



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 3, 2018 – 06:58 PM EST

PDB ID : 5VJ6
EMDB ID: : EMD-8695
Title : BG505 SOSIP.664 in complex with broadly neutralizing antibodies PG9 and 8ANC195
Authors : Wang, H.; Bjorkman, P.J.
Deposited on : 2017-04-18
Resolution : 11.50 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

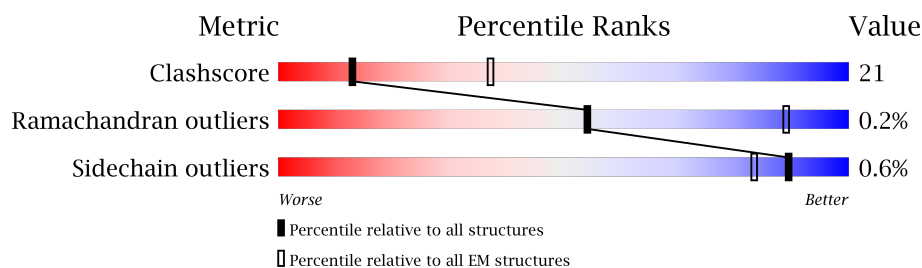
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 11.50 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)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	153	
1	B	153	
1	C	153	
2	D	481	
2	E	481	
2	F	481	
3	H	248	
4	M	233	
4	O	233	

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Mol	Chain	Length	Quality of chain
4	Q	233	 79% 17% .
5	N	215	 86% 13%
5	P	215	 84% 15%
5	R	215	 85% 14%
6	L	216	 71% 26% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26459 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	126	Total	C	N	O	S	0	0
			1001	633	172	190	6		
1	B	126	Total	C	N	O	S	0	0
			1001	633	172	190	6		
1	C	126	Total	C	N	O	S	0	0
			1001	633	172	190	6		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	559	PRO	ILE	engineered mutation	UNP Q2N0S6
A	605	CYS	THR	engineered mutation	UNP Q2N0S6
B	559	PRO	ILE	engineered mutation	UNP Q2N0S6
B	605	CYS	THR	engineered mutation	UNP Q2N0S6
C	559	PRO	ILE	engineered mutation	UNP Q2N0S6
C	605	CYS	THR	engineered mutation	UNP Q2N0S6

- Molecule 2 is a protein called Envelope glycoprotein gp160.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	449	Total	C	N	O	S	0	0
			3532	2217	623	665	27		
2	E	449	Total	C	N	O	S	0	0
			3532	2217	623	665	27		
2	F	449	Total	C	N	O	S	0	0
			3532	2217	623	665	27		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	332	ASN	THR	engineered mutation	UNP Q2N0S6
D	501	CYS	ALA	engineered mutation	UNP Q2N0S6
D	509	ARG	-	expression tag	UNP Q2N0S6

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Chain	Residue	Modelled	Actual	Comment	Reference
D	510	ARG	-	expression tag	UNP Q2N0S6
D	511	ARG	-	expression tag	UNP Q2N0S6
D	512	ARG	-	expression tag	UNP Q2N0S6
D	513	ARG	-	expression tag	UNP Q2N0S6
E	332	ASN	THR	engineered mutation	UNP Q2N0S6
E	501	CYS	ALA	engineered mutation	UNP Q2N0S6
E	509	ARG	-	expression tag	UNP Q2N0S6
E	510	ARG	-	expression tag	UNP Q2N0S6
E	511	ARG	-	expression tag	UNP Q2N0S6
E	512	ARG	-	expression tag	UNP Q2N0S6
E	513	ARG	-	expression tag	UNP Q2N0S6
F	332	ASN	THR	engineered mutation	UNP Q2N0S6
F	501	CYS	ALA	engineered mutation	UNP Q2N0S6
F	509	ARG	-	expression tag	UNP Q2N0S6
F	510	ARG	-	expression tag	UNP Q2N0S6
F	511	ARG	-	expression tag	UNP Q2N0S6
F	512	ARG	-	expression tag	UNP Q2N0S6
F	513	ARG	-	expression tag	UNP Q2N0S6

- Molecule 3 is a protein called PG9 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	229	Total	C	N	O	S	0	0
			1772	1117	297	349	9		

- Molecule 4 is a protein called 8ANC195 Fab heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	224	Total	C	N	O	S	0	0
			1614	1022	269	318	5		
4	O	224	Total	C	N	O	S	0	0
			1614	1022	269	318	5		
4	Q	224	Total	C	N	O	S	0	0
			1614	1022	269	318	5		

- Molecule 5 is a protein called 8ANC195 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	214	Total	C	N	O	S	0	0
			1560	976	260	319	5		
5	P	214	Total	C	N	O	S	0	0
			1560	976	260	319	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	214	Total	C	N	O	S	0	0
			1560	976	260	319	5		

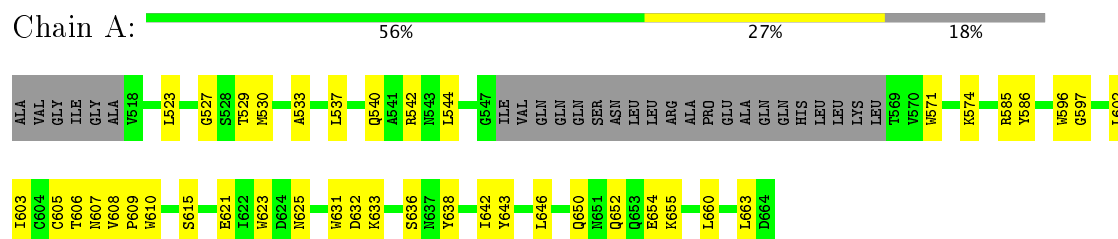
- Molecule 6 is a protein called PG9 Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	211	Total	C	N	O	S	0	0
			1566	974	267	321	4		

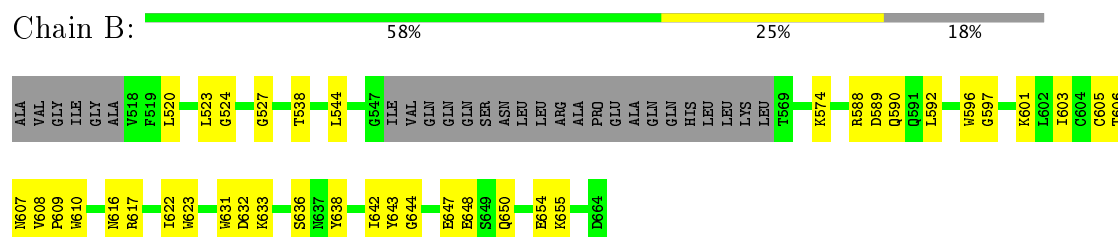
3 Residue-property plots

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. 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. 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.

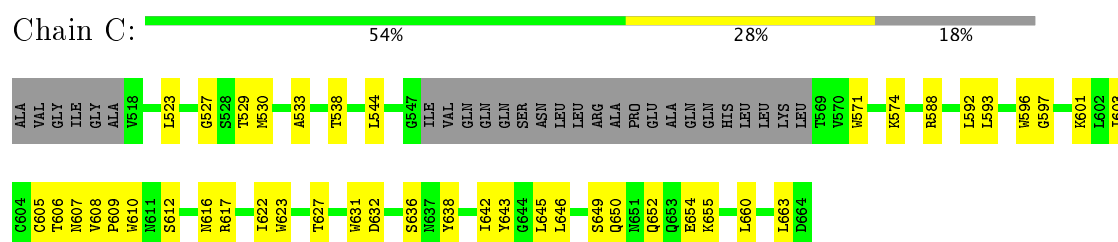
• Molecule 1: Envelope glycoprotein gp160



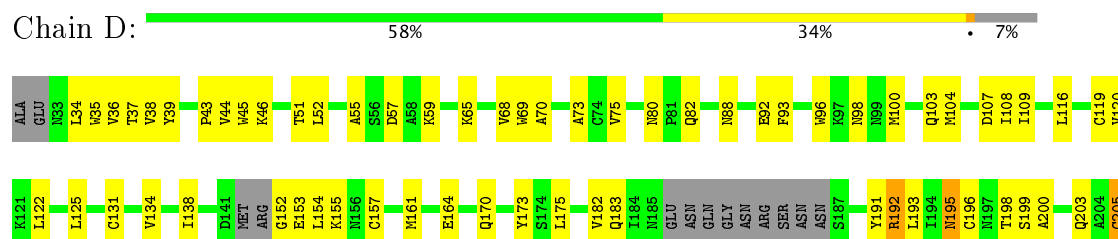
• Molecule 1: Envelope glycoprotein gp160



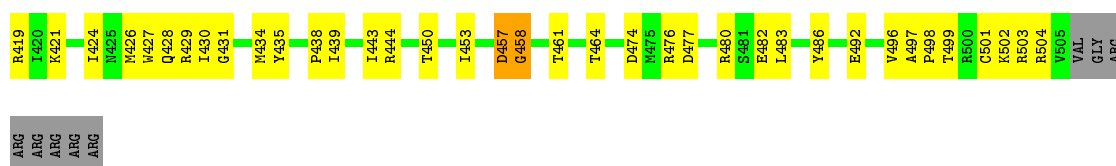
• Molecule 1: Envelope glycoprotein gp160



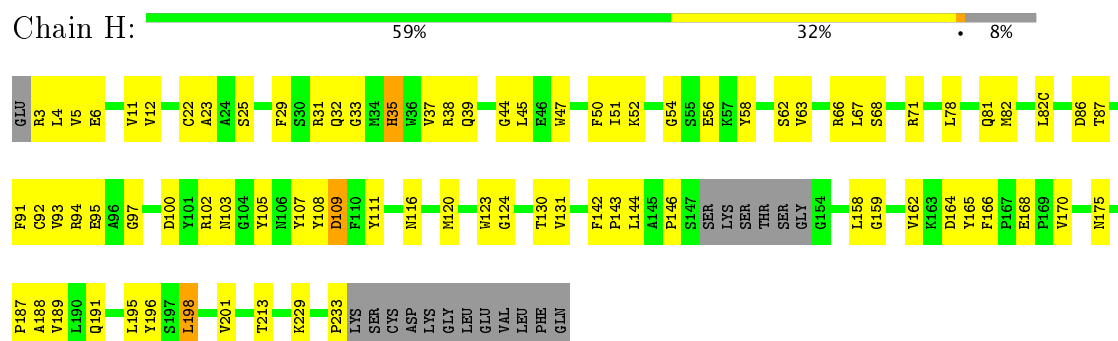
• Molecule 2: Envelope glycoprotein gp160



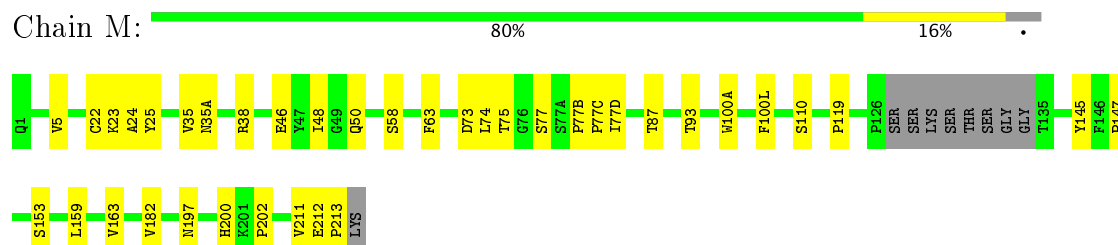




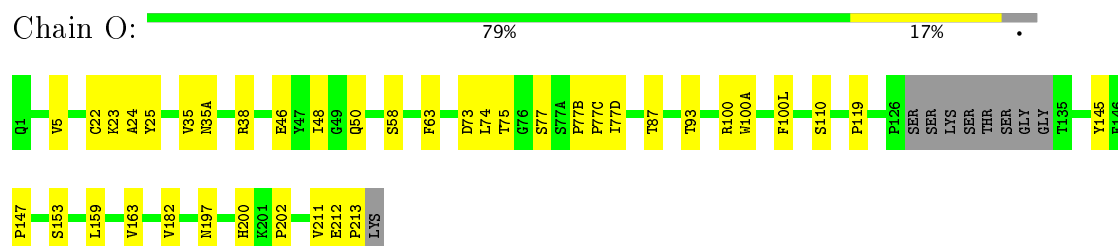
• Molecule 3: PG9 Fab heavy chain



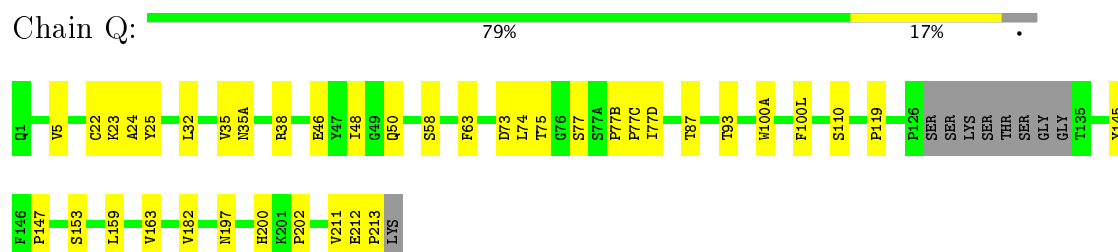
• Molecule 4: 8ANC195 Fab heavy chain




• Molecule 4: 8ANC195 Fab heavy chain



• Molecule 4: 8ANC195 Fab heavy chain




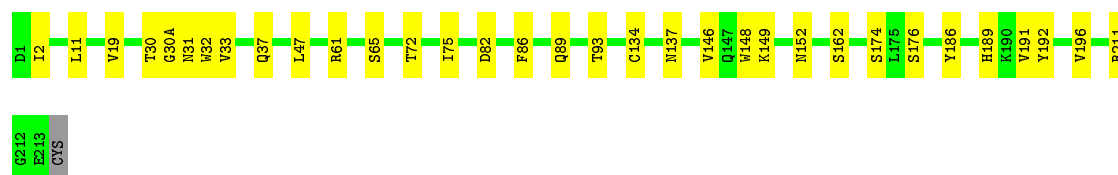
• Molecule 5: 8ANC195 Fab light chain

Chain N:  86% 13%




- Molecule 5: 8ANC195 Fab light chain

Chain P:  84% 15%



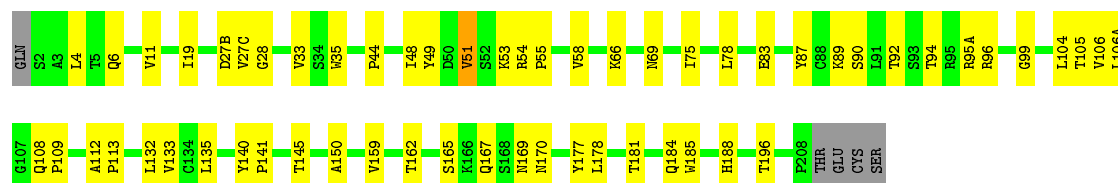
- Molecule 5: 8ANC195 Fab light chain

Chain R:  85% 14%



- Molecule 6: PG9 Fab light chain

Chain L:  71% 26%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	9500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 >2	RMSZ	# Z >2
1	A	0.27	0/1019	0.55	0/1382
1	B	0.27	0/1019	0.58	0/1382
1	C	0.26	0/1019	0.56	0/1382
2	D	0.28	0/3605	0.53	2/4895 (0.0%)
2	E	0.28	0/3605	0.53	2/4895 (0.0%)
2	F	0.28	0/3605	0.53	2/4895 (0.0%)
3	H	0.32	0/1786	0.62	1/2429 (0.0%)
4	M	0.31	1/1656 (0.1%)	0.50	1/2280 (0.0%)
4	O	0.31	1/1656 (0.1%)	0.50	1/2280 (0.0%)
4	Q	0.31	1/1656 (0.1%)	0.50	1/2280 (0.0%)
5	N	0.26	0/1594	0.46	0/2181
5	P	0.26	0/1594	0.46	0/2181
5	R	0.26	0/1594	0.46	0/2181
6	L	0.29	0/1601	0.51	0/2180
All	All	0.28	3/27009 (0.0%)	0.52	10/36823 (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
3	H	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	213	PRO	N-CD	5.22	1.55	1.47
4	Q	213	PRO	N-CD	5.22	1.55	1.47
4	O	213	PRO	N-CD	5.18	1.55	1.47

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	458	GLY	O-C-N	-8.00	109.60	123.20
2	E	458	GLY	O-C-N	-7.99	109.62	123.20
2	F	458	GLY	O-C-N	-7.98	109.64	123.20
3	H	198	LEU	CA-CB-CG	6.12	129.38	115.30
2	E	458	GLY	CA-C-N	5.83	127.85	116.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	35	HIS	Peptide

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	A	1001	0	978	177	0
1	B	1001	0	977	151	0
1	C	1001	0	977	144	0
2	D	3532	0	3480	261	0
2	E	3532	0	3479	261	0
2	F	3532	0	3479	232	0
3	H	1772	0	1670	98	0
4	M	1614	0	1511	46	0
4	O	1614	0	1511	49	0
4	Q	1614	0	1511	47	0
5	N	1560	0	1438	21	0
5	P	1560	0	1438	22	0
5	R	1560	0	1438	27	0
6	L	1566	0	1533	69	0
All	All	26459	0	25420	1072	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 21.

The worst 5 of 1072 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:636:SER:CB	4:O:100(A):TRP:HZ3	1.15	1.58
1:A:605:CYS:SG	2:D:501:CYS:SG	1.47	1.44
3:H:95:GLU:HG3	6:L:89:LYS:NZ	1.30	1.44
1:A:636:SER:CB	4:O:100(A):TRP:CZ3	1.99	1.43
3:H:95:GLU:CG	6:L:89:LYS:NZ	1.79	1.43

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 PDB entries followed by that with respect to all EM entries.

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	122/153 (80%)	112 (92%)	10 (8%)	0	100	100
1	B	122/153 (80%)	110 (90%)	12 (10%)	0	100	100
1	C	122/153 (80%)	114 (93%)	8 (7%)	0	100	100
2	D	441/481 (92%)	406 (92%)	33 (8%)	2 (0%)	32	74
2	E	441/481 (92%)	408 (92%)	31 (7%)	2 (0%)	32	74
2	F	441/481 (92%)	407 (92%)	32 (7%)	2 (0%)	32	74
3	H	223/248 (90%)	201 (90%)	21 (9%)	1 (0%)	38	77
4	M	220/233 (94%)	210 (96%)	10 (4%)	0	100	100
4	O	220/233 (94%)	210 (96%)	10 (4%)	0	100	100
4	Q	220/233 (94%)	210 (96%)	10 (4%)	0	100	100
5	N	212/215 (99%)	209 (99%)	3 (1%)	0	100	100
5	P	212/215 (99%)	209 (99%)	3 (1%)	0	100	100
5	R	212/215 (99%)	209 (99%)	3 (1%)	0	100	100
6	L	209/216 (97%)	204 (98%)	4 (2%)	1 (0%)	32	74
All	All	3417/3710 (92%)	3219 (94%)	190 (6%)	8 (0%)	54	84

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	51	VAL
2	D	138	ILE
2	E	138	ILE
2	F	138	ILE
2	D	457	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	108/129 (84%)	108 (100%)	0	100	100
1	B	108/129 (84%)	108 (100%)	0	100	100
1	C	108/129 (84%)	108 (100%)	0	100	100
2	D	401/428 (94%)	395 (98%)	6 (2%)	70	85
2	E	401/428 (94%)	395 (98%)	6 (2%)	70	85
2	F	401/428 (94%)	395 (98%)	6 (2%)	70	85
3	H	191/208 (92%)	191 (100%)	0	100	100
4	M	175/199 (88%)	175 (100%)	0	100	100
4	O	175/199 (88%)	175 (100%)	0	100	100
4	Q	175/199 (88%)	175 (100%)	0	100	100
5	N	163/182 (90%)	163 (100%)	0	100	100
5	P	163/182 (90%)	163 (100%)	0	100	100
5	R	163/182 (90%)	163 (100%)	0	100	100
6	L	178/183 (97%)	178 (100%)	0	100	100
All	All	2910/3205 (91%)	2892 (99%)	18 (1%)	89	94

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	195	ASN
2	E	205	CYS
2	F	195	ASN

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Mol	Chain	Res	Type
2	E	57	ASP
2	E	192	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	607	ASN
1	C	650	GLN
3	H	184	HIS
1	B	652	GLN
5	N	31	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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$
3	TYS	H	107	3	16,16,17	2.11	3 (18%)	19,22,24	0.85	0
3	TYS	H	108	3	16,16,17	2.08	3 (18%)	19,22,24	1.21	2 (10%)

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
3	TYS	H	107	3	-	0/9/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TYS	H	108	3	-	0/9/11/13	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	107	TYS	OH-S	-5.52	1.53	1.63
3	H	108	TYS	OH-S	-5.37	1.54	1.63
3	H	107	TYS	OH-CZ	-3.54	1.37	1.42
3	H	108	TYS	OH-CZ	-3.32	1.37	1.42
3	H	108	TYS	O1-S	4.87	1.63	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	108	TYS	CG-CB-CA	-3.75	106.74	114.29
3	H	108	TYS	O-C-CA	-2.32	118.61	125.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	107	TYS	2	0
3	H	108	TYS	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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.