W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2023 – 11:02 AM EDT

PDB ID	:	2I5Y
Title	:	Crystal structure of CD4M47, a scorpion-toxin mimic of CD4, in complex with HIV-1 YU2 GP120 envelope glycoprotein and anti-HIV-1 antibody 17B
Authors	:	Huang, C.-C.; Kwong, P.D.
Deposited on	:	2006-08-26
Resolution	:	2.20 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

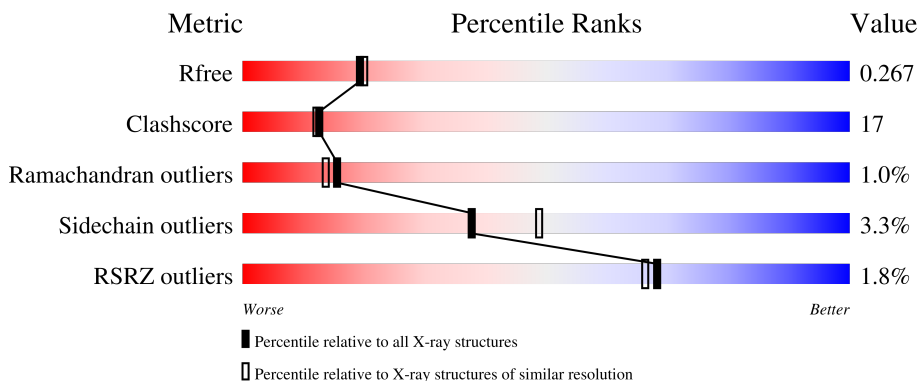|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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	Percentile Ranks	Value
Rfree		0.267
Clashscore		17
Ramachandran outliers		1.0%
Sidechain outliers		3.3%
RSRZ outliers		1.8%

Worse *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	G	313	2%; 71% 24% · ·
1	P	313	5%; 58% 35% · ·
2	L	214	70% 28% ·
2	Q	214	66% 32% ·
3	H	229	%; 71% 24% · ·

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WORLDWIDE PDB PROTEIN DATA BANK

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Mol	Chain	Length	Quality of chain
3	R	229	66% · 31% · ·
4	M	27	70% · 26% ·
4	S	27	81% · 11% · ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	P	741	X	-	-	X
5	NAG	P	789	X	-	-	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 12533 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 Exterior membrane glycoprotein(GP120).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	302	Total 2348	C 1471	N 408	O 449	S 20	0	0	0
1	P	300	Total 2332	C 1463	N 405	O 444	S 20	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	79	GLY	-	cloning artifact	UNP P35961
G	80	ALA	-	cloning artifact	UNP P35961
G	81	ARG	-	cloning artifact	UNP P35961
G	82	SER	-	cloning artifact	UNP P35961
G	128	GLY	-	linker	UNP P35961
G	129	ALA	-	linker	UNP P35961
G	194	GLY	-	linker	UNP P35961
G	298	GLY	-	linker	UNP P35961
G	299	ALA	-	linker	UNP P35961
G	329	GLY	-	linker	UNP P35961
P	79	GLY	-	cloning artifact	UNP P35961
P	80	ALA	-	cloning artifact	UNP P35961
P	81	ARG	-	cloning artifact	UNP P35961
P	82	SER	-	cloning artifact	UNP P35961
P	128	GLY	-	linker	UNP P35961
P	129	ALA	-	linker	UNP P35961
P	194	GLY	-	linker	UNP P35961
P	298	GLY	-	linker	UNP P35961
P	299	ALA	-	linker	UNP P35961
P	329	GLY	-	linker	UNP P35961

- Molecule 2 is a protein called Antibody 17B Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	214	Total 1647	C 1028	N 282	O 332	S 5	0	0	0
2	Q	214	Total 1647	C 1028	N 282	O 332	S 5	0	0	0

- Molecule 3 is a protein called Antibody 17B Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	224	Total 1688	C 1067	N 283	O 333	S 5	0	0	0
3	R	223	Total 1684	C 1065	N 282	O 332	S 5	0	0	0

- Molecule 4 is a protein called CD4M47, SCORPION-TOXIN MIMIC OF CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	27	Total 207	C 132	N 38	O 31	S 6	0	0	0
4	S	27	Total 207	C 132	N 38	O 31	S 6	0	0	0

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
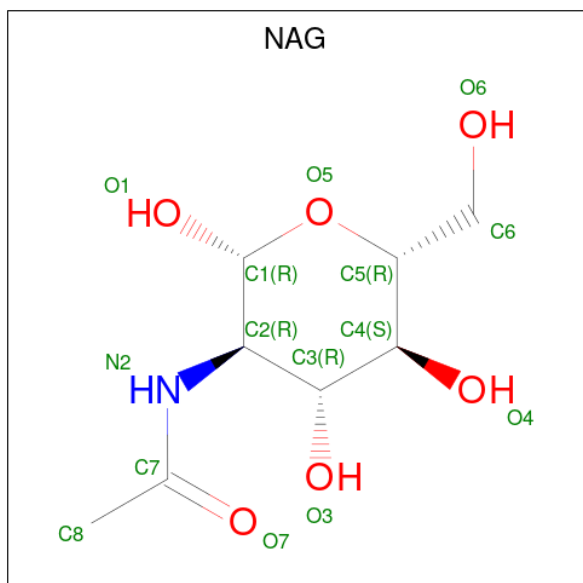
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total 14	C 8	N 1	O 5	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		
5	P	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	106	Total	O	0	0
			106	106		
6	L	120	Total	O	0	0
			120	120		
6	H	119	Total	O	0	0
			119	119		
6	M	4	Total	O	0	0
			4	4		

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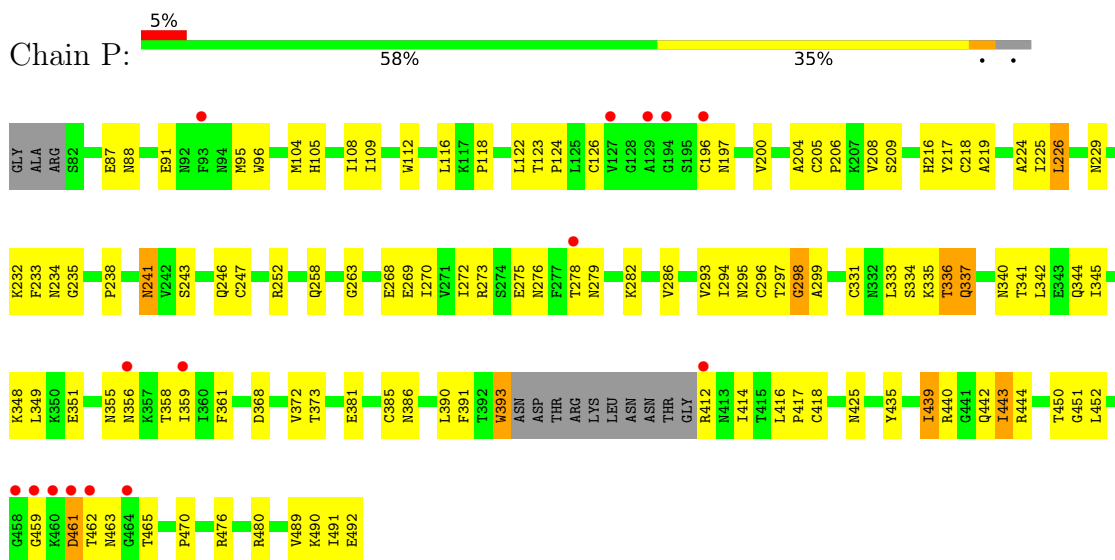| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	P	61	Total 61	O 61	0	0
6	Q	69	Total 69	O 69	0	0
6	R	65	Total 65	O 65	0	0
6	S	5	Total 5	O 5	0	0

3 Residue-property plots ⓘ

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.
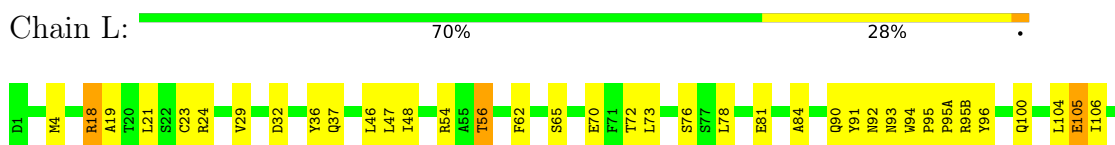
- Molecule 1: Exterior membrane glycoprotein(GP120)

- Molecule 1: Exterior membrane glycoprotein(GP120)

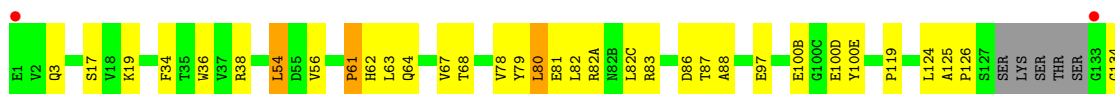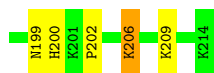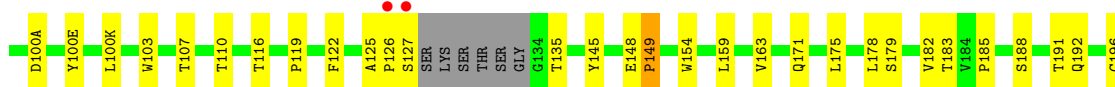- Molecule 2: Antibody 17B Light chain

V110 P113 S121 L125 L135 L136 N137 N138 F139 D151 N152 A153 L154 S159 Q160 Q166 Y173 S174 L175 S176 S177 T178 K183 E187 K188 H189 K190 V191 Y192 A193 Q199 G200 L201 V205 S208 G212

• Molecule 2: Antibody 17B Light chain

Chain Q:

66%   32%

D1 I2 V3 V13 E17 R18 A19 S26 V29 S30 S31 D32 Q37 P44 R45 L46 L47 R54 A55 V58 R61 L73 T74 I75 L78 F83 Q90 Y91 N92 N93 W94 P95 P95A R95B Y96 R103 L104 E105 I106 K107 R108 T109 P113 S114 V115

P120 Q124 L125 A130 S131 V132 L135 N138 F139 Y140 P141 R142 K145 V150 D151 L154 N158 V163 Q166 D167 D170 S171 T172 Y173 S174 L175 S176 L179 K183 E187 K190 V191 Y192 A193 C194 T197 L201 T206 K207 S208 F209

N210 R211 G212

• Molecule 3: Antibody 17B Heavy chain

Chain H:

%
71%   24%

E1 V2 Q3 S17 V18 K19 F34 T35 W36 V37 R38 L54 D55 V56 P61 H62 L63 Q64 V67 T68 V78 Y79 L80 E81 L82 R82A N82B L82C R83 D86 T87 A88 E97 E100B G100C E100D Y100E P119 L124 A125 P126 S127 SER LYS SER THR SER G133 G134

T135 L138 K143 D144 Y145 F146 P147 E148 P149 V150 T151 L159 L175 L178 V182 T183 T193 Y194 I195 C196 N197 V198 N199 H200 K201 P202 S203 N204 T205 K206 K210 V211 E212 P213 K214

• Molecule 3: Antibody 17B Heavy chain

Chain R:

2%
66%   31%

E1 E6 V11 K12 K13 S17 K23 D27 T28 F29 I30 F34 T35 W36 V37 R38 E46 G49 R50 I51 I52 T52A I53 L54 A57 H58 Y59 L63 R66 V67 T68 I69 T70 V78 Y79 L80 E81 L82 R82A R83 S84 D85 D86 T87 A88 A93

D100A Y100E L100K W103 T107 T110 T116 P119 F122 A125 P126 S127 SER LYS SER THR SER GLY G134 T135 Y145 E148 P149 W154 L159 V163 Q171 L175 L178 S179 V182 T183 V184 P185 S188 T191 Q192 C196

N199 H200 K201 P202 K206 K209 K214

• Molecule 4: CD4M47, SCORPION-TOXIN MIMIC OF CD4

Chain M:

70%   26%

MPT1 N2 L3 Q7 L8 R9 C10 K11 S12 L13 R18 F23 X27

• Molecule 4: CD4M47, SCORPION-TOXIN MIMIC OF CD4

Chain S:

81%   11%

MPT1 N2 L3 H4 Q7 F23 X27

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.44Å 158.16Å 109.93Å 90.00° 93.67° 90.00°	Depositor
Resolution (Å)	19.99 – 2.20 38.01 – 2.19	Depositor EDS
% Data completeness (in resolution range)	78.6 (19.99-2.20) 78.1 (38.01-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.273 0.208 , 0.267	Depositor DCC
R_{free} test set	7489 reflections (10.10%)	wwPDB-VP
Wilson B-factor (Å^2)	31.1	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.8	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12533	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 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BIF, DPR, NAG, VLM, MPT

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	G	0.51	0/2393	0.63	0/3242
1	P	0.49	0/2377	0.59	0/3220
2	L	0.52	0/1684	0.70	0/2288
2	Q	0.51	0/1684	0.64	0/2288
3	H	0.52	0/1727	0.69	0/2351
3	R	0.51	0/1723	0.65	0/2346
4	M	0.49	0/169	0.63	0/221
4	S	0.50	0/169	0.59	0/221
All	All	0.51	0/11926	0.65	0/16177

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	G	2348	0	2300	70	0
1	P	2332	0	2289	107	0
2	L	1647	0	1593	55	0
2	Q	1647	0	1593	60	0
3	H	1688	0	1655	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	1684	0	1652	51	0
4	M	207	0	204	9	0
4	S	207	0	204	3	0
5	G	112	0	104	7	0
5	P	112	0	104	7	0
6	G	106	0	0	4	0
6	H	119	0	0	2	0
6	L	120	0	0	3	0
6	M	4	0	0	2	0
6	P	61	0	0	6	0
6	Q	69	0	0	2	0
6	R	65	0	0	0	0
6	S	5	0	0	0	0
All	All	12533	0	11698	396	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 17.

The worst 5 of 396 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)
2:L:29:VAL:HG11	2:L:90:GLN:HB2	1.49	0.94
2:L:113:PRO:HB3	2:L:139:PHE:HB3	1.53	0.90
3:H:63:LEU:HD13	3:H:67:VAL:HG11	1.54	0.87
3:R:135:THR:HG23	3:R:183:THR:HG23	1.58	0.86
1:P:224:ALA:HB2	1:P:491:ILE:HD11	1.60	0.84

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	G	298/313 (95%)	277 (93%)	17 (6%)	4 (1%)	12	9
1	P	296/313 (95%)	266 (90%)	25 (8%)	5 (2%)	9	6
2	L	212/214 (99%)	200 (94%)	11 (5%)	1 (0%)	29	31
2	Q	212/214 (99%)	193 (91%)	18 (8%)	1 (0%)	29	31
3	H	220/229 (96%)	204 (93%)	13 (6%)	3 (1%)	11	8
3	R	219/229 (96%)	208 (95%)	11 (5%)	0	100	100
4	M	23/27 (85%)	22 (96%)	1 (4%)	0	100	100
4	S	23/27 (85%)	22 (96%)	0	1 (4%)	2	1
All	All	1503/1566 (96%)	1392 (93%)	96 (6%)	15 (1%)	15	14

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	62	HIS
1	G	298	GLY
1	G	462	THR
3	H	61	PRO
1	P	268	GLU

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 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	G	267/276 (97%)	261 (98%)	6 (2%)	52	65
1	P	265/276 (96%)	256 (97%)	9 (3%)	37	47
2	L	184/184 (100%)	177 (96%)	7 (4%)	33	42
2	Q	184/184 (100%)	178 (97%)	6 (3%)	38	49
3	H	188/193 (97%)	178 (95%)	10 (5%)	22	27
3	R	188/193 (97%)	184 (98%)	4 (2%)	53	67
4	M	19/19 (100%)	19 (100%)	0	100	100
4	S	19/19 (100%)	18 (95%)	1 (5%)	22	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1314/1344 (98%)	1271 (97%)	43 (3%)	38	49

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	356	ASN
2	Q	90	GLN
1	P	393	TRP
2	Q	31	SER
2	Q	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	Q	166	GLN
2	Q	199	GLN
3	H	164	HIS
3	H	3	GLN
2	Q	210	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\#|Z| > 2$
4	BIF	M	23	4	16,18,19	1.51	3 (18%)	16,23,25	1.63	3 (18%)
4	BIF	S	23	4	16,18,19	1.79	4 (25%)	16,23,25	1.46	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	VLM	S	27	4	6,7,7	1.25	1 (16%)	7,9,9	0.72	0
4	VLM	M	27	4	6,7,7	1.27	1 (16%)	7,9,9	0.16	0

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	BIF	M	23	4	-	0/5/10/12	0/2/2/2
4	BIF	S	23	4	-	0/5/10/12	0/2/2/2
4	VLM	S	27	4	-	0/7/8/8	-
4	VLM	M	27	4	-	0/7/8/8	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	27	VLM	C-NT	-2.99	1.25	1.32
4	S	23	BIF	C8-C13	2.94	1.43	1.36
4	S	27	VLM	C-NT	-2.78	1.25	1.32
4	S	23	BIF	C10-C11	2.75	1.43	1.36
4	S	23	BIF	C13-C12	2.66	1.48	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	23	BIF	CG-CB-CA	3.99	122.19	114.10
4	M	23	BIF	C13-C12-C11	-3.12	115.88	118.65
4	S	23	BIF	C13-C12-C11	-3.10	115.89	118.65
4	S	23	BIF	CG-CB-CA	3.10	120.37	114.10
4	S	23	BIF	CE2-CZ-CE1	-2.90	116.07	118.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	23	BIF	1	0
4	S	23	BIF	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 ligands 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
5	NAG	G	795	1	14,14,15	0.51	0	17,19,21	0.66	0
5	NAG	G	886	1	14,14,15	0.48	0	17,19,21	0.62	0
5	NAG	G	588	1	14,14,15	0.59	0	17,19,21	0.69	0
5	NAG	P	741	1	14,14,15	0.65	0	17,19,21	0.62	0
5	NAG	P	789	1	14,14,15	0.64	0	17,19,21	0.86	1 (5%)
5	NAG	P	588	1	14,14,15	0.54	0	17,19,21	0.83	1 (5%)
5	NAG	G	776	1	14,14,15	0.46	0	17,19,21	0.80	1 (5%)
5	NAG	P	776	1	14,14,15	0.64	0	17,19,21	0.71	1 (5%)
5	NAG	P	734	1	14,14,15	0.65	0	17,19,21	0.72	0
5	NAG	P	795	1	14,14,15	0.56	0	17,19,21	0.63	0
5	NAG	P	762	1	14,14,15	0.55	0	17,19,21	0.82	0
5	NAG	G	789	1	14,14,15	0.53	0	17,19,21	0.67	0
5	NAG	G	741	1	14,14,15	0.62	0	17,19,21	0.60	0
5	NAG	G	762	1	14,14,15	0.47	0	17,19,21	0.70	0
5	NAG	G	734	1	14,14,15	0.50	0	17,19,21	0.68	0
5	NAG	P	886	1	14,14,15	0.51	0	17,19,21	0.67	0

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
5	NAG	G	795	1	-	2/6/23/26	0/1/1/1
5	NAG	P	741	1	1/1/5/7	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	588	1	-	2/6/23/26	0/1/1/1
5	NAG	G	886	1	-	3/6/23/26	0/1/1/1
5	NAG	P	789	1	1/1/5/7	2/6/23/26	0/1/1/1
5	NAG	P	588	1	-	4/6/23/26	0/1/1/1
5	NAG	G	776	1	-	2/6/23/26	0/1/1/1
5	NAG	P	776	1	-	2/6/23/26	0/1/1/1
5	NAG	P	734	1	-	5/6/23/26	0/1/1/1
5	NAG	P	795	1	-	4/6/23/26	0/1/1/1
5	NAG	P	762	1	-	4/6/23/26	0/1/1/1
5	NAG	G	789	1	-	2/6/23/26	0/1/1/1
5	NAG	G	741	1	-	2/6/23/26	0/1/1/1
5	NAG	G	762	1	-	0/6/23/26	0/1/1/1
5	NAG	G	734	1	-	5/6/23/26	0/1/1/1
5	NAG	P	886	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	776	NAG	C2-N2-C7	-2.54	119.29	122.90
5	P	588	NAG	C2-N2-C7	-2.20	119.77	122.90
5	P	776	NAG	C2-N2-C7	-2.13	119.87	122.90
5	P	789	NAG	C2-N2-C7	-2.00	120.06	122.90

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	P	741	NAG	C1
5	P	789	NAG	C1

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	588	NAG	C8-C7-N2-C2
5	G	588	NAG	O7-C7-N2-C2
5	G	734	NAG	C8-C7-N2-C2
5	G	734	NAG	O7-C7-N2-C2
5	G	886	NAG	C8-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	886	NAG	2	0
5	P	789	NAG	1	0
5	P	588	NAG	1	0
5	P	776	NAG	2	0
5	P	795	NAG	1	0
5	P	762	NAG	1	0
5	G	789	NAG	2	0
5	G	762	NAG	1	0
5	G	734	NAG	2	0
5	P	886	NAG	1	0

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, 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	G	302/313 (96%)	0.08	6 (1%)	65	63	19, 36, 66, 78	0
1	P	300/313 (95%)	0.31	15 (5%)	28	27	31, 50, 77, 95	0
2	L	214/214 (100%)	-0.38	0	100	100	16, 31, 46, 52	0
2	Q	214/214 (100%)	-0.12	1 (0%)	91	90	22, 41, 67, 74	0
3	H	224/229 (97%)	-0.29	2 (0%)	84	83	18, 30, 47, 69	0
3	R	223/229 (97%)	-0.21	4 (1%)	68	66	25, 39, 52, 81	0
4	M	23/27 (85%)	0.04	0	100	100	25, 43, 52, 57	0
4	S	23/27 (85%)	-0.01	0	100	100	25, 42, 52, 57	0
All	All	1523/1566 (97%)	-0.06	28 (1%)	68	66	16, 38, 67, 95	0

The worst 5 of 28 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	460	LYS	5.5
1	P	459	GLY	5.3
1	P	458	GLY	4.9
1	P	127	VAL	4.5
1	P	464	GLY	4.5

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

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
4	DPR	S	21	7/8	0.91	0.12	23,27,27,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BIF	S	23	17/18	0.92	0.13	30,32,36,36	0
4	VLM	S	27	8/8	0.93	0.17	44,47,48,48	0
4	VLM	M	27	8/8	0.94	0.15	39,42,42,44	0
4	DPR	M	21	7/8	0.95	0.15	23,27,27,30	0
4	BIF	M	23	17/18	0.96	0.16	19,22,24,24	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
5	NAG	P	741	14/15	0.39	0.41	79,83,87,88	0
5	NAG	P	886	14/15	0.66	0.21	67,70,73,76	0
5	NAG	P	789	14/15	0.71	0.23	78,80,83,83	0
5	NAG	P	734	14/15	0.72	0.33	83,86,88,88	0
5	NAG	G	741	14/15	0.77	0.29	65,67,69,69	0
5	NAG	P	776	14/15	0.80	0.29	58,60,62,64	0
5	NAG	P	588	14/15	0.84	0.20	67,68,69,70	0
5	NAG	G	734	14/15	0.87	0.25	59,63,66,66	0
5	NAG	P	795	14/15	0.87	0.28	63,65,67,68	0
5	NAG	G	886	14/15	0.87	0.12	45,51,54,54	0
5	NAG	G	795	14/15	0.90	0.18	52,57,58,59	0
5	NAG	G	588	14/15	0.91	0.19	60,61,63,63	0
5	NAG	G	789	14/15	0.92	0.09	37,39,42,43	0
5	NAG	G	776	14/15	0.94	0.17	46,49,52,53	0
5	NAG	P	762	14/15	0.95	0.10	43,45,48,49	0
5	NAG	G	762	14/15	0.96	0.10	30,32,34,37	0

6.5 Other polymers ⓘ

There are no such residues in this entry.