Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:21 am BST

PDB ID	:	6DB5
Title	:	Crystal structure of anti-HIV-1 V3 Fab TA6 in complex with a HIV-1 gp120 V3 peptide from NY5 strain
Authors	:	Chan, K.-W.; Kong, X.-P.
Deposited on	:	2018-05-02
Resolution	:	2.60 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:

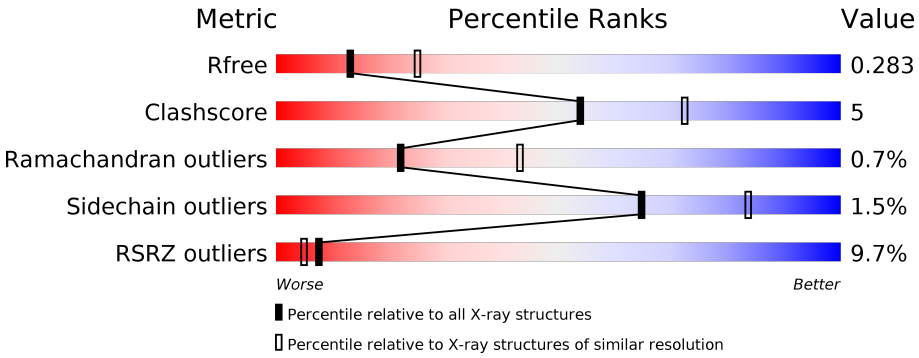
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	H	232	6% 84% 15%
1	I	232	10% 81% 18%
2	L	214	12% 86% 11%
2	M	214	7% 87% 11%
3	P	20	25% 55% 15% 30%
3	Q	20	20% 55% 15% 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7112 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 Human monoclonal anti-HIV-1 gp120 V3 antibody TA6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	228	Total	C	N	O	S	0	0	0
			1710	1074	292	336	8			
1	I	228	Total	C	N	O	S	0	0	0
			1710	1074	292	336	8			

- Molecule 2 is a protein called Human monoclonal anti-HIV-1 gp120 V3 antibody TA6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1591	1001	257	328	5			
2	M	211	Total	C	N	O	S	0	0	0
			1591	1001	257	328	5			

- Molecule 3 is a protein called HIV-1 gp120 V3 peptide from NY5 strain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	14	Total	C	N	O	0	0	0
			101	66	19	16			
3	Q	14	Total	C	N	O	0	0	0
			101	66	19	16			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	75	Total	O	0	0
			75	75		
4	L	81	Total	O	0	0
			81	81		
4	P	6	Total	O	0	0
			6	6		

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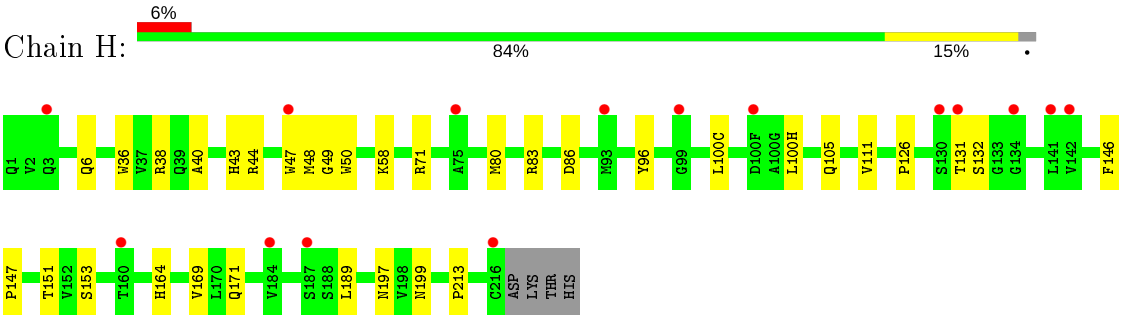
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	I	72	Total O 72 72	0	0
4	M	70	Total O 70 70	0	0
4	Q	4	Total O 4 4	0	0

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.

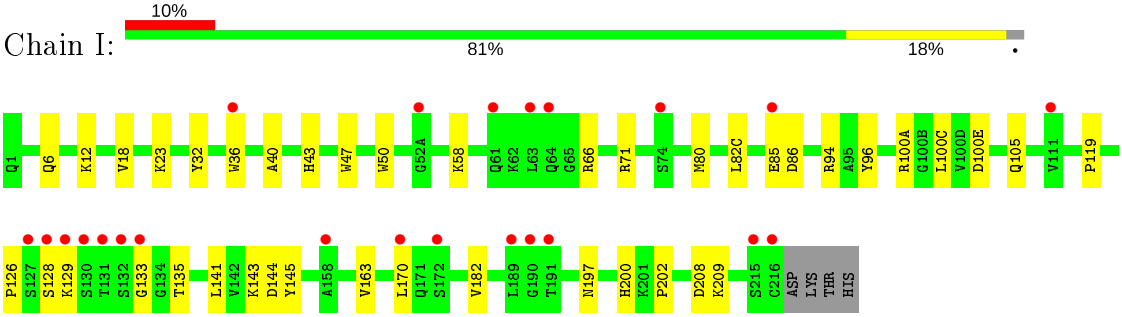
• Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody TA6 Fab heavy chain

Chain H:



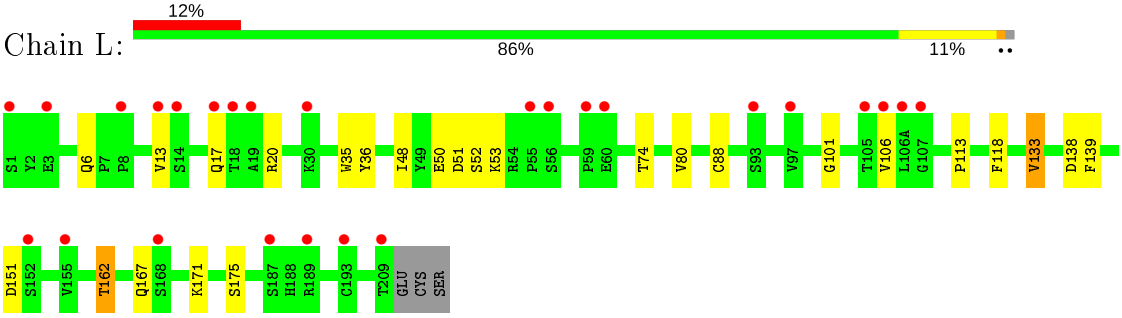
• Molecule 1: Human monoclonal anti-HIV-1 gp120 V3 antibody TA6 Fab heavy chain

Chain I:



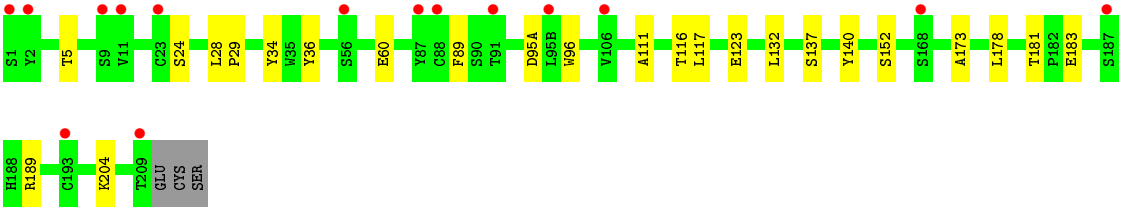
• Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody TA6 Fab light chain

Chain L:

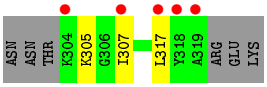


• Molecule 2: Human monoclonal anti-HIV-1 gp120 V3 antibody TA6 Fab light chain

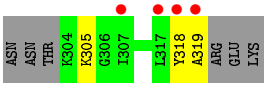
Chain M:



• Molecule 3: HIV-1 gp120 V3 peptide from NY5 strain



• Molecule 3: HIV-1 gp120 V3 peptide from NY5 strain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.62Å 67.36Å 103.04Å 90.00° 100.25° 90.00°	Depositor
Resolution (Å)	29.79 – 2.60 29.79 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.79-2.60) 99.2 (29.79-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.227 , 0.283 0.227 , 0.283	Depositor DCC
R_{free} test set	1998 reflections (6.12%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.771	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7112	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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	H	0.24	0/1750	0.45	0/2382
1	I	0.24	0/1750	0.45	0/2382
2	L	0.24	0/1632	0.43	0/2228
2	M	0.24	0/1632	0.42	0/2228
3	P	0.25	0/102	0.42	0/135
3	Q	0.25	0/102	0.47	0/135
All	All	0.24	0/6968	0.44	0/9490

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	H	1710	0	1681	19	0
1	I	1710	0	1681	25	0
2	L	1591	0	1535	19	0
2	M	1591	0	1535	16	0
3	P	101	0	113	2	0
3	Q	101	0	113	3	0
4	H	75	0	0	2	0
4	I	72	0	0	1	0
4	L	81	0	0	1	0
4	M	70	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	P	6	0	0	0	0
4	Q	4	0	0	1	0
All	All	7112	0	6658	71	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 5.

All (71) 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:I:129:LYS:HE2	2:M:117:LEU:H	1.52	0.75
1:H:153:SER:HB3	1:H:197:ASN:HB2	1.77	0.65
1:H:169:VAL:HG12	2:L:162:THR:HG23	1.80	0.63
3:Q:318:TYR:H	3:Q:319:ALA:HA	1.64	0.63
1:I:40:ALA:HB3	1:I:43:HIS:HB2	1.81	0.63
1:I:58:LYS:HG2	2:M:95(A):ASP:HB3	1.81	0.62
2:L:138:ASP:OD1	2:L:167:GLN:NE2	2.34	0.61
1:I:143:LYS:NZ	4:I:307:HOH:O	2.33	0.59
2:L:80:VAL:HA	2:L:106:VAL:HG21	1.84	0.59
1:I:66:ARG:NH2	1:I:86:ASP:OD2	2.33	0.59
1:I:18:VAL:HG23	1:I:82(C):LEU:HD11	1.87	0.57
3:Q:318:TYR:N	3:Q:319:ALA:HA	2.20	0.56
1:H:40:ALA:HB3	1:H:43:HIS:HB2	1.87	0.56
2:M:132:LEU:HD12	2:M:178:LEU:HD23	1.88	0.55
2:M:5:THR:OG1	2:M:24:SER:OG	2.24	0.55
2:L:6:GLN:OE1	2:L:88:CYS:N	2.40	0.55
1:I:96:TYR:OH	2:M:36:TYR:OH	2.25	0.54
1:H:171:GLN:NE2	4:H:305:HOH:O	2.40	0.53
2:L:118:PHE:HB2	2:L:133:VAL:HG13	1.89	0.53
1:I:119:PRO:HB3	1:I:145:TYR:HB3	1.91	0.52
2:M:34:TYR:HB2	2:M:89:PHE:HB3	1.92	0.52
1:I:197:ASN:ND2	1:I:208:ASP:OD2	2.44	0.51
2:L:20:ARG:NH2	4:L:305:HOH:O	2.42	0.51
1:I:129:LYS:HG2	2:M:116:THR:HG23	1.91	0.51
2:L:167:GLN:HE21	2:L:171:LYS:HB2	1.75	0.50
3:Q:305:LYS:NZ	4:Q:402:HOH:O	2.43	0.50
3:P:307:ILE:HD11	3:P:317:LEU:HD12	1.92	0.50
1:I:32:TYR:OH	1:I:100(E):ASP:OD2	2.17	0.49
1:H:38:ARG:NH2	1:H:86:ASP:OD1	2.44	0.49
1:I:94:ARG:NH2	1:I:100(E):ASP:OD2	2.46	0.48
1:I:129:LYS:HZ1	2:M:204:LYS:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:20:ARG:HG2	2:L:74:THR:HG22	1.97	0.47
1:H:96:TYR:OH	2:L:36:TYR:OH	2.31	0.47
1:H:58:LYS:NZ	2:M:60:GLU:OE2	2.31	0.47
1:H:96:TYR:HH	2:L:36:TYR:HH	1.57	0.47
1:H:44:ARG:HH11	2:L:101:GLY:HA3	1.79	0.47
2:L:35:TRP:HB2	2:L:48:ILE:HB	1.96	0.47
1:H:36:TRP:CE2	1:H:80:MET:HB2	2.50	0.46
1:I:200:HIS:CD2	1:I:202:PRO:HD2	2.50	0.46
1:I:47:TRP:CE2	2:M:96:TRP:HB2	2.51	0.46
1:H:83:ARG:O	1:H:111:VAL:HG11	2.17	0.45
1:H:38:ARG:HD2	1:H:48:MET:HG2	1.99	0.45
1:H:151:THR:HG23	1:H:199:ASN:HB3	1.98	0.45
1:H:126:PRO:HD2	1:H:213:PRO:HA	1.99	0.45
1:I:36:TRP:CE2	1:I:80:MET:HB2	2.53	0.45
2:L:51:ASP:OD2	3:P:305:LYS:NZ	2.38	0.45
2:L:162:THR:HG1	2:L:175:SER:H	1.62	0.44
1:H:44:ARG:NH1	4:H:312:HOH:O	2.50	0.44
1:I:85:GLU:OE2	1:I:85:GLU:N	2.44	0.43
2:L:50:GLU:O	2:L:52:SER:N	2.49	0.43
2:M:28:LEU:N	2:M:29:PRO:HD2	2.34	0.43
2:L:50:GLU:HB2	2:L:53:LYS:HD3	2.01	0.43
2:L:113:PRO:HB3	2:L:139:PHE:HB3	2.01	0.43
1:I:129:LYS:HD2	1:I:129:LYS:HA	1.86	0.42
1:H:126:PRO:HB2	1:H:189:LEU:HD21	2.01	0.42
1:H:47:TRP:CH2	1:H:49:GLY:HA2	2.55	0.42
1:I:23:LYS:HE3	1:I:23:LYS:HB2	1.87	0.42
2:M:181:THR:HG22	2:M:183:GLU:H	1.85	0.42
2:M:111:ALA:HB3	2:M:140:TYR:N	2.34	0.42
1:H:6:GLN:H	1:H:105:GLN:HE22	1.68	0.42
1:I:163:VAL:HG22	1:I:182:VAL:HG12	2.02	0.42
2:M:152:SER:HG	2:M:189:ARG:HH22	1.68	0.42
2:M:137:SER:HA	2:M:173:ALA:HA	2.00	0.42
1:I:133:GLY:HA2	1:I:135:THR:H	1.85	0.42
1:I:6:GLN:H	1:I:105:GLN:HE22	1.68	0.42
1:I:209:LYS:NZ	2:M:123:GLU:OE2	2.51	0.41
1:I:100(A):ARG:HH21	1:I:100(C):LEU:HD11	1.86	0.41
1:H:146:PHE:HA	1:H:147:PRO:HA	1.84	0.41
2:L:13:VAL:HG22	2:L:17:GLN:HB3	2.03	0.41
1:I:12:LYS:HG3	1:I:18:VAL:HG22	2.03	0.41
2:L:167:GLN:HG2	2:L:171:LYS:O	2.21	0.41

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	H	226/232 (97%)	212 (94%)	12 (5%)	2 (1%)	17 35
1	I	226/232 (97%)	211 (93%)	12 (5%)	3 (1%)	12 24
2	L	209/214 (98%)	202 (97%)	6 (3%)	1 (0%)	29 52
2	M	209/214 (98%)	202 (97%)	7 (3%)	0	100 100
3	P	12/20 (60%)	10 (83%)	2 (17%)	0	100 100
3	Q	12/20 (60%)	11 (92%)	1 (8%)	0	100 100
All	All	894/932 (96%)	848 (95%)	40 (4%)	6 (1%)	22 43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	131	THR
1	H	132	SER
1	I	126	PRO
2	L	151	ASP
1	I	128	SER
1	I	144	ASP

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	H	191/195 (98%)	186 (97%)	5 (3%)	46 72
1	I	191/195 (98%)	187 (98%)	4 (2%)	53 77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	179/182 (98%)	177 (99%)	2 (1%)	73 88
2	M	179/182 (98%)	179 (100%)	0	100 100
3	P	9/15 (60%)	9 (100%)	0	100 100
3	Q	9/15 (60%)	9 (100%)	0	100 100
All	All	758/784 (97%)	747 (98%)	11 (2%)	65 83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	50	TRP
1	H	71	ARG
1	H	100(C)	LEU
1	H	100(H)	LEU
1	H	164	HIS
2	L	133	VAL
2	L	162	THR
1	I	50	TRP
1	I	71	ARG
1	I	141	LEU
1	I	170	LEU

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

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	H	228/232 (98%)	0.72	15 (6%) 18 13	24, 36, 49, 81	0
1	I	228/232 (98%)	0.99	23 (10%) 7 4	24, 41, 66, 105	0
2	L	211/214 (98%)	0.93	26 (12%) 4 2	23, 39, 54, 63	0
2	M	211/214 (98%)	0.77	15 (7%) 16 11	24, 39, 52, 63	0
3	P	14/20 (70%)	2.14	5 (35%) 0 0	39, 48, 65, 76	0
3	Q	14/20 (70%)	1.98	4 (28%) 0 0	47, 53, 80, 90	0
All	All	906/932 (97%)	0.89	88 (9%) 7 5	23, 39, 57, 105	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	216	CYS	8.0
3	Q	318	TYR	6.7
3	P	319	ALA	6.6
1	I	127	SER	5.8
2	M	1	SER	5.6
1	I	132	SER	5.6
3	P	318	TYR	5.4
1	H	216	CYS	5.0
1	I	133	GLY	4.9
1	I	215	SER	4.4
1	I	128	SER	4.3
1	I	130	SER	4.2
3	Q	319	ALA	4.1
1	I	189	LEU	3.9
2	M	168	SER	3.9
2	L	106(A)	LEU	3.9
3	P	304	LYS	3.8
2	L	152	SER	3.8
2	L	105	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	I	64	GLN	3.5
1	I	131	THR	3.5
1	I	191	THR	3.5
2	M	56	SER	3.5
2	M	95(B)	LEU	3.4
1	I	61	GLN	3.4
2	L	193	CYS	3.4
2	M	91	THR	3.4
3	Q	307	ILE	3.3
2	M	209	THR	3.3
2	L	19	ALA	3.2
3	Q	317	LEU	3.2
1	H	130	SER	3.2
3	P	307	ILE	3.1
2	M	88	CYS	3.1
2	M	23	CYS	3.0
1	I	158	ALA	2.8
1	H	184	VAL	2.8
1	H	131	THR	2.7
1	H	160	THR	2.7
2	L	93	SER	2.7
2	M	106	VAL	2.7
2	M	193	CYS	2.7
2	L	187	SER	2.6
1	I	170	LEU	2.6
3	P	317	LEU	2.6
1	H	47	TRP	2.6
2	L	17	GLN	2.6
1	I	111	VAL	2.5
1	H	100(F)	ASP	2.5
1	I	190	GLY	2.5
2	L	8	PRO	2.5
2	L	55	PRO	2.5
2	L	18	THR	2.5
2	L	56	SER	2.4
2	L	107	GLY	2.4
2	L	209	THR	2.4
2	L	13	VAL	2.4
2	L	189	ARG	2.4
1	H	99	GLY	2.4
1	I	172	SER	2.4
2	L	30	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	129	LYS	2.4
2	L	59	PRO	2.3
2	L	14	SER	2.3
2	M	87	TYR	2.3
2	L	97	VAL	2.2
2	M	9	SER	2.2
1	I	85	GLU	2.2
2	L	60	GLU	2.2
1	H	3	GLN	2.2
1	H	75	ALA	2.2
2	L	1	SER	2.2
2	M	187	SER	2.2
2	L	155	VAL	2.1
1	H	134	GLY	2.1
1	H	187	SER	2.1
2	M	2	TYR	2.1
1	I	52(A)	GLY	2.1
1	H	141	LEU	2.1
1	I	63	LEU	2.1
1	H	93	MET	2.1
2	L	106	VAL	2.1
1	I	74	SER	2.1
1	H	142	VAL	2.0
2	L	3	GLU	2.0
1	I	36	TRP	2.0
2	L	168	SER	2.0
2	M	11	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 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.