



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:32 am BST

PDB ID : 5VIG
Title : Crystal structure of anti-Zika antibody Z006 bound to Zika virus envelope protein DIII
Authors : Keeffe, J.R.; West Jr., A.P.; Gristick, H.B.; Bjorkman, P.J.
Deposited on : 2017-04-16
Resolution : 3.00 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
Mogul : 1.8.5 (274361), CSD as541be (2020)
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

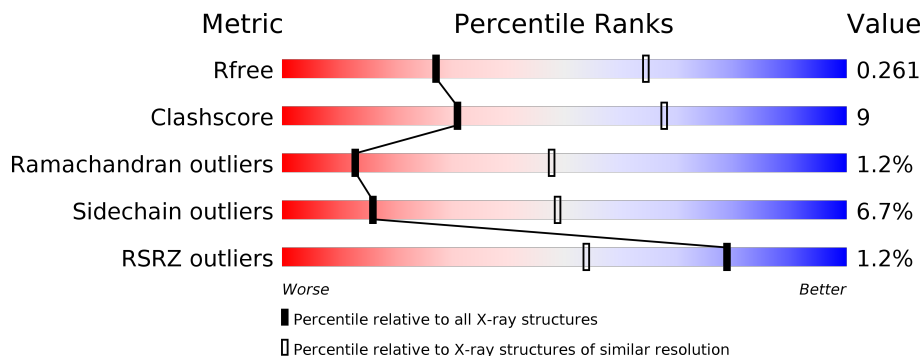
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 $\leq 5\%$. 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	232	
1	H	232	
2	B	213	
2	L	213	
3	G	110	
3	Z	110	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7905 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 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	H	213	1596	1009	273	308	6	0	0	0
1	A	213	1596	1009	273	308	6	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	220	HIS	-	expression tag	UNP S6B291
H	221	HIS	-	expression tag	UNP S6B291
H	222	HIS	-	expression tag	UNP S6B291
H	223	HIS	-	expression tag	UNP S6B291
H	224	HIS	-	expression tag	UNP S6B291
H	225	HIS	-	expression tag	UNP S6B291
A	220	HIS	-	expression tag	UNP S6B291
A	221	HIS	-	expression tag	UNP S6B291
A	222	HIS	-	expression tag	UNP S6B291
A	223	HIS	-	expression tag	UNP S6B291
A	224	HIS	-	expression tag	UNP S6B291
A	225	HIS	-	expression tag	UNP S6B291

- Molecule 2 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	212	1591	997	263	325	6	0	0	0
2	B	212	1591	997	263	325	6	0	0	0

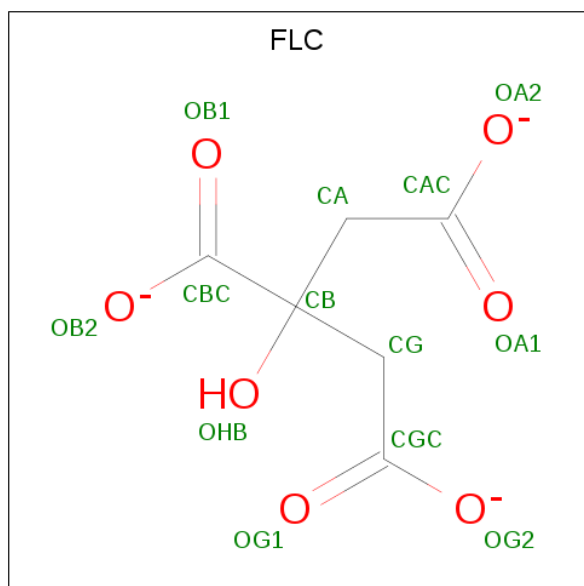
- Molecule 3 is a protein called Zika virus envelope protein DIII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	Z	100	759	482	125	146	6	0	0	0
3	G	100	759	482	125	146	6	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	298	MET	-	initiating methionine	UNP A0A1I9ZK43
G	298	MET	-	initiating methionine	UNP A0A1I9ZK43

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7^-$).

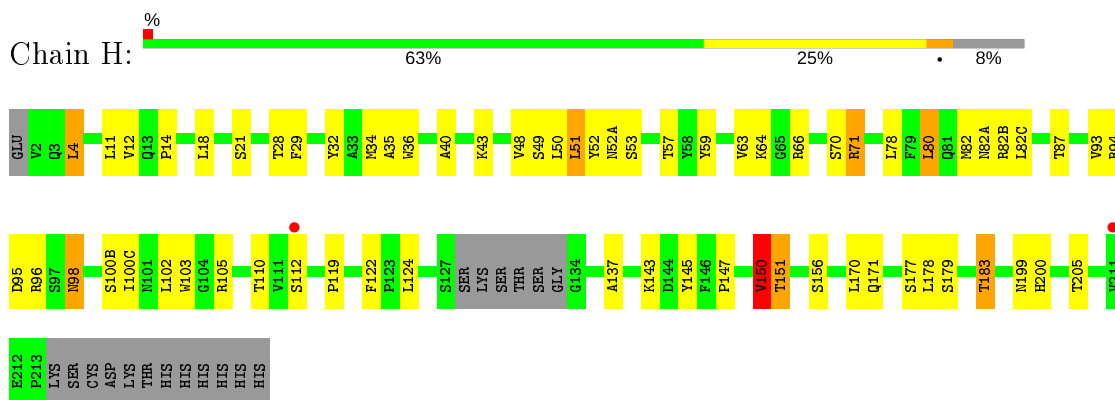


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	13	6	7	0	0

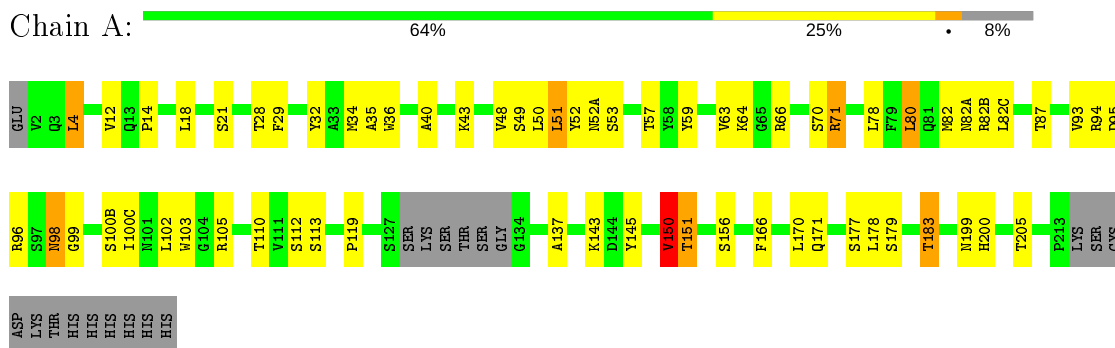
3 Residue-property plots [i](#)

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.

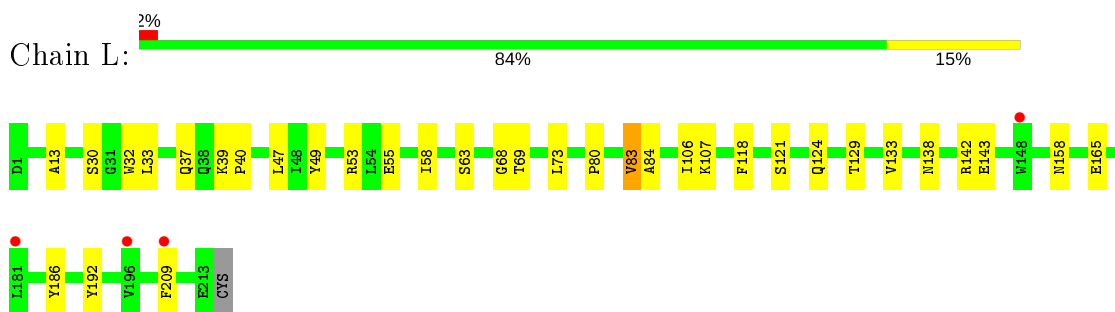
- Molecule 1: Fab heavy chain



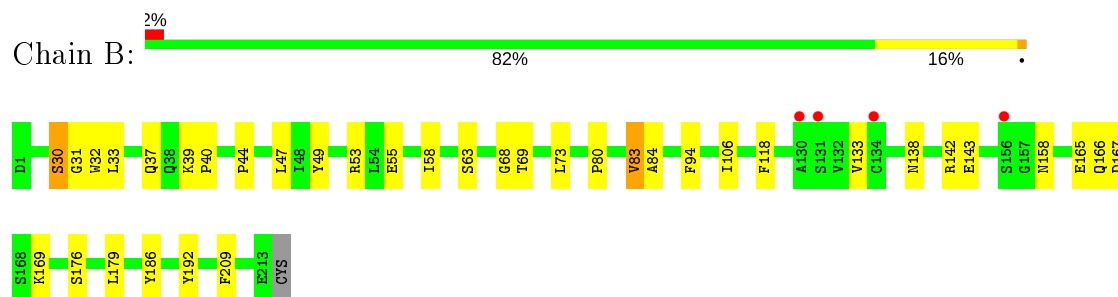
- Molecule 1: Fab heavy chain



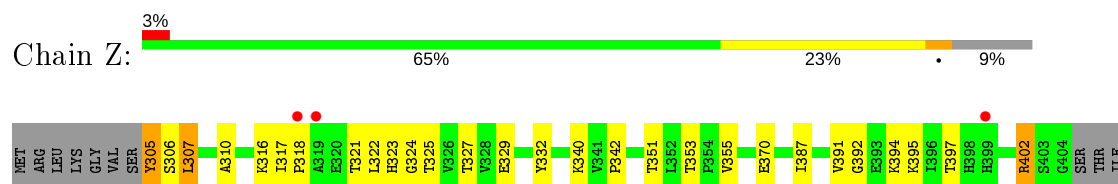
- Molecule 2: Fab light chain



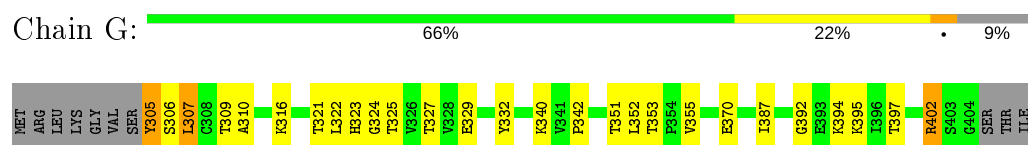
- Molecule 2: Fab light chain



- Molecule 3: Zika virus envelope protein DIII



- Molecule 3: Zika virus envelope protein DIII



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	385.08Å 385.08Å 56.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.75 – 3.00 96.27 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.75-3.00) 98.9 (96.27-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.212 , 0.257 0.216 , 0.261	Depositor DCC
R_{free} test set	1734 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	76.2	Xtrriage
Anisotropy	0.245	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 69.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7905	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: FLC

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	0.40	0/1633	0.57	0/2227
1	H	0.40	0/1633	0.57	0/2227
2	B	0.35	0/1627	0.53	0/2221
2	L	0.35	0/1627	0.53	0/2221
3	G	0.39	0/777	0.57	0/1060
3	Z	0.39	0/777	0.57	0/1060
All	All	0.38	0/8074	0.55	0/11016

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 [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	1596	0	1553	41	0
1	H	1596	0	1553	39	0
2	B	1591	0	1492	24	0
2	L	1591	0	1492	21	0
3	G	759	0	751	16	0
3	Z	759	0	751	14	0
4	A	13	0	5	0	0
All	All	7905	0	7597	141	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 9.

All (141) 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:51:LEU:HD21	1:A:71:ARG:HB2	1.69	0.75
2:L:83:VAL:HG22	2:L:106:ILE:HG13	1.70	0.73
1:H:51:LEU:HD21	1:H:71:ARG:HB2	1.69	0.72
1:A:98:ASN:HB3	3:G:392:GLY:H	1.57	0.69
1:H:32:TYR:CD2	1:H:94:ARG:HD3	2.29	0.68
1:H:87:THR:HG23	1:H:110:THR:HA	1.76	0.68
1:A:32:TYR:CD2	1:A:94:ARG:HD3	2.29	0.67
1:H:98:ASN:HB3	3:Z:392:GLY:H	1.59	0.67
1:A:87:THR:HG23	1:A:110:THR:HA	1.76	0.67
1:A:98:ASN:O	1:A:98:ASN:ND2	2.27	0.67
1:H:98:ASN:O	1:H:98:ASN:ND2	2.27	0.66
2:L:32:TRP:CE2	3:Z:394:LYS:HG2	2.36	0.61
2:L:118:PHE:HB2	2:L:133:VAL:HG23	1.82	0.61
1:H:40:ALA:HB3	1:H:43:LYS:HB2	1.84	0.60
1:A:112:SER:OG	1:A:113:SER:N	2.34	0.60
2:B:118:PHE:HB2	2:B:133:VAL:HG23	1.82	0.60
2:L:80:PRO:HA	2:L:106:ILE:HD12	1.84	0.59
1:A:40:ALA:HB3	1:A:43:LYS:HB2	1.84	0.59
2:B:186:TYR:O	2:B:192:TYR:OH	2.21	0.59
2:L:186:TYR:O	2:L:192:TYR:OH	2.21	0.58
3:Z:321:THR:OG1	3:Z:325:THR:OG1	2.22	0.57
2:B:47:LEU:HD23	2:B:58:ILE:HD12	1.87	0.57
2:L:13:ALA:O	2:L:107:LYS:N	2.31	0.57
1:A:96:ARG:NH2	2:B:55:GLU:OE1	2.37	0.57
3:G:321:THR:HG1	3:G:325:THR:HG1	1.51	0.57
1:A:93:VAL:HG13	1:A:100(C):ILE:HG23	1.87	0.56
1:A:12:VAL:HG11	1:A:82(C):LEU:HD12	1.86	0.56
1:H:119:PRO:HD2	1:H:205:THR:HG21	1.88	0.56
1:A:119:PRO:HD2	1:A:205:THR:HG21	1.87	0.56
1:H:12:VAL:HG11	1:H:82(C):LEU:HD12	1.86	0.56
2:L:47:LEU:HD23	2:L:58:ILE:HD12	1.87	0.56
1:H:93:VAL:HG13	1:H:100(C):ILE:HG23	1.87	0.56
1:H:11:LEU:HD12	1:H:147:PRO:HG3	1.88	0.55
1:A:98:ASN:OD1	3:G:352:LEU:HD12	2.07	0.55
2:B:83:VAL:HG22	2:B:106:ILE:HG13	1.89	0.55
1:A:59:TYR:O	1:A:64:LYS:NZ	2.36	0.54
1:H:59:TYR:O	1:H:64:LYS:NZ	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:307:LEU:HG	3:Z:342:PRO:HG3	1.90	0.54
3:G:307:LEU:HG	3:G:342:PRO:HG3	1.90	0.54
3:G:307:LEU:HD12	3:G:340:LYS:HB3	1.89	0.53
3:Z:307:LEU:HD12	3:Z:340:LYS:HB3	1.89	0.53
2:B:80:PRO:HA	2:B:106:ILE:HD12	1.90	0.53
2:B:32:TRP:CE2	3:G:394:LYS:HG2	2.44	0.53
1:H:96:ARG:NH2	2:L:55:GLU:OE1	2.41	0.52
3:Z:323:HIS:O	3:Z:402:ARG:NH1	2.43	0.52
2:B:143:GLU:OE2	2:B:143:GLU:N	2.42	0.52
3:G:323:HIS:O	3:G:402:ARG:NH1	2.43	0.52
1:H:4:LEU:HD22	1:H:102:LEU:HG	1.92	0.52
1:A:151:THR:HG23	1:A:199:ASN:HB3	1.93	0.51
1:A:4:LEU:HD22	1:A:102:LEU:HG	1.91	0.51
1:A:82:MET:HB2	1:A:82(C):LEU:HD21	1.93	0.51
2:L:143:GLU:OE2	2:L:143:GLU:N	2.42	0.51
1:H:151:THR:HG23	1:H:199:ASN:HB3	1.92	0.51
1:A:53:SER:O	1:A:57:THR:HG23	2.12	0.50
3:G:310:ALA:HB3	3:G:332:TYR:CZ	2.47	0.50
1:H:82:MET:HB2	1:H:82(C):LEU:HD21	1.93	0.50
1:H:143:LYS:NZ	1:H:171:GLN:OE1	2.45	0.50
3:Z:310:ALA:HB3	3:Z:332:TYR:CZ	2.47	0.49
1:H:32:TYR:CG	1:H:94:ARG:HD3	2.47	0.49
1:A:32:TYR:CG	1:A:94:ARG:HD3	2.47	0.49
2:L:49:TYR:O	2:L:53:ARG:HB2	2.12	0.49
1:H:53:SER:O	1:H:57:THR:HG23	2.12	0.49
1:A:143:LYS:NZ	1:A:171:GLN:OE1	2.45	0.48
2:B:49:TYR:O	2:B:53:ARG:HB2	2.12	0.48
1:A:150:VAL:HG12	1:A:200:HIS:HB2	1.95	0.48
2:L:158:ASN:OD1	2:L:158:ASN:N	2.47	0.48
1:H:150:VAL:HG12	1:H:200:HIS:HB2	1.95	0.48
1:H:171:GLN:NE2	1:H:177:SER:HB2	2.28	0.48
2:B:158:ASN:OD1	2:B:158:ASN:N	2.47	0.48
1:H:122:PHE:HB3	2:L:121:SER:OG	2.14	0.47
1:A:171:GLN:NE2	1:A:177:SER:HB2	2.28	0.47
1:H:137:ALA:HB2	1:H:183:THR:HG22	1.97	0.47
1:H:66:ARG:NH1	1:H:82(B):ARG:O	2.47	0.47
2:L:39:LYS:HG2	2:L:84:ALA:HB2	1.97	0.47
1:A:66:ARG:NH1	1:A:82(B):ARG:O	2.47	0.47
1:H:94:ARG:HD2	1:H:95:ASP:O	2.15	0.47
1:A:94:ARG:HD2	1:A:95:ASP:O	2.15	0.46
1:A:48:VAL:HG12	1:A:63:VAL:HG21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:HG2	1:A:82(B):ARG:HB2	1.98	0.46
1:A:99:GLY:O	3:G:392:GLY:HA3	2.15	0.46
2:B:192:TYR:HB2	2:B:209:PHE:CE2	2.51	0.46
2:B:39:LYS:HG2	2:B:84:ALA:HB2	1.97	0.46
1:H:36:TRP:CG	1:H:80:LEU:HD12	2.50	0.46
1:A:36:TRP:CG	1:A:80:LEU:HD12	2.50	0.46
2:L:192:TYR:HB2	2:L:209:PHE:CE2	2.51	0.46
1:A:166:PHE:CE2	2:B:176:SER:HB2	2.51	0.46
1:H:66:ARG:HG2	1:H:82(B):ARG:HB2	1.98	0.46
2:L:40:PRO:HG2	2:L:165:GLU:HG2	1.98	0.46
1:A:137:ALA:HB2	1:A:183:THR:HG22	1.97	0.45
1:H:48:VAL:HG12	1:H:63:VAL:HG21	1.98	0.45
2:B:40:PRO:HG2	2:B:165:GLU:HG2	1.99	0.44
2:B:83:VAL:HG11	2:B:166:GLN:HB3	1.98	0.44
1:H:14:PRO:HD3	1:H:112:SER:O	2.18	0.44
3:Z:387:ILE:O	3:Z:397:THR:HA	2.18	0.44
3:G:387:ILE:O	3:G:397:THR:HA	2.18	0.44
1:A:98:ASN:H	3:G:392:GLY:HA2	1.83	0.44
1:A:150:VAL:HG23	1:A:178:LEU:HD21	2.00	0.43
1:A:14:PRO:HD3	1:A:112:SER:O	2.18	0.43
1:H:51:LEU:HB2	1:H:57:THR:HG22	2.01	0.43
1:A:29:PHE:O	1:A:71:ARG:NH1	2.50	0.43
1:H:124:LEU:HB3	2:L:118:PHE:CD1	2.53	0.43
1:H:150:VAL:HG23	1:H:178:LEU:HD21	2.00	0.43
2:B:80:PRO:O	2:B:83:VAL:HG23	2.19	0.43
1:A:51:LEU:HD13	1:A:57:THR:HG22	2.01	0.42
1:A:52:TYR:CE2	1:A:52(A):ASN:ND2	2.87	0.42
1:H:51:LEU:HD13	1:H:57:THR:HG22	2.02	0.42
2:L:80:PRO:O	2:L:83:VAL:HG23	2.19	0.42
1:H:52:TYR:CE2	1:H:52(A):ASN:ND2	2.87	0.42
2:L:37:GLN:HB2	2:L:47:LEU:HD11	2.01	0.42
3:Z:392:GLY:O	3:Z:395:LYS:HE3	2.19	0.42
1:A:35:ALA:HB2	1:A:50:LEU:HD12	2.02	0.42
1:A:103:TRP:CE3	2:B:44:PRO:HD2	2.55	0.42
2:B:47:LEU:HA	2:B:58:ILE:HG13	2.02	0.42
3:Z:305:TYR:HB2	3:Z:306:SER:H	1.64	0.42
1:A:21:SER:HA	1:A:78:LEU:O	2.20	0.42
2:L:47:LEU:HA	2:L:58:ILE:HG13	2.02	0.42
2:B:37:GLN:HB2	2:B:47:LEU:HD11	2.01	0.42
1:H:29:PHE:O	1:H:71:ARG:NH1	2.50	0.42
1:H:21:SER:HA	1:H:78:LEU:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LEU:HB2	1:A:57:THR:HG22	2.01	0.41
2:B:63:SER:O	2:B:73:LEU:HD12	2.21	0.41
2:L:63:SER:O	2:L:73:LEU:HD12	2.21	0.41
3:G:316:LYS:HG2	3:G:329:GLU:HB3	2.03	0.41
3:G:392:GLY:O	3:G:395:LYS:HE3	2.19	0.41
2:B:94:PHE:CE1	3:G:309:THR:HG21	2.56	0.41
1:H:35:ALA:HB2	1:H:50:LEU:HD12	2.02	0.41
2:B:179:LEU:HA	2:B:179:LEU:HD12	1.90	0.41
3:Z:317:ILE:HG13	3:Z:318:PRO:HD2	2.03	0.41
1:A:34:MET:HB3	1:A:78:LEU:HD22	2.02	0.41
3:Z:342:PRO:HG2	3:Z:391:VAL:HG13	2.03	0.41
3:Z:324:GLY:HA3	3:Z:402:ARG:HH11	1.85	0.41
2:B:167:ASP:OD1	2:B:169:LYS:N	2.34	0.41
3:G:324:GLY:HA3	3:G:402:ARG:HH11	1.85	0.41
2:B:30:SER:HB2	2:B:31:GLY:H	1.59	0.40
1:H:119:PRO:HB3	1:H:145:TYR:HB3	2.02	0.40
1:H:34:MET:HB3	1:H:78:LEU:HD22	2.02	0.40
3:Z:316:LYS:HG2	3:Z:329:GLU:HB3	2.03	0.40
1:A:119:PRO:HB3	1:A:145:TYR:HB3	2.02	0.40
2:L:124:GLN:HG2	2:L:129:THR:O	2.21	0.40
3:G:305:TYR:HB2	3:G:306:SER:H	1.64	0.40
1:H:100(C):ILE:HG22	1:H:103:TRP:NE1	2.36	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	209/232 (90%)	194 (93%)	13 (6%)	2 (1%)	15 53
1	H	209/232 (90%)	194 (93%)	13 (6%)	2 (1%)	15 53
2	B	210/213 (99%)	191 (91%)	16 (8%)	3 (1%)	11 43

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	210/213 (99%)	192 (91%)	15 (7%)	3 (1%)	11	43
3	G	98/110 (89%)	85 (87%)	12 (12%)	1 (1%)	15	53
3	Z	98/110 (89%)	85 (87%)	12 (12%)	1 (1%)	15	53
All	All	1034/1110 (93%)	941 (91%)	81 (8%)	12 (1%)	13	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	28	THR
3	Z	322	LEU
1	A	28	THR
3	G	322	LEU
2	L	138	ASN
2	B	138	ASN
2	L	68	GLY
2	B	68	GLY
1	H	150	VAL
1	A	150	VAL
2	L	83	VAL
2	B	83	VAL

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	177/199 (89%)	160 (90%)	17 (10%)	8	32
1	H	177/199 (89%)	160 (90%)	17 (10%)	8	32
2	B	174/187 (93%)	170 (98%)	4 (2%)	50	80
2	L	174/187 (93%)	170 (98%)	4 (2%)	50	80
3	G	85/94 (90%)	77 (91%)	8 (9%)	8	32
3	Z	85/94 (90%)	77 (91%)	8 (9%)	8	32
All	All	872/960 (91%)	814 (93%)	58 (7%)	16	49

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	4	LEU
1	H	18	LEU
1	H	49	SER
1	H	51	LEU
1	H	70	SER
1	H	71	ARG
1	H	80	LEU
1	H	82(A)	ASN
1	H	98	ASN
1	H	100(B)	SER
1	H	105	ARG
1	H	150	VAL
1	H	151	THR
1	H	156	SER
1	H	170	LEU
1	H	179	SER
1	H	183	THR
2	L	30	SER
2	L	33	LEU
2	L	69	THR
2	L	142	ARG
3	Z	305	TYR
3	Z	307	LEU
3	Z	327	THR
3	Z	351	THR
3	Z	353	THR
3	Z	355	VAL
3	Z	370	GLU
3	Z	402	ARG
1	A	4	LEU
1	A	18	LEU
1	A	49	SER
1	A	51	LEU
1	A	70	SER
1	A	71	ARG
1	A	80	LEU
1	A	82(A)	ASN
1	A	98	ASN
1	A	100(B)	SER
1	A	105	ARG
1	A	150	VAL
1	A	151	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	156	SER
1	A	170	LEU
1	A	179	SER
1	A	183	THR
2	B	30	SER
2	B	33	LEU
2	B	69	THR
2	B	142	ARG
3	G	305	TYR
3	G	307	LEU
3	G	327	THR
3	G	351	THR
3	G	353	THR
3	G	355	VAL
3	G	370	GLU
3	G	402	ARG

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	FLC	A	500	-	3,12,12	1.13	0	3,17,17	1.89	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FLC	A	500	-	-	1/6/16/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	500	FLC	CB-CA-CAC	-3.19	109.88	114.98

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	500	FLC	CBC-CB-CG-CGC

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 [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	213/232 (91%)	-0.12	0 100 100	68, 90, 128, 174	0
1	H	213/232 (91%)	-0.03	2 (0%) 84 63	67, 101, 162, 219	0
2	B	212/213 (99%)	0.02	4 (1%) 66 37	70, 94, 179, 204	0
2	L	212/213 (99%)	-0.05	4 (1%) 66 37	68, 100, 175, 228	0
3	G	100/110 (90%)	0.09	0 100 100	78, 93, 146, 170	0
3	Z	100/110 (90%)	0.23	3 (3%) 50 22	79, 101, 137, 168	0
All	All	1050/1110 (94%)	-0.01	13 (1%) 79 54	67, 96, 166, 228	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	148	TRP	2.9
2	L	209	PHE	2.9
2	B	131	SER	2.6
2	B	156	SER	2.5
1	H	211	VAL	2.5
2	L	196	VAL	2.3
2	B	130	ALA	2.2
2	L	181	LEU	2.2
3	Z	399	HIS	2.2
1	H	112	SER	2.1
3	Z	319	ALA	2.1
3	Z	318	PRO	2.1
2	B	134	CYS	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](#)

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
4	FLC	A	500	13/13	0.77	0.40	120,139,147,150	0

6.5 Other polymers [i](#)

There are no such residues in this entry.