:TRP:HB2	1:C:48:ILE:HB	1.98	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:35:TRP:CD2	1:A:73:PHE:HB2	2.51	0.45
1:A:155:ARG:NH2	1:A:185:GLU:OE1	2.49	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
1:A:163:TRP:NE1	1:A:175:MET:HE2	2.31	0.45
3:F:152:LEU:C	3:F:152:LEU:HD23	2.42	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
3:E:255:LEU:HD12	3:E:255:LEU:C	2.42	0.44
2:D:161:ASN:ND2	2:D:200:THR:H	2.16	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
1:A:144:ILE:HG23	1:A:175:MET:HE3	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:55:TYR:O	1:A:56:THR:C	2.63	0.41
1:A:118:PHE:HA	1:A:119:PRO:HD3	1.85	0.41
1:A:144:ILE:CG2	1:A:175:MET:HE3	2.51	0.41
2:B:11:LEU:HB2	2:B:153:PRO:HG3	2.01	0.41
3:E:81:ILE:HD13	3:E:81:ILE:HA	1.92	0.41
2:D:50:TRP:HZ2	3:F:24:HIS:CD2	2.38	0.41
2:D:177:GLN:O	2:D:178:SER:C	2.64	0.41
1:C:119:PRO:HB3	1:C:209:PHE:CE1	2.56	0.40
1:C:170:ASP:OD2	1:C:170:ASP:C	2.63	0.40
2:D:131:ALA:O	2:D:219:ARG:NH2	2.54	0.40
2:D:183:LEU:HD12	2:D:183:LEU:C	2.46	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
3:E:12:LEU:C	3:E:12:LEU:HD23	2.46	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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%)	6	11
2	D	217/229 (95%)	207 (95%)	10 (5%)	0	100	100
3	E	310/328 (94%)	295 (95%)	13 (4%)	2 (1%)	21	35
3	F	290/328 (88%)	279 (96%)	8 (3%)	3 (1%)	12	22
All	All	1468/1542 (95%)	1393 (95%)	66 (4%)	9 (1%)	21	35

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%)	183 (96%)	7 (4%)	30	54
1	C	190/190 (100%)	181 (95%)	9 (5%)	23	44
2	B	194/194 (100%)	181 (93%)	13 (7%)	15	29
2	D	185/194 (95%)	178 (96%)	7 (4%)	29	53
3	E	278/292 (95%)	263 (95%)	15 (5%)	20	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	F	262/292 (90%)	256 (98%)	6 (2%)	44 69
All	All	1299/1352 (96%)	1242 (96%)	57 (4%)	25 47

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	50	SER
1	A	58	VAL
1	A	93	SER
1	A	97	THR
1	A	122	SER
1	A	181	LEU
2	B	12	VAL
2	B	43	GLN
2	B	50	TRP
2	B	85	SER
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	212	VAL
2	B	217	VAL
2	B	229	HIS
1	C	4	ILE
1	C	83	LEU
1	C	94	THR
1	C	103	LYS
1	C	127	SER
1	C	143	ASP
1	C	168	SER
1	C	181	LEU
1	C	185	GLU
2	D	13	LYS
2	D	67	LYS
2	D	77	SER
2	D	84	SER
2	D	144	LEU
2	D	162	SER
2	D	217	VAL

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Mol	Chain	Res	Type
3	E	70	ASN
3	E	98	SER
3	E	130	THR
3	E	151	THR
3	E	206	GLN
3	E	208	ASP
3	E	225	THR
3	E	228	VAL
3	E	237	ASN
3	E	251	GLN
3	E	255	LEU
3	E	276	LYS
3	E	287	LEU
3	E	288	VAL
3	E	290	ILE
3	F	31	LEU
3	F	141	GLU
3	F	151	THR
3	F	208	ASP
3	F	225	THR
3	F	228	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	79	GLN
1	A	91	HIS
1	A	156	GLN
2	B	161	ASN
1	C	91	HIS
1	C	161	ASN
1	C	189	HIS
1	C	190	ASN
2	D	57	ASN
2	D	161	ASN
3	E	56	HIS
3	E	202	HIS
3	E	206	GLN
3	E	215	ASN
3	E	244	GLN
3	E	254	GLN

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Mol	Chain	Res	Type
3	F	157	ASN
3	F	202	HIS
3	F	244	GLN
3	F	254	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	17,19,21	1.17	2 (11%)
6	NAG	F	401	3	14,14,15	0.47	0	17,19,21	0.80	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	-	1/6/23/26	0/1/1/1
6	NAG	F	401	3	-	2/6/23/26	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	-2.50	107.42	111.29
6	E	401	NAG	C1-O5-C5	2.47	115.50	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	401	NAG	O5-C5-C6-O6
6	F	401	NAG	C4-C5-C6-O6
6	E	401	NAG	O5-C5-C6-O6

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/214 (100%)	-0.42	0 100 100	25, 56, 92, 115	0
1	C	214/214 (100%)	-0.41	1 (0%) 87 85	29, 54, 94, 132	0
2	B	229/229 (100%)	-0.46	4 (1%) 69 66	29, 49, 92, 153	0
2	D	219/229 (95%)	-0.52	0 100 100	27, 49, 74, 119	0
3	E	314/328 (95%)	-0.36	4 (1%) 75 72	30, 51, 124, 204	0
3	F	296/328 (90%)	-0.03	9 (3%) 52 49	27, 59, 178, 219	0
All	All	1486/1542 (96%)	-0.35	18 (1%) 76 74	25, 52, 120, 219	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	288	VAL	6.5
2	B	136	ALA	4.8
3	F	287	LEU	3.6
2	B	229	HIS	3.3
2	B	133	GLY	3.2
3	F	315	LEU	3.1
3	F	272	LEU	3.0
3	E	235	VAL	3.0
3	F	269	ALA	3.0
3	F	255	LEU	2.9
3	E	290	ILE	2.8
3	F	263	VAL	2.5
3	E	96	LYS	2.4
1	C	214	CYS	2.4
3	E	287	LEU	2.3
3	F	241	VAL	2.2
2	B	135	ALA	2.0
3	F	286	PHE	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NAG	F	401	14/15	0.62	0.15	98,166,213,219	0
6	NAG	E	401	14/15	0.93	0.09	63,86,128,134	0
5	CL	D	301	1/1	0.95	0.09	67,67,67,67	0
5	CL	E	402	1/1	0.96	0.14	68,68,68,68	0
4	ZN	B	301	1/1	0.99	0.02	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.