Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 04:05 PM EDT

PDB ID	:	6IEK
Title	:	Structure of RVFV Gn and human monoclonal antibody R12
Authors	:	Wang, Q.H.; Wu, Y.; Gao, F.; Qi, J.X.; Gao, G.F.
Deposited on	:	2018-09-14
Resolution	:	2.70 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

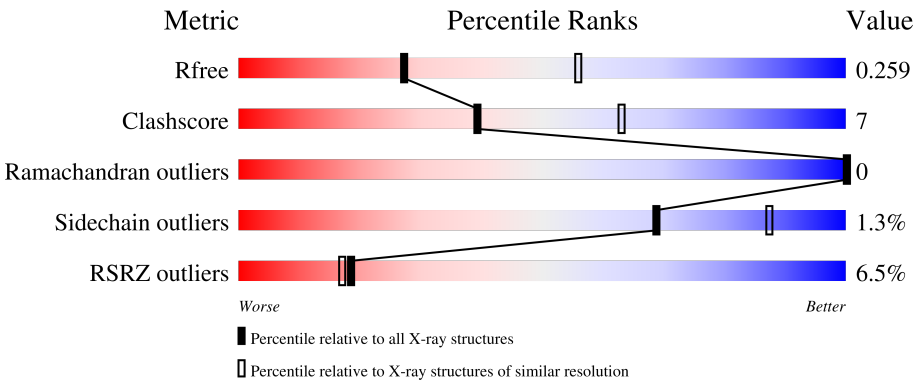
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	316	3%, 77%, 18%, • 5%
1	D	316	9%, 76%, 18%, • 5%
2	B	226	4%, 88%, 11%, •
2	E	226	20%, 77%, 22%, •
3	C	219	%, 88%, 11%, •

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Mol	Chain	Length	Quality of chain
3	F	219	% 79% 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11528 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 NSmGnGc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	301	2324	1456	400	444	24	0	0	0
1	D	301	2324	1456	400	444	24	0	0	0

- Molecule 2 is a protein called Heavy chain of Fab R12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	223	1680	1058	277	337	8	0	0	0
2	E	223	1680	1058	277	337	8	0	0	0

- Molecule 3 is a protein called Light chain of Fab R12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	218	1649	1041	267	336	5	0	0	0
3	F	218	1649	1041	267	336	5	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	50	50	50	0	0
4	B	30	30	30	0	0
4	C	36	36	36	0	0
4	D	52	52	52	0	0

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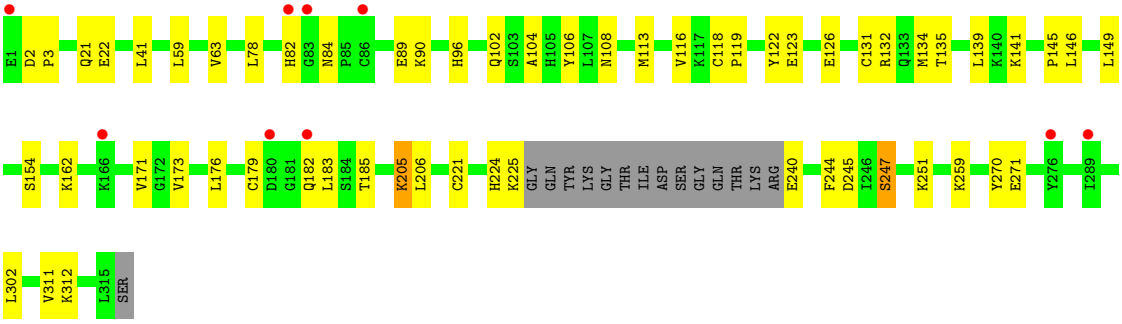
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	E	18	18	18	0	0
			Total	O		
4	F	36	36	36	0	0

3 Residue-property plots (i)

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

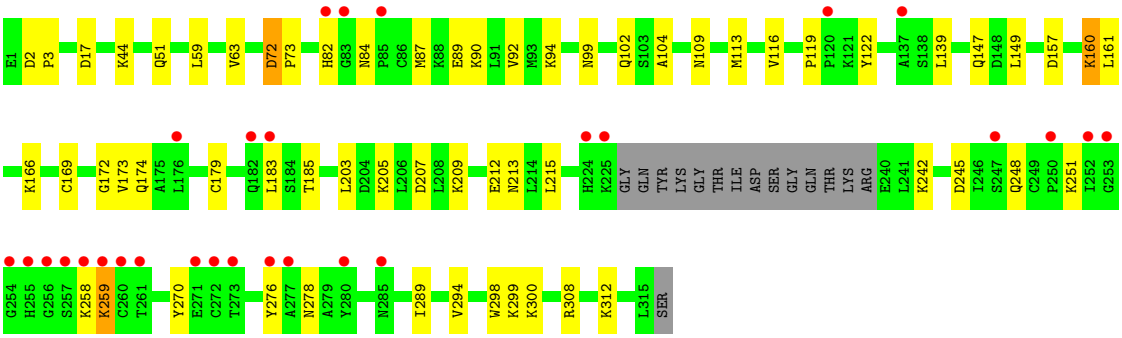
• Molecule 1: NSmGnGc

Chain A:



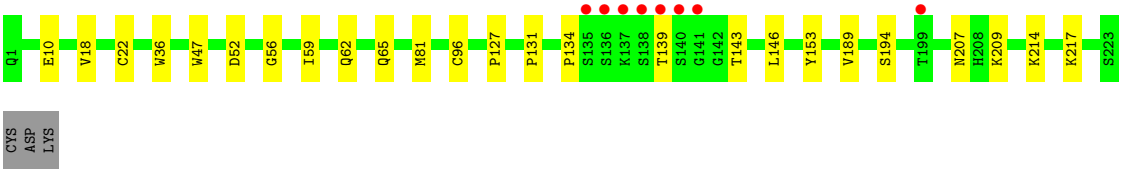
• Molecule 1: NSmGnGc

Chain D:



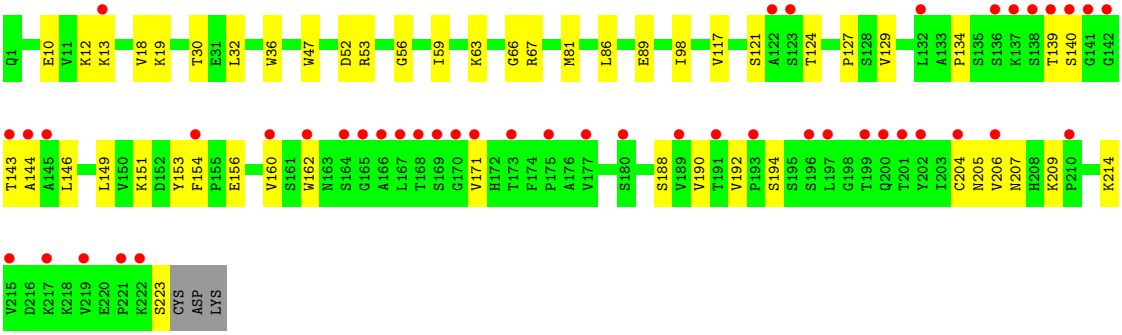
• Molecule 2: Heavy chain of Fab R12

Chain B:



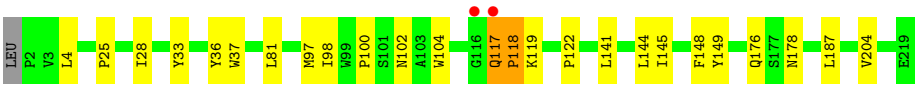
• Molecule 2: Heavy chain of Fab R12

Chain E:



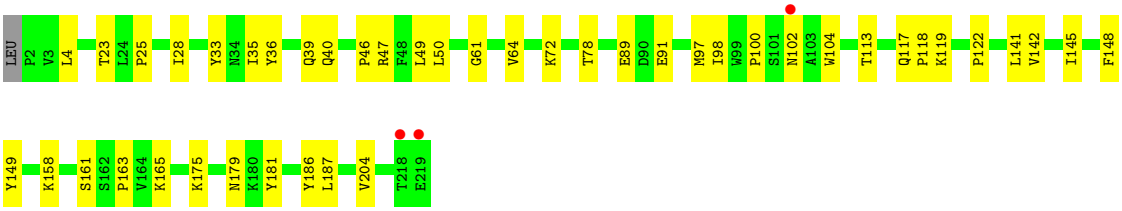
• Molecule 3: Light chain of Fab R12

Chain C:



• Molecule 3: Light chain of Fab R12

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.76Å 108.07Å 107.42Å 90.00° 90.34° 90.00°	Depositor
Resolution (Å)	48.27 – 2.70 48.27 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.8 (48.27-2.70) 90.5 (48.27-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.225 , 0.258 0.226 , 0.259	Depositor DCC
R_{free} test set	2812 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 17.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.030 for -h,-l,-k 0.018 for -h,l,k 0.099 for h,-k,-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11528	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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 (i)

5.1 Standard geometry (i)

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	0.25	0/2374	0.46	0/3198
1	D	0.26	0/2374	0.48	0/3198
2	B	0.24	0/1720	0.46	0/2343
2	E	0.27	0/1720	0.49	0/2343
3	C	0.26	0/1696	0.46	0/2319
3	F	0.25	0/1696	0.46	0/2319
All	All	0.26	0/11580	0.47	0/15720

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
3	C	0	2
3	F	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	117	GLN	Peptide
3	C	118	PRO	Peptide
1	D	72	ASP	Peptide
3	F	117	GLN	Peptide
3	F	118	PRO	Peptide

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	2324	0	2265	37	0
1	D	2324	0	2265	43	0
2	B	1680	0	1636	15	0
2	E	1680	0	1636	36	0
3	C	1649	0	1582	15	0
3	F	1649	0	1582	26	0
4	A	50	0	0	5	0
4	B	30	0	0	0	0
4	C	36	0	0	0	0
4	D	52	0	0	3	0
4	E	18	0	0	4	0
4	F	36	0	0	1	0
All	All	11528	0	10966	165	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 7.

All (165) 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)
1:A:118:CYS:SG	4:A:417:HOH:O	2.29	0.91
2:E:18:VAL:HG23	2:E:86:LEU:HD11	1.54	0.88
1:D:72:ASP:OD2	1:D:73:PRO:HD2	1.77	0.85
1:D:72:ASP:OD2	1:D:73:PRO:CD	2.32	0.77
1:D:258:LYS:HG2	1:D:259:LYS:H	1.49	0.77
1:A:162:LYS:HZ1	1:A:176:LEU:HD22	1.50	0.77
3:C:141:LEU:HD12	3:C:187:LEU:HD23	1.67	0.76
1:D:179:CYS:HB3	1:D:183:LEU:HD21	1.73	0.71
1:D:72:ASP:CG	1:D:73:PRO:HD2	2.12	0.70
2:E:160:VAL:HG12	2:E:206:VAL:HA	1.73	0.70
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.75	0.69
1:A:185:THR:HG22	1:A:312:LYS:HG2	1.73	0.69
1:D:157:ASP:O	1:D:299:LYS:NZ	2.26	0.68
2:E:12:LYS:HG3	2:E:18:VAL:HG22	1.73	0.68
3:C:145:ILE:HG12	3:C:204:VAL:HG11	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:PRO:HB3	2:B:153:TYR:HB3	1.76	0.67
3:F:175:LYS:HE3	3:F:181:TYR:CE2	2.30	0.66
3:F:145:ILE:HG12	3:F:204:VAL:HG11	1.77	0.66
1:D:242:LYS:NZ	4:D:409:HOH:O	2.29	0.65
1:D:203:LEU:HD21	1:D:294:VAL:HG12	1.76	0.65
1:D:84:ASN:HA	1:D:87:MET:HB2	1.79	0.65
1:D:212:GLU:OE2	4:D:401:HOH:O	2.13	0.65
2:E:13:LYS:HG3	2:E:121:SER:HA	1.79	0.65
2:E:129:VAL:HG21	2:E:206:VAL:HG21	1.79	0.65
2:E:144:ALA:HB3	2:E:192:VAL:HG13	1.80	0.64
1:A:22:GLU:HG3	1:A:141:LYS:HD2	1.79	0.63
1:A:123:GLU:HG3	1:A:134:MET:HA	1.80	0.63
3:F:47:ARG:NH1	4:F:308:HOH:O	2.32	0.62
1:A:162:LYS:NZ	1:A:176:LEU:HD22	2.15	0.61
3:C:117:GLN:HB3	3:C:118:PRO:HD3	1.82	0.60
1:A:82:HIS:HD2	1:A:84:ASN:H	1.50	0.60
1:D:251:LYS:HA	1:D:270:TYR:HA	1.83	0.59
2:E:149:LEU:HG	2:E:151:LYS:HG2	1.83	0.59
3:F:141:LEU:HD12	3:F:187:LEU:HD23	1.84	0.59
2:E:32:LEU:HB3	2:E:98:ILE:HD11	1.85	0.58
3:F:158:LYS:HE3	3:F:161:SER:HA	1.84	0.58
2:E:10:GLU:OE1	4:E:301:HOH:O	2.17	0.58
2:B:59:ILE:HG21	3:C:102:ASN:HB3	1.86	0.57
3:F:35:ILE:HD12	3:F:72:LYS:HE2	1.87	0.57
3:F:91:GLU:HG3	3:F:113:THR:HA	1.86	0.57
2:E:162:TRP:NE1	2:E:188:SER:OG	2.38	0.56
2:B:209:LYS:HE2	2:B:209:LYS:HA	1.87	0.56
2:B:131:PRO:HD3	2:B:217:LYS:HE3	1.88	0.55
1:D:258:LYS:HD3	1:D:278:ASN:HB2	1.88	0.55
2:B:189:VAL:HG11	3:C:144:LEU:HD13	1.89	0.54
1:D:99:ASN:ND2	4:D:414:HOH:O	2.33	0.54
1:A:224:HIS:NE2	3:F:179:ASN:OD1	2.41	0.54
1:D:89:GLU:HG3	1:D:173:VAL:HG21	1.90	0.54
1:D:259:LYS:HZ1	1:D:276:TYR:HB2	1.72	0.53
1:A:78:LEU:HB2	1:A:131:CYS:SG	2.49	0.53
1:D:109:ASN:OD1	1:D:174:GLN:NE2	2.39	0.53
1:D:72:ASP:OD2	1:D:73:PRO:N	2.42	0.53
1:D:161:LEU:HD11	1:D:299:LYS:HD3	1.91	0.53
1:A:82:HIS:CD2	1:A:84:ASN:H	2.27	0.53
1:A:205:LYS:NZ	4:A:409:HOH:O	2.36	0.53
3:F:40:GLN:HB2	3:F:46:PRO:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:ASN:HD21	1:D:215:LEU:HB2	1.74	0.53
2:B:139:THR:HA	2:B:143:THR:O	2.09	0.52
1:A:123:GLU:OE1	1:A:135:THR:N	2.37	0.52
1:A:102:GLN:HB2	1:A:139:LEU:HD13	1.92	0.52
3:C:4:LEU:HD11	3:C:98:ILE:HG12	1.92	0.52
3:C:25:PRO:HD2	3:C:28:ILE:HD11	1.92	0.51
1:A:2:ASP:HB3	1:A:3:PRO:HD3	1.92	0.51
1:D:161:LEU:HD13	1:D:294:VAL:HG21	1.93	0.51
2:E:124:THR:HA	2:E:154:PHE:O	2.11	0.51
2:E:18:VAL:HG21	2:E:117:VAL:HG11	1.93	0.50
2:E:223:SER:O	2:E:223:SER:OG	2.28	0.50
1:A:251:LYS:HA	1:A:270:TYR:HA	1.93	0.50
2:B:36:TRP:CE2	2:B:81:MET:HB2	2.46	0.50
1:A:123:GLU:N	1:A:132:ARG:O	2.36	0.50
1:D:289:ILE:HG23	1:D:300:LYS:HD2	1.92	0.50
1:A:104:ALA:HB3	1:A:116:VAL:HG12	1.94	0.50
1:D:259:LYS:CE	1:D:276:TYR:HB2	2.42	0.50
1:D:84:ASN:HA	1:D:87:MET:CB	2.41	0.50
1:D:160:LYS:HE3	1:D:161:LEU:HD23	1.94	0.49
3:F:4:LEU:HD11	3:F:98:ILE:HG12	1.93	0.49
1:D:102:GLN:HB2	1:D:139:LEU:HD13	1.93	0.49
1:D:209:LYS:HE2	1:D:298:TRP:CZ2	2.48	0.49
2:E:209:LYS:HD2	2:E:209:LYS:N	2.26	0.49
2:E:67:ARG:N	4:E:302:HOH:O	2.46	0.49
1:D:147:GLN:HB2	1:D:149:LEU:HD23	1.95	0.48
2:B:134:PRO:HG3	2:B:146:LEU:HB3	1.95	0.48
1:D:2:ASP:HB3	1:D:3:PRO:HD3	1.96	0.48
1:A:89:GLU:HG3	1:A:173:VAL:HG11	1.96	0.48
1:A:179:CYS:HB3	1:A:183:LEU:HD21	1.95	0.47
1:A:245:ASP:OD2	1:A:247:SER:HB3	2.14	0.47
1:D:94:LYS:HG2	1:D:308:ARG:HD2	1.97	0.47
1:D:245:ASP:O	1:D:248:GLN:HG3	2.14	0.47
3:F:119:LYS:H	3:F:149:TYR:HD2	1.62	0.47
1:D:213:ASN:ND2	1:D:215:LEU:HB2	2.29	0.47
3:F:49:LEU:O	3:F:64:VAL:HG21	2.14	0.47
1:A:119:PRO:HB2	1:A:122:TYR:CD1	2.49	0.47
2:E:134:PRO:HG3	2:E:146:LEU:HB3	1.97	0.47
1:A:240:GLU:N	1:A:240:GLU:OE2	2.48	0.47
3:F:23:THR:HG22	3:F:78:THR:HG22	1.95	0.47
2:B:47:TRP:HH2	2:B:59:ILE:HG22	1.79	0.46
1:A:171:VAL:HG23	1:A:311:VAL:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:SER:HB3	1:A:302:LEU:HD23	1.97	0.46
2:E:19:LYS:NZ	4:E:303:HOH:O	2.31	0.46
2:E:66:GLY:N	4:E:302:HOH:O	2.49	0.46
2:E:52:ASP:O	2:E:56:GLY:N	2.49	0.46
2:E:134:PRO:HG3	2:E:146:LEU:HD23	1.98	0.46
1:D:119:PRO:HB2	1:D:122:TYR:CD1	2.51	0.45
1:D:258:LYS:HG2	1:D:259:LYS:N	2.25	0.45
3:F:163:PRO:HB2	3:F:165:LYS:HE2	1.98	0.45
1:A:41:LEU:HD21	1:A:145:PRO:HG2	1.98	0.45
2:B:59:ILE:HG21	3:C:102:ASN:CB	2.46	0.45
3:F:33:TYR:CE1	3:F:100:PRO:HB3	2.52	0.45
1:D:185:THR:HG22	1:D:312:LYS:HG2	1.99	0.45
2:E:30:THR:O	2:E:53:ARG:HD3	2.17	0.45
2:E:36:TRP:CE2	2:E:81:MET:HB2	2.52	0.45
2:B:207:ASN:OD1	2:B:209:LYS:HE3	2.17	0.45
2:E:171:VAL:HG22	2:E:190:VAL:HB	1.98	0.45
2:E:89:GLU:N	2:E:89:GLU:OE2	2.50	0.44
1:D:104:ALA:HB3	1:D:116:VAL:HG12	1.99	0.44
3:C:36:TYR:HB2	3:C:97:MET:HB3	1.99	0.44
1:D:166:LYS:H	1:D:166:LYS:HG2	1.49	0.44
3:F:89:GLU:H	3:F:89:GLU:HG3	1.63	0.44
2:E:63:LYS:HE3	2:E:63:LYS:HB3	1.81	0.44
3:F:142:VAL:HG22	3:F:186:TYR:HD2	1.83	0.44
1:A:221:CYS:HB2	1:A:244:PHE:O	2.18	0.43
2:E:47:TRP:CD1	3:F:104:TRP:HB2	2.53	0.43
1:D:82:HIS:HB3	1:D:84:ASN:HB2	1.99	0.43
1:A:63:VAL:HG21	1:A:113:MET:SD	2.58	0.43
3:C:37:TRP:CD2	3:C:81:LEU:HB2	2.54	0.43
3:C:176:GLN:NE2	3:C:178:ASN:HD21	2.17	0.43
2:E:207:ASN:ND2	2:E:209:LYS:HD3	2.34	0.43
2:E:139:THR:HA	2:E:143:THR:O	2.19	0.43
3:C:33:TYR:CE1	3:C:100:PRO:HB3	2.53	0.43
1:D:44:LYS:HD2	1:D:51:GLN:HE22	1.83	0.43
2:E:206:VAL:O	2:E:214:LYS:HA	2.19	0.43
3:F:119:LYS:HA	3:F:149:TYR:O	2.19	0.42
2:E:143:THR:O	2:E:194:SER:OG	2.38	0.42
1:A:96:HIS:HA	1:A:126:GLU:O	2.20	0.42
3:C:119:LYS:H	3:C:149:TYR:HD2	1.68	0.42
3:F:25:PRO:HD2	3:F:28:ILE:HD11	2.01	0.42
1:A:131:CYS:HA	4:A:417:HOH:O	2.20	0.42
1:D:59:LEU:HB2	1:D:149:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLU:OE1	4:A:401:HOH:O	2.21	0.41
2:E:59:ILE:HG21	3:F:102:ASN:HB2	2.02	0.41
3:F:61:GLY:O	3:F:64:VAL:HG22	2.20	0.41
1:A:59:LEU:HB2	1:A:149:LEU:HD11	2.02	0.41
1:A:82:HIS:HB2	1:A:84:ASN:HB2	2.01	0.41
1:A:106:TYR:HB3	1:A:146:LEU:HD12	2.03	0.41
2:B:62:GLN:HA	2:B:65:GLN:HG2	2.03	0.41
1:A:225:LYS:HA	1:A:225:LYS:HD2	1.80	0.41
2:B:10:GLU:HG2	2:B:18:VAL:HG23	2.02	0.41
2:B:52:ASP:O	2:B:56:GLY:N	2.52	0.41
1:D:92:VAL:HG21	1:D:172:GLY:HA2	2.03	0.41
3:C:122:PRO:HB3	3:C:148:PHE:HB3	2.03	0.41
2:E:140:SER:H	2:E:143:THR:HG23	1.85	0.41
2:E:160:VAL:HA	2:E:205:ASN:O	2.21	0.41
3:F:122:PRO:HB3	3:F:148:PHE:HB3	2.03	0.41
1:A:21:GLN:NE2	4:A:414:HOH:O	2.47	0.41
1:D:63:VAL:HG21	1:D:113:MET:SD	2.60	0.41
1:D:169:CYS:HB3	1:D:179:CYS:HB2	1.89	0.40
1:A:90:LYS:HA	1:A:90:LYS:HD2	1.90	0.40
2:B:47:TRP:CD1	3:C:104:TRP:HB2	2.57	0.40
1:D:259:LYS:NZ	1:D:276:TYR:HB2	2.36	0.40
3:F:36:TYR:HB2	3:F:97:MET:HB3	2.04	0.40
3:F:39:GLN:HB2	3:F:49:LEU:HD11	2.03	0.40
1:A:206:LEU:HD12	1:A:206:LEU:HA	1.85	0.40
2:E:153:TYR:HE2	2:E:156:GLU:HG2	1.85	0.40
3:F:175:LYS:HG2	3:F:179:ASN:HA	2.03	0.40
2:E:162:TRP:CZ2	2:E:204:CYS:HB3	2.57	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	297/316 (94%)	292 (98%)	5 (2%)	0	100	100
1	D	297/316 (94%)	289 (97%)	8 (3%)	0	100	100
2	B	221/226 (98%)	212 (96%)	9 (4%)	0	100	100
2	E	221/226 (98%)	212 (96%)	9 (4%)	0	100	100
3	C	216/219 (99%)	207 (96%)	9 (4%)	0	100	100
3	F	216/219 (99%)	206 (95%)	10 (5%)	0	100	100
All	All	1468/1522 (96%)	1418 (97%)	50 (3%)	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	259/271 (96%)	254 (98%)	5 (2%)	57	82
1	D	259/271 (96%)	253 (98%)	6 (2%)	50	78
2	B	189/193 (98%)	185 (98%)	4 (2%)	53	80
2	E	189/193 (98%)	189 (100%)	0	100	100
3	C	187/188 (100%)	187 (100%)	0	100	100
3	F	187/188 (100%)	186 (100%)	1 (0%)	88	96
All	All	1270/1304 (97%)	1254 (99%)	16 (1%)	69	87

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	ASN
1	A	182	GLN
1	A	205	LYS
1	A	247	SER
1	A	259	LYS
2	B	22	CYS
2	B	96	CYS

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Mol	Chain	Res	Type
2	B	194	SER
2	B	214	LYS
1	D	17	ASP
1	D	90	LYS
1	D	160	LYS
1	D	205	LYS
1	D	207	ASP
1	D	259	LYS
3	F	50	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	285	ASN
1	A	293	GLN
3	C	176	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)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	301/316 (95%)	0.33	9 (2%) 50 51	22, 39, 84, 152	0
1	D	301/316 (95%)	0.73	29 (9%) 8 6	19, 41, 105, 210	0
2	B	223/226 (98%)	0.37	8 (3%) 42 42	23, 40, 82, 262	0
2	E	223/226 (98%)	1.37	46 (20%) 1 0	25, 61, 163, 276	0
3	C	218/219 (99%)	0.13	2 (0%) 84 85	21, 39, 65, 113	0
3	F	218/219 (99%)	0.34	3 (1%) 75 77	19, 38, 63, 152	0
All	All	1484/1522 (97%)	0.54	97 (6%) 18 17	19, 41, 102, 276	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	276	TYR	16.3
2	E	138	SER	13.0
2	B	141	GLY	11.9
2	E	202	TYR	11.6
2	E	168	THR	9.3
2	E	165	GLY	9.2
2	E	167	LEU	8.3
2	B	137	LYS	8.0
1	D	257	SER	7.9
2	E	137	LYS	7.2
3	F	218	THR	6.9
2	E	199	THR	6.7
1	D	255	HIS	6.7
2	E	140	SER	6.2
2	B	136	SER	6.0
2	E	215	VAL	6.0
2	E	162	TRP	5.9
2	E	142	GLY	5.7
2	E	197	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
2	B	139	THR	5.5
2	E	139	THR	5.4
2	E	171	VAL	5.4
2	B	140	SER	5.3
2	B	138	SER	5.3
1	D	137	ALA	5.2
1	D	259	LYS	5.2
2	E	143	THR	5.2
2	E	200	GLN	5.0
1	D	252	ILE	4.8
2	E	222	LYS	4.7
1	D	224	HIS	4.5
2	E	164	SER	4.2
2	E	219	VAL	4.1
2	E	204	CYS	4.1
2	E	196	SER	4.0
1	D	83	GLY	3.9
2	E	123	SER	3.9
1	D	254	GLY	3.9
1	D	256	GLY	3.9
1	D	277	ALA	3.8
1	D	261	THR	3.8
2	E	145	ALA	3.8
1	A	180	ASP	3.8
2	E	154	PHE	3.8
3	F	219	GLU	3.7
1	D	182	GLN	3.7
2	E	210	PRO	3.6
1	A	82	HIS	3.5
2	E	221	PRO	3.5
1	D	271	GLU	3.5
1	D	258	LYS	3.5
2	E	173	THR	3.5
1	D	176	LEU	3.5
2	E	166	ALA	3.4
2	E	206	VAL	3.4
1	D	247	SER	3.1
2	E	144	ALA	3.1
2	B	135	SER	3.0
2	E	189	VAL	3.0
1	A	182	GLN	2.9
2	E	132	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	217	LYS	2.9
2	E	169	SER	2.9
2	E	201	THR	2.8
1	D	273	THR	2.8
2	B	199	THR	2.8
2	E	191	THR	2.7
1	A	83	GLY	2.7
3	C	116	GLY	2.7
1	A	86	CYS	2.7
2	E	180	SER	2.6
2	E	141	GLY	2.6
1	D	250	PRO	2.5
2	E	175	PRO	2.5
2	E	136	SER	2.5
2	E	177	VAL	2.5
1	D	82	HIS	2.5
2	E	170	GLY	2.5
2	E	193	PRO	2.4
1	D	253	GLY	2.4
1	D	260	CYS	2.4
1	D	272	CYS	2.4
1	A	276	TYR	2.4
2	E	160	VAL	2.4
1	A	1	GLU	2.3
1	D	120	PRO	2.3
1	D	225	LYS	2.3
1	A	289	ILE	2.3
1	A	166	LYS	2.2
2	E	122	ALA	2.2
1	D	85	PRO	2.1
1	D	285	ASN	2.1
1	D	183	LEU	2.0
1	D	280	TYR	2.0
2	E	13	LYS	2.0
3	C	117	GLN	2.0
3	F	102	ASN	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.