



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 08:12 AM BST

PDB ID : 5OU7
Title : Crystal structure of the Glycoprotein VI loop truncation mutant PAVS-PAPYKN
Authors : Feitsma, L.J.; Huizinga, E.G.
Deposited on : 2017-08-23
Resolution : 1.90 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	:	2.13.1
buster-report	:	1.1.7 (2018)
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

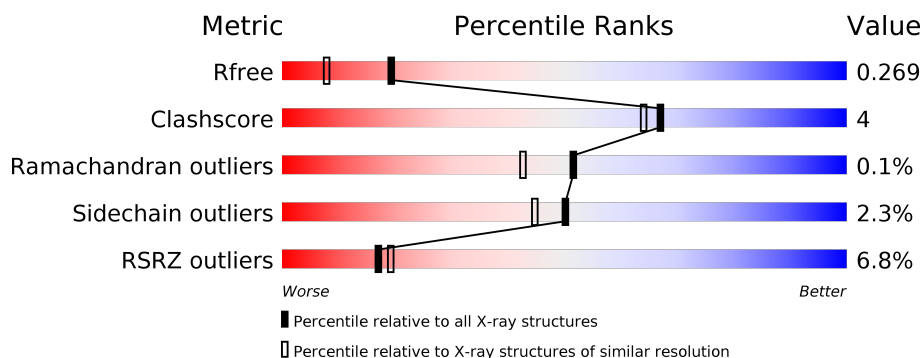
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	A	181	<div> <div>2%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
1	B	181	<div> <div>2%</div> <div>83%</div> <div>13%</div> <div>•</div> </div>
1	C	181	<div> <div>14%</div> <div>90%</div> <div>8%</div> <div>•</div> </div>
1	D	181	<div> <div>8%</div> <div>93%</div> <div>6%</div> <div>•</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	B	203	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6101 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 Platelet glycoprotein VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	13	0
			1422	917	244	256	5			
1	B	173	Total	C	N	O	S	0	15	0
			1433	927	245	256	5			
1	C	178	Total	C	N	O	S	0	4	0
			1398	898	235	260	5			
1	D	178	Total	C	N	O	S	0	4	0
			1392	893	234	260	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9HCN6
A	0	SER	-	expression tag	UNP Q9HCN6
A	?	-	PRO	deletion	UNP Q9HCN6
A	?	-	ALA	deletion	UNP Q9HCN6
A	?	-	VAL	deletion	UNP Q9HCN6
A	?	-	SER	deletion	UNP Q9HCN6
A	?	-	PRO	deletion	UNP Q9HCN6
A	?	-	ALA	deletion	UNP Q9HCN6
A	?	-	PRO	deletion	UNP Q9HCN6
A	?	-	TYR	deletion	UNP Q9HCN6
A	?	-	LYS	deletion	UNP Q9HCN6
A	?	-	ASN	deletion	UNP Q9HCN6
A	177	ALA	-	expression tag	UNP Q9HCN6
A	178	ALA	-	expression tag	UNP Q9HCN6
A	179	ALA	-	expression tag	UNP Q9HCN6
B	-1	GLY	-	expression tag	UNP Q9HCN6
B	0	SER	-	expression tag	UNP Q9HCN6
B	?	-	PRO	deletion	UNP Q9HCN6
B	?	-	ALA	deletion	UNP Q9HCN6
B	?	-	VAL	deletion	UNP Q9HCN6
B	?	-	SER	deletion	UNP Q9HCN6

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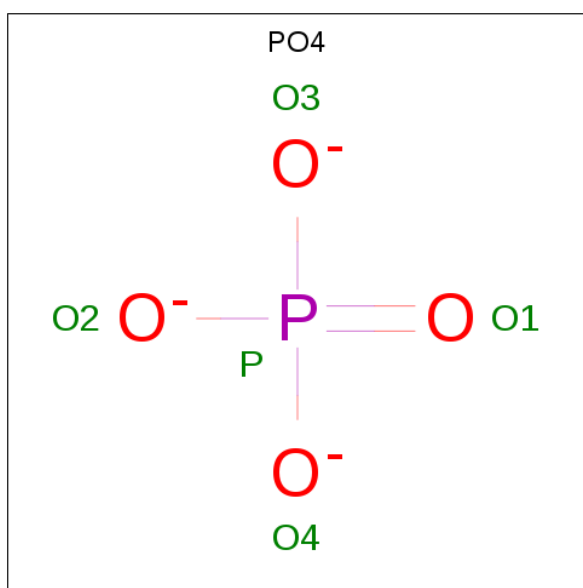
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	deletion	UNP Q9HCN6
B	?	-	ALA	deletion	UNP Q9HCN6
B	?	-	PRO	deletion	UNP Q9HCN6
B	?	-	TYR	deletion	UNP Q9HCN6
B	?	-	LYS	deletion	UNP Q9HCN6
B	?	-	ASN	deletion	UNP Q9HCN6
B	177	ALA	-	expression tag	UNP Q9HCN6
B	178	ALA	-	expression tag	UNP Q9HCN6
B	179	ALA	-	expression tag	UNP Q9HCN6
C	-1	GLY	-	expression tag	UNP Q9HCN6
C	0	SER	-	expression tag	UNP Q9HCN6
C	?	-	PRO	deletion	UNP Q9HCN6
C	?	-	ALA	deletion	UNP Q9HCN6
C	?	-	VAL	deletion	UNP Q9HCN6
C	?	-	SER	deletion	UNP Q9HCN6
C	?	-	PRO	deletion	UNP Q9HCN6
C	?	-	ALA	deletion	UNP Q9HCN6
C	?	-	PRO	deletion	UNP Q9HCN6
C	?	-	TYR	deletion	UNP Q9HCN6
C	?	-	LYS	deletion	UNP Q9HCN6
C	?	-	ASN	deletion	UNP Q9HCN6
C	177	ALA	-	expression tag	UNP Q9HCN6
C	178	ALA	-	expression tag	UNP Q9HCN6
C	179	ALA	-	expression tag	UNP Q9HCN6
D	-1	GLY	-	expression tag	UNP Q9HCN6
D	0	SER	-	expression tag	UNP Q9HCN6
D	?	-	PRO	deletion	UNP Q9HCN6
D	?	-	ALA	deletion	UNP Q9HCN6
D	?	-	VAL	deletion	UNP Q9HCN6
D	?	-	SER	deletion	UNP Q9HCN6
D	?	-	PRO	deletion	UNP Q9HCN6
D	?	-	ALA	deletion	UNP Q9HCN6
D	?	-	PRO	deletion	UNP Q9HCN6
D	?	-	TYR	deletion	UNP Q9HCN6
D	?	-	LYS	deletion	UNP Q9HCN6
D	?	-	ASN	deletion	UNP Q9HCN6
D	177	ALA	-	expression tag	UNP Q9HCN6
D	178	ALA	-	expression tag	UNP Q9HCN6
D	179	ALA	-	expression tag	UNP Q9HCN6

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

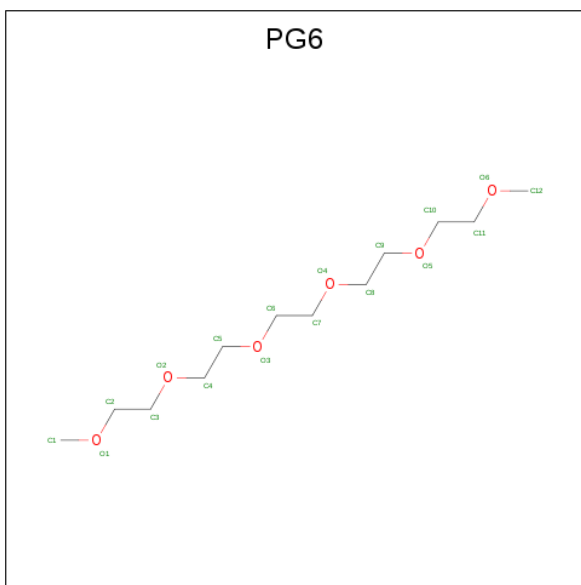
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Cl	0	0
			5	5		
2	A	5	Total	Cl	0	0
			5	5		
2	D	2	Total	Cl	0	0
			2	2		
2	C	2	Total	Cl	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



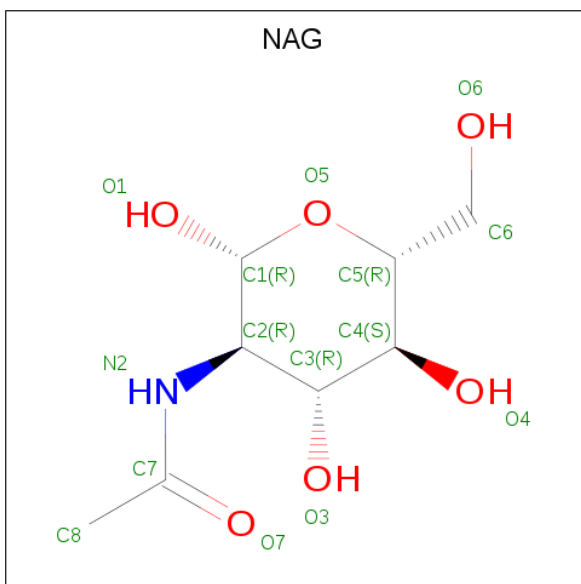
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY)-ETHOXY]-ETHANE (three-letter code: PG6) (formula: C₁₂H₂₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			16	10	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	A	1	Total	C	N	O	0	0
			14	8	1	5		

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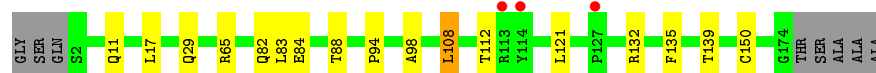
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	114	Total	O	0	0
			114	114		
6	B	108	Total	O	0	0
			108	108		
6	C	63	Total	O	0	0
			63	63		
6	D	59	Total	O	0	0
			59	59		

- Molecule 1: Platelet glycoprotein VI



- | GLY | SER | GIN |
|------|-----|-----|
| S2 | | |
| G3 | | |
| P4 | | |
| R27 | | |
| G28 | | |
| Q29 | | |
| L36 | | |
| L39 | | |
| Q50 | | |
| R65 | | |
| Q71 | | |
| S74 | | |
| Q82 | | |
| P94 | | |
| D105 | | |
| V106 | | |
| T107 | | |
| T112 | | |
| R113 | | |
| Y114 | | |
| L121 | | |
| D126 | | |
| P127 | | |
| R132 | | |
| F135 | | |
| T138 | | |
| T139 | | |
| L168 | | |
| F169 | | |
| L170 | | |
| T173 | | |
| G174 | | |
| SER | | |
| ALA | | |
| ALA | | |

- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|------------|------------|------------|-----------|-----------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|
| GLY | SER | GLN | S2 | P6 | L17 | S45 | R46 | Y47 | R60 | R65 | Y70 | G73 | S74 | L75 | W76 | V90 | S102 | Q111 | T112 | R113 | Y114 | F115 | F116 | E124 | D125 | P127 | R132 | A133 | S134 | F135 | P136 | I137 | V140 | T141 | A142 | A143 | R156 | W161 | L170 | L178 |
|------------|------------|------------|-----------|-----------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|-------------|

- GLY
 SER
 GLN
 S2
 P6
 Q29
 E40
 K41
 L42
 S45
 R46
 R65
 Y70
 G73
 Q82
 S95
 S102
 G103
 R113
 Y114
 G125
 D126
 P127
 F135
 A142
 A143
 R156
 A179

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.65Å 44.05Å 117.66Å 90.00° 104.69° 90.00°	Depositor
Resolution (Å)	113.81 – 1.90 52.38 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.6 (113.81-1.90) 94.6 (52.38-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.90Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.221 , 0.260 0.230 , 0.269	Depositor DCC
R_{free} test set	2967 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtrriage
Anisotropy	0.230	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.56$, $\langle L^2 \rangle = 0.40$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6101	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.10 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.8548e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: PG6, PO4, NAG, CL

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	0.62	0/1500	0.74	0/2041
1	B	0.64	0/1517	0.76	1/2064 (0.0%)
1	C	0.55	0/1451	0.72	0/1980
1	D	0.52	0/1443	0.71	0/1968
All	All	0.59	0/5911	0.73	1/8053 (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
1	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	105	ASP	CB-CG-OD2	-5.27	113.56	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	74	SER	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	1422	0	1457	14	0
1	B	1433	0	1481	17	0
1	C	1398	0	1389	7	0
1	D	1392	0	1390	5	0
2	A	5	0	0	3	0
2	B	5	0	0	4	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	16	0	20	3	0
4	B	16	0	20	4	0
5	A	14	0	13	0	0
5	B	14	0	13	0	0
5	C	14	0	13	0	0
5	D	14	0	13	0	0
6	A	114	0	0	2	1
6	B	108	0	0	2	0
6	C	63	0	0	4	1
6	D	59	0	0	1	0
All	All	6101	0	5809	45	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (45) 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:C:76[B]:TRP:CZ3	6:C:342:HOH:O	2.13	1.00
1:B:132:ARG:HH12	4:B:207:PG6:H72	1.36	0.87
2:B:201:CL:CL	6:B:339:HOH:O	2.30	0.86
1:C:76[B]:TRP:CH2	6:C:342:HOH:O	2.27	0.85
1:B:132:ARG:HH12	4:B:207:PG6:C7	1.96	0.78
1:C:65:ARG:NH2	6:C:301:HOH:O	2.18	0.75
1:A:11[B]:GLN:NE2	6:A:301:HOH:O	2.00	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29[B]:GLN:HG2	2:A:202:CL:CL	2.29	0.69
2:A:201:CL:CL	6:A:313:HOH:O	2.48	0.68
1:B:94:PRO:HB3	1:B:112:THR:HG22	1.78	0.66
1:A:17[B]:LEU:HD21	1:A:88:THR:HG21	1.81	0.63
1:B:121[B]:LEU:HD11	1:B:138:ILE:HD12	1.79	0.62
1:A:121[B]:LEU:HD23	1:A:150:CYS:HB3	1.83	0.59
1:A:94:PRO:HB3	1:A:112:THR:HG22	1.90	0.53
1:A:94:PRO:HB3	1:A:112:THR:CG2	2.39	0.52
1:D:65:ARG:HH11	1:D:82:GLN:HE22	1.58	0.52
1:A:132:ARG:NH1	4:A:207:PG6:H71	2.26	0.50
1:B:27[A]:ARG:HG2	1:B:29[A]:GLN:HG3	1.95	0.49
4:B:207:PG6:H32	6:B:304:HOH:O	2.12	0.49
1:A:65[B]:ARG:HD3	1:A:82:GLN:OE1	2.14	0.48
1:B:94:PRO:HB3	1:B:112:THR:CG2	2.44	0.47
1:D:6:PRO:HB2	1:D:70:TYR:OH	2.14	0.47
1:B:65[B]:ARG:NH1	1:B:82:GLN:OE1	2.48	0.47
1:B:36[B]:LEU:HD22	1:B:71[B]:GLN:HG2	1.97	0.46
1:A:132:ARG:HH12	4:A:207:PG6:H71	1.78	0.46
1:B:121[B]:LEU:CD1	1:B:138:ILE:HD12	2.46	0.46
1:B:65[B]:ARG:HD3	1:B:82:GLN:OE1	2.17	0.45
1:B:4:PRO:O	2:B:205:CL:CL	2.72	0.45
1:B:106:VAL:HG21	1:B:170:LEU:HD21	1.99	0.44
1:C:17[A]:LEU:HD11	1:C:161:TRP:CZ3	2.53	0.44
1:C:6:PRO:HB2	1:C:70:TYR:OH	2.17	0.44
1:A:139:THR:HG23	2:A:203:CL:CL	2.55	0.44
1:C:132:ARG:NH2	6:C:305:HOH:O	2.50	0.44
1:C:60:ARG:HD3	1:C:90:VAL:HG13	2.00	0.43
1:B:173:THR:HG21	1:D:103:GLY:HA2	2.00	0.43
1:A:83[B]:LEU:HD23	1:A:84:GLU:N	2.34	0.43
1:D:65:ARG:NE	1:D:82:GLN:OE1	2.47	0.42
1:D:40:GLU:HG2	6:D:312:HOH:O	2.18	0.42
1:A:98:ALA:HB2	1:A:108:LEU:HD23	2.03	0.41
1:A:17[B]:LEU:CD2	1:A:88:THR:HG21	2.48	0.41
1:A:17[A]:LEU:HD21	4:A:207:PG6:H101	2.03	0.41
1:B:132:ARG:NH1	4:B:207:PG6:C7	2.75	0.40
1:B:139:THR:HG23	2:B:203:CL:CL	2.58	0.40
1:B:107:THR:OG1	2:B:203:CL:CL	2.68	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:395:HOH:O	6:C:359:HOH:O[1_455]	2.03	0.17

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	184/181 (102%)	183 (100%)	1 (0%)	0	100	100
1	B	186/181 (103%)	186 (100%)	0	0	100	100
1	C	180/181 (99%)	175 (97%)	4 (2%)	1 (1%)	25	15
1	D	180/181 (99%)	175 (97%)	5 (3%)	0	100	100
All	All	730/724 (101%)	719 (98%)	10 (1%)	1 (0%)	51	43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	73	GLY

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	161/152 (106%)	159 (99%)	2 (1%)	71	70
1	B	163/152 (107%)	159 (98%)	4 (2%)	47	41
1	C	154/152 (101%)	150 (97%)	4 (3%)	46	39
1	D	154/152 (101%)	150 (97%)	4 (3%)	46	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	632/608 (104%)	618 (98%)	14 (2%)	50 47

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	135	PHE
1	B	50	GLN
1	B	114	TYR
1	B	135	PHE
1	B	168	LEU
1	C	2	SER
1	C	102	SER
1	C	135	PHE
1	C	170	LEU
1	D	29	GLN
1	D	95	SER
1	D	102	SER
1	D	126	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	111	GLN
1	C	82	GLN
1	D	50	GLN

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	$\# Z > 2$
5	NAG	C	203	1	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
5	NAG	B	208	1	14,14,15	0.64	0	17,19,21	0.96	1 (5%)
5	NAG	D	203	1	14,14,15	0.57	0	17,19,21	1.28	2 (11%)
5	NAG	A	208	1	14,14,15	0.57	0	17,19,21	0.95	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	C	203	1	-	0/6/23/26	0/1/1/1
5	NAG	B	208	1	-	2/6/23/26	0/1/1/1
5	NAG	D	203	1	-	2/6/23/26	0/1/1/1
5	NAG	A	208	1	-	0/6/23/26	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(°)	Ideal(°)
5	D	203	NAG	C4-C3-C2	2.76	115.06	111.02
5	B	208	NAG	C4-C3-C2	-2.50	107.35	111.02
5	C	203	NAG	O3-C3-C2	-2.35	104.61	109.47
5	D	203	NAG	C3-C4-C5	2.09	113.97	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	208	NAG	O5-C5-C6-O6
5	B	208	NAG	C4-C5-C6-O6
5	D	203	NAG	C4-C5-C6-O6
5	D	203	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 14 are monoatomic - leaving 8 for Mogul analysis.

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	B	208	1	14,14,15	0.64	0	17,19,21	0.96	1 (5%)
5	NAG	C	203	1	14,14,15	0.73	0	17,19,21	0.91	1 (5%)
5	NAG	D	203	1	14,14,15	0.57	0	17,19,21	1.28	2 (11%)
3	PO4	B	206	-	4,4,4	1.24	1 (25%)	6,6,6	0.78	0
4	PG6	A	207	-	15,15,17	0.38	0	14,14,16	0.45	0
5	NAG	A	208	1	14,14,15	0.57	0	17,19,21	0.95	0
4	PG6	B	207	-	15,15,17	0.34	0	14,14,16	0.93	0
3	PO4	A	206	-	4,4,4	0.94	0	6,6,6	0.56	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	B	208	1	-	2/6/23/26	0/1/1/1
5	NAG	C	203	1	-	0/6/23/26	0/1/1/1
5	NAG	D	203	1	-	2/6/23/26	0/1/1/1
4	PG6	A	207	-	-	9/13/13/15	-
5	NAG	A	208	1	-	0/6/23/26	0/1/1/1
4	PG6	B	207	-	-	8/13/13/15	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	206	PO4	P-O4	-2.18	1.48	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	203	NAG	C4-C3-C2	2.76	115.06	111.02
5	B	208	NAG	C4-C3-C2	-2.50	107.35	111.02
5	C	203	NAG	O3-C3-C2	-2.35	104.61	109.47
5	D	203	NAG	C3-C4-C5	2.09	113.97	110.24

There are no chirality outliers.

All (21) torsion outliers are listed below:

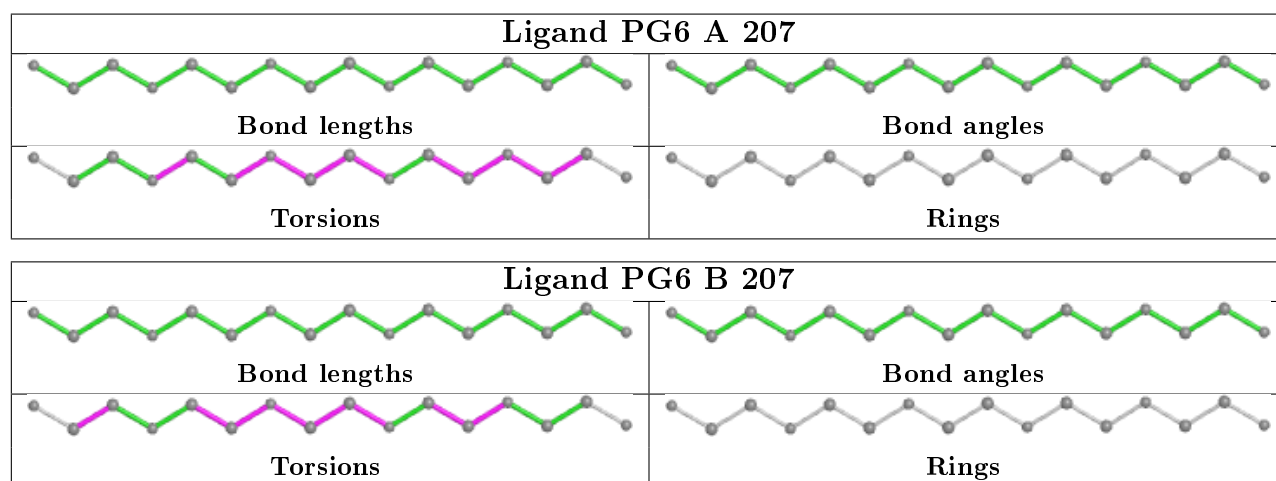
Mol	Chain	Res	Type	Atoms
4	A	207	PG6	O3-C6-C7-O4
5	B	208	NAG	O5-C5-C6-O6
4	B	207	PG6	O5-C10-C11-O6
4	A	207	PG6	O1-C2-C3-O2
4	B	207	PG6	O3-C6-C7-O4
5	B	208	NAG	C4-C5-C6-O6
4	B	207	PG6	O4-C8-C9-O5
5	D	203	NAG	C4-C5-C6-O6
5	D	203	NAG	O5-C5-C6-O6
4	A	207	PG6	C7-C6-O3-C5
4	B	207	PG6	O2-C4-C5-O3
4	B	207	PG6	C9-C8-O4-C7
4	A	207	PG6	C2-C3-O2-C4
4	A	207	PG6	C8-C9-O5-C10
4	A	207	PG6	C5-C4-O2-C3
4	A	207	PG6	O2-C4-C5-O3
4	B	207	PG6	C7-C6-O3-C5
4	B	207	PG6	C5-C4-O2-C3
4	A	207	PG6	C6-C7-O4-C8
4	A	207	PG6	C9-C8-O4-C7
4	B	207	PG6	C6-C7-O4-C8

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	207	PG6	3	0
4	B	207	PG6	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	A	173/181 (95%)	-0.01	3 (1%) 70 72	15, 23, 40, 66	0
1	B	173/181 (95%)	0.03	4 (2%) 60 63	15, 24, 43, 66	0
1	C	178/181 (98%)	0.66	26 (14%) 2 2	20, 38, 70, 92	0
1	D	178/181 (98%)	0.47	15 (8%) 11 12	20, 36, 68, 90	0
All	All	702/724 (96%)	0.29	48 (6%) 17 19	15, 28, 63, 92	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	114	TYR	9.1
1	D	114	TYR	8.7
1	C	127	PRO	6.7
1	D	127	PRO	6.3
1	C	126	ASP	6.3
1	D	126	ASP	6.2
1	C	102	SER	5.6
1	C	76[A]	TRP	5.3
1	C	135	PHE	5.1
1	D	45	SER	4.6
1	C	113	ARG	4.3
1	C	142	ALA	4.1
1	D	102	SER	4.0
1	C	111	GLN	3.6
1	D	113	ARG	3.6
1	C	2	SER	3.5
1	D	135	PHE	3.5
1	C	141	THR	3.5
1	A	114	TYR	3.4
1	B	126	ASP	3.4
1	D	143	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	125	GLY	3.3
1	B	114	TYR	3.3
1	C	45	SER	3.3
1	C	75	LEU	3.1
1	C	143	ALA	3.1
1	B	127	PRO	3.0
1	D	142	ALA	3.0
1	C	73	GLY	2.9
1	C	116	PHE	2.7
1	A	127	PRO	2.7
1	C	47	TYR	2.7
1	B	74	SER	2.6
1	C	125	GLY	2.6
1	A	113	ARG	2.6
1	D	46	ARG	2.5
1	C	137	ILE	2.5
1	C	140	VAL	2.5
1	D	156	ARG	2.4
1	D	73	GLY	2.3
1	D	42	LEU	2.3
1	C	156	ARG	2.3
1	C	74	SER	2.3
1	D	2	SER	2.3
1	C	115	GLY	2.1
1	C	133	ALA	2.1
1	C	179	ALA	2.1
1	C	124	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
5	NAG	C	203	14/15	0.79	0.21	46,55,68,69	0
5	NAG	B	208	14/15	0.80	0.22	58,66,72,74	0
5	NAG	A	208	14/15	0.82	0.20	49,56,62,63	0
5	NAG	D	203	14/15	0.86	0.17	43,52,60,61	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

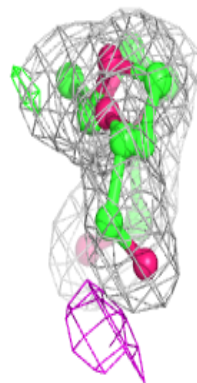
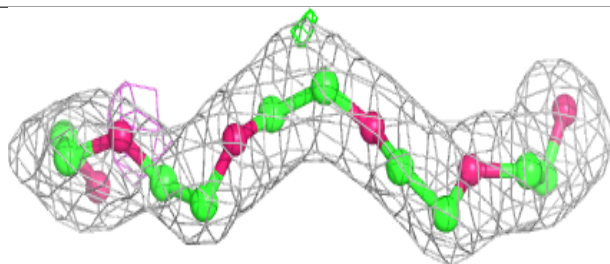
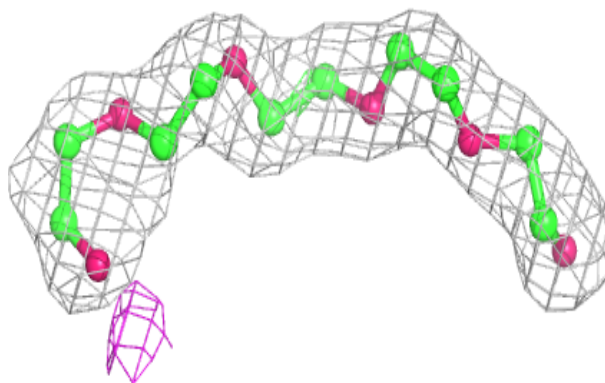
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	203	14/15	0.79	0.21	46,55,68,69	0
5	NAG	B	208	14/15	0.80	0.22	58,66,72,74	0
5	NAG	A	208	14/15	0.82	0.20	49,56,62,63	0
2	CL	B	201	1/1	0.82	0.10	68,68,68,68	0
5	NAG	D	203	14/15	0.86	0.17	43,52,60,61	0
2	CL	A	204	1/1	0.88	0.07	58,58,58,58	0
4	PG6	A	207	16/18	0.90	0.15	30,36,48,49	0
2	CL	C	202	1/1	0.91	0.11	60,60,60,60	0
4	PG6	B	207	16/18	0.92	0.15	30,35,51,55	0
2	CL	D	201	1/1	0.93	0.07	56,56,56,56	0
3	PO4	B	206	5/5	0.93	0.13	42,46,56,57	0
2	CL	B	202	1/1	0.94	0.08	49,49,49,49	0
2	CL	C	201	1/1	0.94	0.09	53,53,53,53	0
3	PO4	A	206	5/5	0.94	0.12	43,44,56,56	0
2	CL	D	202	1/1	0.95	0.14	60,60,60,60	0
2	CL	A	201	1/1	0.95	0.11	58,58,58,58	0
2	CL	A	202	1/1	0.97	0.07	40,40,40,40	0
2	CL	A	205	1/1	0.98	0.06	39,39,39,39	0
2	CL	B	204	1/1	0.98	0.10	59,59,59,59	0
2	CL	A	203	1/1	0.99	0.05	36,36,36,36	0
2	CL	B	205	1/1	0.99	0.10	40,40,40,40	0
2	CL	B	203	1/1	0.99	0.06	39,39,39,39	0

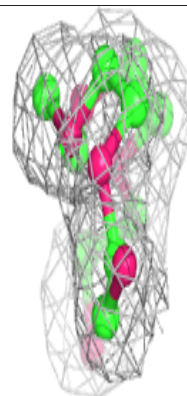
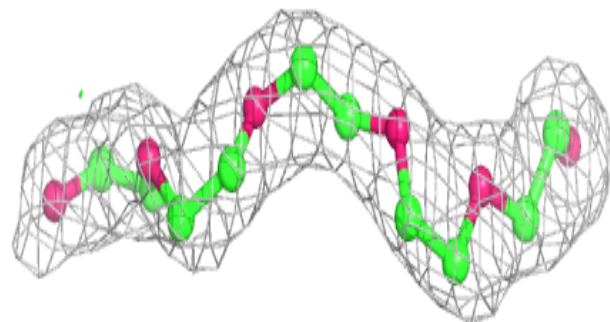
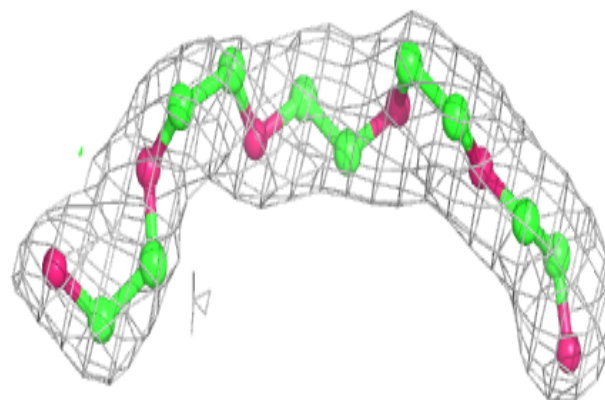
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PG6 A 207:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around PG6 B 207:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers

There are no such residues in this entry.