



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2021 – 12:13 PM EDT

PDB ID : 7LYW
Title : Crystal structure of the HCMV pentamer-specific antibody 2-25
Authors : Wrapp, D.; Mishra, A.K.; McLellan, J.S.
Deposited on : 2021-03-08
Resolution : 2.51 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 : 2.23.1
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) : 2.23.1

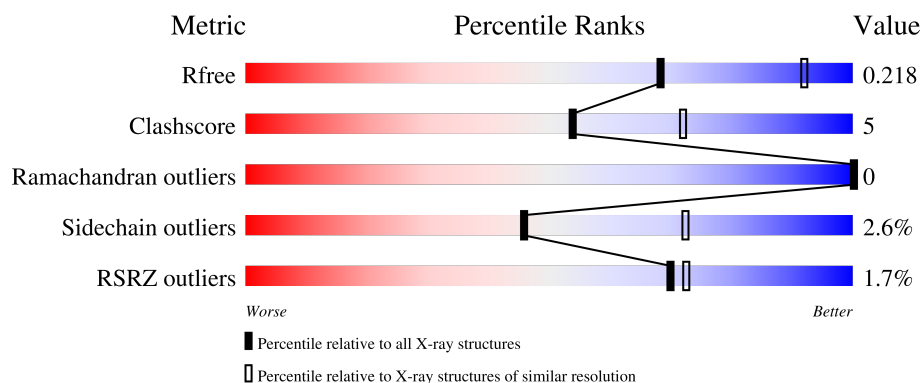
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 $\leq 5\%$. 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	234	
1	C	234	
1	H	234	
2	B	212	
2	D	212	

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Mol	Chain	Length	Quality of chain
2	L	212	 86%13%•

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10140 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 2-25 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1627	1029	273	318	7			
1	C	214	Total	C	N	O	S	0	0	0
			1627	1029	273	318	7			
1	H	214	Total	C	N	O	S	0	0	0
			1627	1029	273	318	7			

- Molecule 2 is a protein called 2-25 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1584	989	259	331	5			
2	D	210	Total	C	N	O	S	0	0	0
			1584	989	259	331	5			
2	L	210	Total	C	N	O	S	0	0	0
			1584	989	259	331	5			

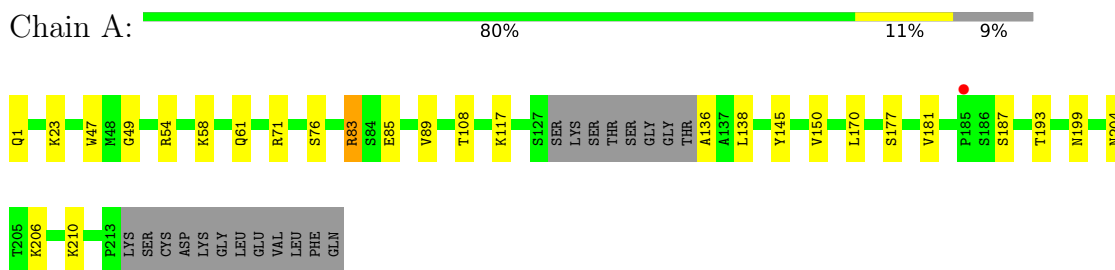
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	106	Total	O	0	0
			106	106		
3	B	99	Total	O	0	0
			99	99		
3	C	73	Total	O	0	0
			73	73		
3	D	54	Total	O	0	0
			54	54		
3	H	100	Total	O	0	0
			100	100		
3	L	75	Total	O	0	0
			75	75		

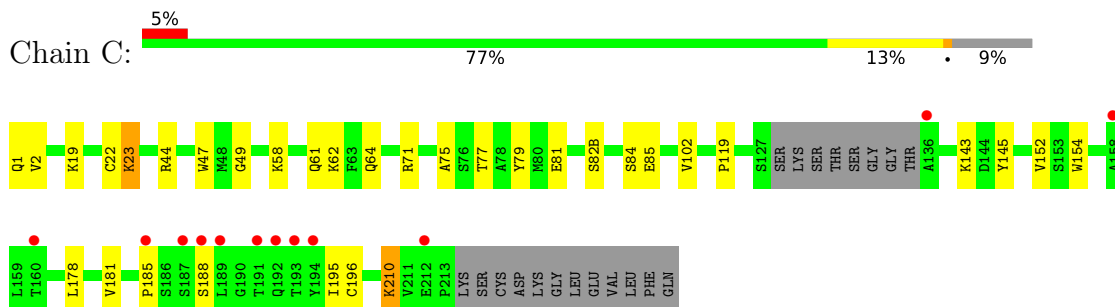
3 Residue-property plots [i](#)

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.

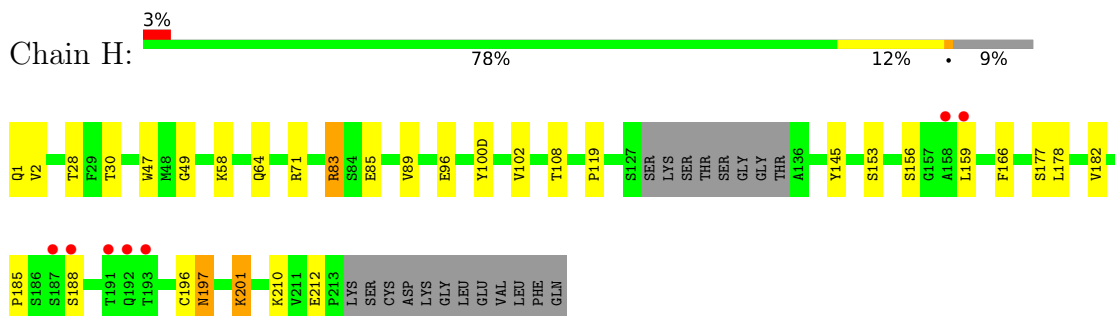
• Molecule 1: 2-25 Fab Heavy Chain



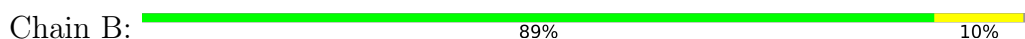
• Molecule 1: 2-25 Fab Heavy Chain

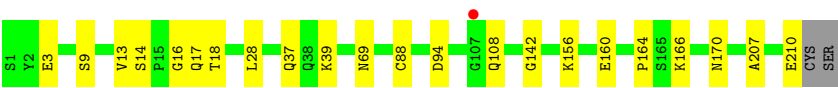


• Molecule 1: 2-25 Fab Heavy Chain

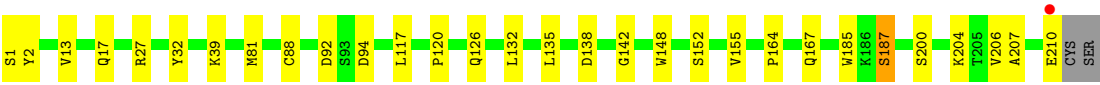
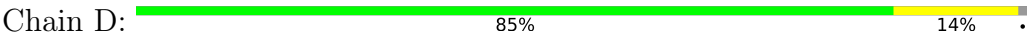


• Molecule 2: 2-25 Fab Light Chain

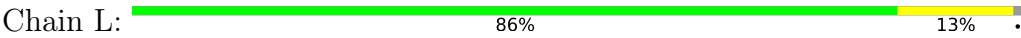




● Molecule 2: 2-25 Fab Light Chain



● Molecule 2: 2-25 Fab Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	180.87Å 180.87Å 138.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.08 – 2.51 58.08 – 2.51	Depositor EDS
% Data completeness (in resolution range)	98.4 (58.08-2.51) 98.4 (58.08-2.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.51Å)	Xtriage
Refinement program	PHENIX dev_3758	Depositor
R, R_{free}	0.187 , 0.219 0.187 , 0.218	Depositor DCC
R_{free} test set	3810 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10140	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 2.34% 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: PCA

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	0.60	0/1660	0.73	1/2262 (0.0%)
1	C	0.57	0/1660	0.75	1/2262 (0.0%)
1	H	0.57	0/1660	0.73	1/2262 (0.0%)
2	B	0.56	0/1623	0.67	0/2219
2	D	0.54	0/1623	0.70	0/2219
2	L	0.56	1/1623 (0.1%)	0.68	0/2219
All	All	0.57	1/9849 (0.0%)	0.71	3/13443 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	13	VAL	C-N	5.24	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	178	LEU	CA-CB-CG	5.55	128.08	115.30
1	H	178	LEU	CA-CB-CG	5.13	127.09	115.30
1	A	54	ARG	NE-CZ-NH2	-5.11	117.74	120.30

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	1627	0	1584	17	0
1	C	1627	0	1584	20	0
1	H	1627	0	1584	18	1
2	B	1584	0	1517	15	0
2	D	1584	0	1517	18	0
2	L	1584	0	1517	21	1
3	A	106	0	0	7	0
3	B	99	0	0	6	1
3	C	73	0	0	4	0
3	D	54	0	0	1	1
3	H	100	0	0	2	0
3	L	75	0	0	8	1
All	All	10140	0	9303	100	3

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 (100) 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:117:LYS:NZ	3:A:301:HOH:O	1.89	1.05
2:B:18:THR:O	3:B:301:HOH:O	1.88	0.91
1:H:156:SER:OG	3:H:301:HOH:O	1.90	0.90
2:B:37:GLN:OE1	3:B:302:HOH:O	1.91	0.86
2:L:66:ASN:O	3:L:303:HOH:O	1.95	0.84
2:L:1:SER:OG	3:L:304:HOH:O	1.98	0.82
2:L:54:ARG:NH1	3:L:302:HOH:O	1.92	0.82
1:C:64:GLN:N	3:C:303:HOH:O	2.15	0.80
1:A:187:SER:OG	3:A:302:HOH:O	1.99	0.79
1:C:181:VAL:HG11	2:D:135:LEU:HD11	1.68	0.74
1:C:79:TYR:OH	3:C:301:HOH:O	2.04	0.72
2:B:3:GLU:OE1	3:B:304:HOH:O	2.08	0.71
2:B:16:GLY:O	3:B:303:HOH:O	2.08	0.71
2:B:13:VAL:HG22	2:B:17:GLN:HB2	1.71	0.71
1:H:159:LEU:HD21	1:H:182:VAL:HG11	1.71	0.70
1:A:170:LEU:O	3:A:303:HOH:O	2.09	0.68
1:C:152:VAL:O	3:C:302:HOH:O	2.11	0.68
1:C:181:VAL:HG11	2:D:135:LEU:CD1	2.24	0.67
1:A:204:ASN:ND2	3:A:306:HOH:O	2.19	0.66
2:L:20:SER:OG	3:L:305:HOH:O	2.13	0.66
1:A:199:ASN:HB2	1:A:206:LYS:NZ	2.12	0.65
2:L:13:VAL:HG22	2:L:17:GLN:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:GLU:OE2	3:A:304:HOH:O	2.15	0.65
1:H:64:GLN:O	3:H:302:HOH:O	2.14	0.65
1:A:193:THR:HG23	1:A:210:LYS:HD2	1.78	0.64
2:D:207:ALA:O	2:D:210:GLU:HG2	1.97	0.64
2:L:140:TYR:OH	3:L:306:HOH:O	2.14	0.64
2:L:197:HIS:ND1	3:L:311:HOH:O	2.31	0.61
2:B:39:LYS:HE3	3:B:302:HOH:O	2.00	0.61
1:A:136:ALA:N	3:A:310:HOH:O	2.34	0.60
1:C:61:GLN:HE22	1:H:83:ARG:HB2	1.67	0.60
1:H:201:LYS:HE2	1:H:201:LYS:HA	1.82	0.60
1:C:23:LYS:HA	1:C:77:THR:HG22	1.85	0.59
1:A:58:LYS:HD2	2:B:94:ASP:HB3	1.85	0.58
1:A:89:VAL:HG22	1:A:108:THR:HG22	1.85	0.58
2:L:120:PRO:HD3	2:L:132:LEU:HD23	1.84	0.58
1:H:201:LYS:HA	1:H:201:LYS:CE	2.35	0.57
2:D:13:VAL:HG13	2:D:17:GLN:HB2	1.88	0.56
2:L:61:ARG:HB2	2:L:76:SER:O	2.06	0.56
1:C:185:PRO:O	1:C:188:SER:OG	2.21	0.55
2:L:189:LYS:NZ	3:L:301:HOH:O	1.83	0.54
2:D:138:ASP:H	2:D:167:GLN:HE22	1.58	0.52
2:L:189:LYS:CE	3:L:301:HOH:O	2.44	0.51
2:L:207:ALA:O	2:L:210:GLU:HG2	2.11	0.51
1:C:119:PRO:HB3	1:C:145:TYR:HB3	1.93	0.51
1:H:210:LYS:HD3	1:H:212:GLU:OE2	2.10	0.50
1:C:195:ILE:HD12	1:C:210:LYS:HG3	1.93	0.50
2:D:138:ASP:H	2:D:167:GLN:NE2	2.08	0.50
2:B:28:LEU:HB3	2:B:69:ASN:HA	1.95	0.49
1:C:2:VAL:HG11	1:C:102:VAL:HG21	1.95	0.49
1:H:89:VAL:HG22	1:H:108:THR:HG22	1.94	0.48
1:C:19:LYS:HE2	1:C:81:GLU:OE2	2.13	0.48
2:B:207:ALA:O	2:B:210:GLU:HG2	2.14	0.48
2:B:14:SER:O	2:B:17:GLN:HG3	2.13	0.47
2:L:54:ARG:HG2	2:L:58:ILE:HB	1.96	0.47
1:C:61:GLN:HE21	1:H:85:GLU:HG2	1.80	0.47
1:H:28:THR:HG22	1:H:30:THR:HG22	1.97	0.47
2:D:39:LYS:HE2	2:D:81:MET:O	2.15	0.47
2:D:185:TRP:HH2	2:D:206:VAL:HG23	1.79	0.47
1:H:185:PRO:O	1:H:188:SER:OG	2.30	0.47
2:L:14:SER:O	2:L:17:GLN:HG3	2.16	0.46
2:D:187:SER:O	2:D:187:SER:OG	2.33	0.46
1:A:23:LYS:NZ	1:A:76:SER:HB2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:120:PRO:HD3	2:D:132:LEU:CD2	2.46	0.46
2:D:32:TYR:O	3:D:301:HOH:O	2.21	0.45
2:D:117:LEU:HD23	2:D:206:VAL:HG13	1.97	0.45
1:H:153:SER:OG	1:H:197:ASN:OD1	2.33	0.45
2:B:160:GLU:OE2	3:B:305:HOH:O	2.21	0.45
1:C:58:LYS:HD2	2:D:94:ASP:HB3	1.98	0.45
1:C:22:CYS:O	1:C:77:THR:HA	2.17	0.45
2:D:120:PRO:HD3	2:D:132:LEU:HD23	1.98	0.45
2:D:1:SER:OG	2:D:2:TYR:N	2.50	0.44
1:C:47:TRP:CZ2	1:C:49:GLY:HA2	2.52	0.44
1:H:166:PHE:CE2	2:L:135:LEU:HD22	2.53	0.44
1:H:96:GLU:HG3	1:H:100(D):TYR:CE1	2.52	0.44
1:H:119:PRO:HB3	1:H:145:TYR:HB3	1.99	0.44
1:C:154:TRP:CZ3	1:C:196:CYS:HB3	2.52	0.44
2:B:108:GLN:NE2	2:B:170:ASN:O	2.39	0.44
1:A:83:ARG:NH2	3:A:304:HOH:O	2.27	0.43
2:D:148:TRP:HB2	2:D:155:VAL:HB	2.00	0.43
2:L:26:ASP:OD2	2:L:27:ARG:HD3	2.19	0.43
2:D:27:ARG:NH2	2:D:92:ASP:OD1	2.52	0.43
1:C:154:TRP:CH2	1:C:196:CYS:HB3	2.54	0.43
2:L:7:PRO:HD2	2:L:22:THR:O	2.19	0.42
1:H:47:TRP:CZ2	1:H:49:GLY:HA2	2.54	0.42
2:D:142:GLY:O	2:D:164:PRO:HG2	2.19	0.42
1:H:201:LYS:HE2	1:H:201:LYS:CA	2.47	0.42
2:B:166:LYS:HE3	2:B:170:ASN:HD22	1.84	0.41
2:L:132:LEU:HD12	2:L:178:LEU:HD23	2.02	0.41
1:C:75:ALA:O	1:C:77:THR:HG23	2.20	0.41
1:A:47:TRP:CZ2	1:A:49:GLY:HA2	2.56	0.41
1:H:2:VAL:HG11	1:H:102:VAL:HG21	2.03	0.41
2:B:156:LYS:HE2	2:L:29:ASP:O	2.20	0.41
2:L:120:PRO:HD3	2:L:132:LEU:CD2	2.49	0.41
1:A:61:GLN:OE1	1:C:85:GLU:HG2	2.20	0.41
2:L:4:LEU:HD11	2:L:90:ALA:HB3	2.02	0.41
1:A:138:LEU:O	1:A:181:VAL:HG23	2.21	0.40
2:B:142:GLY:O	2:B:164:PRO:HG2	2.21	0.40
1:A:58:LYS:HD3	3:C:364:HOH:O	2.22	0.40
1:A:145:TYR:CE2	1:A:150:VAL:HG13	2.56	0.40

All (3) 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)
3:L:369:HOH:O	3:L:372:HOH:O[3_544]	1.88	0.32
3:B:363:HOH:O	3:D:336:HOH:O[4_555]	1.89	0.31
1:H:100(D):TYR:OH	2:L:189:LYS:NZ[4_555]	2.17	0.03

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	210/234 (90%)	204 (97%)	6 (3%)	0	100	100
1	C	210/234 (90%)	204 (97%)	6 (3%)	0	100	100
1	H	210/234 (90%)	204 (97%)	6 (3%)	0	100	100
2	B	208/212 (98%)	206 (99%)	2 (1%)	0	100	100
2	D	208/212 (98%)	206 (99%)	2 (1%)	0	100	100
2	L	208/212 (98%)	206 (99%)	2 (1%)	0	100	100
All	All	1254/1338 (94%)	1230 (98%)	24 (2%)	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	179/196 (91%)	176 (98%)	3 (2%)	60	82
1	C	179/196 (91%)	171 (96%)	8 (4%)	27	51
1	H	179/196 (91%)	172 (96%)	7 (4%)	32	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	179/181 (99%)	177 (99%)	2 (1%)	73	89
2	D	179/181 (99%)	173 (97%)	6 (3%)	37	63
2	L	179/181 (99%)	177 (99%)	2 (1%)	73	89
All	All	1074/1131 (95%)	1046 (97%)	28 (3%)	46	72

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ARG
1	A	83	ARG
1	A	177	SER
2	B	9	SER
2	B	88	CYS
1	C	23	LYS
1	C	44	ARG
1	C	62	LYS
1	C	71	ARG
1	C	82(B)	SER
1	C	84	SER
1	C	143	LYS
1	C	210	LYS
2	D	88	CYS
2	D	126	GLN
2	D	152	SER
2	D	187	SER
2	D	200	SER
2	D	204	LYS
1	H	58	LYS
1	H	71	ARG
1	H	83	ARG
1	H	177	SER
1	H	196	CYS
1	H	197	ASN
1	H	201	LYS
2	L	67	SER
2	L	88	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	126	GLN
2	B	170	ASN
1	C	61	GLN
2	D	167	GLN
2	D	188	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
1	PCA	A	1	1	7,8,9	1.90	1 (14%)	9,10,12	2.68	5 (55%)
1	PCA	C	1	1	7,8,9	1.90	1 (14%)	9,10,12	2.16	5 (55%)
1	PCA	H	1	1	7,8,9	1.89	1 (14%)	9,10,12	2.16	5 (55%)

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
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	C	1	1	-	0/0/11/13	0/1/1/1
1	PCA	H	1	1	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	PCA	CD-N	4.86	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CD-N	4.84	1.47	1.34
1	H	1	PCA	CD-N	4.79	1.47	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	PCA	CB-CA-C	-4.09	107.07	112.70
1	A	1	PCA	CA-N-CD	-3.88	100.28	113.58
1	A	1	PCA	CB-CA-N	3.57	113.54	103.30
1	H	1	PCA	CA-N-CD	-3.46	101.74	113.58
1	C	1	PCA	CA-N-CD	-3.38	102.01	113.58
1	H	1	PCA	CB-CA-N	3.04	112.03	103.30
1	C	1	PCA	CB-CA-N	2.97	111.84	103.30
1	A	1	PCA	OE-CD-CG	-2.90	121.70	126.76
1	C	1	PCA	OE-CD-CG	-2.63	122.18	126.76
1	H	1	PCA	OE-CD-CG	-2.62	122.20	126.76
1	A	1	PCA	CG-CD-N	2.60	115.13	108.39
1	H	1	PCA	CG-CD-N	2.43	114.68	108.39
1	C	1	PCA	CG-CD-N	2.40	114.59	108.39
1	C	1	PCA	CB-CA-C	-2.35	109.47	112.70
1	H	1	PCA	CB-CA-C	-2.05	109.88	112.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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, 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	213/234 (91%)	0.01	1 (0%) 91 91	24, 33, 60, 79	0
1	C	213/234 (91%)	0.29	12 (5%) 24 25	21, 34, 78, 90	0
1	H	213/234 (91%)	0.21	7 (3%) 46 50	22, 33, 59, 76	0
2	B	210/212 (99%)	0.12	1 (0%) 91 91	25, 39, 56, 65	0
2	D	210/212 (99%)	0.24	1 (0%) 91 91	25, 46, 63, 76	0
2	L	210/212 (99%)	0.04	0 100 100	25, 39, 55, 65	0
All	All	1269/1338 (94%)	0.15	22 (1%) 70 72	21, 38, 63, 90	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	191	THR	4.4
1	H	158	ALA	4.1
1	C	191	THR	4.0
1	C	192	GLN	3.5
1	C	194	TYR	3.5
1	C	188	SER	3.3
1	C	185	PRO	3.2
1	C	158	ALA	3.1
1	H	188	SER	3.1
1	C	187	SER	3.0
1	C	189	LEU	3.0
1	A	185	PRO	2.8
1	H	187	SER	2.7
2	D	210	GLU	2.5
1	H	159	LEU	2.5
1	C	136	ALA	2.5
1	H	192	GLN	2.4
1	C	193	THR	2.4
1	C	160	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	107	GLY	2.2
1	H	193	THR	2.1
1	C	212	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	PCA	H	1	8/9	0.82	0.29	48,59,78,88	0
1	PCA	C	1	8/9	0.86	0.28	40,55,66,75	0
1	PCA	A	1	8/9	0.91	0.31	38,53,58,60	0

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.