



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2026 – 02:34 PM EDT

PDB ID : 12QC / pdb_000012qc
Title : Crystal structure of 30G4 Fab in complex with an orthommarburgvirus GP2 peptide
Authors : Niyongabo, A.; Ofek, G.
Deposited on : 2026-04-14
Resolution : 2.08 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
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

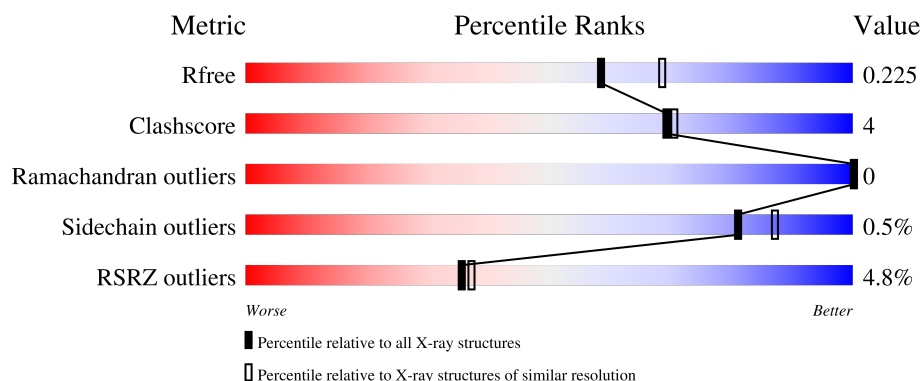
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	19	<div> <div>21%</div> <div>47%</div> <div>53%</div> </div>
1	D	19	<div> <div>26%</div> <div>32%</div> <div>16%</div> <div>53%</div> </div>
1	P	19	<div> <div>16%</div> <div>58%</div> <div>42%</div> </div>
1	Q	19	<div> <div>16%</div> <div>47%</div> <div>53%</div> </div>
2	B	219	<div> <div>3%</div> <div>92%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	219	<div><div></div><div>2%</div><div>92%</div><div>8%</div></div>
2	G	219	<div><div></div><div>3%</div><div>96%</div><div></div><div>.</div></div>
2	L	219	<div><div></div><div>%</div><div>95%</div><div>5%</div></div>
3	C	224	<div><div></div><div>4%</div><div>94%</div><div>.</div><div>..</div></div>
3	F	224	<div><div></div><div>2%</div><div>91%</div><div>7%</div><div>..</div></div>
3	H	224	<div><div></div><div>2%</div><div>95%</div><div>5%</div></div>
3	N	224	<div><div></div><div>16%</div><div>87%</div><div>11%</div><div>.</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 27657 atoms, of which 13057 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 GP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	9	Total	C	H	N	O	0	0	0
			111	42	47	9	13			
1	A	9	Total	C	H	N	O	0	0	0
			119	44	51	9	15			
1	P	11	Total	C	H	N	O	0	0	0
			159	56	71	12	20			
1	D	9	Total	C	H	N	O	0	0	0
			138	47	66	10	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	448	LYS	-	insertion	UNP Q1PDC7
Q	449	LYS	-	insertion	UNP Q1PDC7
Q	465	LYS	-	insertion	UNP Q1PDC7
Q	466	LYS	-	insertion	UNP Q1PDC7
A	448	LYS	-	insertion	UNP Q1PDC7
A	449	LYS	-	insertion	UNP Q1PDC7
A	465	LYS	-	insertion	UNP Q1PDC7
A	466	LYS	-	insertion	UNP Q1PDC7
P	448	LYS	-	insertion	UNP Q1PDC7
P	449	LYS	-	insertion	UNP Q1PDC7
P	465	LYS	-	insertion	UNP Q1PDC7
P	466	LYS	-	insertion	UNP Q1PDC7
D	448	LYS	-	insertion	UNP Q1PDC7
D	449	LYS	-	insertion	UNP Q1PDC7
D	465	LYS	-	insertion	UNP Q1PDC7
D	466	LYS	-	insertion	UNP Q1PDC7

- Molecule 2 is a protein called 30G4 Fab light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	219	Total	C	H	N	O	S	0	0	0
			3278	1051	1604	279	338	6			
2	B	219	Total	C	H	N	O	S	0	0	0
			3258	1047	1590	277	338	6			
2	G	219	Total	C	H	N	O	S	0	0	0
			3278	1051	1603	280	338	6			
2	L	219	Total	C	H	N	O	S	0	0	0
			3289	1053	1611	281	338	6			

- Molecule 3 is a protein called 30G4 Fab heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	222	Total	C	H	N	O	S	0	0	0
			3282	1058	1610	278	329	7			
3	C	222	Total	C	H	N	O	S	0	0	0
			3297	1061	1621	279	329	7			
3	N	220	Total	C	H	N	O	S	0	0	0
			3174	1035	1540	272	320	7			
3	H	224	Total	C	H	N	O	S	0	0	0
			3336	1071	1643	282	332	8			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Q	2	Total	O	0	0
			2	2		
4	E	124	Total	O	0	0
			124	124		
4	F	140	Total	O	0	0
			140	140		
4	A	4	Total	O	0	0
			4	4		
4	B	158	Total	O	0	0
			158	158		
4	C	106	Total	O	0	0
			106	106		
4	G	109	Total	O	0	0
			109	109		
4	N	35	Total	O	0	0
			35	35		
4	P	8	Total	O	0	0
			8	8		
4	L	119	Total	O	0	0
			119	119		

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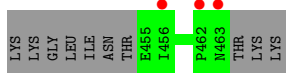
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	130	Total 130	O 130	0	0
4	D	3	Total 3	O 3	0	0

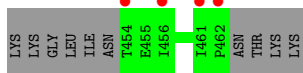
3 Residue-property plots [i](#)

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.

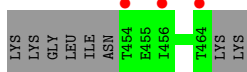
- Molecule 1: GP2



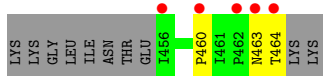
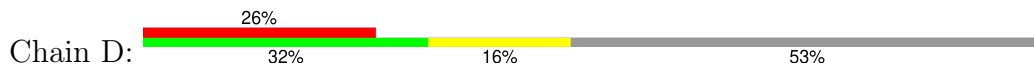
- Molecule 1: GP2



- Molecule 1: GP2



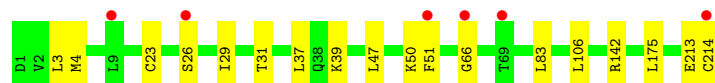
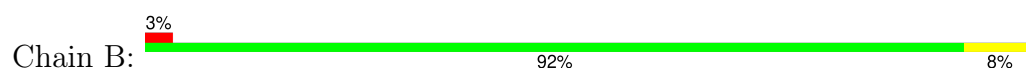
- Molecule 1: GP2



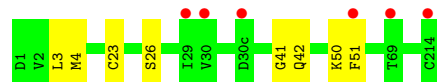
- Molecule 2: 30G4 Fab light chain



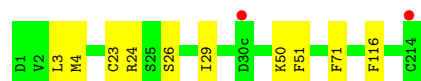
- Molecule 2: 30G4 Fab light chain



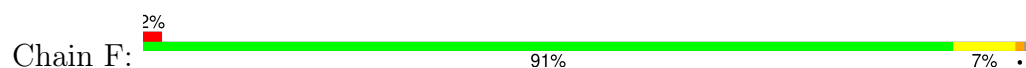
- Molecule 2: 30G4 Fab light chain



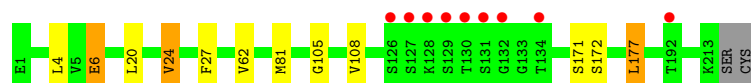
- Molecule 2: 30G4 Fab light chain



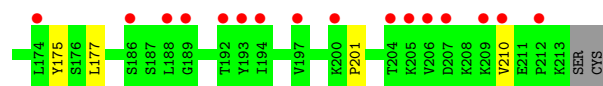
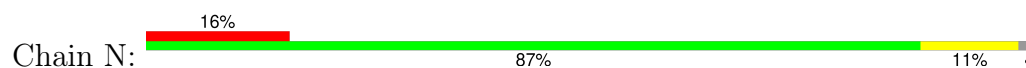
- Molecule 3: 30G4 Fab heavy chain



- Molecule 3: 30G4 Fab heavy chain

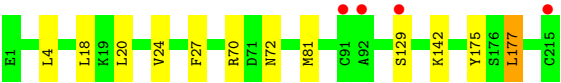


- Molecule 3: 30G4 Fab heavy chain



- Molecule 3: 30G4 Fab heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.75Å 145.08Å 146.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.31 – 2.08 29.31 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.31-2.08) 99.7 (29.31-2.08)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.08Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.193 , 0.223 0.199 , 0.225	Depositor DCC
R_{free} test set	6533 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	27657	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.09 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3865e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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](#)

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	0.20	0/70	0.27	0/96
1	D	0.91	0/74	1.02	0/102
1	P	0.90	0/90	1.15	0/124
1	Q	0.19	0/66	0.29	0/91
2	B	0.26	0/1706	0.46	1/2321 (0.0%)
2	E	0.26	0/1712	0.44	0/2326
2	G	0.14	0/1713	0.33	0/2329
2	L	0.17	0/1716	0.38	0/2332
3	C	0.15	0/1718	0.36	0/2340
3	F	0.17	0/1714	0.37	0/2336
3	H	0.20	0/1735	0.42	0/2361
3	N	0.30	0/1675	0.48	1/2286 (0.0%)
All	All	0.24	0/13989	0.42	2/19044 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	66	GLY	CA-C-O	-6.64	117.65	122.23
3	N	146	PRO	N-CA-C	-5.20	102.93	111.15

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	68	51	51	0	0
1	D	72	66	65	2	0
1	P	88	71	78	0	0
1	Q	64	47	47	0	0
2	B	1668	1590	1590	14	0
2	E	1674	1604	1605	13	0
2	G	1675	1603	1603	7	0
2	L	1678	1611	1611	8	0
3	C	1676	1621	1621	9	0
3	F	1672	1610	1610	13	0
3	H	1693	1643	1643	9	0
3	N	1634	1540	1539	22	0
4	A	4	0	0	0	0
4	B	158	0	0	2	0
4	C	106	0	0	2	0
4	D	3	0	0	0	0
4	E	124	0	0	4	0
4	F	140	0	0	1	0
4	G	109	0	0	4	0
4	H	130	0	0	0	0
4	L	119	0	0	1	0
4	N	35	0	0	0	0
4	P	8	0	0	0	0
4	Q	2	0	0	0	0
All	All	14600	13057	13063	94	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 4.

All (94) 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)
3:F:101:TYR:OH	4:F:301:HOH:O	1.68	1.10
2:B:50:LYS:O	2:B:51:PHE:CD2	2.17	0.96
3:N:86:THR:HG22	3:N:110:VAL:H	1.41	0.83
3:F:86:THR:HG22	3:F:110:VAL:H	1.44	0.82
3:N:115:THR:HG23	3:N:146:PRO:HG2	1.67	0.77
2:B:50:LYS:O	2:B:51:PHE:CG	2.38	0.76
3:H:4:LEU:HD23	3:H:24:VAL:HG22	1.69	0.72
3:C:4:LEU:HD23	3:C:24:VAL:HG22	1.74	0.69
3:N:115:THR:HG23	3:N:146:PRO:CG	2.23	0.68
2:E:33:LEU:HD12	2:E:89:PHE:O	1.96	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:4:LEU:HD23	3:F:24:VAL:HG22	1.79	0.65
3:H:4:LEU:CD2	3:H:24:VAL:HG22	2.28	0.64
3:N:4:LEU:CD2	3:N:24:VAL:HG22	2.27	0.64
2:B:50:LYS:C	2:B:51:PHE:CD2	2.76	0.63
3:C:4:LEU:CD2	3:C:24:VAL:HG22	2.28	0.62
3:N:4:LEU:HD23	3:N:24:VAL:HG22	1.82	0.62
2:B:4:MET:HE3	2:B:23:CYS:SG	2.43	0.59
2:L:29:ILE:HD11	2:L:71:PHE:CZ	2.37	0.58
2:G:42:GLN:N	4:G:304:HOH:O	2.37	0.58
3:F:20:LEU:HG	3:F:81:MET:HE2	1.86	0.58
3:H:20:LEU:HG	3:H:81:MET:HE2	1.85	0.58
2:B:31:THR:HB	2:B:51:PHE:CD2	2.39	0.58
3:F:18:LEU:HB3	3:F:81:MET:HE3	1.85	0.57
3:N:118:PRO:HB2	3:N:141:VAL:HG13	1.85	0.57
3:F:62:VAL:HG13	3:F:66:PHE:CG	2.40	0.57
3:F:4:LEU:CD2	3:F:24:VAL:HG22	2.34	0.57
3:H:142:LYS:O	3:H:175:TYR:O	2.22	0.57
3:N:177:LEU:HD12	3:N:177:LEU:C	2.29	0.57
2:E:105:GLU:OE2	2:E:142:ARG:NH2	2.36	0.56
2:G:41:GLY:N	4:G:304:HOH:O	2.40	0.55
3:N:32:TYR:CG	3:N:93:ARG:HD3	2.42	0.53
3:C:177:LEU:HD12	3:C:177:LEU:C	2.33	0.53
2:G:41:GLY:CA	4:G:304:HOH:O	2.56	0.52
2:E:50:LYS:O	2:E:51:PHE:HB3	2.10	0.52
2:L:29:ILE:HD11	2:L:71:PHE:CE2	2.45	0.52
3:F:83(c):SER:O	3:F:86:THR:HG23	2.10	0.51
2:B:83:LEU:HD11	2:B:106:LEU:HG	1.92	0.51
2:L:50:LYS:O	2:L:51:PHE:HB3	2.09	0.51
2:E:161:GLU:HG3	4:E:347:HOH:O	2.11	0.51
3:N:145:PHE:O	3:N:146:PRO:C	2.53	0.50
3:C:81:MET:HE1	3:C:108:VAL:HG21	1.92	0.50
3:H:177:LEU:C	3:H:177:LEU:HD12	2.37	0.50
2:E:116:PHE:HD1	3:F:129:SER:HA	1.76	0.50
2:L:3:LEU:HB3	2:L:26:SER:OG	2.12	0.50
2:B:29:ILE:O	2:B:29:ILE:HG22	2.11	0.49
2:E:163:VAL:HG22	2:E:175:LEU:HD12	1.93	0.49
3:H:18:LEU:HB3	3:H:81:MET:HE3	1.95	0.48
2:E:126:LYS:NZ	4:E:305:HOH:O	2.46	0.48
3:F:177:LEU:C	3:F:177:LEU:HD12	2.37	0.48
2:G:3:LEU:HB3	2:G:26:SER:OG	2.13	0.48
3:N:146:PRO:HB2	3:N:201:PRO:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:ASN:O	1:D:464:THR:C	2.56	0.48
3:C:20:LEU:HG	3:C:81:MET:HE2	1.95	0.47
3:N:141:VAL:HG12	3:N:144:TYR:CD2	2.48	0.47
3:C:172:SER:N	4:C:308:HOH:O	2.47	0.47
2:E:33:LEU:HD22	2:E:71:PHE:CG	2.49	0.47
2:E:166:GLN:HG2	2:E:171:SER:HA	1.97	0.47
3:N:20:LEU:HG	3:N:81:MET:HE2	1.97	0.47
3:N:129:SER:O	3:N:135:ALA:HA	2.15	0.47
2:E:29:ILE:HD11	2:E:71:PHE:CE2	2.50	0.47
2:B:50:LYS:C	2:B:51:PHE:CG	2.93	0.47
2:G:50:LYS:O	2:G:51:PHE:HB3	2.14	0.47
2:L:3:LEU:HB3	2:L:26:SER:HG	1.79	0.46
3:C:6:GLU:CD	3:C:105:GLY:H	2.23	0.46
4:E:410:HOH:O	3:F:128:LYS:HE3	2.15	0.46
2:B:175:LEU:C	2:B:175:LEU:HD23	2.40	0.46
2:B:142:ARG:NH1	4:B:305:HOH:O	2.47	0.46
3:N:93:ARG:NE	3:N:94:HIS:O	2.50	0.45
2:G:41:GLY:C	4:G:304:HOH:O	2.59	0.45
3:N:33:ALA:HB2	1:D:460:PRO:HB3	1.99	0.45
2:B:37:LEU:HB2	2:B:47:LEU:HD11	1.99	0.44
2:L:4:MET:HE3	2:L:23:CYS:SG	2.57	0.44
3:C:171:SER:HB2	4:C:308:HOH:O	2.18	0.44
2:L:24:ARG:HD2	4:L:304:HOH:O	2.17	0.43
3:F:12:VAL:HG11	3:F:83(a):LEU:HD13	2.00	0.43
3:H:24:VAL:HG13	3:H:27:PHE:CE1	2.54	0.43
2:B:39:LYS:NZ	4:B:310:HOH:O	2.51	0.43
2:E:161:GLU:CG	4:E:347:HOH:O	2.66	0.43
2:B:213:GLU:O	2:B:214:CYS:HB2	2.19	0.42
2:E:175:LEU:C	2:E:175:LEU:HD23	2.45	0.42
2:B:3:LEU:HB3	2:B:26:SER:OG	2.18	0.42
3:N:118:PRO:CB	3:N:141:VAL:HG13	2.49	0.42
3:H:70:ARG:HD3	3:H:72:ASN:OD1	2.19	0.42
2:E:37:LEU:HB2	2:E:47:LEU:HD11	2.02	0.41
3:N:115:THR:HG23	3:N:146:PRO:HG3	2.02	0.41
3:N:24:VAL:HG13	3:N:27:PHE:CZ	2.56	0.41
3:N:24:VAL:HG13	3:N:27:PHE:CE1	2.55	0.41
3:N:137:LEU:HB2	3:N:210:VAL:HG11	2.01	0.41
3:F:190:THR:OG1	3:F:191:GLN:N	2.54	0.41
3:N:145:PHE:HB3	3:N:146:PRO:HD3	2.03	0.41
3:C:24:VAL:HG13	3:C:27:PHE:CZ	2.56	0.41
3:N:142:LYS:O	3:N:175:TYR:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4:MET:HE3	2:G:23:CYS:SG	2.61	0.40
2:L:116:PHE:CD1	3:H:129:SER:HA	2.57	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	7/19 (37%)	7 (100%)	0	0	100	100
1	D	7/19 (37%)	7 (100%)	0	0	100	100
1	P	9/19 (47%)	9 (100%)	0	0	100	100
1	Q	7/19 (37%)	7 (100%)	0	0	100	100
2	B	217/219 (99%)	213 (98%)	4 (2%)	0	100	100
2	E	217/219 (99%)	211 (97%)	6 (3%)	0	100	100
2	G	217/219 (99%)	212 (98%)	5 (2%)	0	100	100
2	L	217/219 (99%)	212 (98%)	5 (2%)	0	100	100
3	C	220/224 (98%)	216 (98%)	4 (2%)	0	100	100
3	F	220/224 (98%)	215 (98%)	5 (2%)	0	100	100
3	H	222/224 (99%)	217 (98%)	5 (2%)	0	100	100
3	N	216/224 (96%)	208 (96%)	8 (4%)	0	100	100
All	All	1776/1848 (96%)	1734 (98%)	42 (2%)	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	7/18 (39%)	7 (100%)	0	100	100
1	D	9/18 (50%)	9 (100%)	0	100	100
1	P	11/18 (61%)	11 (100%)	0	100	100
1	Q	6/18 (33%)	6 (100%)	0	100	100
2	B	189/194 (97%)	189 (100%)	0	100	100
2	E	190/194 (98%)	190 (100%)	0	100	100
2	G	190/194 (98%)	190 (100%)	0	100	100
2	L	191/194 (98%)	191 (100%)	0	100	100
3	C	186/192 (97%)	182 (98%)	4 (2%)	45	51
3	F	185/192 (96%)	183 (99%)	2 (1%)	65	73
3	H	189/192 (98%)	188 (100%)	1 (0%)	81	87
3	N	175/192 (91%)	175 (100%)	0	100	100
All	All	1528/1616 (95%)	1521 (100%)	7 (0%)	81	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	24	VAL
3	F	177	LEU
3	C	6	GLU
3	C	24	VAL
3	C	62	VAL
3	C	177	LEU
3	H	177	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	163	HIS
2	B	38	GLN

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Mol	Chain	Res	Type
3	C	39	GLN
3	C	80	GLN
3	C	163	HIS
2	G	27	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](#)

There are no ligands in this entry.

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	9/19 (47%)	1.78	4 (44%) 0 1	55, 66, 88, 93	0
1	D	9/19 (47%)	2.02	5 (55%) 0 0	43, 75, 116, 128	0
1	P	11/19 (57%)	1.62	3 (27%) 1 1	30, 61, 113, 116	0
1	Q	9/19 (47%)	1.20	3 (33%) 1 1	51, 57, 85, 95	0
2	B	219/219 (100%)	-0.05	6 (2%) 56 58	31, 48, 78, 121	0
2	E	219/219 (100%)	-0.12	4 (1%) 67 70	31, 48, 75, 99	0
2	G	219/219 (100%)	0.01	6 (2%) 56 58	39, 53, 83, 112	0
2	L	219/219 (100%)	-0.11	2 (0%) 81 83	34, 50, 75, 102	0
3	C	222/224 (99%)	0.12	9 (4%) 41 43	32, 55, 93, 160	0
3	F	222/224 (99%)	-0.14	5 (2%) 61 64	30, 48, 76, 116	0
3	H	224/224 (100%)	-0.08	4 (1%) 67 70	34, 51, 69, 92	0
3	N	220/224 (98%)	1.04	35 (15%) 5 5	39, 80, 113, 143	0
All	All	1802/1848 (97%)	0.12	86 (4%) 35 37	30, 53, 93, 160	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	51	PHE	5.9
1	P	464	THR	5.2
2	L	214	CYS	5.0
1	Q	463	ASN	4.9
1	D	456	ILE	4.5
3	F	129	SER	4.4
3	N	130	THR	4.2
1	A	456	ILE	4.0
3	N	145	PHE	4.0
2	B	69	THR	4.0
2	G	214	CYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	464	THR	3.9
3	N	197	VAL	3.8
3	N	129	SER	3.8
1	A	462	PRO	3.8
3	N	188	LEU	3.7
3	N	212	PRO	3.6
3	C	129	SER	3.6
3	N	205	LYS	3.5
3	C	128	LYS	3.5
1	A	454	THR	3.4
3	C	127	SER	3.4
3	C	126	SER	3.4
3	N	204	THR	3.3
3	N	206	VAL	3.3
1	Q	456	ILE	3.2
2	E	214	CYS	3.2
3	N	133	GLY	3.2
3	F	213	LYS	3.2
3	N	210	VAL	3.1
3	C	192	THR	3.1
2	B	214	CYS	3.1
3	H	215	CYS	3.1
3	N	189	GLY	3.0
3	N	146	PRO	3.0
1	P	454	THR	3.0
3	N	17	SER	2.9
3	N	153	TRP	2.9
3	N	12	VAL	2.9
2	E	68	GLY	2.8
1	D	462	PRO	2.8
3	N	148	PRO	2.8
3	C	131	SER	2.7
3	F	128	LYS	2.7
3	C	130	THR	2.7
3	N	11	LEU	2.7
3	H	129	SER	2.6
2	E	30(c)	ASP	2.6
3	N	209	LYS	2.6
2	G	69	THR	2.6
3	N	144	TYR	2.5
3	N	43	LYS	2.5
3	F	130	THR	2.5

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Mol	Chain	Res	Type	RSRZ
3	N	192	THR	2.5
3	H	92	ALA	2.5
3	C	132	GLY	2.5
3	N	193	TYR	2.5
3	N	186	SER	2.5
1	P	456	ILE	2.4
3	N	118	PRO	2.4
3	N	108	VAL	2.4
3	F	127	SER	2.4
2	B	66	GLY	2.3
3	N	207	ASP	2.3
2	E	69	THR	2.3
1	A	461	ILE	2.3
3	N	110	VAL	2.3
3	H	91	CYS	2.3
2	B	26	SER	2.2
3	N	98	TYR	2.2
2	G	29	ILE	2.2
3	N	141	VAL	2.2
3	N	200	LYS	2.2
3	N	174	LEU	2.2
1	D	463	ASN	2.2
2	G	30(c)	ASP	2.2
3	N	125	PRO	2.1
2	G	30	VAL	2.1
1	D	460	PRO	2.1
2	B	9	LEU	2.1
2	L	30(c)	ASP	2.1
3	N	194	ILE	2.1
1	Q	462	PRO	2.0
3	C	134	THR	2.0
2	G	51	PHE	2.0
3	N	119	SER	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.