



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 10:25 AM BST

PDB ID : 2I60
Title : Crystal structure of [Phe23]M47, 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 : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 2.13.1
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) : 2.13.1

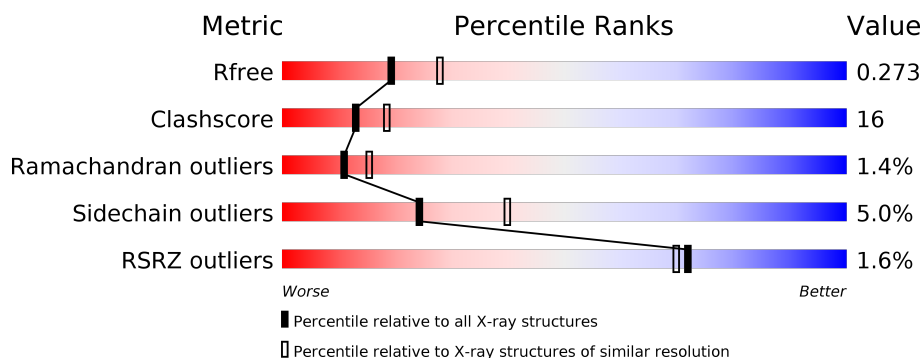
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	G	313	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>29%</div> <div>• •</div> </div> </div>
1	P	313	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>38%</div> <div>• •</div> </div> </div>
2	L	214	<div> <div></div> <div> <div></div> <div>71%</div> <div>28%</div> <div>•</div> </div> </div>
2	Q	214	<div> <div>2%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>5%</div> </div> </div>
3	H	229	<div> <div></div> <div> <div></div> <div>69%</div> <div>24%</div> <div>• •</div> </div> </div>
3	R	229	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	M	27	 70% 30%
4	S	27	 67% 26% 7%

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	G	886	X	-	-	-
5	NAG	P	734	X	-	-	-
5	NAG	P	741	X	-	-	X
5	NAG	P	789	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12434 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	301	Total	C	N	O	S	0	0	0
			2342	1468	407	447	20			
1	P	300	Total	C	N	O	S	0	0	0
			2332	1463	405	444	20			

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	C	N	O	S	0	0	0
			1647	1028	282	332	5			
2	Q	214	Total	C	N	O	S	0	0	0
			1647	1028	282	332	5			

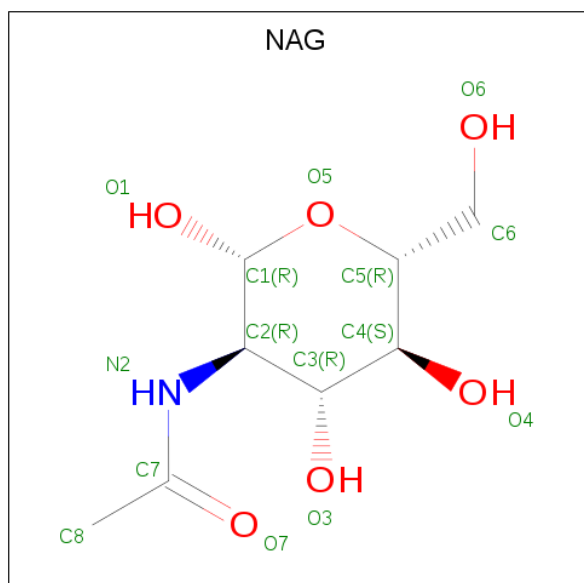
- Molecule 3 is a protein called ANTIBODY 17B HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	221	Total	C	N	O	S	0	0	0
			1669	1057	280	327	5			
3	R	222	Total	C	N	O	S	0	0	0
			1678	1062	281	330	5			

- Molecule 4 is a protein called [PHE23]M47, SCORPION-TOXIN MIMIC OF CD4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	27	Total	C	N	O	S	0	0	0
			201	126	38	31	6			
4	S	27	Total	C	N	O	S	0	0	0
			201	126	38	31	6			

- 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	C	N	O	0	0
			14	8	1	5		

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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		

- Molecule 6 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	G	1	Total	C	O	0	0
			4	3	1		
6	P	1	Total	C	O	0	0
			4	3	1		

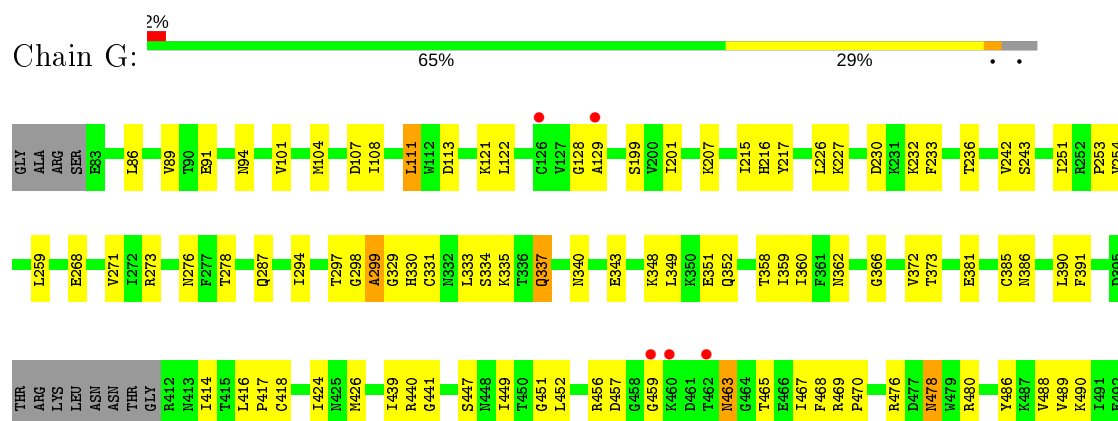
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	83	Total	O	0	0
			83	83		
7	L	85	Total	O	0	0
			85	85		
7	H	112	Total	O	0	0
			112	112		
7	M	7	Total	O	0	0
			7	7		
7	P	59	Total	O	0	0
			59	59		
7	Q	70	Total	O	0	0
			70	70		
7	R	61	Total	O	0	0
			61	61		
7	S	8	Total	O	0	0
			8	8		

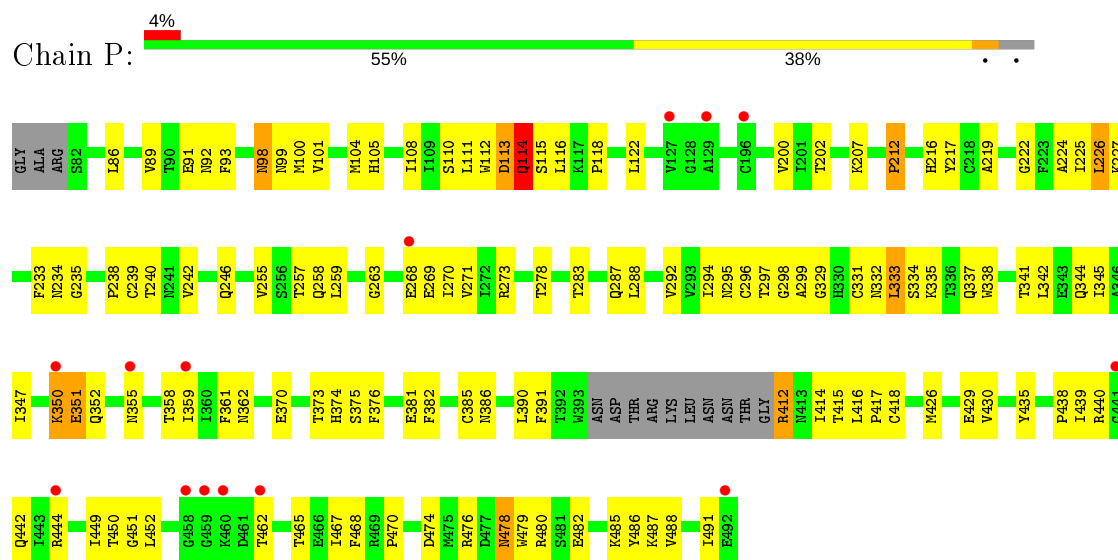
3 Residue-property plots [i](#)

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.

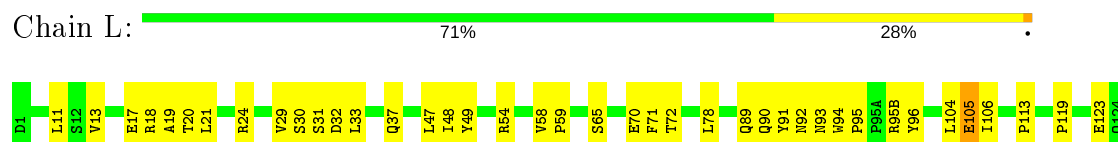
• Molecule 1: EXTERIOR MEMBRANE GLYCOPROTEIN(GP120)



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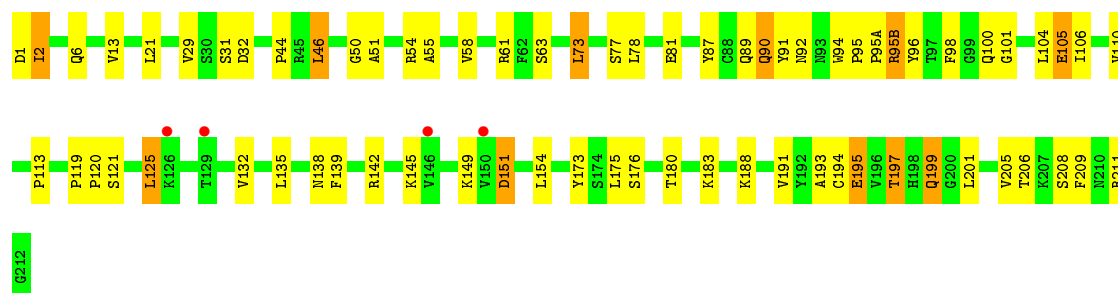


• Molecule 2: ANTIBODY 17B LIGHT CHAIN

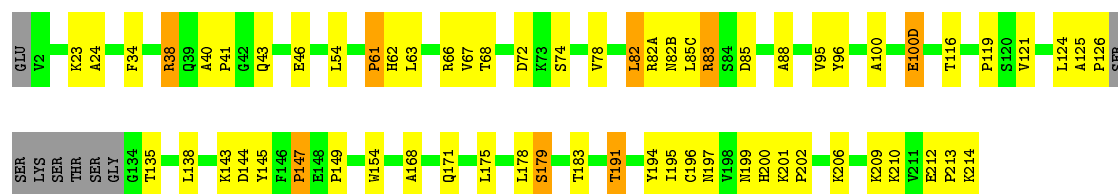




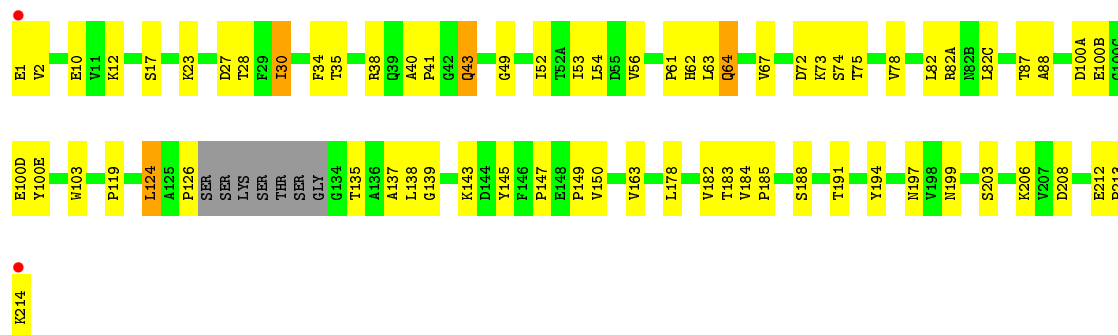
• Molecule 2: ANTIBODY 17B LIGHT CHAIN



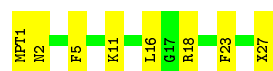
• Molecule 3: ANTIBODY 17B HEAVY CHAIN



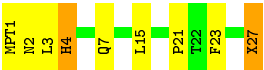
• Molecule 3: ANTIBODY 17B HEAVY CHAIN



• Molecule 4: [PHE23]M47, SCORPION-TOXIN MIMIC OF CD4



• Molecule 4: [PHE23]M47, SCORPION-TOXIN MIMIC OF CD4



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 157.76Å 109.85Å 90.00° 93.74° 90.00°	Depositor
Resolution (Å)	19.98 – 2.40 45.65 – 2.08	Depositor EDS
% Data completeness (in resolution range)	83.6 (19.98-2.40) 61.7 (45.65-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.215 , 0.281 0.207 , 0.273	Depositor DCC
R_{free} test set	6863 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	28.0	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12434	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: MPT, IPA, VLM, NAG, DPR

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	0.35	0/2387	0.63	0/3234
1	P	0.32	0/2377	0.59	0/3220
2	L	0.40	0/1684	0.64	0/2288
2	Q	0.37	0/1684	0.64	0/2288
3	H	0.39	0/1708	0.67	0/2326
3	R	0.37	0/1717	0.62	0/2338
4	M	0.40	0/182	0.62	0/240
4	S	0.39	0/182	0.68	0/240
All	All	0.37	0/11921	0.63	0/16174

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 [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	G	2342	0	2294	73	0
1	P	2332	0	2289	120	0
2	L	1647	0	1593	46	0
2	Q	1647	0	1593	53	0
3	H	1669	0	1638	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	1678	0	1647	40	0
4	M	201	0	201	7	0
4	S	201	0	201	7	0
5	G	112	0	104	7	0
5	P	112	0	104	12	0
6	G	4	0	8	0	0
6	P	4	0	8	2	0
7	G	83	0	0	2	0
7	H	112	0	0	1	0
7	L	85	0	0	3	0
7	M	7	0	0	0	0
7	P	59	0	0	5	0
7	Q	70	0	0	1	0
7	R	61	0	0	2	0
7	S	8	0	0	0	0
All	All	12434	0	11680	388	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 16.

The worst 5 of 388 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:P:439:ILE:HG13	1:P:440:ARG:H	1.18	1.04
3:H:199:ASN:HD21	3:H:206:LYS:HG3	1.30	0.94
3:H:199:ASN:ND2	3:H:206:LYS:HG3	1.84	0.92
1:P:442:GLN:HE21	1:P:444:ARG:HD2	1.33	0.92
2:L:106:ILE:H	2:L:166:GLN:HE22	1.20	0.88

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	G	297/313 (95%)	279 (94%)	12 (4%)	6 (2%)	7	9
1	P	296/313 (95%)	266 (90%)	25 (8%)	5 (2%)	9	11
2	L	212/214 (99%)	200 (94%)	11 (5%)	1 (0%)	29	41
2	Q	212/214 (99%)	194 (92%)	15 (7%)	3 (1%)	11	15
3	H	217/229 (95%)	203 (94%)	11 (5%)	3 (1%)	11	15
3	R	218/229 (95%)	203 (93%)	12 (6%)	3 (1%)	11	15
4	M	24/27 (89%)	23 (96%)	1 (4%)	0	100	100
4	S	24/27 (89%)	23 (96%)	1 (4%)	0	100	100
All	All	1500/1566 (96%)	1391 (93%)	88 (6%)	21 (1%)	11	15

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	H	62	HIS
1	P	114	GLN
2	Q	138	ASN
3	R	62	HIS
3	R	64	GLN

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	266/276 (96%)	259 (97%)	7 (3%)	46	66
1	P	265/276 (96%)	250 (94%)	15 (6%)	20	33
2	L	184/184 (100%)	179 (97%)	5 (3%)	44	65
2	Q	184/184 (100%)	170 (92%)	14 (8%)	13	20
3	H	186/193 (96%)	174 (94%)	12 (6%)	17	27
3	R	187/193 (97%)	176 (94%)	11 (6%)	19	32
4	M	20/20 (100%)	19 (95%)	1 (5%)	24	40
4	S	20/20 (100%)	19 (95%)	1 (5%)	24	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1312/1346 (98%)	1246 (95%)	66 (5%)	24	40

5 of 66 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	216	HIS
1	P	374	HIS
3	R	124	LEU
1	P	226	LEU
1	P	350	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	99	ASN
1	P	340	ASN
3	R	192	GLN
1	P	203	GLN
1	P	216	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	VLM	M	27	4	6,7,7	1.55	1 (16%)	7,9,9	0.66	0
4	VLM	S	27	4	6,7,7	1.30	1 (16%)	7,9,9	0.63	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	VLM	M	27	4	-	0/7/8/8	-
4	VLM	S	27	4	-	0/7/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	27	VLM	C-NT	-3.78	1.23	1.32
4	S	27	VLM	C-NT	-3.03	1.25	1.32

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	S	27	VLM	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

18 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	588	1	14,14,15	0.55	0	17,19,21	0.67	1 (5%)
5	NAG	P	588	1	14,14,15	0.65	0	17,19,21	0.68	0
5	NAG	P	789	1	14,14,15	0.65	0	17,19,21	0.83	1 (5%)
5	NAG	G	795	1	14,14,15	0.57	0	17,19,21	0.81	1 (5%)
6	IPA	G	501	-	3,3,3	0.65	0	3,3,3	0.31	0
5	NAG	G	741	1	14,14,15	0.55	0	17,19,21	0.70	0
5	NAG	P	741	1	14,14,15	0.65	0	17,19,21	0.72	0
5	NAG	P	734	1	14,14,15	0.63	0	17,19,21	0.67	0
5	NAG	G	734	1	14,14,15	0.53	0	17,19,21	0.68	0
5	NAG	G	762	1	14,14,15	0.50	0	17,19,21	0.76	0
5	NAG	G	776	1	14,14,15	0.51	0	17,19,21	0.77	0
5	NAG	P	795	1	14,14,15	0.58	0	17,19,21	0.81	1 (5%)
6	IPA	P	502	-	3,3,3	0.61	0	3,3,3	0.35	0
5	NAG	P	776	1	14,14,15	0.55	0	17,19,21	0.67	1 (5%)
5	NAG	P	762	1	14,14,15	0.51	0	17,19,21	0.71	0
5	NAG	G	789	1	14,14,15	0.45	0	17,19,21	0.72	0
5	NAG	P	886	1	14,14,15	0.54	0	17,19,21	0.75	1 (5%)
5	NAG	G	886	1	14,14,15	0.89	1 (7%)	17,19,21	0.83	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	P	741	1	1/1/5/7	4/6/23/26	0/1/1/1
5	NAG	P	588	1	-	3/6/23/26	0/1/1/1
5	NAG	P	789	1	1/1/5/7	3/6/23/26	0/1/1/1
5	NAG	G	795	1	-	4/6/23/26	0/1/1/1
5	NAG	G	741	1	-	0/6/23/26	0/1/1/1
5	NAG	G	588	1	-	4/6/23/26	0/1/1/1
5	NAG	P	734	1	1/1/5/7	6/6/23/26	0/1/1/1
5	NAG	G	734	1	-	5/6/23/26	0/1/1/1
5	NAG	G	762	1	-	4/6/23/26	0/1/1/1
5	NAG	G	776	1	-	4/6/23/26	0/1/1/1
5	NAG	P	795	1	-	4/6/23/26	0/1/1/1
5	NAG	P	776	1	-	4/6/23/26	0/1/1/1
5	NAG	P	762	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	G	789	1	-	0/6/23/26	0/1/1/1
5	NAG	P	886	1	-	4/6/23/26	0/1/1/1
5	NAG	G	886	1	1/1/5/7	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	886	NAG	C1-C2	2.83	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	795	NAG	C2-N2-C7	-2.40	119.48	122.90
5	P	795	NAG	C2-N2-C7	-2.39	119.50	122.90
5	P	789	NAG	C2-N2-C7	-2.29	119.64	122.90
5	P	886	NAG	C2-N2-C7	-2.08	119.94	122.90
5	P	776	NAG	C2-N2-C7	-2.07	119.96	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	P	789	NAG	C1
5	P	741	NAG	C1
5	P	734	NAG	C1
5	G	886	NAG	C1

5 of 54 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	P	789	NAG	C8-C7-N2-C2
5	P	789	NAG	O7-C7-N2-C2
5	G	795	NAG	C8-C7-N2-C2

There are no ring outliers.

13 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	588	NAG	2	0
5	P	789	NAG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	795	NAG	1	0
5	G	741	NAG	1	0
5	P	734	NAG	1	0
5	G	762	NAG	1	0
5	G	776	NAG	1	0
5	P	795	NAG	1	0
6	P	502	IPA	2	0
5	P	776	NAG	1	0
5	P	762	NAG	1	0
5	P	886	NAG	3	0
5	G	886	NAG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	301/313 (96%)	-0.13	5 (1%) 70 68	17, 35, 65, 76	0
1	P	300/313 (95%)	0.17	14 (4%) 31 30	28, 48, 73, 87	0
2	L	214/214 (100%)	-0.53	0 100 100	14, 29, 42, 48	0
2	Q	214/214 (100%)	-0.24	4 (1%) 66 64	19, 36, 59, 68	0
3	H	221/229 (96%)	-0.52	0 100 100	15, 25, 41, 73	0
3	R	222/229 (96%)	-0.41	2 (0%) 84 82	15, 33, 48, 75	0
4	M	24/27 (88%)	0.04	0 100 100	27, 40, 51, 59	0
4	S	24/27 (88%)	-0.25	0 100 100	32, 38, 47, 58	0
All	All	1520/1566 (97%)	-0.24	25 (1%) 72 70	14, 35, 64, 87	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	459	GLY	7.0
1	P	462	THR	5.1
1	P	441	GLY	4.9
1	P	458	GLY	4.3
1	P	129	ALA	4.2

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	VLM	M	27	8/8	0.85	0.19	35,36,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DPR	S	21	7/8	0.93	0.14	31,32,34,35	0
4	VLM	S	27	8/8	0.93	0.15	40,41,43,44	0
4	DPR	M	21	7/8	0.96	0.12	26,27,28,30	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [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(\AA^2)	Q<0.9
5	NAG	P	741	14/15	0.38	0.53	77,80,80,81	0
5	NAG	P	795	14/15	0.56	0.33	71,74,75,77	0
5	NAG	P	588	14/15	0.62	0.23	61,65,65,66	0
5	NAG	P	734	14/15	0.68	0.29	81,83,84,84	0
5	NAG	P	776	14/15	0.71	0.26	63,65,67,67	0
5	NAG	G	795	14/15	0.78	0.20	52,54,55,55	0
5	NAG	G	741	14/15	0.78	0.28	65,67,70,70	0
5	NAG	G	886	14/15	0.78	0.17	49,52,56,56	0
5	NAG	P	886	14/15	0.79	0.23	63,67,69,71	0
5	NAG	G	734	14/15	0.82	0.17	66,67,69,69	0
5	NAG	P	789	14/15	0.84	0.22	65,69,74,75	0
5	NAG	G	588	14/15	0.88	0.18	66,67,69,70	0
6	IPA	G	501	4/4	0.90	0.28	44,47,48,48	0
5	NAG	G	762	14/15	0.91	0.18	32,34,38,39	0
5	NAG	G	776	14/15	0.91	0.13	42,44,47,48	0
5	NAG	G	789	14/15	0.92	0.11	40,42,44,45	0
5	NAG	P	762	14/15	0.94	0.13	40,42,45,46	0
6	IPA	P	502	4/4	0.94	0.31	46,47,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.