



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2021 – 12:05 PM 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : 1.13
EDS : 2.18
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

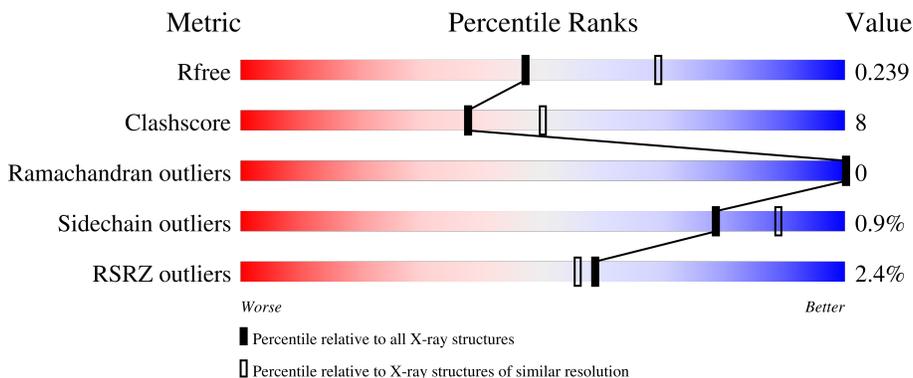
1 Overall quality at a glance i

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}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (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 ≥ 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 style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 85%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 13%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">85% 13% .</p>
1	C	215	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 84%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">84% 14% .</p>
1	E	215	<div style="display: flex; align-items: center;"> <div style="width: 10%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 74%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 21%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">74% 21% 5%</p>
1	L	215	<div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> <p style="margin-left: 10px;">87% 12% .</p>
2	B	244	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 16%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 10px;">77% 16% 7%</p>

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

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

- Molecule 2 is a protein called Fab heavy chain.

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

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

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

- Molecule 4 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fab light chain

Chain L: 



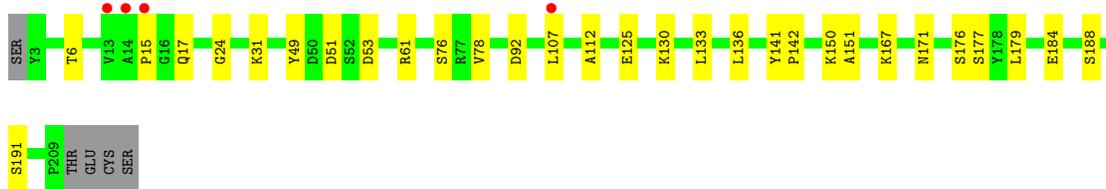
- Molecule 1: Fab light chain

Chain A: 



- Molecule 1: Fab light chain

Chain C: 



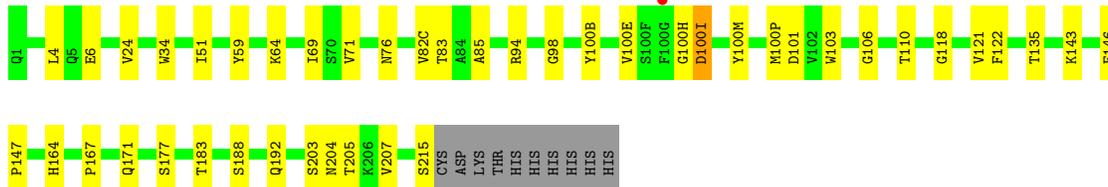
- Molecule 1: Fab light chain

Chain E: 



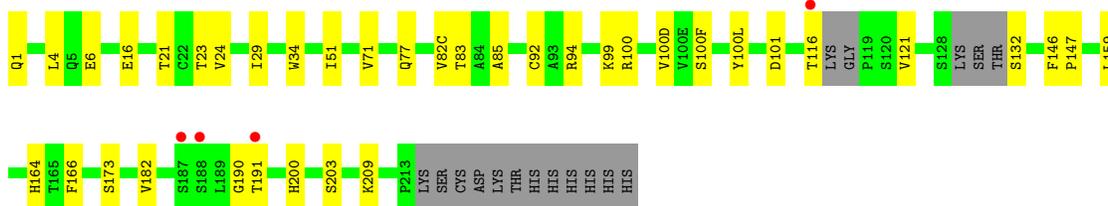
- Molecule 2: Fab heavy chain

Chain H:  78% 18%



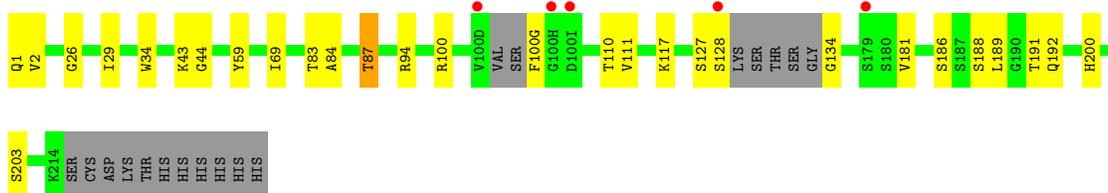
- Molecule 2: Fab heavy chain

Chain B:  2% 77% 16% 7%



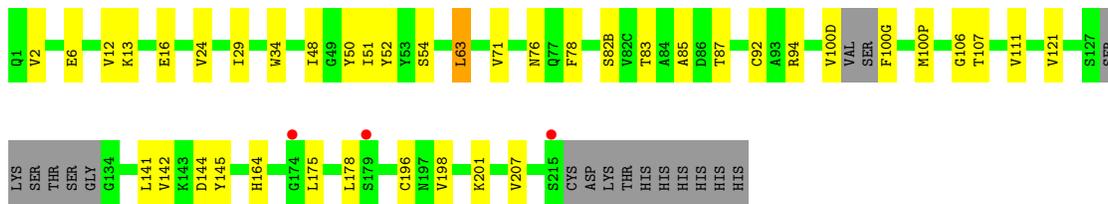
- Molecule 2: Fab heavy chain

Chain D:  2% 81% 11% 7%



- Molecule 2: Fab heavy chain

Chain F:  76% 16% 7%



4 Data and refinement statistics i

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	1.02 (at 2.42Å)	Xtrriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.194 , 0.237 0.196 , 0.239	Depositor DCC
R_{free} test set	1992 reflections (2.68%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtrriage
Anisotropy	0.246	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.009 for l,k,-h 0.066 for h,-k,-l 0.035 for l,-k,h	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section:
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 [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	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 [i](#)

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%)	86	93
1	C	177/182 (97%)	176 (99%)	1 (1%)	86	93
1	E	174/182 (96%)	174 (100%)	0	100	100
1	L	180/182 (99%)	178 (99%)	2 (1%)	73	86
2	B	197/213 (92%)	196 (100%)	1 (0%)	88	95
2	D	196/213 (92%)	194 (99%)	2 (1%)	76	87
2	F	196/213 (92%)	192 (98%)	4 (2%)	55	72
2	H	203/213 (95%)	201 (99%)	2 (1%)	76	87
All	All	1501/1580 (95%)	1488 (99%)	13 (1%)	78	89

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 monosaccharides 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, 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%)	-0.00	3 (1%) 75 73	27, 48, 83, 105	7 (3%)
1	C	210/215 (97%)	-0.10	4 (1%) 66 64	32, 51, 76, 94	3 (1%)
1	E	205/215 (95%)	0.49	21 (10%) 6 5	30, 69, 110, 146	6 (2%)
1	L	213/215 (99%)	-0.09	1 (0%) 91 89	26, 40, 67, 90	1 (0%)
2	B	227/244 (93%)	0.14	4 (1%) 68 65	34, 54, 88, 113	9 (3%)
2	D	226/244 (92%)	-0.15	5 (2%) 62 59	25, 40, 73, 108	4 (1%)
2	F	226/244 (92%)	0.15	3 (1%) 77 75	34, 56, 84, 110	6 (2%)
2	H	234/244 (95%)	-0.27	1 (0%) 92 91	24, 41, 66, 102	2 (0%)
All	All	1752/1836 (95%)	0.02	42 (2%) 59 56	24, 49, 88, 146	38 (2%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	191	THR	5.4
1	E	107	LEU	5.1
1	E	151	ALA	4.8
1	E	181	LEU	4.5
1	E	182	THR	4.4
1	E	13	VAL	3.7
2	B	188	SER	3.5
1	L	107	LEU	3.4
1	E	193	SER	3.4
1	E	208	ALA	3.3
1	E	190	ARG	3.2
1	A	182	THR	3.0
1	E	179	LEU	2.9
1	E	191	SER	2.9
1	E	192	TYR	2.8
1	E	145	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	107	LEU	2.8
1	E	152	ASP	2.8
1	E	185	GLN	2.8
2	F	215	SER	2.8
1	E	141	TYR	2.7
1	C	13	VAL	2.6
1	E	160	VAL	2.6
2	F	174	GLY	2.6
1	C	14	ALA	2.5
1	E	188	SER	2.5
2	B	116	THR	2.5
1	E	11	VAL	2.4
2	D	179	SER	2.4
2	F	179	SER	2.4
2	D	100(I)	ASP	2.3
2	D	100(H)	GLY	2.3
1	C	15	PRO	2.2
1	A	183	PRO	2.2
1	E	12	SER	2.2
2	D	128	SER	2.2
2	H	100(G)	PHE	2.2
1	E	149	TRP	2.1
2	B	187	SER	2.1
1	E	150	LYS	2.1
1	A	152	ASP	2.0
2	D	100(D)	VAL	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	L	400	1/1	0.88	0.29	44,44,44,44	0
3	NA	D	400	1/1	0.91	0.37	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.