Full wwPDB X-ray Structure Validation Report (i)

May 15, 2016 – 05:51 AM EDT

PDB ID	:	5I8E
Title	:	Crystal Structure of Broadly Neutralizing HIV-1 Fusion Peptide-Targeting Antibody VRC34.01 Fab
Authors	:	Xu, K.; Zhou, T.; Liu, K.; Kwong, P.D.
Deposited on	:	2016-02-18
Resolution	:	2.65 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 (i) symbol.

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

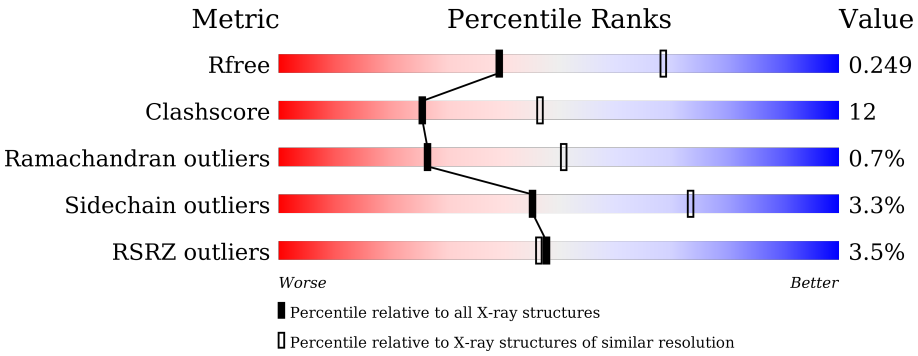
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027457
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

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 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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 <=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	222	8% 74% 23%
1	C	222	81% 15%
2	B	210	3% 70% 24%
2	D	210	2% 65% 32%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6546 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 VRC34.01 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1633	1031	277	319	6			
1	C	216	Total	C	N	O	S	0	0	0
			1627	1027	276	318	6			

- Molecule 2 is a protein called VRC34.01 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	203	Total	C	N	O	S	0	0	0
			1541	976	258	302	5			
2	D	210	Total	C	N	O	S	0	0	0
			1610	1015	269	321	5			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	4	Total	Zn	0	0
			4	4		
3	D	1	Total	Zn	0	0
			1	1		
3	C	4	Total	Zn	0	0
			4	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total	O	0	0
			33	33		
4	B	31	Total	O	0	0
			31	31		

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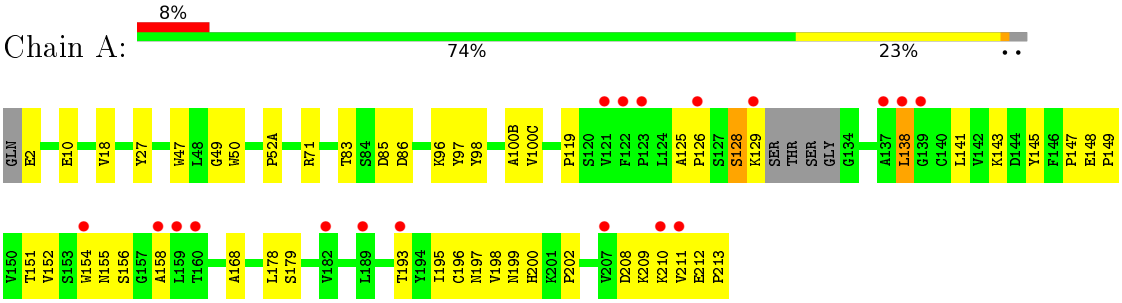
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	31	Total O 31 31	0	0
4	D	30	Total O 30 30	0	0

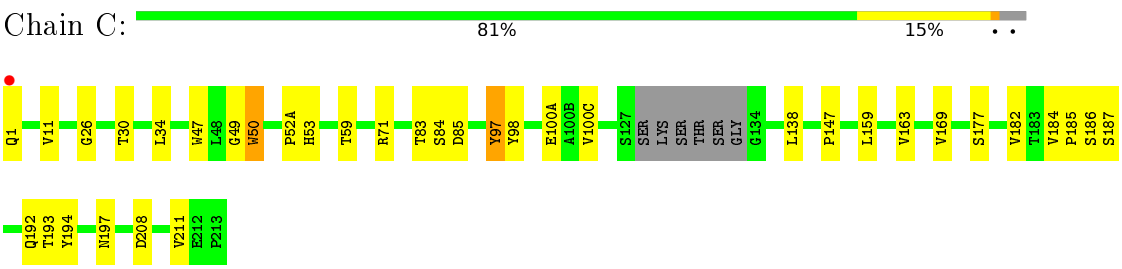
3 Residue-property plots (i)

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.

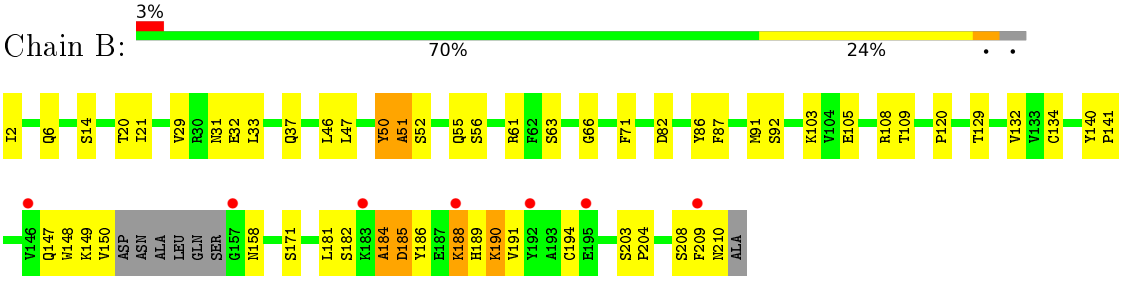
- Molecule 1: VRC34.01 Fab heavy chain



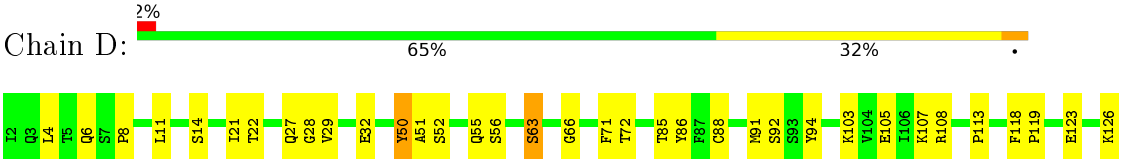
- Molecule 1: VRC34.01 Fab heavy chain



- Molecule 2: VRC34.01 Fab light chain



- Molecule 2: VRC34.01 Fab light chain




S127
G128
L136
F139
Y140
K145
Y146
Q147
W148
K149
Y150
D151
N152
A153
L154
Q155
S156
G157
N158
S159
D167
D170
S171
T172
Y173
S174
L175
K183
A184
D185
Y186
E187
K188
H189
K190
V191
Y192
A193
C194
E195
V196
T197
L201
S202
S203
P204
V205
S208
F209
N210
A211

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	114.61Å 114.61Å 174.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.31 – 2.65 37.31 – 2.66	Depositor EDS
% Data completeness (in resolution range)	92.9 (37.31-2.65) 92.9 (37.31-2.66)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.40 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.186 , 0.248 0.187 , 0.249	Depositor DCC
R_{free} test set	1536 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	64.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.116 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6546	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.46	0/1673	0.71	0/2280
1	C	0.51	0/1667	0.66	0/2273
2	B	0.54	0/1577	0.77	0/2145
2	D	0.51	0/1647	0.76	1/2239 (0.0%)
All	All	0.51	0/6564	0.73	1/8937 (0.0%)

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
2	B	0	3
2	D	0	3
All	All	0	6

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	157	GLY	N-CA-C	5.78	127.56	113.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	185	ASP	Peptide
2	B	190	LYS	Peptide
2	B	50	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	D	150	VAL	Peptide
2	D	187	GLU	Peptide
2	D	50	TYR	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	1633	0	1593	41	0
1	C	1627	0	1586	22	0
2	B	1541	0	1487	44	0
2	D	1610	0	1569	54	0
3	A	4	0	0	0	0
3	B	1	0	0	0	0
3	C	4	0	0	0	0
3	D	1	0	0	0	0
4	A	33	0	0	0	0
4	B	31	0	0	0	0
4	C	31	0	0	0	0
4	D	30	0	0	1	0
All	All	6546	0	6235	158	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 12.

All (158) 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:D:29:VAL:HG13	2:D:92:SER:HB3	1.50	0.92
2:B:186:TYR:HD1	2:B:188:LYS:HD2	1.36	0.88
2:B:129:THR:HG23	2:B:182:SER:HB2	1.57	0.86
1:C:138:LEU:HD13	1:C:211:VAL:HG21	1.57	0.85
2:B:186:TYR:CD1	2:B:188:LYS:HD2	2.11	0.85
1:A:52(A):PRO:HA	1:A:71:ARG:HD2	1.61	0.82
2:B:181:LEU:HD13	2:B:186:TYR:HB2	1.64	0.80
2:D:190:LYS:HG3	2:D:191:VAL:N	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:THR:HG22	1:C:85:ASP:H	1.46	0.79
1:C:197:ASN:ND2	1:C:208:ASP:OD1	2.16	0.79
2:D:148:TRP:O	2:D:154:LEU:HD12	1.82	0.79
2:D:190:LYS:HG3	2:D:191:VAL:H	1.49	0.78
2:D:154:LEU:HD23	2:D:155:GLN:N	1.99	0.77
2:B:29:VAL:HG13	2:B:92:SER:HB2	1.70	0.73
2:D:191:VAL:HG22	2:D:210:ASN:HA	1.70	0.72
2:B:32:GLU:HB3	2:B:91:MET:HB2	1.73	0.71
2:B:186:TYR:CD1	2:B:188:LYS:HB3	2.27	0.70
2:B:33:LEU:HB3	2:B:51:ALA:HB2	1.74	0.70
1:C:184:VAL:HG21	1:C:194:TYR:OH	1.93	0.69
2:B:150:VAL:HG13	2:B:188:LYS:HE2	1.77	0.67
2:D:150:VAL:HG23	2:D:151:ASP:H	1.59	0.67
2:D:151:ASP:HA	2:D:190:LYS:HD3	1.78	0.66
2:D:184:ALA:O	2:D:188:LYS:HG3	1.95	0.66
2:D:123:GLU:HA	2:D:126:LYS:HD2	1.77	0.66
1:C:52(A):PRO:HA	1:C:71:ARG:HD2	1.77	0.65
1:A:155:ASN:HA	1:A:195:ILE:HG13	1.79	0.64
2:D:191:VAL:HG13	2:D:209:PHE:O	1.97	0.64
2:D:128:GLY:HA2	2:D:183:LYS:HD3	1.79	0.63
1:A:152:VAL:HG22	1:A:198:VAL:HG22	1.81	0.62
1:C:11:VAL:HG21	1:C:147:PRO:HG3	1.79	0.62
2:B:186:TYR:CE1	2:B:188:LYS:HB3	2.34	0.62
2:D:150:VAL:O	2:D:190:LYS:HG2	2.00	0.61
2:D:105:GLU:OE1	2:D:173:TYR:OH	2.15	0.61
1:A:155:ASN:HA	1:A:195:ILE:CG1	2.30	0.61
2:B:6:GLN:HE22	2:B:87:PHE:HA	1.66	0.61
2:D:190:LYS:HE3	2:D:191:VAL:O	2.01	0.61
2:D:148:TRP:HB2	2:D:154:LEU:HD11	1.81	0.60
2:D:186:TYR:O	2:D:192:TYR:OH	2.09	0.60
1:C:159:LEU:HD21	1:C:182:VAL:HG11	1.84	0.60
1:A:209:LYS:HZ1	1:A:211:VAL:HG13	1.67	0.59
2:B:103:LYS:HE2	2:B:105:GLU:HG2	1.84	0.59
2:B:189:HIS:O	2:B:189:HIS:ND1	2.36	0.59
1:A:2:GLU:HG2	1:A:27:TYR:HB3	1.85	0.58
1:A:155:ASN:HA	1:A:195:ILE:HB	1.86	0.58
1:C:71:ARG:HH21	1:C:71:ARG:HG2	1.69	0.57
2:D:123:GLU:N	2:D:123:GLU:OE1	2.35	0.56
2:B:108:ARG:NH1	2:B:109:THR:O	2.38	0.56
1:A:195:ILE:HD13	1:A:210:LYS:NZ	2.21	0.56
2:B:66:GLY:HA3	2:B:71:PHE:CD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:149:LYS:NZ	2:D:152:ASN:O	2.25	0.56
2:D:148:TRP:C	2:D:154:LEU:HD12	2.25	0.56
1:A:197:ASN:ND2	1:A:208:ASP:OD1	2.38	0.55
1:A:155:ASN:HB3	1:A:158:ALA:HB3	1.88	0.55
1:C:1:GLN:O	1:C:26:GLY:HA3	2.07	0.54
2:D:11:LEU:HD22	2:D:21:ILE:HD11	1.89	0.54
2:B:150:VAL:HG12	2:B:191:VAL:O	2.06	0.54
2:B:50:TYR:O	2:B:52:SER:N	2.39	0.54
2:D:145:LYS:HB3	2:D:197:THR:OG1	2.08	0.54
2:D:190:LYS:CG	2:D:191:VAL:N	2.71	0.53
1:A:96:LYS:HE3	2:B:55:GLN:HE21	1.74	0.53
2:D:29:VAL:HG12	2:D:32:GLU:H	1.74	0.52
2:B:55:GLN:HG2	2:B:56:SER:N	2.25	0.52
1:A:151:THR:O	1:A:198:VAL:HA	2.10	0.52
1:A:147:PRO:O	1:A:200:HIS:NE2	2.31	0.52
1:C:1:GLN:HG3	1:C:1:GLN:O	2.07	0.52
2:B:134:CYS:HB2	2:B:148:TRP:CZ2	2.44	0.52
2:D:22:THR:HG22	2:D:72:THR:HG22	1.92	0.52
1:C:71:ARG:HG2	1:C:71:ARG:NH2	2.25	0.52
2:B:29:VAL:HG12	2:B:32:GLU:H	1.75	0.51
2:D:154:LEU:HD23	2:D:155:GLN:H	1.75	0.51
1:A:155:ASN:HA	1:A:195:ILE:CB	2.40	0.51
1:A:71:ARG:HG2	1:A:71:ARG:HH21	1.76	0.51
1:C:163:VAL:HG22	1:C:182:VAL:HG22	1.92	0.51
2:D:8:PRO:HD2	2:D:21:ILE:HD12	1.93	0.51
1:A:141:LEU:HD21	1:A:143:LYS:HD2	1.93	0.50
2:B:108:ARG:HD2	2:B:171:SER:O	2.12	0.50
2:B:46:LEU:HD23	2:B:47:LEU:N	2.26	0.50
2:D:136:LEU:HB2	2:D:175:LEU:HB3	1.93	0.50
2:B:6:GLN:HE22	2:B:87:PHE:CA	2.24	0.50
1:A:126:PRO:HG3	1:A:138:LEU:HG	1.94	0.50
2:D:50:TYR:O	2:D:52:SER:N	2.43	0.49
2:D:63:SER:HB3	4:D:404:HOH:O	2.13	0.49
2:B:150:VAL:CG2	2:B:188:LYS:HG3	2.42	0.49
1:C:47:TRP:CH2	1:C:49:GLY:HA2	2.47	0.49
2:B:189:HIS:O	2:B:189:HIS:CG	2.65	0.49
2:D:85:THR:OG1	2:D:103:LYS:HD3	2.13	0.49
2:D:108:ARG:HD2	2:D:171:SER:HB2	1.94	0.49
1:A:128:SER:O	1:A:128:SER:OG	2.21	0.49
2:D:203:SER:OG	2:D:204:PRO:HD2	2.13	0.48
1:C:50:TRP:HZ2	2:D:94:TYR:HH	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100(B):ALA:O	2:B:91:MET:HG3	2.13	0.48
1:A:156:SER:N	1:A:195:ILE:HG21	2.29	0.48
1:C:169:VAL:HG22	1:C:177:SER:O	2.14	0.48
2:D:136:LEU:HD13	2:D:175:LEU:HD22	1.96	0.48
2:D:197:THR:HG22	2:D:204:PRO:HG3	1.96	0.48
2:D:193:ALA:HB2	2:D:208:SER:HB2	1.97	0.47
1:A:148:GLU:HG2	1:A:149:PRO:HA	1.97	0.47
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.96	0.47
2:D:150:VAL:HG21	2:D:155:GLN:OE1	2.15	0.47
2:D:167:ASP:HB3	2:D:170:ASP:OD1	2.15	0.47
1:A:168:ALA:HA	1:A:178:LEU:HB3	1.97	0.47
2:D:4:LEU:HD13	2:D:88:CYS:SG	2.55	0.46
2:B:6:GLN:NE2	2:B:86:TYR:O	2.49	0.46
1:A:119:PRO:HB3	1:A:145:TYR:HB3	1.95	0.46
2:D:148:TRP:HB2	2:D:154:LEU:CD1	2.46	0.46
1:A:47:TRP:CH2	1:A:49:GLY:HA2	2.50	0.46
1:A:83:THR:HG22	1:A:86:ASP:OD2	2.15	0.46
1:A:83:THR:HG23	1:A:85:ASP:HB2	1.98	0.46
1:A:10:GLU:HG2	1:A:18:VAL:HG23	1.97	0.46
1:A:200:HIS:CE1	1:A:202:PRO:HB2	2.51	0.46
2:B:147:GLN:O	2:B:194:CYS:HA	2.16	0.46
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.98	0.46
1:A:98:TYR:HB2	1:A:100(C):VAL:HG21	1.98	0.45
2:B:186:TYR:C	2:B:188:LYS:N	2.70	0.45
2:D:55:GLN:HG2	2:D:56:SER:N	2.31	0.45
2:D:66:GLY:HA3	2:D:71:PHE:CD1	2.52	0.45
1:C:47:TRP:CZ2	1:C:49:GLY:HA2	2.51	0.45
2:B:190:LYS:NZ	2:B:210:ASN:O	2.32	0.45
2:B:209:PHE:CD2	2:B:210:ASN:N	2.85	0.45
2:B:208:SER:OG	2:B:209:PHE:N	2.51	0.44
2:D:6:GLN:NE2	2:D:86:TYR:O	2.51	0.44
2:B:150:VAL:HG21	2:B:188:LYS:HG3	2.00	0.44
1:A:196:CYS:O	1:A:208:ASP:HA	2.17	0.43
2:B:190:LYS:HA	2:B:190:LYS:HD2	1.57	0.43
1:C:98:TYR:HB2	1:C:100(C):VAL:HG21	1.99	0.43
2:D:108:ARG:NE	2:D:170:ASP:O	2.51	0.43
1:A:195:ILE:HD13	1:A:210:LYS:CE	2.49	0.43
2:D:201:LEU:HD22	2:D:205:VAL:HG23	2.00	0.43
1:A:155:ASN:CB	1:A:158:ALA:HB3	2.49	0.43
1:A:141:LEU:HD23	1:A:143:LYS:HB2	2.00	0.43
1:A:125:ALA:HA	1:A:126:PRO:HD3	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:PRO:HB3	2:D:139:PHE:HB3	2.00	0.43
2:D:118:PHE:HA	2:D:119:PRO:HD3	1.86	0.43
2:D:147:GLN:HB2	2:D:195:GLU:HG2	2.01	0.42
1:A:156:SER:H	1:A:195:ILE:HG21	1.83	0.42
2:B:184:ALA:O	2:B:185:ASP:C	2.55	0.42
2:B:140:TYR:CG	2:B:141:PRO:HA	2.54	0.42
1:C:184:VAL:HG22	1:C:185:PRO:HD2	2.00	0.42
1:A:154:TRP:CE3	1:A:195:ILE:O	2.73	0.42
2:D:158:ASN:OD1	2:D:158:ASN:N	2.45	0.42
1:C:97:TYR:HA	1:C:100(A):GLU:O	2.20	0.42
1:A:128:SER:HA	1:A:129:LYS:HA	1.89	0.42
2:B:20:THR:O	2:B:21:ILE:HD13	2.19	0.41
2:B:61:ARG:NE	2:B:82:ASP:OD2	2.47	0.41
2:B:203:SER:HB3	2:B:204:PRO:HD2	2.03	0.41
2:D:108:ARG:HD2	2:D:171:SER:O	2.20	0.41
2:D:27:GLN:HG2	2:D:28:GLY:N	2.36	0.41
1:A:212:GLU:HG2	1:A:213:PRO:HD3	2.03	0.41
1:C:30:THR:HB	1:C:53:HIS:HB2	2.03	0.41
2:D:107:LYS:HA	2:D:140:TYR:OH	2.21	0.41
1:A:155:ASN:H	1:A:195:ILE:HB	1.86	0.41
1:C:34:LEU:HA	1:C:34:LEU:HD23	1.91	0.41
1:A:141:LEU:CD2	1:A:143:LYS:HB2	2.51	0.40
2:D:150:VAL:HG23	2:D:151:ASP:N	2.30	0.40
2:B:134:CYS:HB2	2:B:148:TRP:CH2	2.57	0.40
1:C:192:GLN:OE1	1:C:193:THR:N	2.54	0.40
1:A:147:PRO:HD2	1:A:202:PRO:CB	2.51	0.40
2:B:185:ASP:O	2:B:186:TYR:C	2.60	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	213/222 (96%)	204 (96%)	9 (4%)	0	100 100
1	C	212/222 (96%)	203 (96%)	9 (4%)	0	100 100
2	B	199/210 (95%)	188 (94%)	7 (4%)	4 (2%)	9 21
2	D	208/210 (99%)	197 (95%)	9 (4%)	2 (1%)	19 41
All	All	832/864 (96%)	792 (95%)	34 (4%)	6 (1%)	26 51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	ALA
2	D	51	ALA
2	B	31	ASN
2	D	190	LYS
2	B	149	LYS
2	B	184	ALA

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	182/186 (98%)	175 (96%)	7 (4%)	40 68
1	C	181/186 (97%)	175 (97%)	6 (3%)	45 73
2	B	171/183 (93%)	166 (97%)	5 (3%)	50 77
2	D	183/183 (100%)	177 (97%)	6 (3%)	45 73
All	All	717/738 (97%)	693 (97%)	24 (3%)	45 73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	TRP
1	A	97	TYR
1	A	128	SER
1	A	138	LEU
1	A	179	SER

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Mol	Chain	Res	Type
1	A	193	THR
1	A	199	ASN
2	B	2	ILE
2	B	14	SER
2	B	63	SER
2	B	158	ASN
2	B	188	LYS
1	C	50	TRP
1	C	59	THR
1	C	84	SER
1	C	97	TYR
1	C	186	SER
1	C	187	SER
2	D	14	SER
2	D	63	SER
2	D	91	MET
2	D	155	GLN
2	D	158	ASN
2	D	159	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	155	ASN
2	B	6	GLN
2	B	38	GLN
2	B	55	GLN
2	B	138	ASN
1	C	199	ASN
2	D	147	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 10 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, 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	A	217/222 (97%)	0.08	18 (8%) 14 11	40, 73, 167, 214	0
1	C	216/222 (97%)	-0.23	1 (0%) 91 92	39, 69, 109, 134	0
2	B	203/210 (96%)	-0.01	7 (3%) 49 47	40, 71, 166, 229	0
2	D	210/210 (100%)	-0.11	4 (1%) 70 69	41, 79, 152, 210	0
All	All	846/864 (97%)	-0.07	30 (3%) 48 46	39, 74, 156, 229	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	157	GLY	7.8
1	A	129	LYS	4.6
1	A	137	ALA	4.5
1	A	138	LEU	4.3
1	A	158	ALA	4.1
1	A	182	VAL	4.1
1	A	139	GLY	3.9
1	A	211	VAL	3.5
1	A	189	LEU	3.5
1	A	154	TRP	3.5
2	B	195	GLU	3.4
2	D	192	TYR	3.4
2	B	192	TYR	3.4
1	A	121	VAL	3.4
1	A	193	THR	3.3
1	A	122	PHE	3.1
2	D	153	ALA	3.0
1	A	160	THR	3.0
2	B	146	VAL	2.9
2	B	209	PHE	2.9
1	A	126	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	183	LYS	2.7
2	B	188	LYS	2.6
1	A	210	LYS	2.5
1	A	207	VAL	2.4
2	D	155	GLN	2.3
1	C	1	GLN	2.2
1	A	159	LEU	2.1
2	D	209	PHE	2.1
1	A	123	PRO	2.1

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)

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, 95^{th} 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(Å^2)	Q<0.9
3	ZN	A	303	1/1	0.98	0.18	1.23	51,51,51,51	0
3	ZN	C	303	1/1	0.99	0.14	0.23	49,49,49,49	0
3	ZN	C	304	1/1	0.97	0.16	-0.03	103,103,103,103	0
3	ZN	A	304	1/1	0.97	0.14	-0.13	109,109,109,109	0
3	ZN	A	301	1/1	0.92	0.12	-0.81	118,118,118,118	0
3	ZN	C	301	1/1	0.87	0.09	-2.64	113,113,113,113	0
3	ZN	B	301	1/1	1.00	0.22	-	94,94,94,94	0
3	ZN	C	302	1/1	0.99	0.16	-	72,72,72,72	0
3	ZN	A	302	1/1	0.99	0.24	-	81,81,81,81	0
3	ZN	D	301	1/1	0.99	0.23	-	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.