Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 01:16 am BST

PDB ID	:	6IEB
Title	:	Structure of RVFV Gn and human monoclonal antibody R15
Authors	:	Wang, Q.H.; Wu, Y.; Gao, F.; Qi, J.X.; Gao, G.F.
Deposited on	:	2018-09-13
Resolution	:	2.41 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 ①) were used in the production of this report:

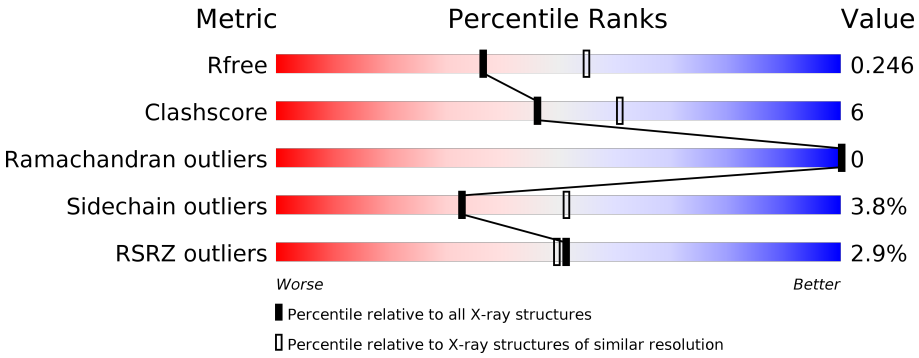
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.41 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 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 <=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	E	218	6% 67% 17% 17%
1	H	218	80% 17% •
2	F	207	6% 78% 19% ••
2	L	207	% 81% 19%
3	A	316	2% 81% 12% • 7%
3	B	316	2% 84% 8% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10916 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 R15 H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	211	Total	C	N	O	S	0	0	0
			1594	1017	257	316	4			
1	E	182	Total	C	N	O	S	0	0	0
			1390	889	223	274	4			

- Molecule 2 is a protein called R15 L chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	207	Total	C	N	O	S	0	0	0
			1537	961	254	315	7			
2	F	204	Total	C	N	O	S	0	0	0
			1515	945	251	312	7			

- Molecule 3 is a protein called NSmGnGc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	293	Total	C	N	O	S	0	0	0
			2264	1421	386	433	24			
3	A	295	Total	C	N	O	S	0	0	0
			2275	1427	388	436	24			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	63	Total	O	0	0
			63	63		
4	L	28	Total	O	0	0
			28	28		
4	B	95	Total	O	0	0
			95	95		
4	A	109	Total	O	0	0
			109	109		

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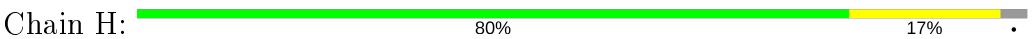
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	34	Total O 34 34	0	0
4	F	12	Total O 12 12	0	0

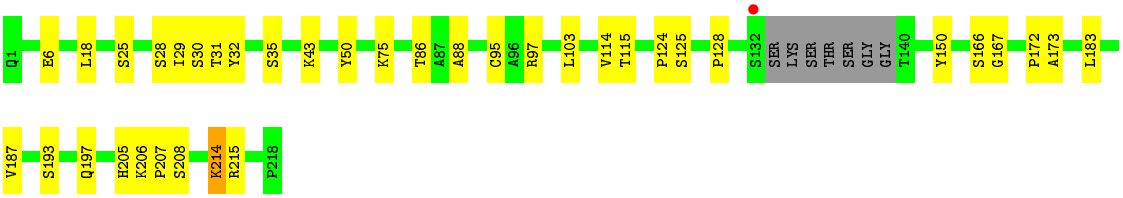
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: R15 H chain

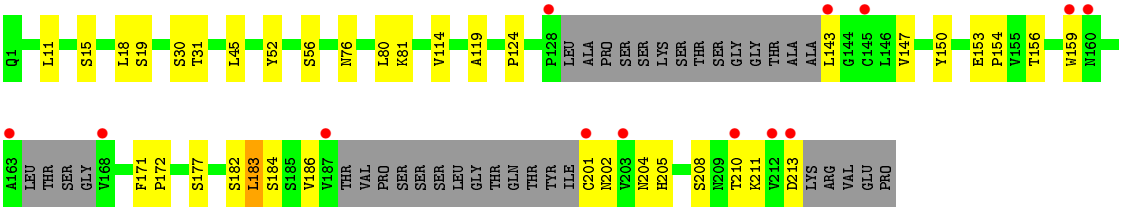
Chain H:





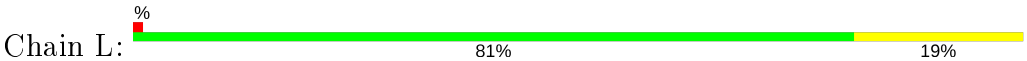
- Molecule 1: R15 H chain

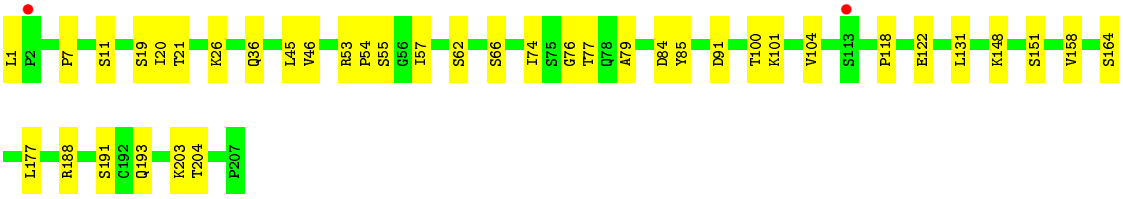
Chain E:



- Molecule 2: R15 L chain

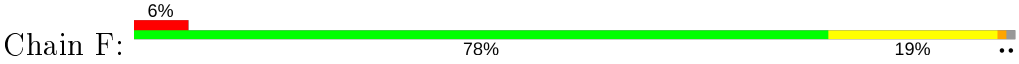
Chain L:

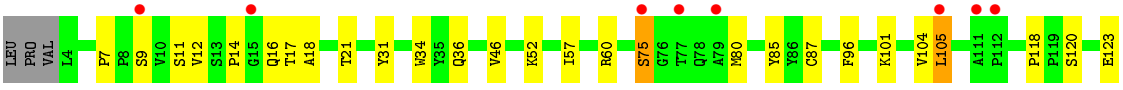


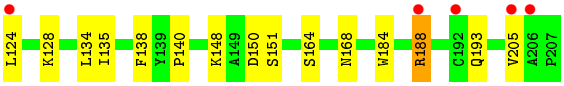


- Molecule 2: R15 L chain

Chain F:

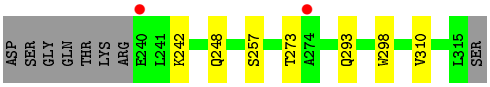






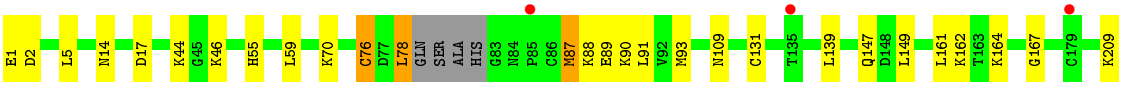
- Molecule 3: NSmGnGc

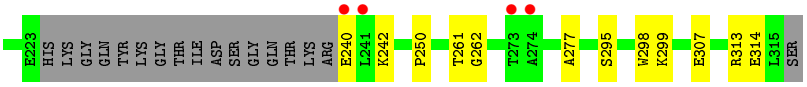
Chain B:



- Molecule 3: NSmGnGc

Chain A:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.00Å 70.52Å 99.33Å 85.09° 84.71° 70.70°	Depositor
Resolution (Å)	38.56 – 2.41 38.56 – 2.41	Depositor EDS
% Data completeness (in resolution range)	91.2 (38.56-2.41) 91.2 (38.56-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.96 (at 2.42Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.195 , 0.246 0.195 , 0.246	Depositor DCC
R_{free} test set	3077 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10916	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	E	0.42	0/1426	0.64	0/1947
1	H	0.56	0/1636	0.68	0/2239
2	F	0.39	0/1551	0.58	0/2118
2	L	0.45	0/1574	0.63	0/2151
3	A	0.56	0/2322	0.66	0/3127
3	B	0.51	0/2310	0.64	0/3109
All	All	0.50	0/10819	0.64	0/14691

There are no bond length outliers.

There are no bond angle outliers.

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	E	1390	0	1345	24	0
1	H	1594	0	1560	18	0
2	F	1515	0	1468	29	0
2	L	1537	0	1498	20	0
3	A	2275	0	2219	30	0
3	B	2264	0	2208	17	0
4	A	109	0	0	8	0
4	B	95	0	0	4	0
4	E	34	0	0	3	0
4	F	12	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	63	0	0	4	0
4	L	28	0	0	3	0
All	All	10916	0	10298	132	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 6.

All (132) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:14:ASN:ND2	4:A:403:HOH:O	2.12	0.79
2:F:46:VAL:HA	2:F:57:ILE:HD13	1.67	0.74
1:H:86:THR:HG22	1:H:88:ALA:H	1.55	0.72
1:E:147:VAL:CG1	1:E:183:LEU:HD23	2.23	0.68
1:H:18:LEU:HD13	1:H:114:VAL:HG11	1.76	0.67
1:H:43:LYS:NZ	4:H:303:HOH:O	2.27	0.67
3:A:78:LEU:HD13	3:A:131:CYS:SG	2.35	0.67
1:H:124:PRO:HB3	1:H:150:TYR:HB3	1.78	0.65
3:B:293:GLN:O	4:B:401:HOH:O	2.14	0.64
2:L:1:LEU:N	4:L:301:HOH:O	2.15	0.64
1:E:18:LEU:HD13	1:E:114:VAL:HG11	1.78	0.64
3:A:147:GLN:NE2	3:A:307:GLU:OE1	2.28	0.64
3:A:2:ASP:HB3	3:A:5:LEU:CD1	2.27	0.64
3:B:98:PRO:O	4:B:402:HOH:O	2.15	0.64
2:F:17:THR:HG22	2:F:75:SER:HA	1.80	0.64
1:E:159:TRP:CZ3	1:E:201:CYS:HB3	2.34	0.63
2:L:191:SER:OG	2:L:204:THR:HG22	2.00	0.62
3:B:149:LEU:HD12	3:B:149:LEU:C	2.20	0.62
2:F:96:PHE:HB2	4:F:309:HOH:O	1.99	0.61
1:E:208:SER:HB2	1:E:210:THR:HG23	1.82	0.61
3:B:188:GLU:OE1	4:B:403:HOH:O	2.17	0.59
1:E:202:ASN:ND2	1:E:213:ASP:OD2	2.19	0.59
1:H:166:SER:HA	4:H:301:HOH:O	2.02	0.58
2:L:54:PRO:HD2	2:L:57:ILE:HD12	1.85	0.58
2:L:76:GLY:N	4:L:302:HOH:O	2.17	0.58
3:A:2:ASP:HB3	3:A:5:LEU:HD11	1.87	0.57
3:B:248:GLN:HB3	3:B:257:SER:HB3	1.87	0.56
2:L:26:LYS:HA	2:L:26:LYS:HE2	1.87	0.56
3:A:164:LYS:NZ	4:A:408:HOH:O	2.37	0.56
1:E:45:LEU:N	4:E:305:HOH:O	2.38	0.56
1:H:128:PRO:HD3	1:H:214:LYS:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:124:LEU:HD21	2:F:184:TRP:CD1	2.41	0.55
1:E:124:PRO:HB3	1:E:150:TYR:HB3	1.88	0.55
2:L:46:VAL:HA	2:L:57:ILE:HD13	1.88	0.55
1:E:172:PRO:HG2	2:F:164:SER:OG	2.07	0.55
3:A:78:LEU:N	3:A:78:LEU:HD12	2.22	0.55
3:A:164:LYS:NZ	4:A:402:HOH:O	1.91	0.54
3:B:273:THR:OG1	3:B:273:THR:O	2.22	0.53
2:F:120:SER:O	2:F:124:LEU:HD12	2.09	0.53
3:A:242:LYS:NZ	4:A:412:HOH:O	2.42	0.53
2:F:16:GLN:HG2	2:F:17:THR:H	1.73	0.53
3:A:162:LYS:O	3:A:164:LYS:HE2	2.09	0.53
2:L:46:VAL:HA	2:L:57:ILE:CD1	2.38	0.53
2:F:120:SER:C	2:F:124:LEU:HD12	2.30	0.52
3:B:164:LYS:NZ	4:B:409:HOH:O	2.43	0.51
2:L:118:PRO:HA	2:L:131:LEU:HD23	1.93	0.51
3:A:17:ASP:OD2	3:A:70:LYS:NZ	2.28	0.51
1:E:183:LEU:HG	1:E:184:SER:N	2.26	0.50
1:E:186:VAL:HG21	2:F:134:LEU:HD13	1.94	0.50
3:A:161:LEU:HD11	3:A:299:LYS:HE3	1.94	0.50
1:E:205:HIS:HB3	1:E:210:THR:OG1	2.12	0.50
2:F:36:GLN:HG2	4:F:302:HOH:O	2.12	0.49
1:H:193:SER:HB2	1:H:197:GLN:OE1	2.11	0.49
1:E:124:PRO:HB2	1:E:147:VAL:HG23	1.94	0.49
2:L:131:LEU:HD12	2:L:177:LEU:HD23	1.94	0.49
3:A:89:GLU:OE1	3:A:109:ASN:N	2.42	0.49
3:B:92:VAL:O	3:B:310:VAL:HG23	2.13	0.49
3:A:313:ARG:NH1	4:A:401:HOH:O	1.90	0.49
2:F:7:PRO:HD3	2:F:21:THR:HG22	1.95	0.49
2:L:148:LYS:HE2	2:L:193:GLN:OE1	2.13	0.49
3:A:261:THR:HG22	3:A:262:GLY:H	1.78	0.48
3:B:126:GLU:OE1	3:B:132:ARG:NH2	2.47	0.48
1:E:30:SER:OG	1:E:31:THR:N	2.45	0.48
3:B:137:ALA:O	2:F:52:LYS:NZ	2.36	0.48
2:F:150:ASP:CG	2:F:188:ARG:HB2	2.33	0.48
2:F:135:ILE:HG22	2:F:138:PHE:CE1	2.49	0.48
1:H:205:HIS:ND1	1:H:208:SER:OG	2.33	0.48
3:A:261:THR:OG1	3:A:277:ALA:HB2	2.14	0.48
1:H:50:TYR:CD2	1:H:103:LEU:HD21	2.49	0.48
2:L:79:ALA:HA	2:L:104:VAL:HG11	1.96	0.48
3:A:87:MET:O	3:A:91:LEU:HB2	2.13	0.47
1:H:206:LYS:HB2	1:H:207:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:143:LEU:N	4:E:306:HOH:O	2.46	0.47
2:L:20:ILE:HD12	2:L:100:THR:HG21	1.96	0.47
2:L:74:ILE:HB	2:L:77:THR:HG22	1.95	0.47
1:H:115:THR:HG21	4:H:329:HOH:O	2.13	0.47
2:F:9:SER:HA	2:F:101:LYS:O	2.14	0.47
2:L:122:GLU:OE2	2:L:122:GLU:N	2.44	0.47
1:E:52:TYR:CZ	1:E:56:SER:HB2	2.49	0.47
1:H:167:GLY:N	4:H:301:HOH:O	2.03	0.47
3:B:77:ASP:HA	3:B:117:LYS:O	2.15	0.47
2:L:203:LYS:HB3	2:L:203:LYS:HE3	1.69	0.47
1:E:147:VAL:HG11	1:E:183:LEU:HD23	1.95	0.46
2:F:118:PRO:HB3	2:F:205:VAL:HG11	1.97	0.46
3:A:55:HIS:ND1	4:A:407:HOH:O	2.36	0.46
2:L:84:ASP:OD2	4:L:303:HOH:O	2.21	0.46
1:E:201:CYS:O	1:E:213:ASP:HA	2.16	0.45
1:E:171:PHE:O	1:E:183:LEU:HD12	2.16	0.45
1:E:81:LYS:NZ	4:E:308:HOH:O	2.50	0.45
2:F:60:ARG:HB2	2:F:75:SER:O	2.16	0.45
3:B:149:LEU:C	3:B:149:LEU:CD1	2.86	0.44
3:A:161:LEU:HA	4:A:402:HOH:O	2.18	0.44
2:F:36:GLN:HB2	2:F:85:TYR:CE1	2.52	0.44
1:H:173:ALA:HA	1:H:183:LEU:HB3	1.99	0.44
3:B:209:LYS:HG2	3:B:298:TRP:CZ3	2.53	0.44
3:A:139:LEU:HD23	3:A:139:LEU:HA	1.85	0.44
2:L:36:GLN:HB2	2:L:85:TYR:CE1	2.53	0.44
1:E:153:GLU:OE2	1:E:154:PRO:HA	2.18	0.43
3:A:209:LYS:HG2	3:A:298:TRP:CZ3	2.53	0.43
3:A:162:LYS:HA	3:A:162:LYS:HD2	1.83	0.43
3:A:90:LYS:O	3:A:93:MET:HG2	2.18	0.43
1:H:167:GLY:O	1:H:187:VAL:HA	2.19	0.43
2:F:34:TRP:CZ3	2:F:87:CYS:HB3	2.53	0.43
3:A:59:LEU:HB2	3:A:149:LEU:HD11	2.00	0.43
3:A:250:PRO:HD2	4:A:438:HOH:O	2.18	0.43
2:F:11:SER:HB3	2:F:105:LEU:HD11	2.01	0.43
1:H:6:GLU:HG3	1:H:95:CYS:SG	2.59	0.42
2:L:45:LEU:O	2:L:57:ILE:HD11	2.20	0.42
1:E:11:LEU:HD21	1:E:119:ALA:O	2.19	0.42
3:A:87:MET:HA	3:A:90:LYS:HB3	2.00	0.42
1:E:156:THR:HB	1:E:204:ASN:HB3	2.01	0.42
3:A:167:GLY:O	3:A:314:GLU:HG2	2.19	0.42
3:A:149:LEU:C	3:A:149:LEU:HD12	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:24:ALA:HA	1:E:52:TYR:CE2	2.55	0.41
2:F:14:PRO:HD3	2:F:105:LEU:O	2.20	0.41
3:A:2:ASP:HB3	3:A:5:LEU:HD13	2.01	0.41
2:F:16:GLN:HG2	2:F:17:THR:N	2.34	0.41
2:F:12:VAL:HG21	2:F:18:ALA:HB2	2.03	0.41
2:F:148:LYS:NZ	4:F:301:HOH:O	2.01	0.41
3:A:76:CYS:SG	3:A:76:CYS:O	2.78	0.41
3:B:84:ASN:C	3:B:86:CYS:H	2.24	0.41
2:F:12:VAL:O	2:F:104:VAL:HA	2.20	0.41
1:H:30:SER:OG	1:H:31:THR:N	2.53	0.41
1:E:19:SER:HA	1:E:80:LEU:O	2.20	0.40
2:L:7:PRO:HD3	2:L:21:THR:HG22	2.03	0.40
3:B:121:LYS:HE2	2:F:31:TYR:CD1	2.56	0.40
1:H:172:PRO:HG2	2:L:164:SER:OG	2.22	0.40
3:B:90:LYS:O	3:B:93:MET:HG2	2.20	0.40
2:F:148:LYS:HG3	2:F:193:GLN:NE2	2.37	0.40
2:F:123:GLU:HG2	2:F:128:LYS:O	2.22	0.40
2:F:168:ASN:OD1	2:F:168:ASN:C	2.60	0.40
1:H:32:TYR:CG	1:H:97:ARG:HD2	2.56	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	E	174/218 (80%)	163 (94%)	11 (6%)	0	100	100
1	H	207/218 (95%)	203 (98%)	4 (2%)	0	100	100
2	F	202/207 (98%)	191 (95%)	11 (5%)	0	100	100
2	L	205/207 (99%)	195 (95%)	10 (5%)	0	100	100
3	A	289/316 (92%)	279 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	285/316 (90%)	276 (97%)	9 (3%)	0	100	100
All	All	1362/1482 (92%)	1307 (96%)	55 (4%)	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	E	160/189 (85%)	154 (96%)	6 (4%)	33	51
1	H	184/189 (97%)	176 (96%)	8 (4%)	29	46
2	F	173/176 (98%)	167 (96%)	6 (4%)	36	55
2	L	176/176 (100%)	165 (94%)	11 (6%)	18	28
3	A	254/271 (94%)	245 (96%)	9 (4%)	36	55
3	B	253/271 (93%)	248 (98%)	5 (2%)	55	74
All	All	1200/1272 (94%)	1155 (96%)	45 (4%)	33	51

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	25	SER
1	H	28	SER
1	H	29	ILE
1	H	35	SER
1	H	75	LYS
1	H	125	SER
1	H	214	LYS
1	H	215	ARG
2	L	11	SER
2	L	19	SER
2	L	53	ARG
2	L	55	SER
2	L	62	SER

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Mol	Chain	Res	Type
2	L	66	SER
2	L	91	ASP
2	L	101	LYS
2	L	151	SER
2	L	158	VAL
2	L	188	ARG
3	B	44	LYS
3	B	132	ARG
3	B	149	LEU
3	B	207	ASP
3	B	242	LYS
3	A	1	GLU
3	A	44	LYS
3	A	46	LYS
3	A	76	CYS
3	A	78	LEU
3	A	87	MET
3	A	88	LYS
3	A	240	GLU
3	A	295	SER
1	E	15	SER
1	E	76	ASN
1	E	177	SER
1	E	182	SER
1	E	183	LEU
1	E	211	LYS
2	F	75	SER
2	F	80	MET
2	F	105	LEU
2	F	140	PRO
2	F	151	SER
2	F	188	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 95^{th} 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	E	182/218 (83%)	0.26	13 (7%) 16 14	31, 47, 84, 104	0
1	H	211/218 (96%)	-0.25	1 (0%) 91 89	20, 33, 57, 67	0
2	F	204/207 (98%)	0.50	13 (6%) 19 18	38, 65, 82, 90	0
2	L	207/207 (100%)	-0.04	2 (0%) 82 80	24, 42, 57, 72	0
3	A	295/316 (93%)	-0.04	7 (2%) 59 57	19, 31, 61, 79	0
3	B	293/316 (92%)	-0.08	5 (1%) 70 68	26, 38, 62, 80	0
All	All	1392/1482 (93%)	0.04	41 (2%) 51 50	19, 41, 74, 104	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	159	TRP	4.5
1	E	213	ASP	4.2
1	E	210	THR	3.6
1	E	143	LEU	3.5
2	L	2	PRO	3.5
1	E	203	VAL	3.4
3	B	274	ALA	3.3
2	F	206	ALA	3.3
1	E	160	ASN	3.2
2	F	105	LEU	3.2
2	F	9	SER	3.2
1	E	201	CYS	3.1
1	E	163	ALA	3.1
1	E	145	CYS	2.9
2	F	15	GLY	2.9
2	F	188	ARG	2.8
2	F	205	VAL	2.7
2	F	79	ALA	2.7
2	F	112	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	240	GLU	2.6
2	F	111	ALA	2.5
1	E	187	VAL	2.5
2	F	192	CYS	2.5
3	B	240	GLU	2.5
3	A	179	CYS	2.4
1	E	128	PRO	2.4
3	A	241	LEU	2.4
3	A	273	THR	2.3
2	F	124	LEU	2.3
1	E	212	VAL	2.2
3	B	85	PRO	2.2
3	A	135	THR	2.2
3	B	180	ASP	2.2
2	F	77	THR	2.1
1	H	132	SER	2.1
2	F	75	SER	2.1
1	E	168	VAL	2.1
2	L	113	SER	2.1
3	B	179	CYS	2.1
3	A	274	ALA	2.0
3	A	85	PRO	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 carbohydrates 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.