



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2024 – 12:10 AM EDT

PDB ID : 4FQQ  
Title : Crystal Structure of Germline Antibody PGT121-GL Fab  
Authors : Scharf, L.; Bjorkman, P.J.  
Deposited on : 2012-06-25  
Resolution : 2.42 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

<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>.

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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
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

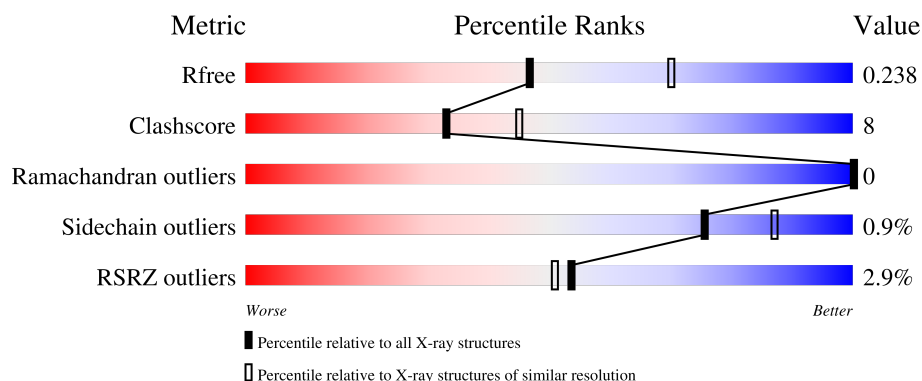
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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))
$R_{free}$	164625	5670 (2.44-2.40)
Clashscore	180529	6299 (2.44-2.40)
Ramachandran outliers	177936	6232 (2.44-2.40)
Sidechain outliers	177891	6233 (2.44-2.40)
RSRZ outliers	164620	5670 (2.44-2.40)

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  $\geq 3$ , 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	215	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>
1	C	215	<div> <div>0%</div> <div>84%</div> <div>14%</div> <div>•</div> </div>
1	E	215	<div> <div>8%</div> <div>74%</div> <div>21%</div> <div>5%</div> </div>
1	L	215	<div> <div>0%</div> <div>87%</div> <div>12%</div> <div>•</div> </div>
2	B	244	<div> <div>3%</div> <div>77%</div> <div>16%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	244	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>81%</div><div>11%</div><div>7%</div></div></div>
2	F	244	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>76%</div><div>16%</div><div>7%</div></div></div>
2	H	244	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>78%</div><div>18%</div><div>•</div></div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13753 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 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	4	0	0
			1600	1000	270	325	5			
1	A	211	Total	C	N	O	S	30	0	0
			1585	992	268	321	4			
1	C	210	Total	C	N	O	S	15	0	0
			1578	988	267	319	4			
1	E	205	Total	C	N	O	S	28	0	0
			1546	967	261	314	4			

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	234	Total	C	N	O	S	4	0	0
			1776	1132	288	351	5			
2	B	227	Total	C	N	O	S	35	0	0
			1726	1102	278	341	5			
2	D	226	Total	C	N	O	S	14	0	0
			1725	1103	279	338	5			
2	F	226	Total	C	N	O	S	22	0	0
			1725	1103	279	338	5			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		


- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	80	Total	O	0	0
			80	80		
4	H	76	Total	O	0	0
			76	76		
4	A	51	Total	O	0	0
			51	51		
4	B	46	Total	O	0	0
			46	46		
4	C	56	Total	O	0	0
			56	56		
4	D	88	Total	O	0	0
			88	88		
4	E	45	Total	O	0	0
			45	45		
4	F	48	Total	O	0	0
			48	48		

### 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 light chain

Chain L: 




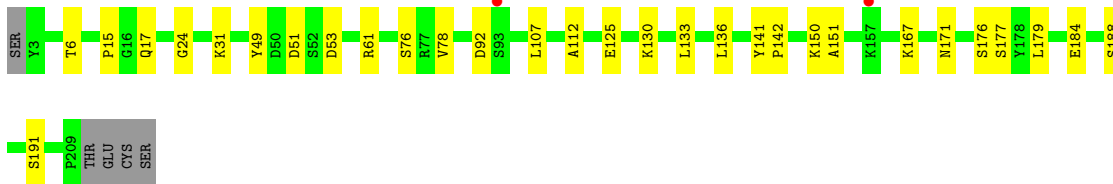
- Molecule 1: Fab light chain

Chain A: 



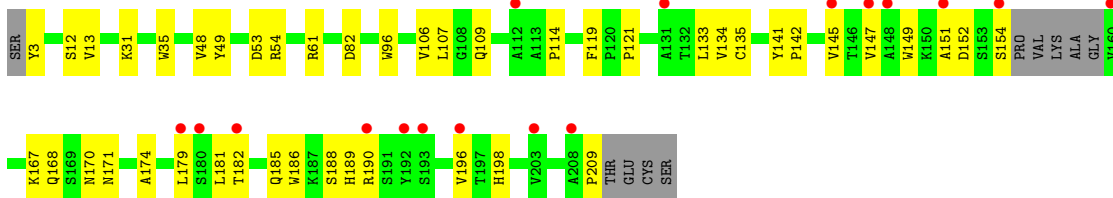
- Molecule 1: Fab light chain

Chain C: 

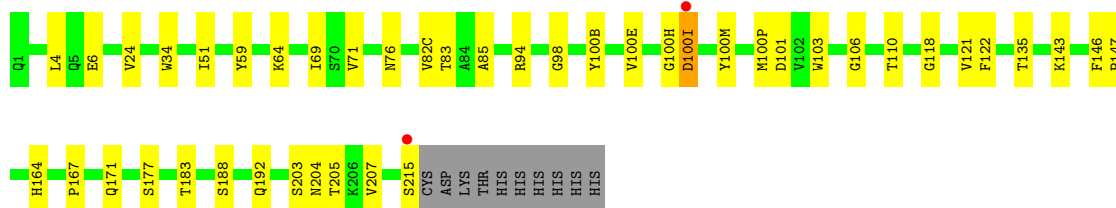
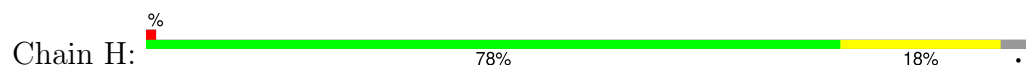


- Molecule 1: Fab light chain

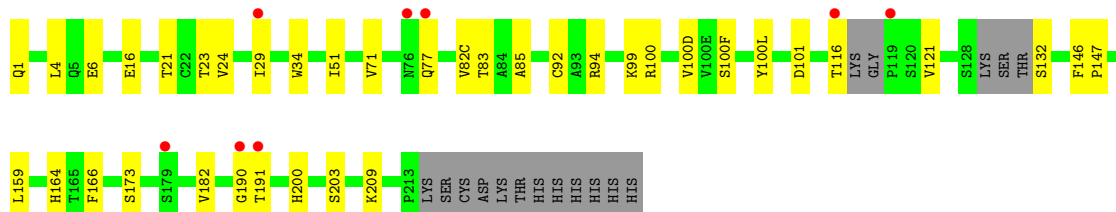
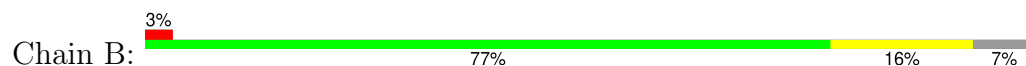
Chain E: 



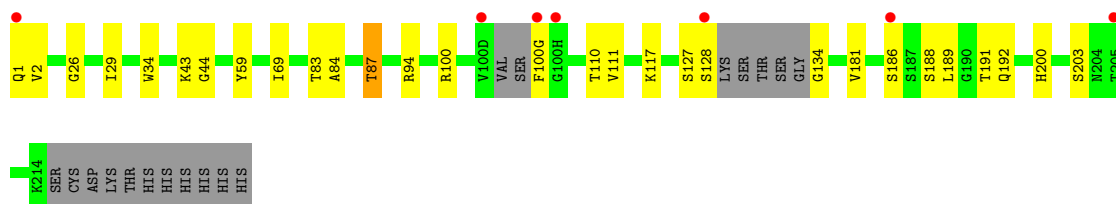
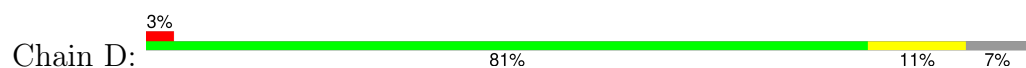
- Molecule 2: Fab heavy chain



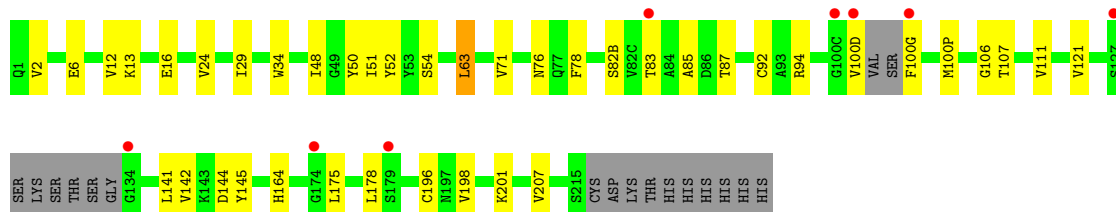
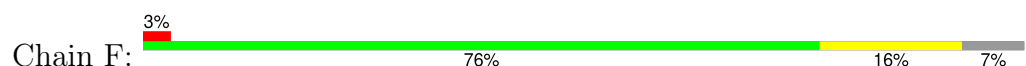
• Molecule 2: Fab heavy chain



• Molecule 2: Fab heavy chain



• Molecule 2: Fab heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.93Å 344.74Å 55.23Å 90.00° 91.95° 90.00°	Depositor
Resolution (Å)	37.44 – 2.42 37.44 – 2.42	Depositor EDS
% Data completeness (in resolution range)	95.5 (37.44-2.42) 91.6 (37.44-2.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.02 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, $R_{free}$	0.194 , 0.237 0.200 , 0.238	Depositor DCC
$R_{free}$ test set	1992 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 52.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.009 for l,k,-h 0.066 for h,-k,-l 0.035 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13753	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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: NA

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	0.23	0/1628	0.45	0/2230
1	C	0.43	0/1621	0.51	0/2220
1	E	0.30	0/1587	0.54	0/2172
1	L	0.27	0/1643	0.46	0/2250
2	B	0.31	0/1772	0.51	0/2420
2	D	0.24	0/1771	0.49	0/2417
2	F	0.46	0/1771	0.54	0/2417
2	H	0.34	0/1824	0.52	1/2491 (0.0%)
All	All	0.33	0/13617	0.50	1/18617 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	100(I)	ASP	CB-CG-OD2	5.20	122.97	118.30

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	1585	0	1519	18	0
1	C	1578	0	1512	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1546	0	1474	36	0
1	L	1600	0	1530	20	0
2	B	1726	0	1682	32	0
2	D	1725	0	1688	23	0
2	F	1725	0	1688	30	0
2	H	1776	0	1742	34	0
3	D	1	0	0	0	0
3	L	1	0	0	0	0
4	A	51	0	0	2	0
4	B	46	0	0	1	0
4	C	56	0	0	1	0
4	D	88	0	0	5	0
4	E	45	0	0	2	0
4	F	48	0	0	1	0
4	H	76	0	0	2	0
4	L	80	0	0	4	0
All	All	13753	0	12835	198	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 8.

All (198) 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)
2:H:4:LEU:HG	2:H:24:VAL:HG12	1.48	0.95
2:B:164:HIS:HD2	2:B:166:PHE:CE1	1.88	0.92
2:B:116:THR:HG21	2:B:147:PRO:HD3	1.51	0.89
2:H:203:SER:OG	2:H:205:THR:HG23	1.73	0.89
2:F:87:THR:HG22	2:F:111:VAL:H	1.40	0.85
2:B:164:HIS:CD2	2:B:166:PHE:CE1	2.69	0.80
2:B:116:THR:CG2	2:B:147:PRO:HD3	2.12	0.79
2:B:29:ILE:HG13	2:B:34:TRP:NE1	1.98	0.77
2:D:87:THR:HG22	2:D:111:VAL:HG13	1.68	0.76
2:F:121:VAL:HG11	2:F:198:VAL:HG21	1.67	0.76
1:E:12:SER:HB3	1:E:107:LEU:HD11	1.69	0.75
2:H:51:ILE:HD13	2:H:71:VAL:HG13	1.68	0.74
1:E:147:VAL:HG12	1:E:196:VAL:HG22	1.69	0.73
2:D:1:GLN:NE2	4:D:584:HOH:O	2.21	0.72
1:L:111:LYS:HD2	1:L:142:PRO:HD3	1.72	0.72
2:D:188:SER:HA	2:D:191:THR:OG1	1.90	0.71
2:B:132:SER:N	4:B:322:HOH:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:CYS:HB2	1:E:149:TRP:CH2	2.27	0.69
1:C:141:TYR:CG	1:C:142:PRO:HA	2.30	0.66
2:B:121:VAL:O	2:B:209:LYS:NZ	2.28	0.66
1:L:103:LYS:NZ	4:L:575:HOH:O	2.28	0.66
2:D:87:THR:HG22	2:D:111:VAL:H	1.59	0.66
2:B:83:THR:HG23	2:B:85:ALA:H	1.60	0.66
1:E:182:THR:H	1:E:185:GLN:HG2	1.60	0.66
2:F:6:GLU:HB2	2:F:107:THR:HG23	1.78	0.66
2:B:190:GLY:O	2:B:191:THR:HG22	1.96	0.66
2:B:23:THR:HA	2:B:77:GLN:HG2	1.78	0.64
2:D:188:SER:HB2	2:D:192:GLN:HG2	1.78	0.64
2:B:164:HIS:HD2	2:B:166:PHE:CZ	2.16	0.64
1:E:151:ALA:O	1:E:154:SER:HB2	1.98	0.63
1:A:3:TYR:N	4:A:314:HOH:O	2.32	0.63
2:H:51:ILE:CD1	2:H:71:VAL:HG13	2.29	0.63
2:B:51:ILE:HD13	2:B:71:VAL:HG13	1.83	0.61
1:C:167:LYS:HE2	1:C:171:ASN:HA	1.83	0.61
1:E:96:TRP:CZ2	2:F:100(P):MET:CE	2.84	0.61
2:F:100(D):VAL:C	2:F:100(G):PHE:HA	2.20	0.61
1:E:133:LEU:HB2	1:E:179:LEU:HB3	1.82	0.60
1:E:151:ALA:O	1:E:154:SER:N	2.26	0.60
2:H:83:THR:HG22	2:H:85:ALA:H	1.65	0.60
2:D:117:LYS:NZ	4:D:546:HOH:O	2.33	0.60
1:A:61:ARG:NH1	1:A:82:ASP:OD2	2.34	0.60
1:E:96:TRP:HZ2	2:F:100(P):MET:HE2	1.67	0.59
2:B:116:THR:HG22	2:B:146:PHE:O	2.02	0.59
2:B:164:HIS:CD2	2:B:166:PHE:CZ	2.90	0.59
2:F:121:VAL:HG12	2:F:142:VAL:HA	1.84	0.59
2:H:94:ARG:HD2	2:H:101:ASP:OD1	2.02	0.58
1:A:152:ASP:O	1:A:153:SER:OG	2.17	0.58
2:H:135:THR:OG1	2:H:183:THR:HG22	2.03	0.58
2:B:116:THR:HG21	2:B:147:PRO:CD	2.29	0.57
1:E:61:ARG:NH1	1:E:82:ASP:OD2	2.35	0.57
2:H:4:LEU:HG	2:H:24:VAL:CG1	2.29	0.56
2:H:98:GLY:HA3	2:H:100(M):TYR:CZ	2.41	0.55
1:A:49:TYR:O	1:A:53:ASP:HB2	2.06	0.55
1:L:212:CYS:HB2	2:H:215:SER:O	2.07	0.55
1:E:135:CYS:HB2	1:E:149:TRP:CZ2	2.43	0.54
1:E:190:ARG:O	1:E:209:PRO:HD2	2.08	0.54
2:H:135:THR:OG1	2:H:183:THR:CG2	2.55	0.54
2:H:203:SER:OG	2:H:205:THR:CG2	2.53	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:GLN:OE1	1:E:174:ALA:HB2	2.08	0.54
1:L:15:PRO:HD3	1:L:107:LEU:O	2.09	0.53
2:B:51:ILE:CD1	2:B:71:VAL:HG13	2.39	0.53
2:B:1:GLN:O	2:B:1:GLN:HG3	2.08	0.53
1:C:51:ASP:OD2	2:D:100:ARG:NH2	2.32	0.53
2:B:200:HIS:ND1	2:B:203:SER:OG	2.31	0.53
1:E:96:TRP:HZ2	2:F:100(P):MET:CE	2.20	0.53
1:E:106:VAL:HG22	1:E:109:GLN:HE21	1.74	0.53
1:E:96:TRP:CZ2	2:F:100(P):MET:HE1	2.43	0.53
2:F:2:VAL:HG21	2:F:94:ARG:NH2	2.24	0.53
2:H:121:VAL:CG1	2:H:207:VAL:HG11	2.40	0.52
1:A:83:GLU:HG3	1:A:106:VAL:HG23	1.91	0.52
1:E:181:LEU:HA	1:E:185:GLN:HE21	1.75	0.52
2:B:29:ILE:HA	2:B:34:TRP:CZ2	2.44	0.52
2:B:100(D):VAL:HG12	2:B:100(F):SER:H	1.74	0.52
2:B:29:ILE:HG13	2:B:34:TRP:CE2	2.45	0.51
2:D:110:THR:HG23	4:D:551:HOH:O	2.09	0.51
1:E:96:TRP:CZ2	2:F:100(P):MET:HE2	2.44	0.51
1:A:109:GLN:HB2	1:A:141:TYR:CE1	2.45	0.51
1:A:182:THR:HG22	1:A:184:GLU:H	1.75	0.51
2:F:83:THR:HG23	2:F:85:ALA:H	1.75	0.51
2:F:78:PHE:CZ	2:F:92:CYS:HB2	2.45	0.51
2:D:2:VAL:HG21	2:D:94:ARG:NH2	2.26	0.51
2:D:59:TYR:HE1	2:D:69:ILE:HG13	1.76	0.51
1:E:31:LYS:O	4:E:306:HOH:O	2.20	0.51
2:F:121:VAL:CG2	2:F:207:VAL:HG11	2.40	0.51
1:L:96:TRP:HZ2	2:H:100(P):MET:CE	2.24	0.51
2:H:100(E):VAL:O	2:H:100(H):GLY:N	2.39	0.50
2:D:134:GLY:O	2:D:186:SER:N	2.42	0.50
2:F:29:ILE:HA	2:F:34:TRP:CZ2	2.46	0.50
1:L:96:TRP:CZ2	2:H:100(P):MET:CE	2.95	0.50
2:H:171:GLN:NE2	2:H:177:SER:OG	2.45	0.50
1:C:125:GLU:HG2	1:C:130:LYS:HB2	1.93	0.50
1:A:15:PRO:HD3	1:A:107:LEU:O	2.12	0.50
1:C:150:LYS:NZ	4:C:354:HOH:O	2.36	0.50
1:E:35:TRP:HB2	1:E:48:VAL:HB	1.93	0.49
2:D:43:LYS:HG2	2:D:44:GLY:H	1.76	0.49
1:E:168:GLN:NE2	1:E:170:ASN:OD1	2.45	0.49
2:F:6:GLU:CB	2:F:107:THR:HG23	2.43	0.49
1:L:212:CYS:O	4:L:558:HOH:O	2.20	0.49
1:C:141:TYR:CD1	1:C:142:PRO:HA	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:NH2	4:A:346:HOH:O	2.45	0.49
2:H:24:VAL:HG23	2:H:76:ASN:ND2	2.28	0.49
2:H:122:PHE:HE2	2:H:143:LYS:HD3	1.78	0.48
2:D:26:GLY:O	4:D:562:HOH:O	2.20	0.48
1:E:145:VAL:CG2	1:E:196:VAL:HG13	2.44	0.48
1:C:31:LYS:NZ	1:C:92:ASP:OD1	2.46	0.48
2:H:4:LEU:CG	2:H:24:VAL:HG12	2.32	0.48
1:L:49:TYR:O	1:L:53:ASP:HB2	2.13	0.48
1:L:109:GLN:HB2	1:L:141:TYR:CZ	2.49	0.48
1:C:151:ALA:O	1:C:191:SER:O	2.31	0.48
2:F:13:LYS:O	2:F:16:GLU:HG2	2.13	0.48
1:L:3:TYR:N	1:L:95:SER:HG	2.11	0.47
2:H:110:THR:HG23	4:H:307:HOH:O	2.14	0.47
1:L:109:GLN:HB2	1:L:141:TYR:CE1	2.49	0.47
2:F:145:TYR:OH	2:F:178:LEU:HD23	2.14	0.47
1:A:5:LEU:HD11	1:A:90:VAL:HG12	1.96	0.47
1:C:136:LEU:HD13	2:D:181:VAL:HG21	1.95	0.47
1:E:151:ALA:O	1:E:152:ASP:HB2	2.13	0.47
1:E:109:GLN:HB2	1:E:141:TYR:CE2	2.49	0.47
1:E:188:SER:OG	1:E:189:HIS:ND1	2.35	0.47
2:F:24:VAL:HG13	2:F:76:ASN:ND2	2.29	0.47
1:E:49:TYR:O	1:E:53:ASP:HB2	2.15	0.47
1:E:141:TYR:CD1	1:E:142:PRO:HA	2.49	0.47
2:B:21:THR:HG21	2:B:77:GLN:NE2	2.30	0.47
1:A:150:LYS:HD2	1:A:195:GLN:OE1	2.14	0.47
2:B:190:GLY:O	2:B:191:THR:CG2	2.64	0.46
2:B:94:ARG:HD2	2:B:101:ASP:OD1	2.15	0.46
2:D:29:ILE:HA	2:D:34:TRP:CZ2	2.51	0.46
1:E:167:LYS:HE2	1:E:171:ASN:HA	1.96	0.46
2:F:121:VAL:HG22	2:F:207:VAL:HG11	1.97	0.46
1:L:166:SER:OG	2:H:167:PRO:HG2	2.16	0.46
2:H:118:GLY:HA3	2:H:205:THR:HG21	1.98	0.46
2:D:127:SER:OG	2:D:128:SER:N	2.48	0.46
2:F:51:ILE:HD13	2:F:71:VAL:HG13	1.97	0.46
2:D:188:SER:HB2	2:D:192:GLN:CG	2.46	0.46
2:H:204:ASN:HA	4:H:351:HOH:O	2.16	0.46
2:H:24:VAL:HG11	2:H:34:TRP:CZ3	2.52	0.45
2:H:188:SER:O	2:H:192:GLN:HG2	2.16	0.45
2:F:144:ASP:HB3	2:F:175:LEU:HD13	1.96	0.45
2:F:201:LYS:NZ	4:F:342:HOH:O	2.45	0.45
1:C:15:PRO:HD3	1:C:107:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:3:TYR:CE1	1:E:31:LYS:HE3	2.51	0.45
1:L:63:SER:OG	1:L:74:THR:HB	2.16	0.45
2:F:82(B):SER:O	2:F:82(B):SER:OG	2.33	0.45
2:H:100(B):TYR:CE1	2:H:100(I):ASP:HB3	2.51	0.45
2:F:48:ILE:HG23	2:F:63:LEU:HD23	1.99	0.45
2:H:59:TYR:HE1	2:H:69:ILE:HG13	1.82	0.45
1:L:96:TRP:HZ2	2:H:100(P):MET:HE2	1.81	0.44
2:D:84:ALA:O	2:D:87:THR:HG23	2.17	0.44
2:H:64:LYS:NZ	1:A:50:ASP:OD2	2.50	0.44
1:A:50:ASP:OD1	2:B:100:ARG:NH2	2.49	0.44
1:E:151:ALA:O	1:E:154:SER:CB	2.63	0.44
1:L:95(A):ASP:O	1:L:95(C):PRO:HD3	2.17	0.44
1:A:116:VAL:O	1:A:205:LYS:HE3	2.16	0.44
1:C:133:LEU:HB2	1:C:179:LEU:HB3	1.98	0.44
1:E:121:PRO:HD2	1:E:186:TRP:CZ2	2.53	0.44
1:L:124:GLU:HG3	4:L:535:HOH:O	2.18	0.44
2:H:6:GLU:CD	2:H:106:GLY:H	2.21	0.44
2:D:200:HIS:CE1	2:D:203:SER:HG	2.34	0.43
1:C:61:ARG:HG2	1:C:76:SER:O	2.18	0.43
2:B:4:LEU:HG	2:B:24:VAL:HG12	2.01	0.43
1:L:29:GLY:O	4:L:518:HOH:O	2.21	0.43
2:H:100(P):MET:HE3	2:H:103:TRP:CZ2	2.54	0.42
1:A:152:ASP:OD2	1:A:190:ARG:N	2.38	0.42
1:C:136:LEU:HD23	1:C:176:SER:HB3	2.01	0.42
1:L:35:TRP:HB2	1:L:48:VAL:HB	2.02	0.42
2:B:99:LYS:HE2	2:B:100(L):TYR:CE2	2.55	0.42
2:F:78:PHE:HZ	2:F:92:CYS:HB2	1.83	0.42
1:A:195:GLN:HG2	1:A:202:THR:HG21	2.01	0.42
1:C:141:TYR:HA	1:C:142:PRO:C	2.38	0.42
2:D:189:LEU:HD23	2:D:189:LEU:HA	1.89	0.42
2:F:121:VAL:HA	2:F:141:LEU:O	2.18	0.42
2:D:83:THR:OG1	4:D:556:HOH:O	2.21	0.42
2:F:12:VAL:O	2:F:111:VAL:HA	2.20	0.42
2:B:159:LEU:HD21	2:B:182:VAL:HG21	2.00	0.42
1:C:49:TYR:O	1:C:53:ASP:HB2	2.20	0.42
2:B:29:ILE:CG1	2:B:34:TRP:NE1	2.78	0.42
1:C:184:GLU:O	1:C:188:SER:HB3	2.19	0.42
1:A:95(A):ASP:O	1:A:95(C):PRO:HD3	2.20	0.41
1:E:119:PHE:HB2	1:E:134:VAL:HB	2.00	0.41
1:A:8:PRO:HA	1:A:9:PRO:HD3	1.90	0.41
2:D:87:THR:HB	2:D:110:THR:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:122:PHE:CE2	2:H:143:LYS:HD3	2.54	0.41
2:B:16:GLU:O	2:B:82(C):VAL:HG23	2.21	0.41
1:E:114:PRO:HD3	1:E:198:HIS:ND1	2.35	0.41
1:L:95(B):HIS:CE1	1:L:97:VAL:HG22	2.56	0.41
2:F:6:GLU:CD	2:F:106:GLY:H	2.23	0.41
2:B:6:GLU:HG3	2:B:92:CYS:SG	2.61	0.41
1:C:6:THR:HG22	1:C:24:GLY:O	2.21	0.41
1:C:17:GLN:O	1:C:78:VAL:HG23	2.21	0.41
1:E:54:ARG:NE	4:E:309:HOH:O	2.54	0.41
1:C:112:ALA:HB3	1:C:141:TYR:N	2.35	0.40
2:B:116:THR:CG2	2:B:146:PHE:O	2.69	0.40
1:E:13:VAL:O	1:E:106:VAL:HA	2.22	0.40
1:L:167:LYS:HE3	1:L:171:ASN:HA	2.02	0.40
2:H:146:PHE:HA	2:H:147:PRO:HA	1.84	0.40
2:D:1:GLN:HB2	2:D:2:VAL:H	1.69	0.40
1:E:188:SER:OG	1:E:189:HIS:N	2.55	0.40
2:F:52:TYR:HD2	2:F:54:SER:HG	1.68	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	209/215 (97%)	206 (99%)	3 (1%)	0	100	100
1	C	208/215 (97%)	202 (97%)	6 (3%)	0	100	100
1	E	201/215 (94%)	194 (96%)	7 (4%)	0	100	100
1	L	211/215 (98%)	207 (98%)	4 (2%)	0	100	100
2	B	221/244 (91%)	218 (99%)	3 (1%)	0	100	100
2	D	220/244 (90%)	218 (99%)	2 (1%)	0	100	100
2	F	220/244 (90%)	218 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	232/244 (95%)	227 (98%)	5 (2%)	0	100	100
All	All	1722/1836 (94%)	1690 (98%)	32 (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	178/182 (98%)	177 (99%)	1 (1%)	84	92
1	C	177/182 (97%)	176 (99%)	1 (1%)	84	92
1	E	174/182 (96%)	174 (100%)	0	100	100
1	L	180/182 (99%)	178 (99%)	2 (1%)	70	84
2	B	197/213 (92%)	196 (100%)	1 (0%)	86	94
2	D	196/213 (92%)	194 (99%)	2 (1%)	73	85
2	F	196/213 (92%)	192 (98%)	4 (2%)	50	68
2	H	203/213 (95%)	201 (99%)	2 (1%)	73	85
All	All	1501/1580 (95%)	1488 (99%)	13 (1%)	75	87

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	95(B)	HIS
1	L	184	GLU
2	H	82(C)	VAL
2	H	164	HIS
1	A	152	ASP
2	B	173	SER
1	C	177	SER
2	D	87	THR
2	D	100(G)	PHE
2	F	50	TYR

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Mol	Chain	Res	Type
2	F	63	LEU
2	F	164	HIS
2	F	196	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	171	GLN
2	B	1	GLN
2	B	76	ASN
2	B	164	HIS
1	E	185	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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	211/215 (98%)	-0.16	5 (2%) 59 57	27, 48, 82, 105	7 (3%)
1	C	210/215 (97%)	-0.11	2 (0%) 79 77	27, 51, 76, 94	3 (1%)
1	E	205/215 (95%)	0.43	17 (8%) 19 17	24, 67, 109, 146	6 (2%)
1	L	213/215 (99%)	-0.41	1 (0%) 87 86	26, 40, 67, 90	1 (0%)
2	B	227/244 (93%)	0.14	8 (3%) 47 45	24, 53, 88, 113	9 (3%)
2	D	226/244 (92%)	-0.22	7 (3%) 51 49	16, 40, 72, 108	4 (1%)
2	F	226/244 (92%)	0.12	8 (3%) 47 45	27, 55, 84, 110	6 (2%)
2	H	234/244 (95%)	-0.35	2 (0%) 81 79	18, 41, 66, 102	2 (0%)
All	All	1752/1836 (95%)	-0.07	50 (2%) 54 51	16, 48, 86, 146	38 (2%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	179	SER	3.5
2	D	100(H)	GLY	3.5
2	D	100(G)	PHE	3.2
2	B	119	PRO	3.1
2	H	215	SER	3.0
1	A	95(A)	ASP	3.0
1	E	147	VAL	3.0
1	A	95(B)	HIS	2.9
2	B	29	ILE	2.8
1	E	131	ALA	2.8
2	F	100(G)	PHE	2.7
2	F	127	SER	2.7
2	B	191	THR	2.7
2	D	205	THR	2.7
2	F	100(D)	VAL	2.7
1	E	148	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	100(I)	ASP	2.6
1	E	112	ALA	2.6
1	L	95(B)	HIS	2.6
1	E	180	SER	2.5
1	E	154	SER	2.5
2	B	77	GLN	2.5
2	B	116	THR	2.5
2	F	100(C)	GLY	2.5
2	F	174	GLY	2.5
2	B	179	SER	2.5
1	C	157	LYS	2.5
2	F	134	GLY	2.5
1	E	151	ALA	2.4
1	C	93	SER	2.3
1	E	179	LEU	2.3
1	E	192	TYR	2.3
1	E	193	SER	2.3
1	E	203	VAL	2.3
1	A	210	THR	2.2
2	D	128	SER	2.2
2	F	83	THR	2.2
1	E	160	VAL	2.2
1	E	182	THR	2.1
2	B	190	GLY	2.1
2	D	186	SER	2.1
2	B	76	ASN	2.1
2	D	100(D)	VAL	2.1
1	E	208	ALA	2.1
2	D	1	GLN	2.1
1	A	93	SER	2.0
1	A	152	ASP	2.0
1	E	145	VAL	2.0
1	E	196	VAL	2.0
1	E	190	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NA	L	400	1/1	0.88	0.19	44,44,44,44	0
3	NA	D	400	1/1	0.92	0.22	47,47,47,47	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.