



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:41 PM UTC

PDB ID : 9CMC / pdb_00009cmc
Title : Crystal structure of the peanut allergen Ara h 2 with two human derived Fab antibodies 22S1 and 23P34
Authors : Pedersen, L.C.; Mueller, G.A.; Min, J.
Deposited on : 2024-07-14
Resolution : 2.95 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

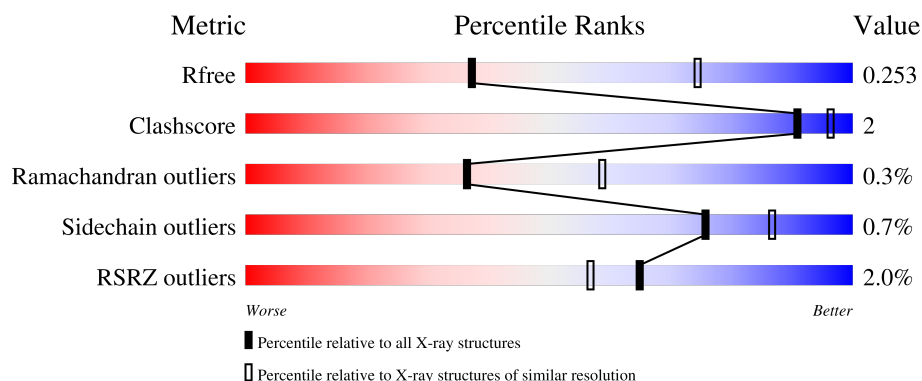
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	225	3% 46% 5% 48%
1	F	225	8% 87% 5% 8%
1	K	225	% 87% 7% 6%
1	P	225	4% 90% 5% 5%
2	B	218	% 46% . 50%

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Mol	Chain	Length	Quality of chain
2	G	218	
2	L	218	
2	Q	218	
3	C	228	
3	H	228	
3	M	228	
3	R	228	
4	D	214	
4	I	214	
4	N	214	
4	V	214	
5	E	140	
5	J	140	
5	O	140	
5	T	140	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25639 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 Fab 23P34 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	116	Total	C	N	O	S	0	0	0
			804	520	135	145	4			
1	F	207	Total	C	N	O	S	0	0	0
			1450	927	246	271	6			
1	K	212	Total	C	N	O	S	0	0	0
			1488	953	247	282	6			
1	P	213	Total	C	N	O	S	0	0	0
			1528	977	259	286	6			

- Molecule 2 is a protein called Fab 23P34 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	110	Total	C	N	O	S	0	0	0
			770	489	132	145	4			
2	G	139	Total	C	N	O	S	0	0	0
			1016	642	168	202	4			
2	L	217	Total	C	N	O	S	0	0	0
			1591	1005	263	317	6			
2	Q	217	Total	C	N	O	S	0	0	0
			1555	983	260	306	6			

- Molecule 3 is a protein called Fab 22S1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	217	Total	C	N	O	S	0	0	0
			1588	1008	257	317	6			
3	H	215	Total	C	N	O	S	0	0	0
			1587	1005	260	316	6			
3	M	217	Total	C	N	O	S	0	0	0
			1573	998	257	312	6			
3	R	216	Total	C	N	O	S	0	0	0
			1579	999	255	319	6			

- Molecule 4 is a protein called Fab 22S1 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	214	Total	C	N	O	S	0	0	0
			1579	992	268	314	5			
4	I	213	Total	C	N	O	S	0	0	0
			1576	991	267	313	5			
4	N	212	Total	C	N	O	S	0	0	0
			1574	992	267	310	5			
4	V	213	Total	C	N	O	S	0	0	0
			1583	996	269	313	5			

- Molecule 5 is a protein called Ara h 2 allergen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	87	Total	C	N	O	S	0	0	0
			658	394	127	127	10			
5	J	93	Total	C	N	O	S	0	1	0
			705	421	136	137	11			
5	O	92	Total	C	N	O	S	0	0	0
			699	418	136	134	11			
5	T	95	Total	C	N	O	S	0	0	0
			713	426	138	138	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	21	GLY	-	expression tag	UNP A0A445BYI5
E	22	SER	-	expression tag	UNP A0A445BYI5
E	23	ALA	-	expression tag	UNP A0A445BYI5
E	24	ALA	-	expression tag	UNP A0A445BYI5
E	25	ALA	-	expression tag	UNP A0A445BYI5
J	21	GLY	-	expression tag	UNP A0A445BYI5
J	22	SER	-	expression tag	UNP A0A445BYI5
J	23	ALA	-	expression tag	UNP A0A445BYI5
J	24	ALA	-	expression tag	UNP A0A445BYI5
J	25	ALA	-	expression tag	UNP A0A445BYI5
O	21	GLY	-	expression tag	UNP A0A445BYI5
O	22	SER	-	expression tag	UNP A0A445BYI5
O	23	ALA	-	expression tag	UNP A0A445BYI5
O	24	ALA	-	expression tag	UNP A0A445BYI5
O	25	ALA	-	expression tag	UNP A0A445BYI5
T	21	GLY	-	expression tag	UNP A0A445BYI5
T	22	SER	-	expression tag	UNP A0A445BYI5
T	23	ALA	-	expression tag	UNP A0A445BYI5

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Chain	Residue	Modelled	Actual	Comment	Reference
T	24	ALA	-	expression tag	UNP A0A445BYI5
T	25	ALA	-	expression tag	UNP A0A445BYI5

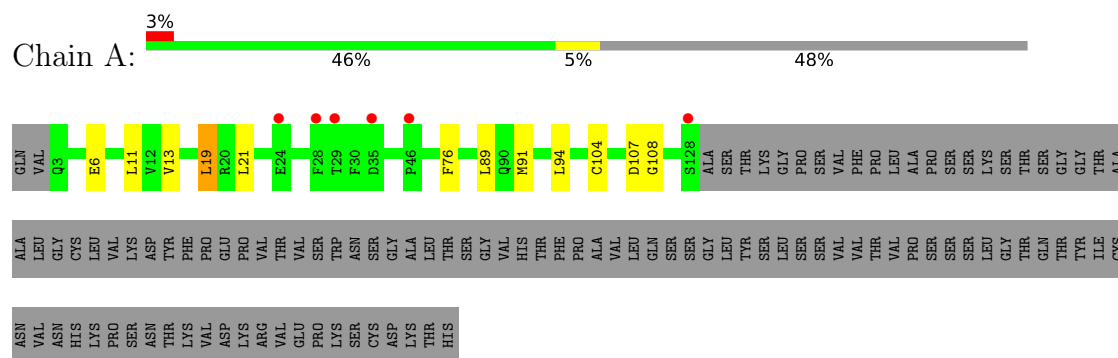
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O 1 1	0	0
6	G	3	Total O 3 3	0	0
6	I	1	Total O 1 1	0	0
6	K	3	Total O 3 3	0	0
6	L	4	Total O 4 4	0	0
6	N	2	Total O 2 2	0	0
6	P	1	Total O 1 1	0	0
6	Q	1	Total O 1 1	0	0
6	R	6	Total O 6 6	0	0
6	T	1	Total O 1 1	0	0

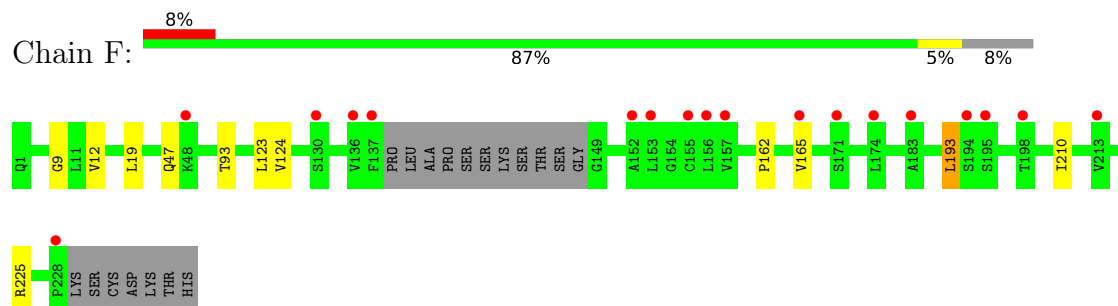
3 Residue-property plots [i](#)

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.

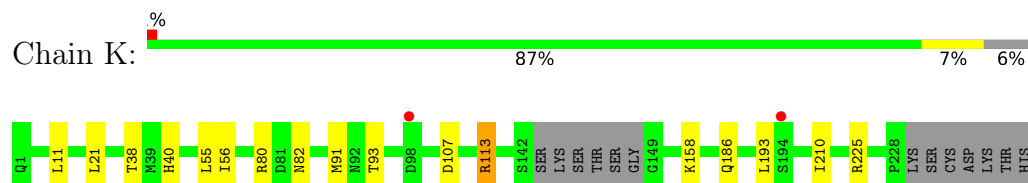
- Molecule 1: Fab 23P34 heavy chain



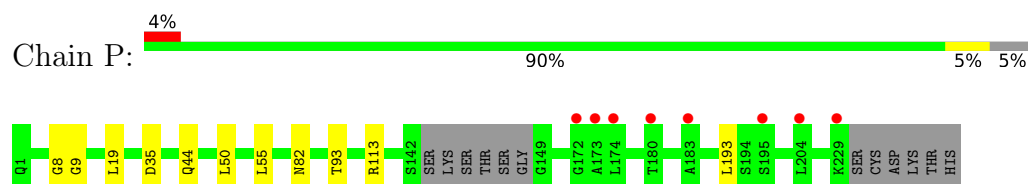
- Molecule 1: Fab 23P34 heavy chain



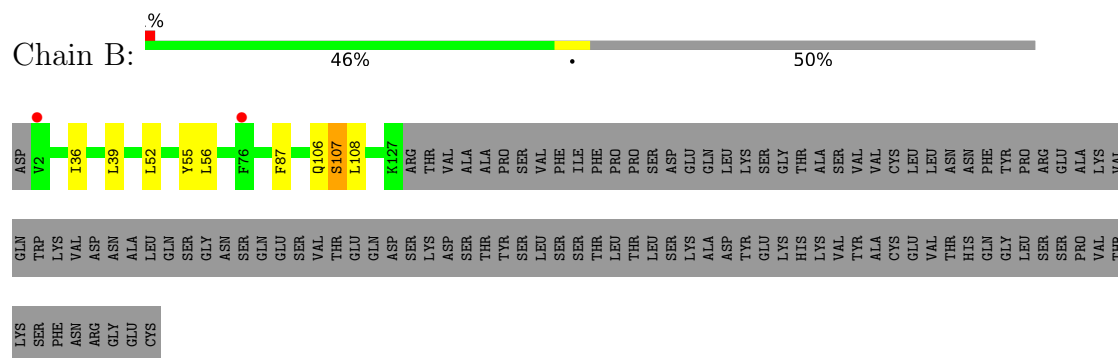
- Molecule 1: Fab 23P34 heavy chain



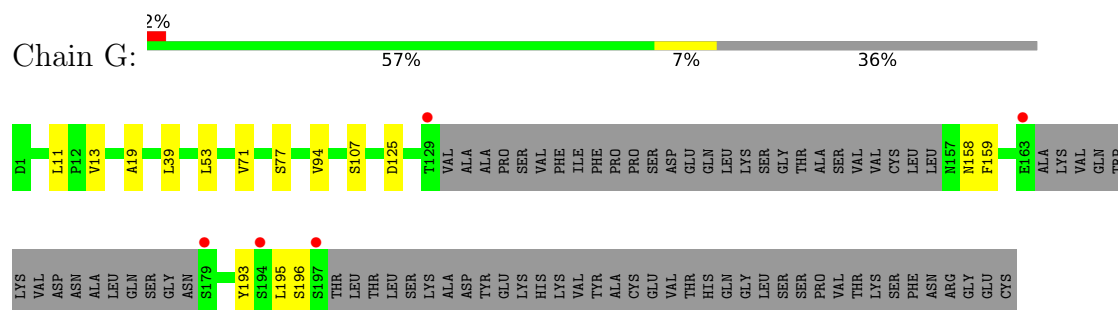
- Molecule 1: Fab 23P34 heavy chain



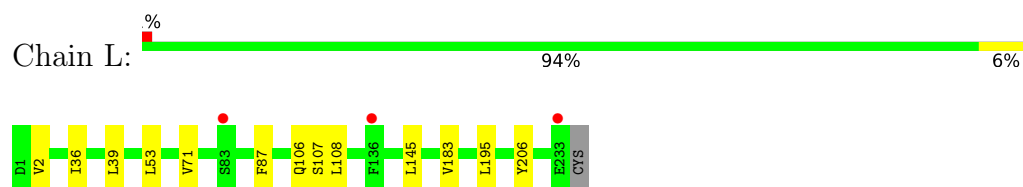
- Molecule 2: Fab 23P34 light chain



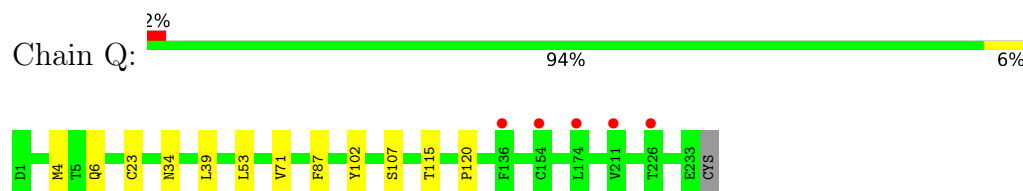
- Molecule 2: Fab 23P34 light chain



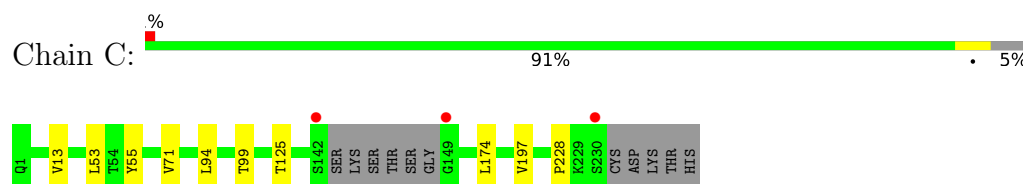
- Molecule 2: Fab 23P34 light chain



- Molecule 2: Fab 23P34 light chain

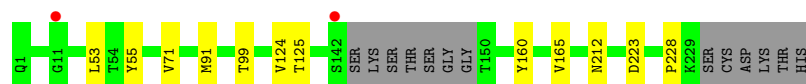


- Molecule 3: Fab 22S1 heavy chain

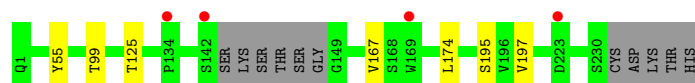


- Molecule 3: Fab 22S1 heavy chain

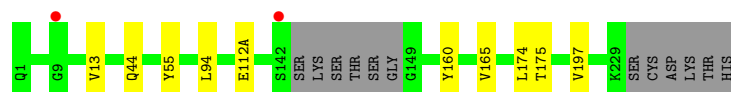
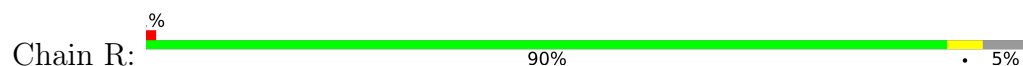




- Molecule 3: Fab 22S1 heavy chain



- Molecule 3: Fab 22S1 heavy chain



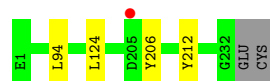
- Molecule 4: Fab 22S1 light chain



- Molecule 4: Fab 22S1 light chain



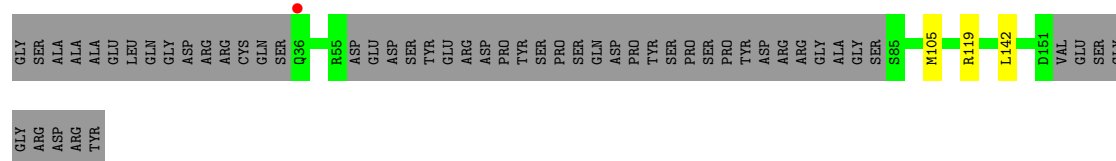
- Molecule 4: Fab 22S1 light chain



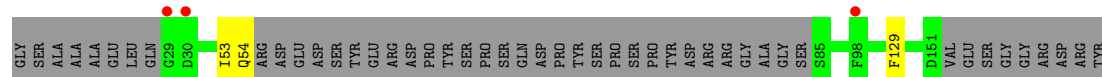
- Molecule 4: Fab 22S1 light chain



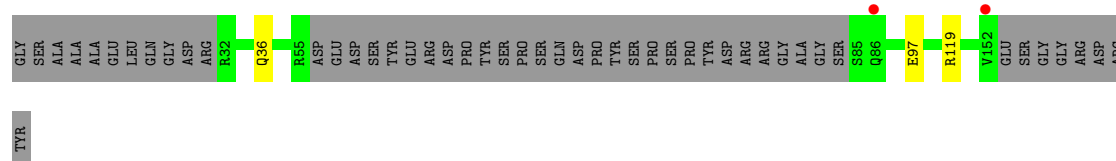
- Molecule 5: Ara h 2 allergen



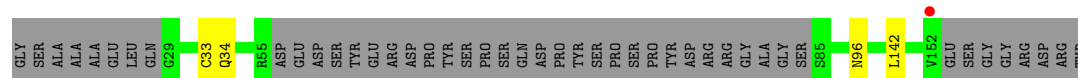
- Molecule 5: Ara h 2 allergen



- Molecule 5: Ara h 2 allergen



- Molecule 5: Ara h 2 allergen



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.91Å 165.01Å 164.64Å 90.00° 105.93° 90.00°	Depositor
Resolution (Å)	49.53 – 2.95 49.53 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.53-2.95) 98.8 (49.53-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.213 , 0.253 0.213 , 0.253	Depositor DCC
R_{free} test set	1996 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25639	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% 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

5.1 Standard geometry

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	0.28	0/825	0.43	0/1130
1	F	0.30	0/1487	0.72	0/2041
1	K	0.38	1/1527 (0.1%)	0.73	0/2097
1	P	0.33	0/1567	0.71	1/2146 (0.0%)
2	B	0.28	0/790	0.47	0/1081
2	G	0.36	0/1038	0.57	0/1414
2	L	0.36	0/1628	0.71	1/2228 (0.0%)
2	Q	0.32	0/1592	0.71	2/2183 (0.1%)
3	C	0.34	0/1625	0.58	0/2217
3	H	0.29	0/1624	0.53	0/2216
3	M	0.29	0/1610	0.55	0/2199
3	R	0.33	0/1616	0.54	0/2207
4	D	0.34	0/1615	0.59	0/2210
4	I	0.33	0/1612	0.55	0/2206
4	N	0.31	0/1610	0.56	0/2202
4	V	0.34	0/1619	0.57	0/2214
5	E	0.35	0/663	0.70	0/890
5	J	0.33	0/710	0.63	0/953
5	O	0.31	0/704	0.65	0/945
5	T	0.34	0/718	0.66	0/964
All	All	0.33	1/26180 (0.0%)	0.62	4/35743 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	107	ASP	C-O	-5.00	1.18	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	115	THR	N-CA-C	-9.19	91.23	110.80
1	P	8	GLY	N-CA-C	-5.93	102.04	112.77
2	L	36	ILE	N-CA-C	5.26	117.43	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	115	THR	N-CA-CB	5.08	119.07	110.49

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	804	0	640	9	0
1	F	1450	0	1240	7	0
1	K	1488	0	1295	8	0
1	P	1528	0	1360	6	0
2	B	770	0	672	6	0
2	G	1016	0	923	5	0
2	L	1591	0	1466	7	0
2	Q	1555	0	1404	5	0
3	C	1588	0	1501	4	0
3	H	1587	0	1512	5	0
3	M	1573	0	1475	3	0
3	R	1579	0	1482	6	0
4	D	1579	0	1450	3	0
4	I	1576	0	1455	1	0
4	N	1574	0	1460	2	0
4	V	1583	0	1469	4	0
5	E	658	0	576	2	0
5	J	705	0	615	2	0
5	O	699	0	621	3	0
5	T	713	0	626	1	0
6	C	1	0	0	0	0
6	G	3	0	0	0	0
6	I	1	0	0	0	0
6	K	3	0	0	1	0
6	L	4	0	0	0	0
6	N	2	0	0	0	0
6	P	1	0	0	1	0
6	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	6	0	0	1	0
6	T	1	0	0	0	0
All	All	25639	0	23242	83	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 2.

All (83) 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)
4:D:94:LEU:HD11	4:D:124:LEU:HD21	1.68	0.76
2:B:36:ILE:HG21	2:B:56:LEU:HD22	1.73	0.70
2:L:39:LEU:HD22	2:L:87:PHE:CG	2.34	0.62
4:I:94:LEU:HD11	4:I:124:LEU:HD21	1.83	0.59
1:F:165:VAL:HG22	1:F:193:LEU:HD21	1.85	0.59
2:G:125:ASP:OD1	2:G:193:TYR:OH	2.20	0.58
1:K:158:LYS:NZ	1:K:186:GLN:OE1	2.37	0.58
2:Q:39:LEU:HD22	2:Q:87:PHE:CG	2.38	0.58
1:A:21:LEU:HD13	1:A:91:MET:HE2	1.86	0.57
3:C:53:LEU:HD22	3:C:71:VAL:HG21	1.86	0.57
2:L:145:LEU:HD21	2:L:206:TYR:CD2	2.40	0.57
2:L:53:LEU:HA	2:L:71:VAL:HG21	1.85	0.56
1:P:113:ARG:NH1	2:Q:107:SER:O	2.38	0.56
3:R:13:VAL:HG11	3:R:94:LEU:HD13	1.87	0.56
1:A:21:LEU:CD1	1:A:91:MET:HE2	2.37	0.55
2:B:39:LEU:HD22	2:B:87:PHE:CG	2.43	0.54
5:O:36:GLN:NE2	5:O:97:GLU:O	2.40	0.54
1:P:35:ASP:OD1	1:P:82:ASN:ND2	2.41	0.54
1:K:40:HIS:CE1	1:K:55:LEU:HD12	2.43	0.53
2:Q:6:GLN:NE2	2:Q:102:TYR:O	2.36	0.53
2:G:195:LEU:HD23	2:G:196:SER:N	2.24	0.53
4:V:94:LEU:HD11	4:V:124:LEU:HD21	1.89	0.52
1:K:80:ARG:NE	1:K:82:ASN:OD1	2.39	0.52
3:R:175:THR:OG1	6:R:301:HOH:O	2.19	0.52
2:L:2:VAL:HG21	2:L:106:GLN:CD	2.35	0.51
1:P:113:ARG:NH2	6:P:301:HOH:O	2.44	0.51
1:A:13:VAL:HG11	1:A:94:LEU:HD12	1.91	0.51
3:M:99:THR:HG23	3:M:125:THR:HA	1.93	0.51
1:K:210:ILE:HD13	1:K:225:ARG:HA	1.94	0.50
2:Q:53:LEU:HA	2:Q:71:VAL:HG21	1.93	0.50
1:A:6:GLU:OE1	1:A:104:CYS:N	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:93:THR:HG22	1:K:93:THR:O	2.13	0.49
2:B:107:SER:O	5:E:119:ARG:NH1	2.42	0.49
1:A:13:VAL:HG22	1:A:19:LEU:HD13	1.95	0.49
3:H:91:MET:HE1	3:H:124:VAL:HG21	1.94	0.49
1:F:93:THR:HG22	1:F:93:THR:O	2.13	0.49
4:N:94:LEU:HD11	4:N:124:LEU:HD21	1.93	0.48
5:J:53:ILE:HD11	5:J:129:PHE:HA	1.95	0.48
1:P:93:THR:O	1:P:93:THR:HG22	2.13	0.48
3:C:99:THR:HG23	3:C:125:THR:HA	1.94	0.48
1:F:165:VAL:CG2	1:F:193:LEU:HD21	2.42	0.47
5:T:96:ASN:OD1	5:T:142:LEU:HD21	2.15	0.47
1:F:123:LEU:HD23	1:F:124:VAL:N	2.30	0.46
2:B:106:GLN:OE1	2:B:108:LEU:N	2.44	0.46
1:A:76:PHE:HB3	1:A:89:LEU:HD11	1.98	0.46
3:R:174:LEU:HD21	3:R:197:VAL:HG21	1.98	0.46
3:C:13:VAL:HG11	3:C:94:LEU:HD13	1.98	0.45
1:K:113:ARG:NH2	6:K:302:HOH:O	2.49	0.45
1:P:9:GLY:HA2	1:P:19:LEU:HD21	1.99	0.45
5:J:53:ILE:HD11	5:J:129:PHE:CA	2.47	0.45
2:L:107:SER:O	5:O:119:ARG:NH1	2.50	0.45
3:M:167:VAL:HG11	3:M:195:SER:CB	2.47	0.45
1:A:13:VAL:CG2	1:A:19:LEU:HD13	2.47	0.45
1:F:9:GLY:HA2	1:F:19:LEU:HD21	1.98	0.45
2:B:52:LEU:HD11	2:B:55:TYR:HB3	1.99	0.44
3:H:53:LEU:HD22	3:H:71:VAL:HG21	1.99	0.44
3:R:160:TYR:CE1	3:R:165:VAL:HG13	2.53	0.44
1:K:21:LEU:HG	1:K:91:MET:HE2	2.00	0.43
3:H:99:THR:HG23	3:H:125:THR:HA	1.99	0.43
2:G:11:LEU:HD21	2:G:19:ALA:HB1	2.00	0.43
1:K:38:THR:HG23	1:K:56:ILE:O	2.18	0.43
3:R:44:GLN:OE1	4:V:44:GLN:NE2	2.52	0.43
1:F:12:VAL:HG21	1:F:162:PRO:HB3	2.00	0.42
5:E:105:MET:HE1	5:E:142:LEU:HD13	2.00	0.42
1:A:107:ASP:OD1	1:A:108:GLY:N	2.52	0.42
3:C:174:LEU:HD21	3:C:197:VAL:HG21	2.00	0.42
2:G:13:VAL:HG21	2:G:94:VAL:HG11	2.00	0.42
2:B:39:LEU:HD22	2:B:87:PHE:CB	2.49	0.42
2:Q:4:MET:HE3	2:Q:23:CYS:SG	2.59	0.42
4:N:206:TYR:O	4:N:212:TYR:OH	2.35	0.42
4:D:19:VAL:HG21	4:D:94:LEU:HD13	2.01	0.42
1:A:91:MET:HB3	1:A:94:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1:GLU:HG2	4:D:115:PRO:HG2	2.01	0.41
1:P:44:GLN:HB2	1:P:50:LEU:HD23	2.02	0.41
3:R:112(A):GLU:O	4:V:116:ARG:NH2	2.52	0.41
3:H:160:TYR:CE2	3:H:165:VAL:HG13	2.54	0.41
2:G:53:LEU:HA	2:G:71:VAL:HG21	2.02	0.41
3:H:212:ASN:ND2	3:H:223:ASP:OD2	2.48	0.41
4:V:19:VAL:HG21	4:V:94:LEU:HD13	2.02	0.41
3:M:174:LEU:HD21	3:M:197:VAL:HG21	2.03	0.41
2:L:108:LEU:O	5:O:119:ARG:NH2	2.38	0.41
1:F:210:ILE:HD13	1:F:225:ARG:HA	2.03	0.40
2:L:183:VAL:HG22	2:L:195:LEU:HD12	2.03	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	114/225 (51%)	106 (93%)	8 (7%)	0	100	100
1	F	203/225 (90%)	193 (95%)	9 (4%)	1 (0%)	24	49
1	K	208/225 (92%)	201 (97%)	5 (2%)	2 (1%)	12	32
1	P	209/225 (93%)	201 (96%)	8 (4%)	0	100	100
2	B	108/218 (50%)	97 (90%)	11 (10%)	0	100	100
2	G	133/218 (61%)	125 (94%)	7 (5%)	1 (1%)	16	37
2	L	215/218 (99%)	210 (98%)	5 (2%)	0	100	100
2	Q	215/218 (99%)	210 (98%)	4 (2%)	1 (0%)	24	49
3	C	213/228 (93%)	206 (97%)	6 (3%)	1 (0%)	24	49
3	H	211/228 (92%)	205 (97%)	5 (2%)	1 (0%)	24	49
3	M	213/228 (93%)	207 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R	212/228 (93%)	207 (98%)	5 (2%)	0	100	100
4	D	212/214 (99%)	207 (98%)	5 (2%)	0	100	100
4	I	211/214 (99%)	205 (97%)	6 (3%)	0	100	100
4	N	210/214 (98%)	204 (97%)	6 (3%)	0	100	100
4	V	211/214 (99%)	204 (97%)	7 (3%)	0	100	100
5	E	83/140 (59%)	82 (99%)	1 (1%)	0	100	100
5	J	90/140 (64%)	88 (98%)	2 (2%)	0	100	100
5	O	88/140 (63%)	86 (98%)	2 (2%)	0	100	100
5	T	91/140 (65%)	88 (97%)	1 (1%)	2 (2%)	5	15
All	All	3450/4100 (84%)	3332 (97%)	109 (3%)	9 (0%)	36	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	47	GLN
5	T	34	GLN
2	G	158	ASN
1	K	11	LEU
2	Q	34	ASN
3	C	228	PRO
1	K	113	ARG
5	T	33	CYS
3	H	228	PRO

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	59/195 (30%)	57 (97%)	2 (3%)	32	58
1	F	127/195 (65%)	126 (99%)	1 (1%)	73	85
1	K	136/195 (70%)	135 (99%)	1 (1%)	76	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	143/195 (73%)	141 (99%)	2 (1%)	59	77
2	B	71/193 (37%)	70 (99%)	1 (1%)	59	77
2	G	105/193 (54%)	101 (96%)	4 (4%)	29	55
2	L	167/193 (86%)	167 (100%)	0	100	100
2	Q	157/193 (81%)	156 (99%)	1 (1%)	78	89
3	C	169/194 (87%)	168 (99%)	1 (1%)	78	89
3	H	172/194 (89%)	171 (99%)	1 (1%)	78	89
3	M	165/194 (85%)	164 (99%)	1 (1%)	78	89
3	R	169/194 (87%)	168 (99%)	1 (1%)	78	89
4	D	163/188 (87%)	162 (99%)	1 (1%)	78	89
4	I	164/188 (87%)	164 (100%)	0	100	100
4	N	163/188 (87%)	163 (100%)	0	100	100
4	V	165/188 (88%)	164 (99%)	1 (1%)	78	89
5	E	64/125 (51%)	64 (100%)	0	100	100
5	J	69/125 (55%)	68 (99%)	1 (1%)	59	77
5	O	70/125 (56%)	70 (100%)	0	100	100
5	T	70/125 (56%)	70 (100%)	0	100	100
All	All	2568/3580 (72%)	2549 (99%)	19 (1%)	76	87

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	19	LEU
2	B	107	SER
3	C	55	TYR
4	D	134	SER
1	F	193	LEU
2	G	39	LEU
2	G	77	SER
2	G	107	SER
2	G	159	PHE
3	H	55	TYR
5	J	54	GLN
1	K	193	LEU
3	M	55	TYR

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Mol	Chain	Res	Type
1	P	55	LEU
1	P	193	LEU
2	Q	120	PRO
3	R	55	TYR
4	V	210	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
2	B	44	GLN
4	D	157	ASN
5	E	47	GLN
5	E	87	HIS
1	F	90	GLN
2	G	180	GLN
3	H	82	ASN
3	H	214	ASN
1	K	90	GLN
1	K	92	ASN
1	K	214	ASN
2	L	209	HIS
3	M	215	HIS
5	O	48	HIS
1	P	44	GLN
2	Q	44	GLN
2	Q	180	GLN
2	Q	209	HIS
5	T	138	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 [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	116/225 (51%)	0.61	6 (5%) 33 28	79, 103, 127, 171	0
1	F	207/225 (92%)	0.79	18 (8%) 16 14	60, 110, 157, 183	0
1	K	212/225 (94%)	0.39	2 (0%) 81 76	61, 93, 120, 146	0
1	P	213/225 (94%)	0.36	8 (3%) 44 36	54, 87, 174, 200	0
2	B	110/218 (50%)	0.17	2 (1%) 67 59	56, 85, 144, 155	0
2	G	139/218 (63%)	-0.04	5 (3%) 46 38	46, 64, 110, 141	0
2	L	217/218 (99%)	0.09	3 (1%) 73 67	45, 75, 131, 161	0
2	Q	217/218 (99%)	0.27	5 (2%) 61 53	53, 110, 162, 185	0
3	C	217/228 (95%)	-0.11	3 (1%) 73 67	49, 67, 106, 140	0
3	H	215/228 (94%)	-0.06	2 (0%) 81 76	59, 82, 105, 126	0
3	M	217/228 (95%)	0.23	4 (1%) 67 59	59, 98, 148, 180	0
3	R	216/228 (94%)	-0.07	2 (0%) 81 76	50, 71, 119, 143	0
4	D	214/214 (100%)	-0.18	1 (0%) 87 83	55, 69, 90, 122	0
4	I	213/214 (99%)	-0.16	1 (0%) 87 83	57, 69, 90, 119	0
4	N	212/214 (99%)	-0.10	1 (0%) 87 83	60, 75, 109, 137	0
4	V	213/214 (99%)	-0.18	0 100 100	50, 68, 92, 127	0
5	E	87/140 (62%)	0.13	1 (1%) 78 73	65, 83, 115, 145	0
5	J	93/140 (66%)	0.28	3 (3%) 50 43	37, 81, 117, 133	1 (1%)
5	O	92/140 (65%)	0.18	2 (2%) 62 54	63, 86, 118, 139	0
5	T	95/140 (67%)	0.16	1 (1%) 78 73	60, 80, 126, 152	0
All	All	3515/4100 (85%)	0.12	70 (1%) 65 57	37, 80, 137, 200	1 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	O	152	VAL	4.3
3	R	9	GLY	3.7
3	H	142	SER	3.7
3	M	134	PRO	3.6
1	F	153	LEU	3.6
1	F	213	VAL	3.5
1	F	155	CYS	3.4
1	F	194	SER	3.3
5	T	152	VAL	3.3
3	M	142	SER	3.2
1	A	28	PHE	3.1
1	P	173	ALA	3.0
5	O	86	GLN	3.0
1	F	165	VAL	3.0
5	J	98	PHE	2.9
1	F	156	LEU	2.9
1	F	195	SER	2.9
5	E	36	GLN	2.9
1	P	183	ALA	2.9
2	B	2	VAL	2.8
1	F	130	SER	2.8
3	H	11	GLY	2.8
1	F	136	VAL	2.8
1	P	229	LYS	2.7
2	Q	211	VAL	2.7
1	F	152	ALA	2.7
1	P	180	THR	2.7
1	P	172	GLY	2.6
1	F	198	THR	2.6
1	F	137	PHE	2.6
2	G	163	GLU	2.5
2	L	136	PHE	2.5
2	G	194	SER	2.5
1	P	174	LEU	2.5
3	C	149	GLY	2.5
1	F	174	LEU	2.5
2	L	233	GLU	2.5
3	M	223	ASP	2.5
1	F	171	SER	2.5
1	P	195	SER	2.5
2	Q	174	LEU	2.4
2	B	76	PHE	2.4
1	A	35	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	Q	136	PHE	2.4
1	F	48	LYS	2.3
3	C	230	SER	2.3
3	C	142	SER	2.3
3	R	142	SER	2.3
1	A	128	SER	2.3
4	D	234	CYS	2.2
2	G	129	THR	2.2
2	G	179	SER	2.2
1	F	183	ALA	2.2
1	K	98	ASP	2.2
1	A	29	THR	2.2
1	K	194	SER	2.2
4	I	233	GLU	2.2
2	G	197	SER	2.1
2	L	83	SER	2.1
1	F	157	VAL	2.1
1	A	46	PRO	2.1
1	P	204	LEU	2.1
4	N	205	ASP	2.1
1	A	24	GLU	2.1
5	J	29	GLY	2.0
2	Q	226	THR	2.0
1	F	228	PRO	2.0
2	Q	154	CYS	2.0
5	J	30	ASP	2.0
3	M	169	TRP	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.