



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:40 PM GMT

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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

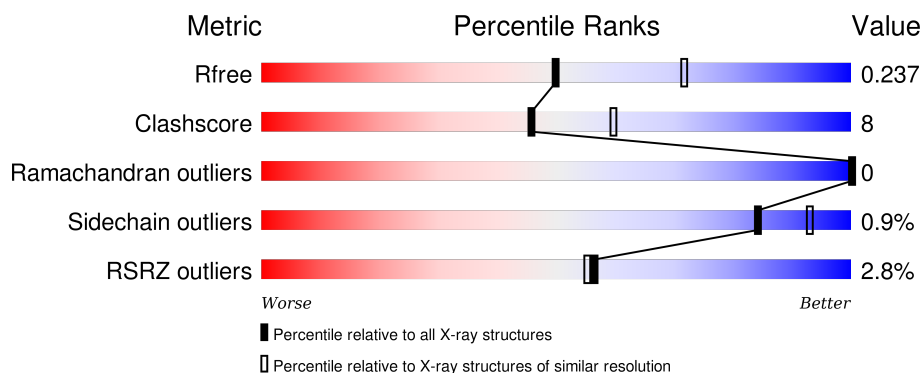
1 Overall quality at a glance ⓘ

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}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>•</div> </div>
1	C	215	<div> <div>2%</div> <div>84%</div> <div>14%</div> <div>•</div> </div>
1	E	215	<div> <div>11%</div> <div>74%</div> <div>21%</div> <div>5%</div> </div>
1	L	215	<div> <div>%</div> <div>87%</div> <div>12%</div> <div>•</div> </div>
2	B	244	<div> <div>2%</div> <div>77%</div> <div>16%</div> <div>7%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	244	
2	F	244	
2	H	244	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NA	D	400	-	-	-	X
3	NA	L	400	-	-	-	X

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	D	1	Total	Na	0	0
			1	1		
3	L	1	Total	Na	0	0
			1	1		

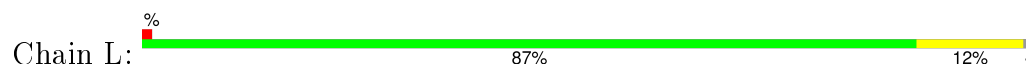
- Molecule 4 is water.

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

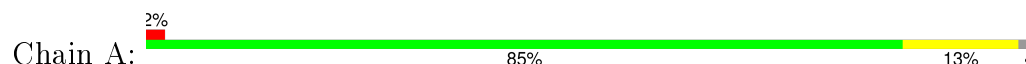
3 Residue-property plots [i](#)

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

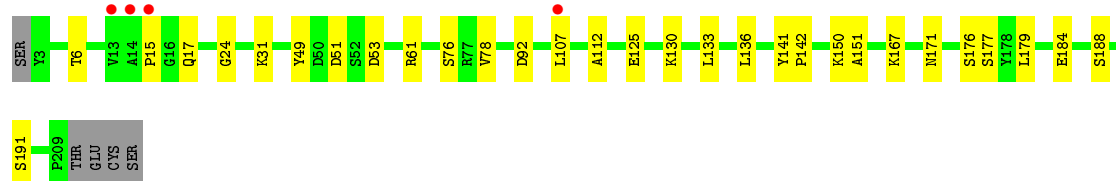
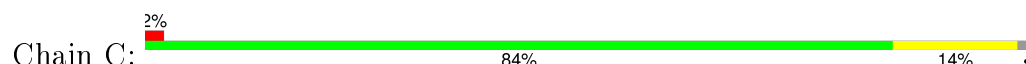
- Molecule 1: Fab light chain



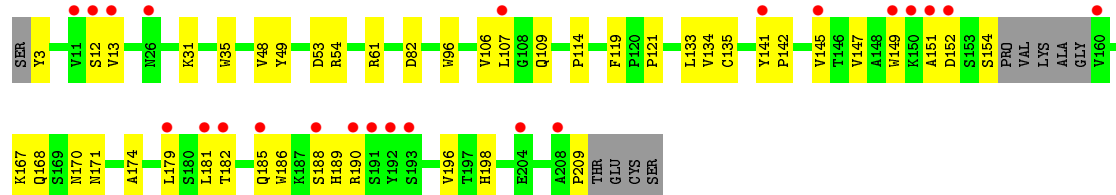
- Molecule 1: Fab light chain



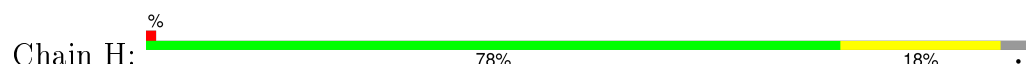
- Molecule 1: Fab light chain

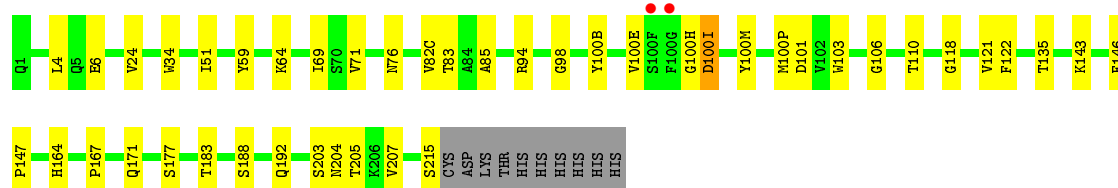


- Molecule 1: Fab light chain

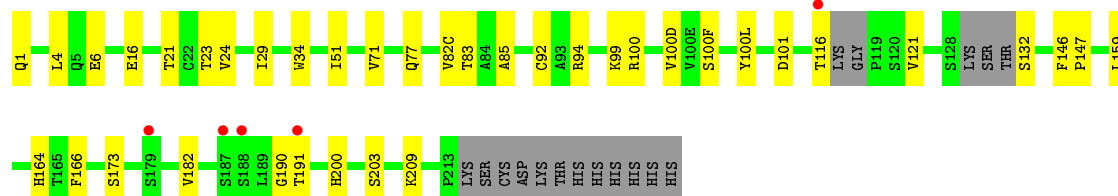
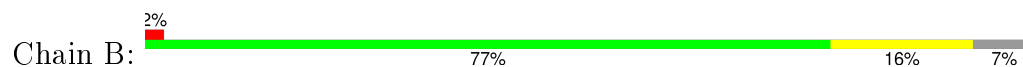


- Molecule 2: Fab heavy chain

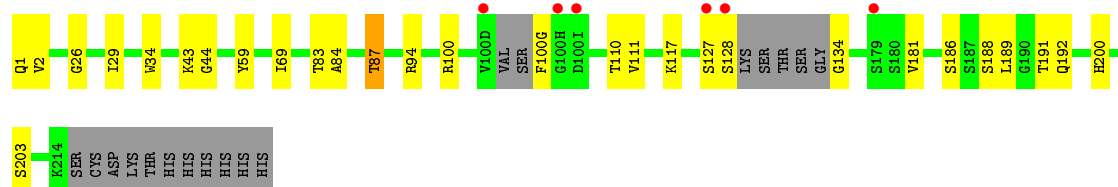
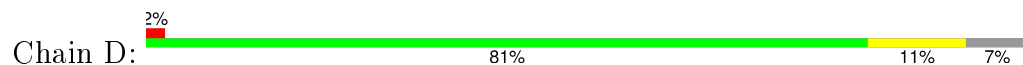




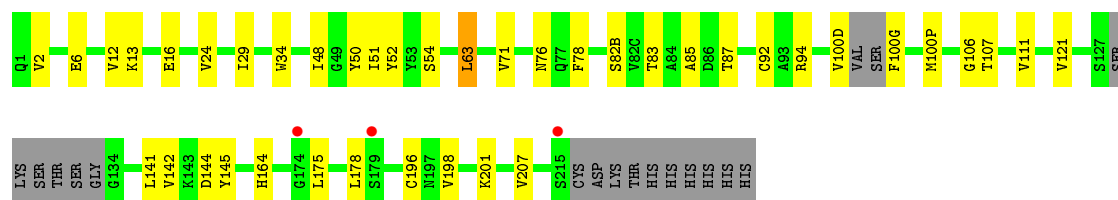
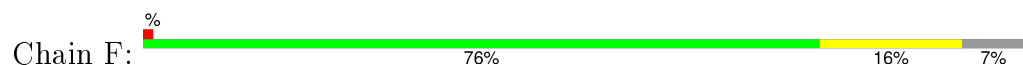
• Molecule 2: Fab heavy chain



• 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, α , β , γ	54.93Å 344.74Å 55.23Å 90.00° 91.95° 90.00°	Depositor
Resolution (Å)	37.44 – 2.42 38.05 – 2.42	Depositor EDS
% Data completeness (in resolution range)	95.5 (37.44-2.42) 91.5 (38.05-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.42Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8 _1069)	Depositor
R, R_{free}	0.194 , 0.237 0.194 , 0.237	Depositor DCC
R_{free} test set	1907 reflections (2.68%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.6	EDS
Estimated twinning fraction	0.008 for l,k,-h 0.066 for h,-k,-l 0.035 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 74257 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13753	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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, 0.375 respectively for untwinned datasets, and 0.333, 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
2:D:87:THR:HG22	2:D:111:VAL:H	1.59	0.66
1:L:103:LYS:NZ	4:L:575:HOH:O	2.28	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:D:188:SER:HB2	2:D:192:GLN:HG2	1.78	0.64
2:B:23:THR:HA	2:B:77: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:E:96:TRP:CZ2	2:F:100(P):MET:CE	2.84	0.61
1:C:167:LYS:HE2	1:C:171:ASN:HA	1.83	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
1:A:49:TYR:O	1:A:53:ASP:HB2	2.06	0.55
2:H:98:GLY:HA3	2:H:100(M):TYR:CZ	2.41	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:GLN:OE1	1:E:174:ALA:HB2	2.08	0.54
2:B:51:ILE:CD1	2:B:71:VAL:HG13	2.39	0.53
1:L:15:PRO:HD3	1:L:107:LEU:O	2.09	0.53
2:B:1:GLN:HG3	2:B:1:GLN:O	2.08	0.53
1:C:51:ASP:OD2	2:D:100:ARG:NH2	2.32	0.53
1:E:96:TRP:HZ2	2:F:100(P):MET:CE	2.20	0.53
2:B:200:HIS:ND1	2:B:203:SER:OG	2.31	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
1:A:83:GLU:HG3	1:A:106:VAL:HG23	1.91	0.52
2:H:121:VAL:CG1	2:H:207:VAL:HG11	2.40	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
2:F:83:THR:HG23	2:F:85:ALA:H	1.75	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:78:PHE:CZ	2:F:92:CYS:HB2	2.45	0.51
2:F:121:VAL:CG2	2:F:207:VAL:HG11	2.40	0.51
2:D:2:VAL:HG21	2:D:94:ARG:NH2	2.26	0.51
1:E:31:LYS:O	4:E:306:HOH:O	2.20	0.51
2:D:59:TYR:HE1	2:D:69:ILE:HG13	1.76	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:F:29:ILE:HA	2:F:34:TRP:CZ2	2.46	0.50
2:D:134:GLY:O	2:D:186:SER:N	2.42	0.50
1:L:96:TRP:CZ2	2:H:100(P):MET:CE	2.95	0.50
1:C:125:GLU:HG2	1:C:130:LYS:HB2	1.93	0.50
2:H:171:GLN:NE2	2:H:177:SER:OG	2.45	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

Continued on next page...

Continued from previous page...

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:E:151:ALA:O	1:E:152:ASP:HB2	2.13	0.47
1:C:136:LEU:HD13	2:D:181:VAL:HG21	1.95	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:141:TYR:CD1	1:E:142:PRO:HA	2.49	0.47
1:E:49:TYR:O	1:E:53:ASP:HB2	2.15	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:F:121:VAL:HG22	2:F:207:VAL:HG11	1.97	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:B:94:ARG:HD2	2:B:101:ASP:OD1	2.15	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
1:L:166:SER:OG	2:H:167:PRO:HG2	2.16	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:E:3:TYR:CE1	1:E:31:LYS:HE3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:PRO:HD3	1:C:107:LEU:O	2.16	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
2:D:84:ALA:O	2:D:87:THR:HG23	2.17	0.44
1:L:96:TRP:HZ2	2:H:100(P):MET:HE2	1.81	0.44
1:E:151:ALA:O	1:E:154:SER:CB	2.63	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:C:133:LEU:HB2	1:C:179:LEU:HB3	1.98	0.44
1:A:116:VAL:O	1:A:205:LYS:HE3	2.16	0.44
1:L:95(A):ASP:O	1:L:95(C):PRO:HD3	2.17	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
1:A:152:ASP:OD2	1:A:190:ARG:N	2.38	0.42
2:H:100(P):MET:HE3	2:H:103:TRP:CZ2	2.54	0.42
1:C:136:LEU:HD23	1:C:176:SER:HB3	2.01	0.42
2:F:78:PHE:HZ	2:F:92:CYS:HB2	1.83	0.42
2:B:99:LYS:HE2	2:B:100(L):TYR:CE2	2.55	0.42
1:L:35:TRP:HB2	1:L:48:VAL:HB	2.02	0.42
1:C:141:TYR:HA	1:C:142:PRO:C	2.38	0.42
1:A:195:GLN:HG2	1:A:202:THR:HG21	2.01	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:F:12:VAL:O	2:F:111:VAL:HA	2.20	0.42
2:D:83:THR:OG1	4:D:556:HOH:O	2.21	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:E:119:PHE:HB2	1:E:134:VAL:HB	2.00	0.41
1:A:95(A):ASP:O	1:A:95(C):PRO:HD3	2.20	0.41
2:D:87:THR:HB	2:D:110:THR:HA	2.01	0.41
1:A:8:PRO:HA	1:A:9:PRO:HD3	1.90	0.41

Continued on next page...

Continued from previous page...

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
2:F:6:GLU:CD	2:F:106:GLY:H	2.23	0.41
1:L:95(B):HIS:CE1	1:L:97:VAL:HG22	2.56	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
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
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: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

Continued on next page...

Continued from previous page...

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%)	90	96
1	C	177/182 (97%)	176 (99%)	1 (1%)	90	96
1	E	174/182 (96%)	174 (100%)	0	100	100
1	L	180/182 (99%)	178 (99%)	2 (1%)	80	91
2	B	197/213 (92%)	196 (100%)	1 (0%)	92	97
2	D	196/213 (92%)	194 (99%)	2 (1%)	82	92
2	F	196/213 (92%)	192 (98%)	4 (2%)	63	80
2	H	203/213 (95%)	201 (99%)	2 (1%)	82	92
All	All	1501/1580 (95%)	1488 (99%)	13 (1%)	84	93

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

Continued on next page...

Continued from previous page...

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

Some 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 carbohydrates 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	211/215 (98%)	0.05	4 (1%) 70 69	27, 48, 83, 105	7 (3%)
1	C	210/215 (97%)	-0.05	4 (1%) 70 69	32, 51, 76, 94	3 (1%)
1	E	205/215 (95%)	0.56	23 (11%) 7 7	30, 69, 110, 146	6 (2%)
1	L	213/215 (99%)	-0.04	2 (0%) 85 85	26, 40, 67, 90	1 (0%)
2	B	227/244 (93%)	0.20	5 (2%) 65 64	34, 54, 88, 113	9 (3%)
2	D	226/244 (92%)	-0.09	6 (2%) 58 57	25, 40, 73, 108	4 (1%)
2	F	226/244 (92%)	0.21	3 (1%) 79 79	34, 56, 84, 110	6 (2%)
2	H	234/244 (95%)	-0.22	2 (0%) 85 85	24, 41, 66, 102	2 (0%)
All	All	1752/1836 (95%)	0.07	49 (2%) 56 55	24, 49, 88, 146	38 (2%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	191	THR	5.7
1	E	107	LEU	5.2
1	E	151	ALA	5.1
1	E	181	LEU	4.7
1	E	182	THR	4.6
1	E	13	VAL	3.9
2	B	188	SER	3.7
1	L	107	LEU	3.6
1	E	208	ALA	3.5
1	E	193	SER	3.5
1	E	190	ARG	3.4
1	A	182	THR	3.1
1	E	191	SER	3.1
1	E	179	LEU	3.0
1	E	145	VAL	3.0
1	E	152	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	107	LEU	2.9
1	E	185	GLN	2.9
1	E	192	TYR	2.9
2	F	215	SER	2.9
1	E	141	TYR	2.8
1	C	13	VAL	2.8
1	E	160	VAL	2.8
2	F	174	GLY	2.7
1	C	14	ALA	2.7
1	E	188	SER	2.6
2	B	116	THR	2.6
1	E	11	VAL	2.6
2	D	179	SER	2.6
2	F	179	SER	2.5
2	D	100(I)	ASP	2.4
1	C	15	PRO	2.4
2	D	100(H)	GLY	2.4
1	A	183	PRO	2.4
1	E	12	SER	2.3
2	H	100(G)	PHE	2.2
2	D	128	SER	2.2
2	D	100(D)	VAL	2.2
1	A	152	ASP	2.2
1	E	150	LYS	2.2
2	B	187	SER	2.2
1	E	149	TRP	2.1
1	E	26	ASN	2.1
2	H	100(F)	SER	2.1
1	E	204	GLU	2.1
2	B	179	SER	2.1
1	L	13	VAL	2.0
1	A	151	ALA	2.0
2	D	127	SER	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
3	NA	D	400	1/1	0.91	0.37	11.60	47,47,47,47	0
3	NA	L	400	1/1	0.88	0.29	7.74	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.