



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:55 PM UTC

PDB ID : 2NR9 / pdb_00002nr9
Title : Crystal structure of GlpG, Rhomboid Peptidase from Haemophilus influenzae
Authors : Lemieux, M.J.; Fischer, S.J.; Cherney, M.M.; Bateman, K.S.; James, M.N.G.
Deposited on : 2006-11-01
Resolution : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

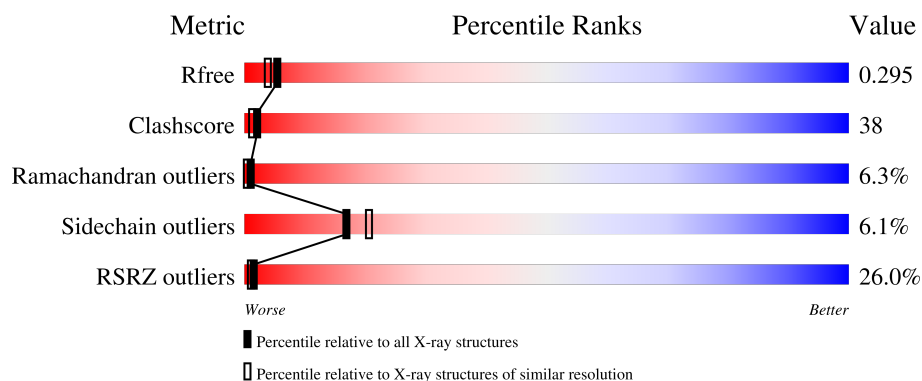
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 $\leq 5\%$. 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	196	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1754 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.

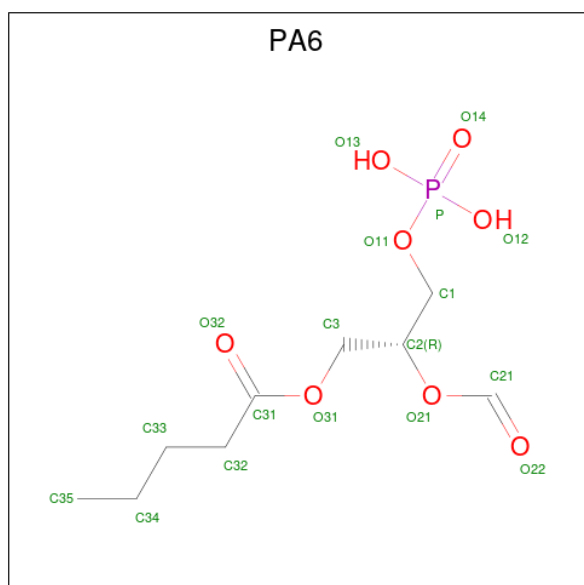
- Molecule 1 is a protein called Protein glpG homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	192	1554	1046	240	261	7	0	7	0

There are 6 discrepancies between the modelled and reference sequences:

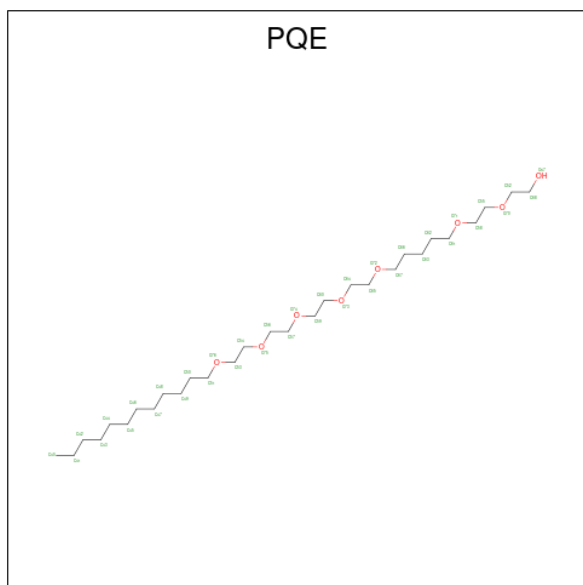
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLU	LYS	engineered mutation	UNP P44783
A	24	ILE	LEU	engineered mutation	UNP P44783
A	193	LEU	-	cloning artifact	UNP P44783
A	194	VAL	-	cloning artifact	UNP P44783
A	195	PRO	-	cloning artifact	UNP P44783
A	196	ARG	-	cloning artifact	UNP P44783

- Molecule 2 is (R)-2-(FORMYLOXY)-3-(PHOSPHONOOXY)PROPYL PENTANOATE (CCD ID: PA6) (formula: C₉H₁₇O₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			18	9	8	1		
2	A	1	Total	C	O	P	0	0
			18	9	8	1		
2	A	1	Total	C	O	P	0	0
			18	9	8	1		

- Molecule 3 is 3,6,12,15,18,21,24-HEPTAOXAHEXATRIACONTAN-1-OL (CCD ID: PQE) (formula: $C_{29}H_{60}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			37	29	8		
3	A	1	Total	C	O	0	1
			47	36	11		

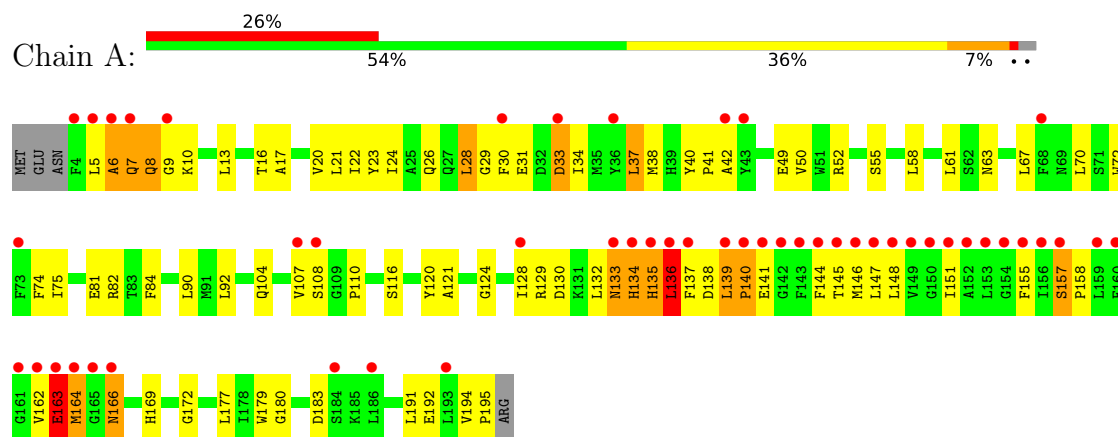
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		

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: Protein glpG homolog



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	121.29Å 35.05Å 52.93Å 90.00° 104.02° 90.00°	Depositor
Resolution (Å)	25.00 – 2.20 25.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.0 (25.00-2.20) 94.9 (25.00-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.233 , 0.295 0.237 , 0.295	Depositor DCC
R_{free} test set	513 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 96.5	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	0.92	EDS
Total number of atoms	1754	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.93% 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: PQE, PA6

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	0.41	0/1628	0.82	3/2213 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	50	VAL	N-CA-C	6.55	119.24	111.05
1	A	157	SER	CA-C-N	6.02	127.36	119.84
1	A	157	SER	C-N-CA	6.02	127.36	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1554	0	1571	123	0
2	A	54	0	45	4	0
3	A	84	0	94	12	0
4	A	62	0	0	4	0
All	All	1754	0	1710	130	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 38.

All (130) 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:128[A]:ILE:HD11	1:A:180:GLY:HA3	1.34	1.07
1:A:155:PHE:HB2	1:A:166:ASN:HB3	1.03	1.03
1:A:37:LEU:HD23	1:A:37:LEU:O	1.57	1.02
1:A:155:PHE:CB	1:A:166:ASN:HB3	1.87	1.02
1:A:61:LEU:HD12	1:A:163:GLU:HB2	1.42	1.01
1:A:155:PHE:HB2	1:A:166:ASN:CB	1.94	0.97
1:A:26:GLN:HB3	1:A:31:GLU:HG2	1.44	0.97
3:A:205[B]:PQE:H662	3:A:205[B]:PQE:H582	1.50	0.90
1:A:128[A]:ILE:HD12	1:A:129:ARG:N	1.87	0.88
1:A:191:LEU:O	1:A:194[A]:VAL:HG22	1.74	0.87
1:A:30:PHE:CE1	1:A:33:ASP:CB	2.60	0.85
1:A:61:LEU:HD12	1:A:163:GLU:CB	2.05	0.85
1:A:166:ASN:HD21	3:A:204:PQE:H482	1.42	0.85
1:A:30:PHE:CE1	1:A:33:ASP:HB3	2.12	0.84
1:A:128[A]:ILE:CD1	1:A:180:GLY:HA3	2.09	0.83
1:A:166:ASN:ND2	3:A:204:PQE:H491	1.95	0.82
1:A:194[B]:VAL:HG13	1:A:195:PRO:HD2	1.58	0.82
1:A:166:ASN:ND2	3:A:204:PQE:H482	2.00	0.77
1:A:194[B]:VAL:CG1	1:A:195:PRO:HD2	2.16	0.74
1:A:146:MET:O	1:A:148:LEU:N	2.20	0.73
1:A:146:MET:C	1:A:148:LEU:H	1.96	0.73
1:A:8:GLN:NE2	1:A:8:GLN:H	1.87	0.72
1:A:49:GLU:OE1	1:A:52:ARG:NE	2.20	0.71
1:A:136:LEU:HD13	1:A:137:PHE:CD1	2.26	0.71
1:A:30:PHE:HE1	1:A:33:ASP:HB2	1.56	0.70
1:A:140:PRO:HG2	1:A:145:THR:OG1	1.93	0.69
1:A:37:LEU:HD23	1:A:37:LEU:C	2.18	0.68
1:A:5:LEU:HD23	1:A:7:GLN:H	1.58	0.68
1:A:30:PHE:HE1	1:A:33:ASP:CB	2.04	0.68
1:A:116:SER:CB	1:A:162:VAL:HG11	2.25	0.67
1:A:30:PHE:CE1	1:A:33:ASP:HB2	2.28	0.66
1:A:26:GLN:CB	1:A:31:GLU:HG2	2.24	0.66
1:A:136:LEU:HD13	1:A:137:PHE:CE1	2.31	0.66
1:A:55:SER:HB3	2:A:201:PA6:H331	1.77	0.66
1:A:192:GLU:HB3	4:A:239:HOH:O	1.96	0.66
1:A:128[A]:ILE:HG23	1:A:177:LEU:CD2	2.26	0.65
1:A:30:PHE:HD1	1:A:33:ASP:H	1.47	0.63
1:A:37:LEU:O	1:A:37:LEU:CD2	2.42	0.62
1:A:166:ASN:HD22	3:A:204:PQE:H491	1.62	0.62
1:A:61:LEU:CD1	1:A:163:GLU:HB2	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ALA:CB	1:A:110:PRO:HG3	2.31	0.61
1:A:166:ASN:ND2	3:A:204:PQE:C48	2.62	0.61
1:A:129:ARG:NH2	1:A:183:ASP:HB3	2.15	0.61
1:A:37:LEU:C	1:A:37:LEU:CD2	2.73	0.61
1:A:166:ASN:ND2	3:A:204:PQE:C49	2.63	0.60
1:A:128[A]:ILE:CG2	1:A:177:LEU:HD22	2.33	0.59
1:A:5:LEU:C	1:A:7:GLN:H	2.11	0.58
1:A:8:GLN:H	1:A:8:GLN:HE21	1.53	0.57
1:A:128[A]:ILE:HG23	1:A:177:LEU:HD22	1.86	0.56
1:A:23:TYR:OH	1:A:63:ASN:ND2	2.38	0.56
1:A:61:LEU:HD12	1:A:163:GLU:CG	2.35	0.56
1:A:5:LEU:CD2	1:A:6:ALA:N	2.68	0.55
1:A:9:GLY:HA3	1:A:81:GLU:CD	2.33	0.54
1:A:72:TRP:CH2	1:A:144:PHE:HD2	2.26	0.54
1:A:128[A]:ILE:HD12	1:A:129:ARG:H	1.67	0.54
1:A:157:SER:HB3	4:A:226:HOH:O	2.08	0.54
2:A:203:PA6:O31	2:A:203:PA6:H21	2.09	0.53
1:A:9:GLY:HA3	1:A:81:GLU:OE1	2.09	0.53
1:A:61:LEU:HD12	1:A:163:GLU:HG3	1.90	0.53
1:A:5:LEU:HD23	1:A:7:GLN:N	2.24	0.53
1:A:146:MET:C	1:A:148:LEU:N	2.63	0.52
1:A:116:SER:HB3	1:A:162:VAL:HG11	1.90	0.52
1:A:155:PHE:CG	1:A:166:ASN:HB3	2.42	0.52
1:A:162:VAL:HB	1:A:169:HIS:CE1	2.44	0.52
1:A:61:LEU:HB2	1:A:163:GLU:HG3	1.91	0.51
1:A:5:LEU:C	1:A:7:GLN:N	2.68	0.51
1:A:84:PHE:CE2	1:A:136:LEU:HD22	2.46	0.51
1:A:42:ALA:HB1	1:A:110:PRO:HG3	1.93	0.51
1:A:24:ILE:HG22	1:A:28:LEU:HD11	1.94	0.50
1:A:135:HIS:C	1:A:137:PHE:H	2.19	0.50
1:A:162:VAL:O	1:A:163:GLU:C	2.54	0.50
1:A:116:SER:OG	1:A:162:VAL:HG11	2.11	0.50
1:A:138:ASP:O	1:A:139:LEU:HB2	2.12	0.50
1:A:40:TYR:CD2	1:A:41:PRO:HD2	2.47	0.49
1:A:13[A]:LEU:HD23	1:A:74:PHE:HE1	1.77	0.49
1:A:5:LEU:HD11	1:A:10:LYS:HG2	1.94	0.49
1:A:130:ASP:O	1:A:134[A]:HIS:HB2	2.13	0.49
2:A:203:PA6:O13	2:A:203:PA6:H341	2.13	0.49
1:A:16:THR:HG23	1:A:70:LEU:HD13	1.94	0.49
1:A:92[A]:LEU:HD23	1:A:179:TRP:CE3	2.47	0.49
1:A:136:LEU:CD1	1:A:137:PHE:CD1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ALA:HB2	1:A:110:PRO:HG3	1.96	0.47
1:A:166:ASN:OD1	1:A:166:ASN:N	2.45	0.47
1:A:26:GLN:HB3	1:A:31:GLU:CG	2.32	0.47
1:A:121:ALA:HA	1:A:172:GLY:O	2.14	0.47
1:A:162:VAL:O	1:A:164:MET:N	2.48	0.47
3:A:205[A]:PQE:H661	3:A:205[A]:PQE:H611	1.44	0.47
1:A:130:ASP:O	1:A:134[B]:HIS:HB3	2.15	0.47
1:A:84:PHE:CZ	1:A:136:LEU:HD22	2.50	0.46
1:A:29:GLY:O	1:A:30:PHE:HB3	2.16	0.46
1:A:17:ALA:O	1:A:21:LEU:HG	2.16	0.46
1:A:42:ALA:HB2	1:A:110:PRO:CG	2.45	0.46
1:A:63:ASN:CG	3:A:205[A]:PQE:H551	2.40	0.46
1:A:8:GLN:NE2	1:A:8:GLN:N	2.62	0.46
1:A:42:ALA:HB2	1:A:110:PRO:CB	2.45	0.46
1:A:135:HIS:C	1:A:137:PHE:N	2.75	0.45
1:A:40:TYR:CG	1:A:41:PRO:HD2	2.51	0.44
1:A:120:TYR:OH	1:A:151:ILE:CD1	2.65	0.43
2:A:203:PA6:O31	2:A:203:PA6:C21	2.66	0.43
1:A:128[A]:ILE:CG2	1:A:177:LEU:CD2	2.94	0.43
1:A:34:ILE:O	1:A:38:MET:CG	2.67	0.43
3:A:205[A]:PQE:C55	3:A:205[A]:PQE:H622	2.49	0.42
1:A:5:LEU:HD22	1:A:6:ALA:N	2.34	0.42
1:A:124:GLY:O	1:A:128[A]:ILE:HG13	2.20	0.42
1:A:135:HIS:O	1:A:137:PHE:N	2.53	0.42
1:A:63:ASN:H	3:A:205[A]:PQE:H552	1.84	0.42
1:A:104:GLN:HE21	1:A:108:SER:HB2	1.85	0.42
3:A:204:PQE:H671	3:A:204:PQE:H641	1.58	0.41
1:A:20:VAL:O	1:A:24:ILE:HG12	2.21	0.41
1:A:82:ARG:NH2	4:A:222:HOH:O	2.52	0.41
1:A:128[A]:ILE:HG23	1:A:177:LEU:HD23	2.01	0.41
1:A:140:PRO:HB2	1:A:141:GLU:H	1.71	0.41
1:A:194[B]:VAL:CG1	1:A:195:PRO:CD	2.95	0.41
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.87	0.40
1:A:5:LEU:O	1:A:7:GLN:N	2.55	0.40
1:A:22:ILE:O	1:A:26:GLN:HG3	2.22	0.40
1:A:148:LEU:C	1:A:151:ILE:HG22	2.46	0.40
1:A:164:MET:HE1	4:A:232:HOH:O	2.21	0.40

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	A	197/196 (100%)	169 (86%)	15 (8%)	13 (7%)	1 0

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	163	GLU
1	A	140	PRO
1	A	133	ASN
1	A	134[A]	HIS
1	A	134[B]	HIS
1	A	135	HIS
1	A	136	LEU
1	A	158	PRO
1	A	164	MET
1	A	6	ALA
1	A	7	GLN
1	A	139	LEU

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	170/167 (102%)	160 (94%)	10 (6%)	18 22

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	28	LEU
1	A	33	ASP
1	A	37	LEU
1	A	58	LEU
1	A	90	LEU
1	A	107	VAL
1	A	136	LEU
1	A	163	GLU
1	A	166	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	56	HIS
1	A	63	ASN
1	A	69	ASN
1	A	104	GLN
1	A	133	ASN
1	A	135	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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
2	PA6	A	203	-	17,17,17	1.96	3 (17%)	18,21,21	1.49	2 (11%)
3	PQE	A	204	-	36,36,36	0.40	0	35,35,35	0.41	0
3	PQE	A	205[A]	-	36,36,36	0.42	0	35,35,35	0.38	0
2	PA6	A	201	-	17,17,17	1.96	3 (17%)	18,21,21	1.56	2 (11%)
3	PQE	A	205[B]	-	36,36,36	0.41	0	35,35,35	0.40	0
2	PA6	A	202	-	17,17,17	1.95	3 (17%)	18,21,21	1.54	2 (11%)

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
2	PA6	A	203	-	-	11/18/18/18	-
3	PQE	A	204	-	-	21/34/34/34	-
3	PQE	A	205[A]	-	-	18/34/34/34	-
2	PA6	A	201	-	-	9/18/18/18	-
3	PQE	A	205[B]	-	-	18/34/34/34	-
2	PA6	A	202	-	-	16/18/18/18	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	203	PA6	O21-C21	6.01	1.46	1.33
2	A	201	PA6	O21-C21	5.96	1.45	1.33
2	A	202	PA6	O21-C21	5.94	1.45	1.33
2	A	201	PA6	O31-C31	4.43	1.46	1.33
2	A	203	PA6	O31-C31	4.31	1.45	1.33
2	A	202	PA6	O31-C31	4.26	1.45	1.33
2	A	202	PA6	O21-C2	-2.74	1.43	1.46
2	A	201	PA6	O21-C2	-2.57	1.43	1.46
2	A	203	PA6	O21-C2	-2.49	1.43	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	202	PA6	O21-C21-O22	-4.46	119.98	125.70
2	A	201	PA6	O21-C21-O22	-4.36	120.11	125.70
2	A	203	PA6	O21-C21-O22	-4.28	120.21	125.70
2	A	201	PA6	O31-C31-C32	2.87	120.59	111.83
2	A	202	PA6	O31-C31-C32	2.77	120.28	111.83
2	A	203	PA6	O31-C31-C32	2.66	119.95	111.83

There are no chirality outliers.

All (93) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	PA6	C1-C2-O21-C21
2	A	201	PA6	O22-C21-O21-C2
2	A	202	PA6	O22-C21-O21-C2
2	A	202	PA6	C1-O11-P-O13
2	A	202	PA6	C1-O11-P-O12
2	A	203	PA6	C1-C2-O21-C21
2	A	203	PA6	O22-C21-O21-C2
2	A	203	PA6	C1-O11-P-O13
2	A	203	PA6	C1-O11-P-O12
2	A	201	PA6	O32-C31-O31-C3
2	A	201	PA6	C32-C31-O31-C3
3	A	205[A]	PQE	C56-C57-O74-C59
3	A	205[B]	PQE	C56-C57-O74-C59
3	A	204	PQE	O70-C55-C58-O71
3	A	205[A]	PQE	O76-C53-C54-O75
3	A	205[B]	PQE	O76-C53-C54-O75
3	A	205[A]	PQE	C62-C61-O71-C58
3	A	205[B]	PQE	O70-C52-C68-O47
3	A	205[B]	PQE	O70-C55-C58-O71
3	A	204	PQE	O75-C56-C57-O74
3	A	204	PQE	C64-C65-O72-C67
3	A	205[A]	PQE	O75-C56-C57-O74
3	A	205[B]	PQE	O75-C56-C57-O74
3	A	205[B]	PQE	O71-C61-C62-C63
2	A	203	PA6	C31-C32-C33-C34
3	A	205[A]	PQE	C61-C62-C63-C66
3	A	204	PQE	O74-C59-C60-O73
3	A	204	PQE	C63-C66-C67-O72
3	A	205[A]	PQE	O71-C61-C62-C63
2	A	202	PA6	C31-C32-C33-C34
3	A	205[A]	PQE	C46-C47-C48-C49
3	A	205[B]	PQE	C46-C47-C48-C49

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Mol	Chain	Res	Type	Atoms
3	A	205[A]	PQE	C48-C49-C50-C51
3	A	205[B]	PQE	C48-C49-C50-C51
2	A	201	PA6	C1-C2-C3-O31
3	A	204	PQE	C48-C49-C50-C51
3	A	204	PQE	C45-C46-C47-C48
2	A	202	PA6	C32-C31-O31-C3
3	A	204	PQE	C41-C42-C43-C44
2	A	202	PA6	C32-C33-C34-C35
3	A	205[B]	PQE	C62-C63-C66-C67
3	A	205[A]	PQE	C42-C43-C44-C45
3	A	205[B]	PQE	C42-C43-C44-C45
3	A	204	PQE	C47-C48-C49-C50
2	A	202	PA6	O32-C31-O31-C3
3	A	204	PQE	O70-C52-C68-O47
2	A	202	PA6	C1-C2-C3-O31
3	A	204	PQE	C62-C63-C66-C67
2	A	202	PA6	C1-O11-P-O14
2	A	203	PA6	C1-O11-P-O14
3	A	205[A]	PQE	C62-C63-C66-C67
2	A	202	PA6	O11-C1-C2-C3
2	A	203	PA6	C32-C33-C34-C35
3	A	205[A]	PQE	C65-C64-O73-C60
3	A	205[B]	PQE	C65-C64-O73-C60
3	A	204	PQE	C40-C41-C42-C43
3	A	204	PQE	C49-C50-C51-O76
3	A	205[A]	PQE	C41-C42-C43-C44
3	A	205[B]	PQE	C41-C42-C43-C44
2	A	202	PA6	O11-C1-C2-O21
3	A	205[B]	PQE	C62-C61-O71-C58
3	A	205[A]	PQE	O70-C55-C58-O71
2	A	201	PA6	O11-C1-C2-C3
3	A	205[A]	PQE	C40-C41-C42-C43
3	A	205[B]	PQE	C40-C41-C42-C43
3	A	204	PQE	C53-C54-O75-C56
2	A	201	PA6	O21-C2-C3-O31
2	A	202	PA6	O21-C2-C3-O31
3	A	205[A]	PQE	C55-C58-O71-C61
3	A	204	PQE	C62-C61-O71-C58
2	A	201	PA6	O11-C1-C2-O21
3	A	204	PQE	C44-C45-C46-C47
3	A	205[A]	PQE	C54-C53-O76-C51
3	A	205[B]	PQE	C54-C53-O76-C51

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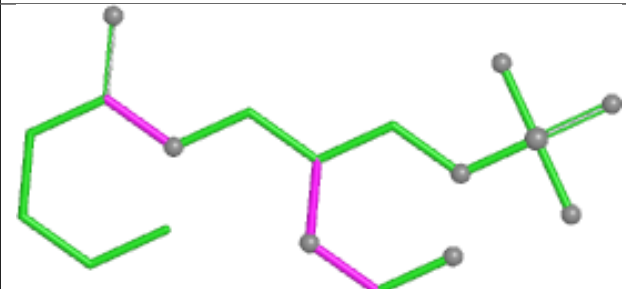
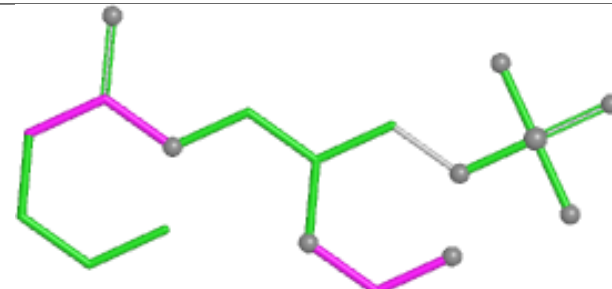
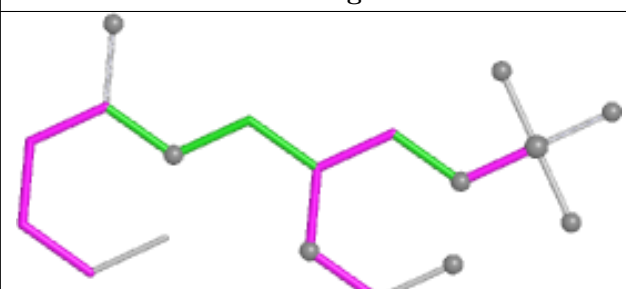
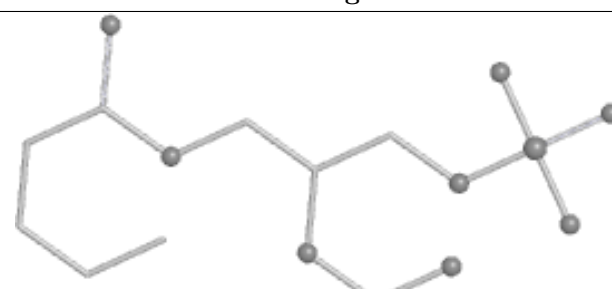
Mol	Chain	Res	Type	Atoms
3	A	205[A]	PQE	C59-C60-O73-C64
3	A	205[B]	PQE	C59-C60-O73-C64
3	A	204	PQE	C56-C57-O74-C59
3	A	204	PQE	C66-C67-O72-C65
3	A	204	PQE	C55-C58-O71-C61
2	A	201	PA6	C32-C33-C34-C35
2	A	202	PA6	C3-C2-O21-C21
2	A	202	PA6	C1-C2-O21-C21
2	A	203	PA6	C3-C2-O21-C21
2	A	203	PA6	O11-C1-C2-O21
2	A	203	PA6	O31-C31-C32-C33
2	A	202	PA6	O31-C31-C32-C33
3	A	205[A]	PQE	O73-C64-C65-O72
3	A	205[B]	PQE	O73-C64-C65-O72
3	A	204	PQE	O73-C64-C65-O72
3	A	205[B]	PQE	C61-C62-C63-C66
3	A	204	PQE	O76-C53-C54-O75
2	A	203	PA6	O32-C31-C32-C33
2	A	202	PA6	O32-C31-C32-C33

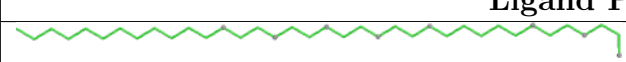
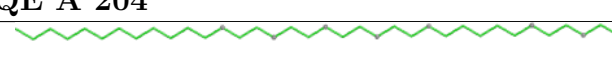
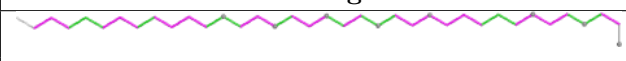
There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	203	PA6	3	0
3	A	204	PQE	7	0
3	A	205[A]	PQE	4	0
2	A	201	PA6	1	0
3	A	205[B]	PQE	1	0

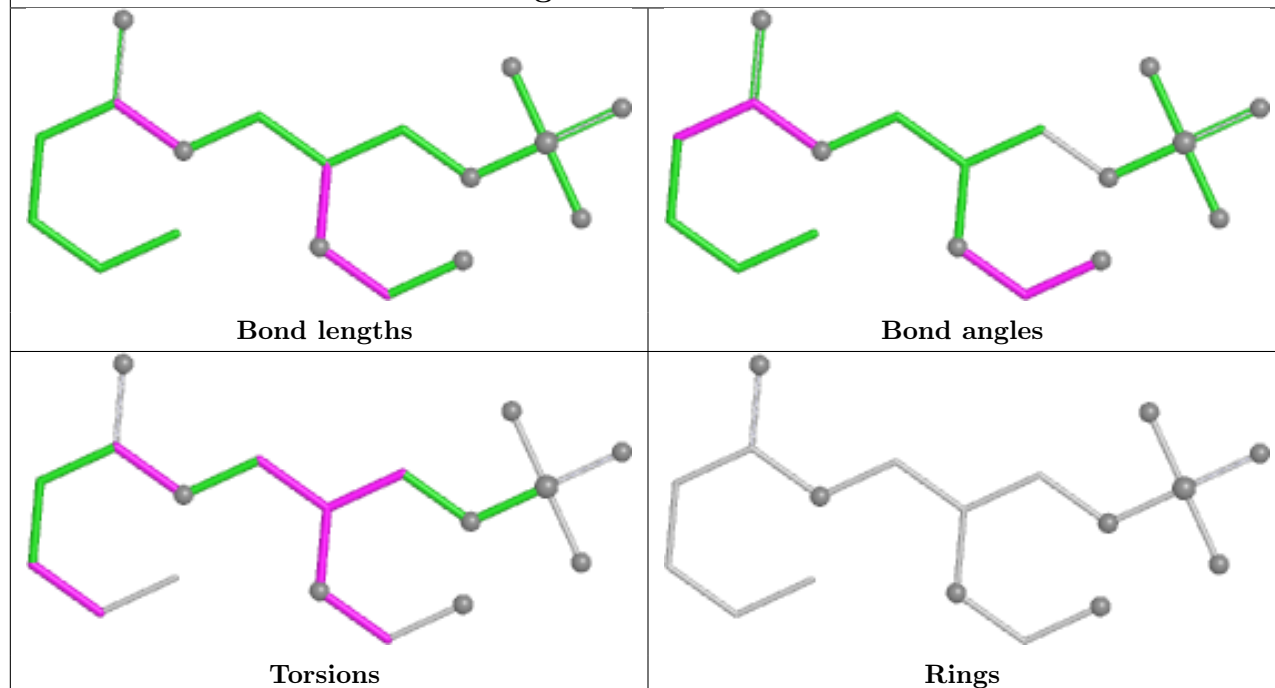
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand PA6 A 203	
	Bond lengths
	Bond angles
	Torsions
	Rings

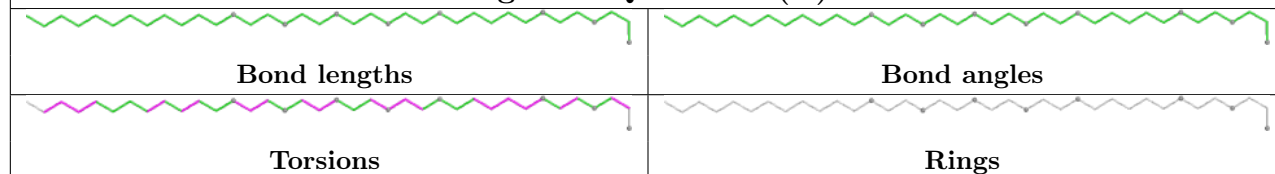
Ligand PQE A 204	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand PQE A 205 (A)	
	Bond lengths
	Bond angles
	Torsions
	Rings

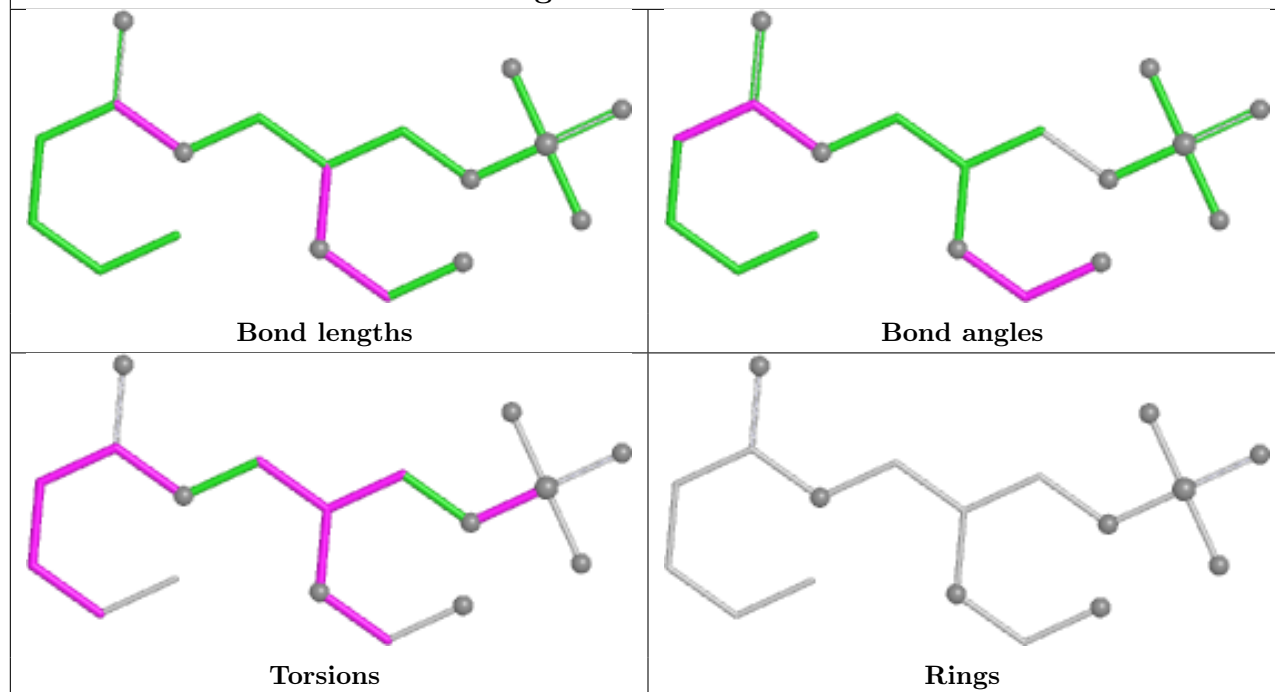
Ligand PA6 A 201



Ligand PQE A 205 (B)



Ligand PA6 A 202



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	A	192/196 (97%)	1.44	50 (26%) 1 1	27, 54, 125, 128	7 (3%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	PHE	5.5
1	A	154	GLY	5.5
1	A	164	MET	5.2
1	A	139	LEU	5.1
1	A	4	PHE	5.0
1	A	136	LEU	4.7
1	A	140	PRO	4.7
1	A	133	ASN	4.5
1	A	134[A]	HIS	4.3
1	A	184	SER	4.2
1	A	9	GLY	4.1
1	A	165	GLY	4.1
1	A	160	PHE	4.0
1	A	33	ASP	4.0
1	A	135	HIS	4.0
1	A	30	PHE	3.9
1	A	137	PHE	3.8
1	A	150	GLY	3.5
1	A	156	ILE	3.4
1	A	143	PHE	3.4
1	A	162	VAL	3.3
1	A	152	ALA	3.2
1	A	193	LEU	3.1
1	A	161	GLY	3.0
1	A	145	THR	2.9
1	A	5	LEU	2.9
1	A	144	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	147	LEU	2.9
1	A	68	PHE	2.8
1	A	6	ALA	2.7
1	A	159	LEU	2.6
1	A	186	LEU	2.6
1	A	141	GLU	2.6
1	A	163	GLU	2.6
1	A	43	TYR	2.6
1	A	73	PHE	2.5
1	A	157	SER	2.5
1	A	153	LEU	2.5
1	A	166	ASN	2.4
1	A	7	GLN	2.4
1	A	148	LEU	2.4
1	A	149	VAL	2.3
1	A	146	MET	2.3
1	A	151	ILE	2.3
1	A	128[A]	ILE	2.2
1	A	108	SER	2.2
1	A	36	TYR	2.2
1	A	107	VAL	2.1
1	A	142	GLY	2.0
1	A	42	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.

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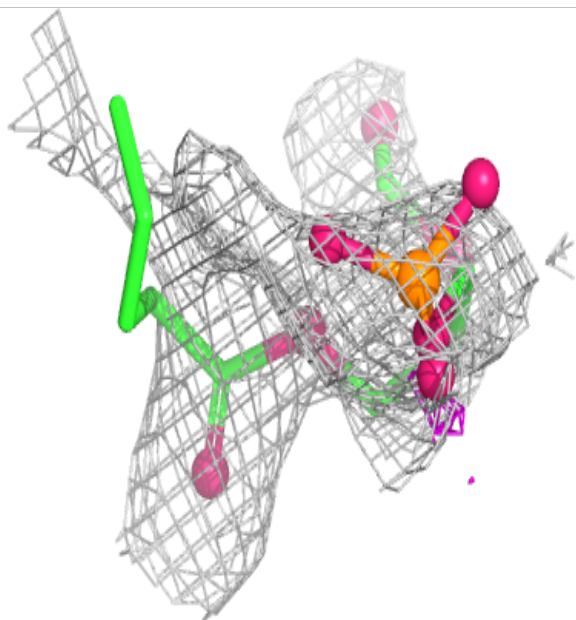
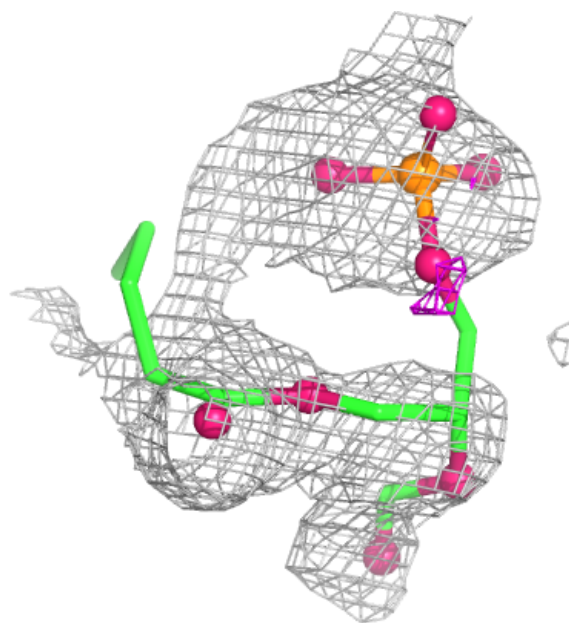
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PA6	A	203	18/18	0.59	0.17	126,126,127,127	0
2	PA6	A	202	18/18	0.67	0.17	100,103,105,105	0
3	PQE	A	205[A]	37/37	0.74	0.18	57,72,85,85	10
3	PQE	A	205[B]	37/37	0.74	0.18	61,72,85,85	10
3	PQE	A	204	37/37	0.75	0.15	73,77,91,91	0
2	PA6	A	201	18/18	0.76	0.14	94,98,99,99	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.

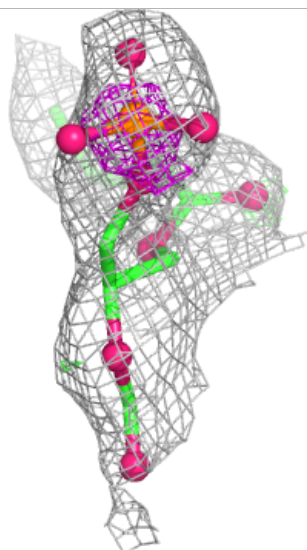
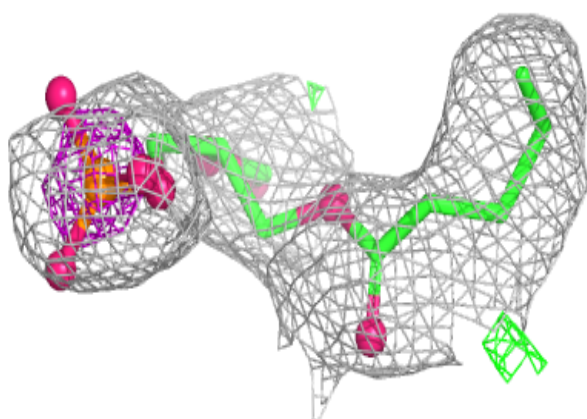
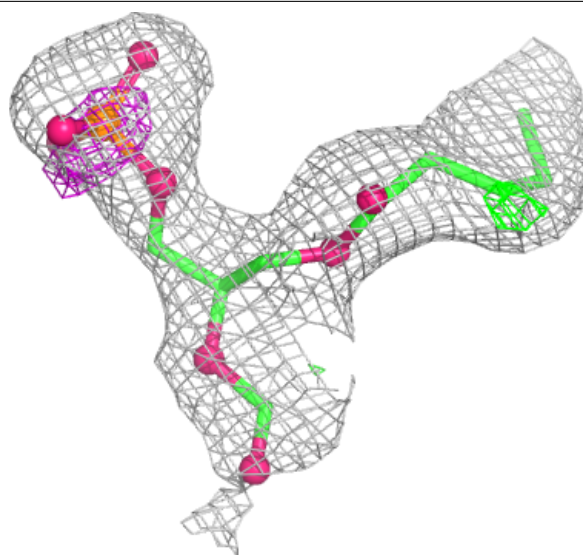
Electron density around PA6 A 203:

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



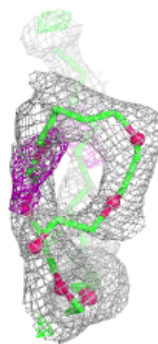
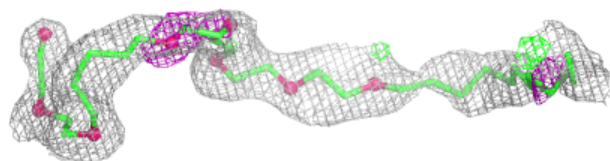
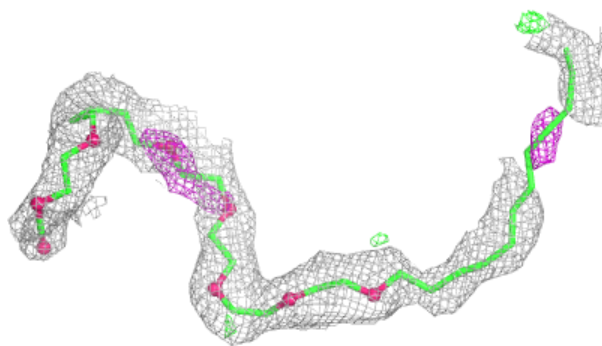
Electron density around PA6 A 202:

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



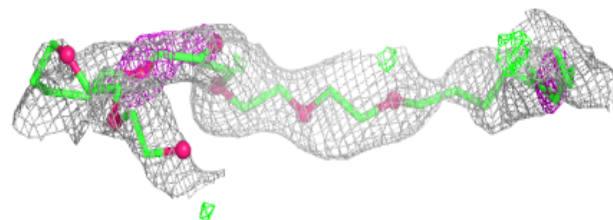
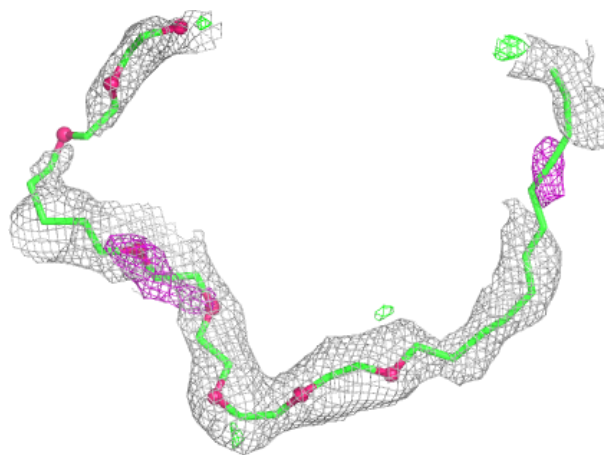
Electron density around PQE A 205 (A):

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



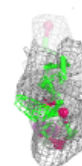
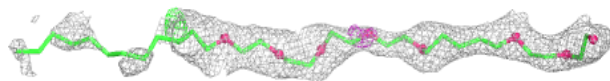
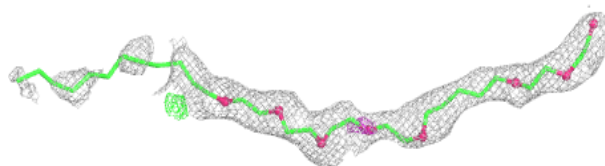
Electron density around PQE A 205 (B):

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

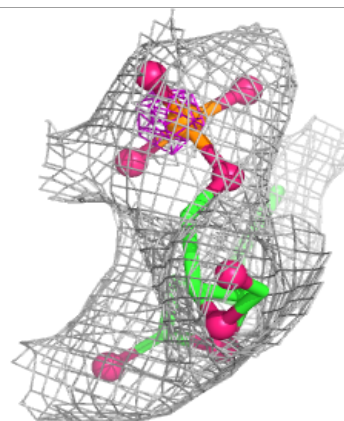
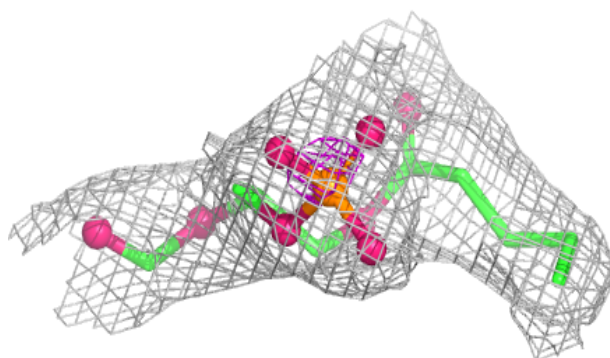
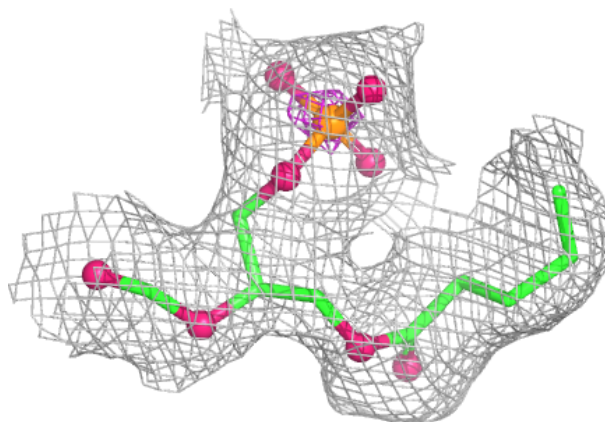


Electron density around PQE A 204:

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

**Electron density around PA6 A 201:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.