Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 08:09 pm GMT

PDB ID	:	5LDN
Title	:	A viral capsid:antibody complex
Authors	:	James, L.
Deposited on	:	2016-06-27
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:

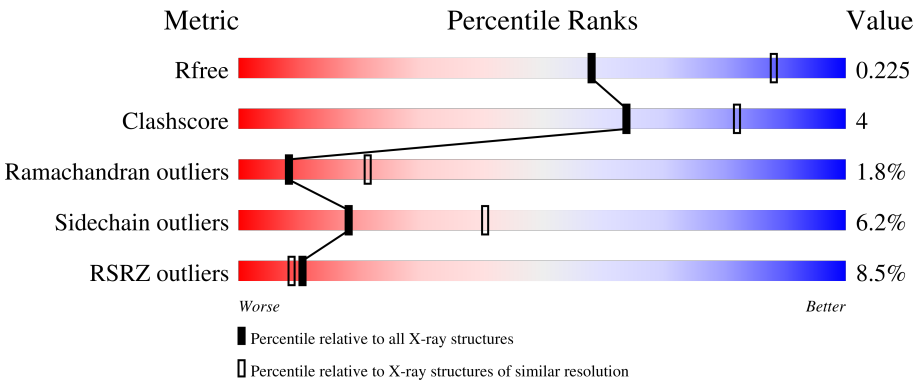
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	927	2% 88% 10% •
2	L	213	23% 81% 16% •
3	H	218	24% 79% 19% ••

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11253 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 Hexon protein,hexon capsid.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	927	7481	4750	1272	1420	39	0	14	0

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLU	deletion	UNP P04133
A	?	-	GLU	deletion	UNP P04133
A	?	-	GLU	deletion	UNP P04133
A	?	-	ASP	deletion	UNP P04133
A	?	-	ASP	deletion	UNP P04133
A	?	-	ASP	deletion	UNP P04133
A	?	-	ASN	deletion	UNP P04133
A	?	-	GLU	deletion	UNP P04133
A	?	-	ASP	deletion	UNP P04133
A	?	-	GLU	deletion	UNP P04133
A	?	-	VAL	deletion	UNP P04133
A	?	-	ASP	deletion	UNP P04133
A	?	-	GLU	deletion	UNP P04133
A	159	ALA	GLN	linker	UNP P04133
A	160	GLN	ALA	linker	UNP P04133
A	161	ALA	GLU	linker	UNP P04133
A	162	GLU	GLN	linker	UNP P04133

- Molecule 2 is a protein called antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	213	1652	1036	274	336	6	0	0	0

- Molecule 3 is a protein called antibody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	218	1637	1037	279	313	8	0	0	0

- Molecule 4 is water.

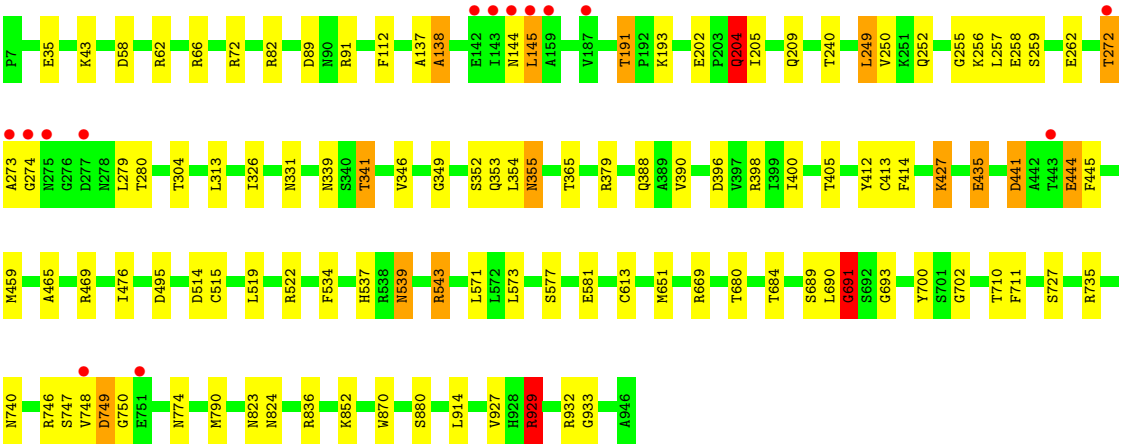
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	441	441	441	0	0
4	L	21	21	21	0	0
4	H	21	21	21	0	0

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.

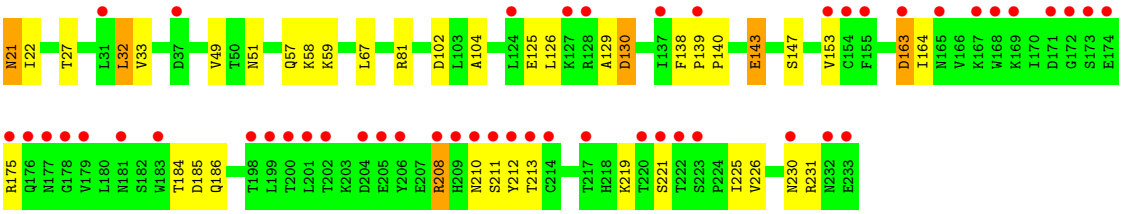
• Molecule 1: Hexon protein,hexon capsid

Chain A:



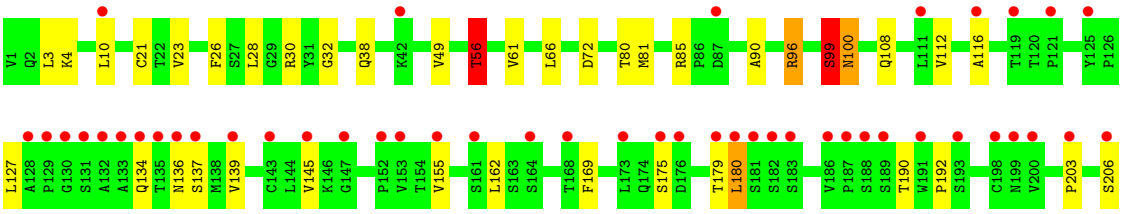
• Molecule 2: antibody

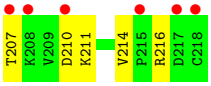
Chain L:



• Molecule 3: antibody

Chain H:




T207
K208
V209
D210
K211
V214
P215
R216
D217
C218

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	157.00Å 157.00Å 144.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	78.50 – 2.70 78.50 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (78.50-2.70) 99.9 (78.50-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.164 , 0.223 0.173 , 0.225	Depositor DCC
R_{free} test set	2821 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 64.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11253	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% 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	0.73	0/7686	0.87	13/10454 (0.1%)
2	L	0.61	0/1690	0.73	1/2298 (0.0%)
3	H	0.60	0/1679	0.84	2/2293 (0.1%)
All	All	0.69	0/11055	0.84	16/15045 (0.1%)

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	A	0	1
2	L	0	1
3	H	0	1
All	All	0	3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	543	ARG	NE-CZ-NH1	7.13	123.87	120.30
3	H	96	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	543	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	669	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	735	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	396	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	522	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	A	204	GLN	CB-CA-C	-5.63	99.13	110.40
1	A	669	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	379	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	929	ARG	NE-CZ-NH1	5.51	123.06	120.30
3	H	99	SER	C-N-CA	5.37	135.12	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	32	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	379	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	145	LEU	CA-CB-CG	5.16	127.18	115.30
1	A	72	ARG	NE-CZ-NH2	-5.15	117.73	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	691	GLY	Peptide
3	H	81	MET	Peptide
2	L	21	ASN	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	7481	0	7152	61	1
2	L	1652	0	1580	17	0
3	H	1637	0	1610	15	1
4	A	441	0	0	7	0
4	H	21	0	0	1	0
4	L	21	0	0	0	0
All	All	11253	0	10342	89	1

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 4.

All (89) 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:469[A]:ARG:HG3	1:A:515[A]:CYS:SG	1.80	1.21
1:A:137:ALA:HB1	1:A:138:ALA:HB2	1.44	0.98
2:L:143:GLU:O	2:L:143:GLU:OE2	1.81	0.96
1:A:469[A]:ARG:CG	1:A:515[A]:CYS:SG	2.55	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469[A]:ARG:HG3	1:A:515[A]:CYS:HG	1.46	0.79
1:A:774:ASN:HD21	1:A:880:SER:H	1.35	0.75
1:A:262:GLU:CB	4:A:1429:HOH:O	2.34	0.74
1:A:469[B]:ARG:NH1	4:A:1001:HOH:O	2.24	0.70
1:A:202:GLU:HB2	1:A:205:ILE:HD12	1.78	0.65
1:A:390:VAL:HG21	1:A:790[B]:MET:HE1	1.79	0.65
1:A:413[A]:CYS:SG	1:A:459:MET:HB2	2.37	0.65
1:A:405:THR:HG21	1:A:465:ALA:HA	1.79	0.64
1:A:573:LEU:HD12	1:A:929:ARG:NH2	2.13	0.63
1:A:137:ALA:CB	1:A:138:ALA:HB2	2.27	0.60
2:L:213:THR:HG23	2:L:226:VAL:HG13	1.82	0.60
1:A:137:ALA:HB1	1:A:138:ALA:CB	2.27	0.60
2:L:57:GLN:HB2	2:L:67:LEU:HD11	1.83	0.60
1:A:339:ASN:HD21	1:A:365:THR:H	1.48	0.59
1:A:746:ARG:HE	1:A:750:GLY:CA	2.16	0.59
1:A:573:LEU:HD12	1:A:929:ARG:HH21	1.69	0.58
3:H:99:SER:CB	3:H:100:ASN:HB2	2.34	0.58
1:A:749:ASP:OD1	1:A:750:GLY:N	2.36	0.57
2:L:153:VAL:HG21	3:H:127:LEU:HD11	1.87	0.56
1:A:684:THR:HG22	1:A:914:LEU:HG	1.88	0.55
1:A:746:ARG:HE	1:A:750:GLY:HA3	1.70	0.55
1:A:534:PHE:CD2	1:A:710:THR:HB	2.42	0.55
1:A:444:GLU:HG2	1:A:445:PHE:HD1	1.72	0.54
2:L:21:ASN:N	2:L:22:ILE:HA	2.21	0.54
1:A:112:PHE:HB2	1:A:326:ILE:HD12	1.91	0.53
1:A:89:ASP:O	1:A:91:ARG:NH1	2.42	0.52
1:A:272:THR:HG23	1:A:273:ALA:H	1.74	0.52
2:L:59:LYS:HE3	2:L:104:ALA:HB2	1.92	0.52
1:A:689:SER:O	1:A:691:GLY:N	2.42	0.52
2:L:58:LYS:O	2:L:104:ALA:HB1	2.10	0.52
2:L:211:SER:HB2	2:L:230:ASN:HD22	1.75	0.51
1:A:82:ARG:NH1	1:A:581:GLU:OE1	2.44	0.51
3:H:49:VAL:O	3:H:56:THR:HA	2.11	0.51
3:H:116:ALA:N	4:H:301:HOH:O	2.35	0.51
1:A:441:ASP:HB3	1:A:444:GLU:OE1	2.12	0.50
1:A:539:ASN:HD22	1:A:539:ASN:C	2.15	0.50
1:A:272:THR:HG23	1:A:273:ALA:N	2.28	0.49
1:A:257:LEU:CB	1:A:258:GLU:HA	2.43	0.49
2:L:81:ARG:NH1	2:L:102:ASP:OD2	2.45	0.48
1:A:341:THR:HA	4:A:1350:HOH:O	2.13	0.48
2:L:211:SER:CB	2:L:230:ASN:HD22	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469[B]:ARG:HD2	1:A:514:ASP:OD1	2.14	0.48
1:A:740[B]:ASN:OD1	1:A:740[B]:ASN:N	2.44	0.47
2:L:138:PHE:CE2	3:H:127:LEU:HB3	2.49	0.47
2:L:164:ILE:O	2:L:164:ILE:HG23	2.15	0.47
1:A:412:TYR:HB2	1:A:414:PHE:CZ	2.49	0.47
1:A:680:THR:HG21	1:A:711:PHE:CD1	2.50	0.47
1:A:790[B]:MET:HE3	1:A:790[B]:MET:HB3	1.81	0.47
1:A:202:GLU:HB3	1:A:204:GLN:OE1	2.16	0.46
1:A:240:THR:HB	1:A:249:LEU:HD22	1.98	0.46
3:H:134:GLN:HE21	3:H:139:VAL:HG21	1.80	0.46
1:A:398:ARG:HD2	4:A:1257:HOH:O	2.15	0.46
1:A:346:VAL:HA	1:A:355:ASN:HD21	1.81	0.45
2:L:143:GLU:OE2	2:L:143:GLU:C	2.50	0.45
3:H:99:SER:HB2	3:H:100:ASN:HB2	1.99	0.45
1:A:400:ILE:HD11	1:A:476:ILE:HD13	1.98	0.45
2:L:221:SER:HB3	2:L:225:ILE:HD11	1.98	0.45
1:A:256:LYS:HB3	1:A:257:LEU:HA	1.97	0.45
1:A:444:GLU:HG2	1:A:445:PHE:CD1	2.50	0.44
3:H:66:LEU:HD12	3:H:80:THR:O	2.18	0.44
3:H:23:VAL:HG13	3:H:26:PHE:CE1	2.52	0.44
1:A:62:ARG:NE	4:A:1014:HOH:O	2.51	0.43
3:H:38:GLN:O	3:H:90:ALA:HB1	2.19	0.43
3:H:3:LEU:HD23	3:H:21:CYS:SG	2.59	0.43
2:L:126:LEU:HB3	2:L:186:GLN:HE22	1.84	0.43
1:A:191:THR:HG22	3:H:72:ASP:HB2	2.01	0.42
3:H:155:VAL:HG21	3:H:180:LEU:HD21	2.01	0.42
1:A:58:ASP:HB2	4:A:1290:HOH:O	2.19	0.42
1:A:346:VAL:HB	1:A:581:GLU:HB3	2.01	0.42
1:A:823:ASN:O	1:A:824:ASN:HB2	2.19	0.42
2:L:184:THR:HG23	3:H:169:PHE:CD1	2.55	0.42
1:A:747:SER:O	1:A:749:ASP:OD2	2.38	0.42
2:L:143:GLU:OE2	2:L:143:GLU:CA	2.68	0.42
1:A:537:HIS:O	1:A:543:ARG:HD2	2.20	0.41
1:A:349:GLY:HA3	1:A:933:GLY:O	2.20	0.41
1:A:62:ARG:NH2	4:A:1014:HOH:O	2.53	0.41
1:A:427:LYS:HB3	1:A:441:ASP:HB2	2.02	0.41
1:A:331:ASN:HD21	1:A:388:GLN:HG3	1.86	0.41
1:A:469[A]:ARG:HG2	1:A:515[A]:CYS:SG	2.56	0.41
1:A:870:TRP:HA	1:A:870:TRP:CE3	2.56	0.41
3:H:23:VAL:HG13	3:H:26:PHE:CZ	2.56	0.40
1:A:571:LEU:HD11	1:A:927:VAL:HG11	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ARG:NH1	1:A:613:CYS:SG	2.94	0.40
1:A:700:TYR:CZ	1:A:702:GLY:HA3	2.56	0.40
1:A:746:ARG:NE	1:A:750:GLY:HA3	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:GLU:OE2	3:H:32:GLY:N[2_545]	2.16	0.04

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	937/927 (101%)	870 (93%)	56 (6%)	11 (1%)	13 32
2	L	211/213 (99%)	182 (86%)	22 (10%)	7 (3%)	4 8
3	H	216/218 (99%)	183 (85%)	27 (12%)	6 (3%)	5 11
All	All	1364/1358 (100%)	1235 (90%)	105 (8%)	24 (2%)	8 21

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	691	GLY
2	L	33	VAL
3	H	100	ASN
3	H	192	PRO
1	A	138	ALA
1	A	272	THR
1	A	353	GLN
1	A	690	LEU
1	A	727	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	749	ASP
2	L	163	ASP
3	H	206	SER
1	A	352	SER
2	L	129	ALA
2	L	139	PRO
2	L	140	PRO
3	H	175	SER
1	A	693	GLY
2	L	130	ASP
2	L	208	ARG
3	H	56	THR
1	A	274	GLY
1	A	255	GLY
3	H	203	PRO

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	810/806 (100%)	776 (96%)	34 (4%)	30 58
2	L	187/188 (100%)	171 (91%)	16 (9%)	10 24
3	H	186/188 (99%)	163 (88%)	23 (12%)	4 11
All	All	1183/1182 (100%)	1110 (94%)	73 (6%)	18 40

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	43	LYS
1	A	144	ASN
1	A	145	LEU
1	A	191	THR
1	A	193	LYS
1	A	204	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	209	GLN
1	A	249	LEU
1	A	250	VAL
1	A	252	GLN
1	A	259	SER
1	A	279	LEU
1	A	280	THR
1	A	304	THR
1	A	313	LEU
1	A	341	THR
1	A	354	LEU
1	A	355	ASN
1	A	427	LYS
1	A	435	GLU
1	A	441	ASP
1	A	444	GLU
1	A	495	ASP
1	A	519	LEU
1	A	539	ASN
1	A	577	SER
1	A	651[A]	MET
1	A	651[B]	MET
1	A	748	VAL
1	A	836	ARG
1	A	852	LYS
1	A	929	ARG
1	A	932	ARG
2	L	27	THR
2	L	32	LEU
2	L	49	VAL
2	L	51	ASN
2	L	125	GLU
2	L	130	ASP
2	L	143	GLU
2	L	147	SER
2	L	163	ASP
2	L	175	ARG
2	L	185	ASP
2	L	208	ARG
2	L	210	ASN
2	L	212	TYR
2	L	219	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	231	ARG
3	H	4	LYS
3	H	10	LEU
3	H	28	LEU
3	H	30	ARG
3	H	56	THR
3	H	61	VAL
3	H	85	ARG
3	H	96	ARG
3	H	99	SER
3	H	108	GLN
3	H	112	VAL
3	H	136	ASN
3	H	137	SER
3	H	145	VAL
3	H	162	LEU
3	H	179	THR
3	H	180	LEU
3	H	190	THR
3	H	207	THR
3	H	210	ASP
3	H	211	LYS
3	H	214	VAL
3	H	216	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	61	GLN
1	A	278	ASN
1	A	331	ASN
1	A	339	ASN
1	A	355	ASN
1	A	370	GLN
1	A	464	ASN
1	A	470	ASN
1	A	539	ASN
1	A	570	ASN
1	A	670	ASN
1	A	774	ASN
1	A	798	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	51	ASN
2	L	99	GLN
2	L	186	GLN
2	L	230	ASN
3	H	34	HIS
3	H	134	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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	145:LEU	C	159:ALA	N	19.97

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	927/927 (100%)	-0.07	14 (1%)	73	76	23, 43, 85, 180	0
2	L	213/213 (100%)	1.34	49 (23%)	0	0	46, 121, 188, 215	7 (3%)
3	H	218/218 (100%)	1.27	53 (24%)	0	0	42, 106, 198, 259	0
All	All	1358/1358 (100%)	0.37	116 (8%)	10	9	23, 54, 178, 259	7 (0%)

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	LEU	12.9
2	L	233	GLU	11.2
2	L	173	SER	10.6
2	L	172	GLY	10.5
1	A	748	VAL	8.9
1	A	159	ALA	8.8
3	H	133	ALA	8.2
1	A	143	ILE	7.8
3	H	132	ALA	7.8
2	L	174	GLU	7.7
3	H	218	CYS	7.7
1	A	144	ASN	7.3
3	H	135	THR	6.4
3	H	189	SER	6.0
2	L	176	GLN	5.9
3	H	143	CYS	5.2
2	L	209	HIS	5.2
2	L	137	ILE	5.1
2	L	230	ASN	5.0
2	L	199	LEU	5.0
1	A	142	GLU	4.9
3	H	198	CYS	4.9
2	L	201	LEU	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	131	SER	4.8
3	H	187	PRO	4.7
3	H	134	GLN	4.7
2	L	232	ASN	4.6
2	L	168	TRP	4.4
1	A	751	GLU	4.2
3	H	173	LEU	4.2
2	L	165	ASN	4.2
2	L	210	ASN	4.2
2	L	163	ASP	4.1
3	H	136	ASN	4.1
2	L	217	THR	4.1
1	A	443	THR	4.0
2	L	222	THR	4.0
3	H	176	ASP	3.9
3	H	217	ASP	3.9
3	H	193	SER	3.9
2	L	213	THR	3.8
2	L	202	THR	3.7
3	H	130	GLY	3.6
3	H	164	SER	3.5
2	L	212	TYR	3.5
3	H	145	VAL	3.4
2	L	214	CYS	3.4
2	L	208	ARG	3.4
3	H	182	SER	3.4
3	H	153	VAL	3.4
2	L	171	ASP	3.3
2	L	167	LYS	3.3
1	A	275	ASN	3.3
3	H	137	SER	3.3
2	L	169	LYS	3.3
3	H	116	ALA	3.3
2	L	200	THR	3.2
1	A	274	GLY	3.2
2	L	155	PHE	3.2
3	H	181	SER	3.2
3	H	191	TRP	3.1
2	L	211	SER	3.1
2	L	127	LYS	3.1
3	H	147	GLY	3.0
3	H	125	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	183	SER	2.9
2	L	183	TRP	2.9
3	H	203	PRO	2.9
2	L	178	GLY	2.9
3	H	119	THR	2.9
3	H	129	PRO	2.8
3	H	207	THR	2.8
2	L	221	SER	2.8
3	H	128	ALA	2.8
2	L	175	ARG	2.8
2	L	153	VAL	2.8
3	H	111	LEU	2.7
3	H	215	PRO	2.7
3	H	139	VAL	2.7
2	L	177	ASN	2.7
2	L	204	ASP	2.6
2	L	128	ARG	2.6
3	H	180	LEU	2.6
2	L	154	CYS	2.6
1	A	272	THR	2.5
3	H	188	SER	2.5
2	L	181	ASN	2.5
3	H	155	VAL	2.5
2	L	220	THR	2.5
3	H	186	VAL	2.5
3	H	10	LEU	2.5
3	H	210	ASP	2.4
3	H	179	THR	2.4
3	H	200	VAL	2.4
3	H	161	SER	2.3
2	L	124	LEU	2.3
2	L	31	LEU	2.3
3	H	199	ASN	2.3
2	L	37	ASP	2.3
3	H	206	SER	2.3
2	L	205	GLU	2.3
2	L	139	PRO	2.2
3	H	87	ASP	2.2
3	H	175	SER	2.2
3	H	42	LYS	2.2
1	A	273	ALA	2.1
3	H	168	THR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	L	198	THR	2.1
3	H	208	LYS	2.1
1	A	277	ASP	2.1
3	H	152	PRO	2.1
2	L	223	SER	2.1
2	L	179	VAL	2.0
1	A	187	VAL	2.0
3	H	121	PRO	2.0
2	L	206	TYR	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.