



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 08:04 PM UTC

PDB ID : 4R5O / pdb_00004r5o
Title : Crystal structure of a Quinonprotein alcohol dehydrogenase-like protein (BT1487) from Bacteroides thetaiotaomicron VPI-5482 at 2.64 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2014-08-21
Resolution : 2.64 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

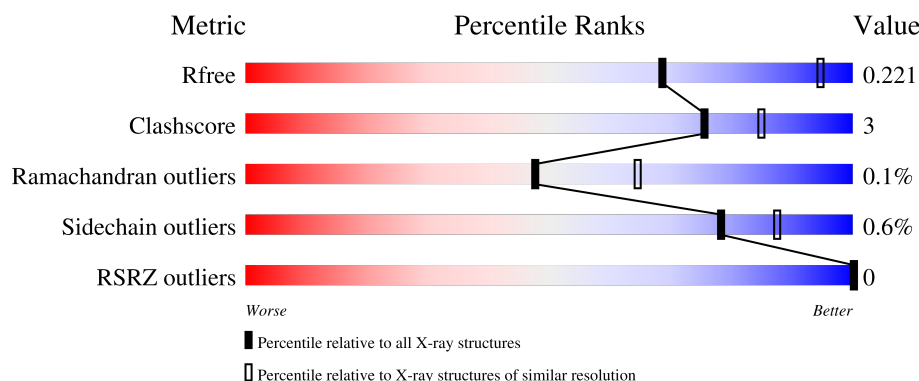
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	427	90% 9%
1	B	427	88% 9% .
1	C	427	90% 7% .
1	D	427	91% 8%

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
3	ACT	B	507	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13489 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.

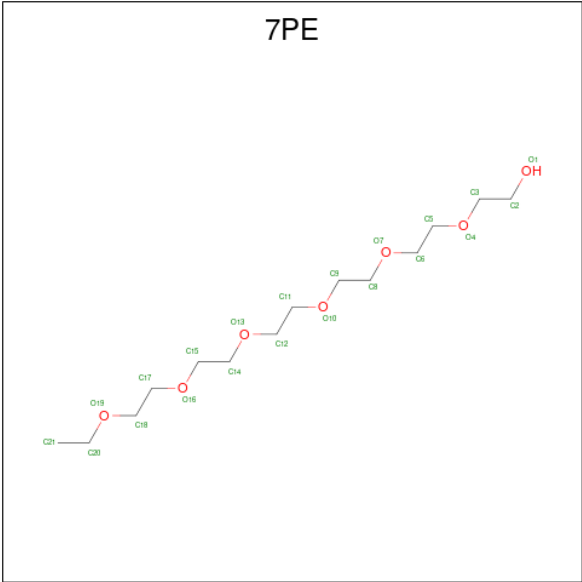
- Molecule 1 is a protein called Quinonprotein alcohol dehydrogenase-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	Se	0	3	0
			3323	2105	535	674	7	2			
1	B	416	Total	C	N	O	S	Se	0	0	0
			3230	2050	522	650	6	2			
1	C	416	Total	C	N	O	S	Se	0	3	0
			3214	2039	517	650	6	2			
1	D	425	Total	C	N	O	S	Se	0	0	0
			3239	2056	519	655	7	2			

There are 4 discrepancies between the modelled and reference sequences:

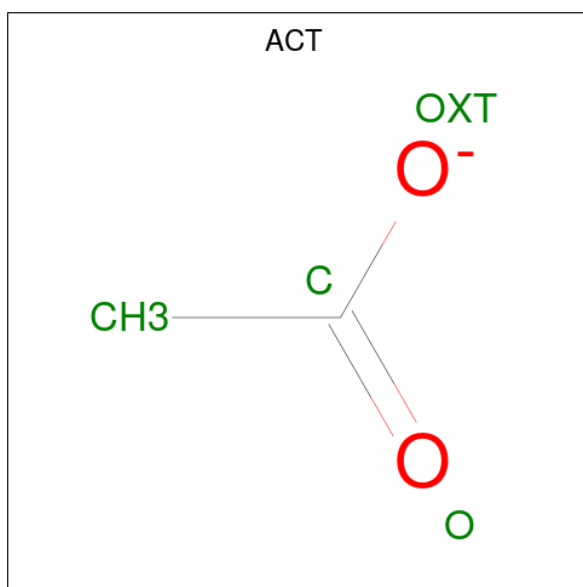
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q8A7N7
B	0	GLY	-	expression tag	UNP Q8A7N7
C	0	GLY	-	expression tag	UNP Q8A7N7
D	0	GLY	-	expression tag	UNP Q8A7N7

- Molecule 2 is 2-(2-(2-(2-(2-ETHOXYETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHOXY)ETHANOL (CCD ID: 7PE) (formula: C₁₄H₃₀O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	A	1	Total	C	O	0	0
			13	8	5		
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			11	7	4		
2	B	1	Total	C	O	0	0
			13	8	5		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Ca 4 4	0	0
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	92	Total 92	O 92	0	0
6	B	115	Total 116	O 116	0	1
6	C	92	Total 92	O 92	0	0
6	D	45	Total 45	O 45	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	155.54Å 155.54Å 94.64Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.39 – 2.64 29.39 – 2.64	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.39-2.64) 98.6 (29.39-2.64)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.64Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.176 , 0.203 0.190 , 0.221	Depositor DCC
R_{free} test set	3712 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l 0.177 for h,-h-k,-l 0.048 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13489	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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: CA, ACT, 7PE, 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	0.85	0/3393	1.21	8/4605 (0.2%)
1	B	0.86	1/3292 (0.0%)	1.21	12/4465 (0.3%)
1	C	0.86	1/3282 (0.0%)	1.20	7/4461 (0.2%)
1	D	0.82	0/3300	1.20	13/4483 (0.3%)
All	All	0.85	2/13267 (0.0%)	1.20	40/18014 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	111	MSE	SE-CE	-5.34	1.79	1.95
1	B	168	ILE	CG1-CD1	-5.08	1.31	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	PHE	CA-CB-CG	8.49	122.29	113.80
1	C	247	PHE	CA-CB-CG	8.18	121.98	113.80
1	B	247	PHE	CA-CB-CG	8.14	121.94	113.80
1	D	247	PHE	CA-CB-CG	7.63	121.43	113.80
1	B	259	SER	CA-C-N	6.43	132.83	123.13
1	B	259	SER	C-N-CA	6.43	132.83	123.13
1	D	91	ASP	CA-CB-CG	6.31	118.91	112.60
1	A	350	ILE	CA-C-N	6.22	126.25	120.34
1	A	350	ILE	C-N-CA	6.22	126.25	120.34
1	D	104	ASN	CA-CB-CG	6.01	118.61	112.60
1	B	413	GLU	CA-C-N	5.96	128.58	120.54
1	B	413	GLU	C-N-CA	5.96	128.58	120.54
1	A	447	ASN	CA-CB-CG	5.86	118.46	112.60
1	A	367	ASP	CA-CB-CG	5.79	118.39	112.60
1	C	104	ASN	CA-CB-CG	5.79	118.39	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	350	ILE	CA-C-N	5.61	125.67	120.34
1	D	350	ILE	C-N-CA	5.61	125.67	120.34
1	B	367	ASP	CA-CB-CG	5.52	118.12	112.60
1	B	418	GLU	CB-CG-CD	5.50	121.95	112.60
1	B	379	ASP	CA-CB-CG	5.47	118.07	112.60
1	D	413	GLU	CA-C-N	5.47	127.92	120.54
1	D	413	GLU	C-N-CA	5.47	127.92	120.54
1	D	238	ARG	CA-C-N	5.46	128.55	120.74
1	D	238	ARG	C-N-CA	5.46	128.55	120.74
1	D	367	ASP	CA-CB-CG	5.42	118.02	112.60
1	C	350	ILE	CA-C-N	5.41	125.48	120.34
1	C	350	ILE	C-N-CA	5.41	125.48	120.34
1	A	104	ASN	CA-CB-CG	5.26	117.86	112.60
1	B	130	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	344	TYR	CA-C-N	5.15	127.70	120.28
1	B	344	TYR	C-N-CA	5.15	127.70	120.28
1	C	91	ASP	CA-CB-CG	5.14	117.74	112.60
1	C	344	TYR	CA-C-N	5.13	127.66	120.28
1	C	344	TYR	C-N-CA	5.13	127.66	120.28
1	D	218	TYR	CA-C-N	5.10	126.11	121.82
1	D	218	TYR	C-N-CA	5.10	126.11	121.82
1	B	91	ASP	CA-CB-CG	5.09	117.69	112.60
1	D	327	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	261	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	32	ASN	CA-CB-CG	5.07	117.67	112.60

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	A	3323	0	3190	26	0
1	B	3230	0	3128	21	0
1	C	3214	0	3068	17	0
1	D	3239	0	3083	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	33	0	43	4	0
2	B	45	0	57	2	0
2	C	30	0	39	5	0
2	D	7	0	9	0	0
3	A	8	0	6	0	0
3	B	8	0	6	2	0
4	A	4	0	0	0	0
4	B	1	0	0	0	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	92	0	0	1	0
6	B	116	0	0	1	0
6	C	92	0	0	0	0
6	D	45	0	0	0	0
All	All	13489	0	12629	77	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 3.

All (77) 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:408:TYR:HD1	1:A:423:VAL:HG22	1.37	0.90
1:A:349:THR:HB	2:A:503:7PE:H82	1.64	0.80
1:A:408:TYR:CD1	1:A:423:VAL:HG22	2.21	0.76
1:A:408:TYR:HE2	1:A:446:PHE:HZ	1.34	0.74
1:B:40:LEU:O	1:B:43:THR:HG22	1.89	0.73
1:B:228:ARG:NH1	1:B:239:ILE:HD11	2.04	0.71
1:D:40:LEU:O	1:D:43:THR:HG22	1.92	0.69
1:C:119:HIS:HA	2:C:501:7PE:H62	1.77	0.65
1:D:128:VAL:HG21	1:D:167:ILE:HD12	1.80	0.62
1:A:408:TYR:HE2	1:A:446:PHE:CZ	2.16	0.60
1:A:190:ILE:HD11	1:A:234:LEU:HD21	1.83	0.59
1:D:190:ILE:HD11	1:D:234:LEU:HD21	1.84	0.58
1:B:190:ILE:HD11	1:B:234:LEU:HD21	1.85	0.58
1:B:43:THR:HG21	1:B:62:GLU:H	1.68	0.58
1:C:190:ILE:HD11	1:C:234:LEU:HD21	1.85	0.57
1:D:43:THR:HG21	1:D:62:GLU:H	1.69	0.57
1:A:45:PRO:HG2	1:A:113:THR:HG21	1.86	0.56
1:D:159:ILE:HD13	1:D:165:ALA:HB2	1.88	0.56
1:A:43:THR:HG21	1:A:62:GLU:H	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:LEU:O	1:A:43:THR:HG22	2.05	0.55
1:D:258:LEU:HD23	1:D:271:TYR:HB3	1.88	0.55
1:B:294:ILE:HG21	2:B:505:7PE:H61	1.87	0.55
1:B:258:LEU:HD23	1:B:271:TYR:HB3	1.88	0.55
1:C:258:LEU:HD23	1:C:271:TYR:HB3	1.89	0.55
1:A:397:PRO:HG3	2:A:503:7PE:H81	1.88	0.54
1:C:315:ALA:HB1	2:C:503:7PE:H92	1.88	0.54
1:B:281:LYS:HG2	1:D:281:LYS:HD2	1.90	0.54
1:A:258:LEU:HD23	1:A:271:TYR:HB3	1.90	0.53
1:D:239:ILE:HG22	1:D:286:PRO:HD3	1.91	0.53
1:B:220:LEU:HD11	1:B:277:LEU:HD13	1.91	0.52
1:B:80:TYR:OH	2:B:503:7PE:H52	2.10	0.52
1:B:128:VAL:HG21	1:B:167:ILE:HD12	1.91	0.52
1:D:220:LEU:HD11	1:D:277:LEU:HD13	1.92	0.52
1:A:220:LEU:HD11	1:A:277:LEU:HD13	1.92	0.51
1:C:220:LEU:HD11	1:C:277:LEU:HD13	1.92	0.51
1:B:425:SER:OG	1:B:429:LYS:HG2	2.11	0.51
1:B:159:ILE:HD13	1:B:165:ALA:HB2	1.94	0.50
1:A:159:ILE:HD13	1:A:165:ALA:HB2	1.94	0.49
1:A:58:GLU:HA	1:A:86:PHE:O	2.13	0.48
1:D:310:TYR:HA	1:D:322:VAL:O	2.13	0.48
1:A:238:ARG:HG3	6:A:618:HOH:O	2.12	0.48
1:B:239:ILE:HG22	1:B:286:PRO:HD3	1.95	0.47
1:D:239:ILE:CG2	1:D:286:PRO:HD3	2.45	0.47
1:C:292:ASP:HB2	2:C:502:7PE:H61	1.96	0.47
1:C:120:ASN:H	2:C:501:7PE:C8	2.28	0.46
1:A:128:VAL:HG21	1:A:167:ILE:HD12	1.98	0.46
1:C:128:VAL:O	1:C:441:PRO:HA	2.16	0.46
1:B:348:PRO:HG2	6:B:657:HOH:O	2.16	0.46
1:C:128:VAL:HG21	1:C:167:ILE:HD12	1.98	0.46
1:A:39:VAL:HG13	1:A:43:THR:CG2	2.46	0.46
1:D:396:ALA:HB3	1:D:410:THR:HB	1.98	0.45
1:C:120:ASN:H	2:C:501:7PE:H82	1.81	0.44
1:C:194:LYS:HA	1:C:447:ASN:HB2	1.99	0.44
1:B:401:ASN:HB2	1:B:408:TYR:HE1	1.83	0.44
1:A:43:THR:CG2	1:A:62:GLU:H	2.30	0.43
1:B:402:GLN:H	3:B:507:ACT:CH3	2.31	0.43
1:B:277:LEU:HD23	1:B:286:PRO:HG3	2.00	0.43
1:B:402:GLN:H	3:B:507:ACT:H1	1.84	0.43
1:A:349:THR:OG1	2:A:503:7PE:H51	2.19	0.43
1:C:228:ARG:HB2	1:C:239:ILE:HD11	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:THR:HG23	1:A:61:PRO:HA	1.99	0.43
1:C:396:ALA:HB3	1:C:410:THR:HB	2.01	0.43
1:D:277:LEU:HD23	1:D:286:PRO:HG3	1.99	0.43
1:A:257:VAL:O	1:A:271:TYR:HA	2.19	0.42
1:A:322:VAL:HG22	1:A:332:LYS:HG2	2.00	0.42
1:A:248:TYR:O	2:A:503:7PE:H52	2.20	0.42
1:D:257:VAL:O	1:D:271:TYR:HA	2.20	0.42
1:A:140:LYS:HA	1:C:55:GLU:HG2	2.02	0.41
1:D:408:TYR:CD2	1:D:423:VAL:HG22	2.55	0.41
1:A:436:CYS:SG	1:A:441:PRO:HG3	2.61	0.41
1:C:322:VAL:HG22	1:C:332:LYS:HG2	2.01	0.41
1:B:257:VAL:O	1:B:271:TYR:HA	2.20	0.41
1:B:396:ALA:HB3	1:B:410:THR:HB	2.02	0.41
1:A:55:GLU:HG2	1:C:140:LYS:HA	2.03	0.41
1:D:256:LYS:HD3	1:D:273:ASP:HA	2.02	0.41
1:B:239:ILE:CG2	1:B:286:PRO:HD3	2.51	0.41
1:C:63:LEU:HD21	1:C:102:ILE:HG21	2.03	0.40

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	A	427/427 (100%)	409 (96%)	18 (4%)	0	100	100
1	B	414/427 (97%)	401 (97%)	13 (3%)	0	100	100
1	C	417/427 (98%)	406 (97%)	11 (3%)	0	100	100
1	D	423/427 (99%)	409 (97%)	13 (3%)	1 (0%)	43	58
All	All	1681/1708 (98%)	1625 (97%)	55 (3%)	1 (0%)	48	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	264	LYS

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	A	365/369 (99%)	363 (100%)	2 (0%)	81	89
1	B	355/369 (96%)	353 (99%)	2 (1%)	78	87
1	C	349/369 (95%)	348 (100%)	1 (0%)	86	93
1	D	347/369 (94%)	344 (99%)	3 (1%)	70	82
All	All	1416/1476 (96%)	1408 (99%)	8 (1%)	78	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	367	ASP
1	B	367	ASP
1	B	415	ARG
1	C	83	GLU
1	D	78	LYS
1	D	363	LEU
1	D	367	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	GLN
1	A	308	ASN
1	A	326	ASN
1	B	217	GLN
1	B	448	ASN
1	C	320	ASN
1	C	448	ASN
1	D	338	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	448	ASN

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](#)

Of 23 ligands modelled in this entry, 7 are monoatomic - leaving 16 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	$\# Z > 2$
2	7PE	B	501	-	10,10,20	0.36	0	9,9,19	0.48	0
3	ACT	B	506	-	3,3,3	1.14	0	3,3,3	0.92	0
2	7PE	B	505	-	6,6,20	0.31	0	5,5,19	0.45	0
2	7PE	A	501	-	9,9,20	0.28	0	8,8,19	0.32	0
2	7PE	B	502	-	12,12,20	0.21	0	11,11,19	0.44	0
3	ACT	A	504	-	3,3,3	1.00	0	3,3,3	1.17	0
3	ACT	B	507	-	3,3,3	1.08	0	3,3,3	0.83	0
2	7PE	D	501	-	6,6,20	0.11	0	5,5,19	0.31	0
2	7PE	A	502	-	12,12,20	0.21	0	11,11,19	0.44	0
2	7PE	C	501	-	9,9,20	0.25	0	8,8,19	0.30	0
3	ACT	A	505	-	3,3,3	1.33	1 (33%)	3,3,3	0.76	0
2	7PE	C	503	-	9,9,20	0.21	0	8,8,19	0.33	0
2	7PE	B	503	-	6,6,20	0.20	0	5,5,19	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	7PE	A	503	-	9,9,20	0.25	0	8,8,19	0.43	0
2	7PE	C	502	-	9,9,20	0.14	0	8,8,19	0.19	0
2	7PE	B	504	-	6,6,20	0.32	0	5,5,19	0.23	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
2	7PE	B	501	-	-	3/8/8/18	-
2	7PE	B	505	-	-	2/4/4/18	-
2	7PE	A	501	-	-	4/7/7/18	-
2	7PE	B	502	-	-	4/10/10/18	-
2	7PE	D	501	-	-	1/4/4/18	-
2	7PE	A	502	-	-	3/10/10/18	-
2	7PE	C	501	-	-	3/7/7/18	-
2	7PE	C	503	-	-	3/7/7/18	-
2	7PE	B	503	-	-	0/4/4/18	-
2	7PE	A	503	-	-	3/7/7/18	-
2	7PE	C	502	-	-	2/7/7/18	-
2	7PE	B	504	-	-	0/4/4/18	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	505	ACT	CH3-C	2.01	1.57	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	7PE	C9-C8-O7-C6
2	C	501	7PE	O4-C5-C6-O7
2	C	502	7PE	C5-C6-O7-C8
2	A	501	7PE	C2-C3-O4-C5
2	B	505	7PE	C6-C5-O4-C3
2	B	501	7PE	C5-C6-O7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	503	7PE	C9-C8-O7-C6
2	A	503	7PE	C2-C3-O4-C5
2	B	502	7PE	C9-C8-O7-C6
2	D	501	7PE	C2-C3-O4-C5
2	C	502	7PE	C9-C8-O7-C6
2	A	501	7PE	C9-C8-O7-C6
2	A	502	7PE	C5-C6-O7-C8
2	A	503	7PE	C5-C6-O7-C8
2	C	501	7PE	C9-C8-O7-C6
2	B	502	7PE	C6-C5-O4-C3
2	A	501	7PE	C6-C5-O4-C3
2	B	505	7PE	O1-C2-C3-O4
2	A	502	7PE	C12-C11-O10-C9
2	B	501	7PE	C2-C3-O4-C5
2	A	502	7PE	C2-C3-O4-C5
2	C	503	7PE	C2-C3-O4-C5
2	C	503	7PE	C5-C6-O7-C8
2	B	501	7PE	C8-C9-O10-C11
2	C	501	7PE	C5-C6-O7-C8
2	B	502	7PE	C8-C9-O10-C11
2	B	502	7PE	O4-C5-C6-O7
2	A	501	7PE	O4-C5-C6-O7

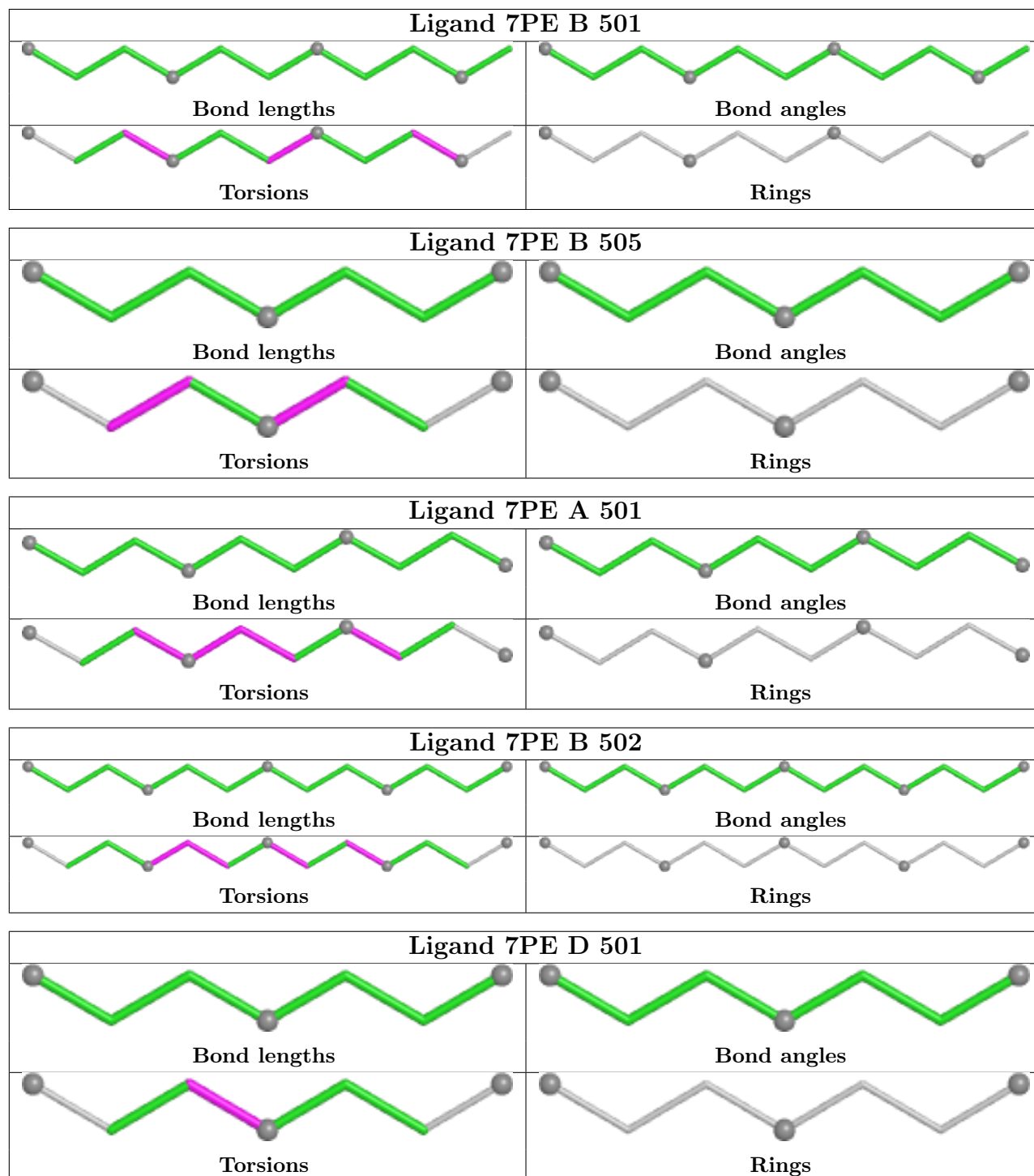
There are no ring outliers.

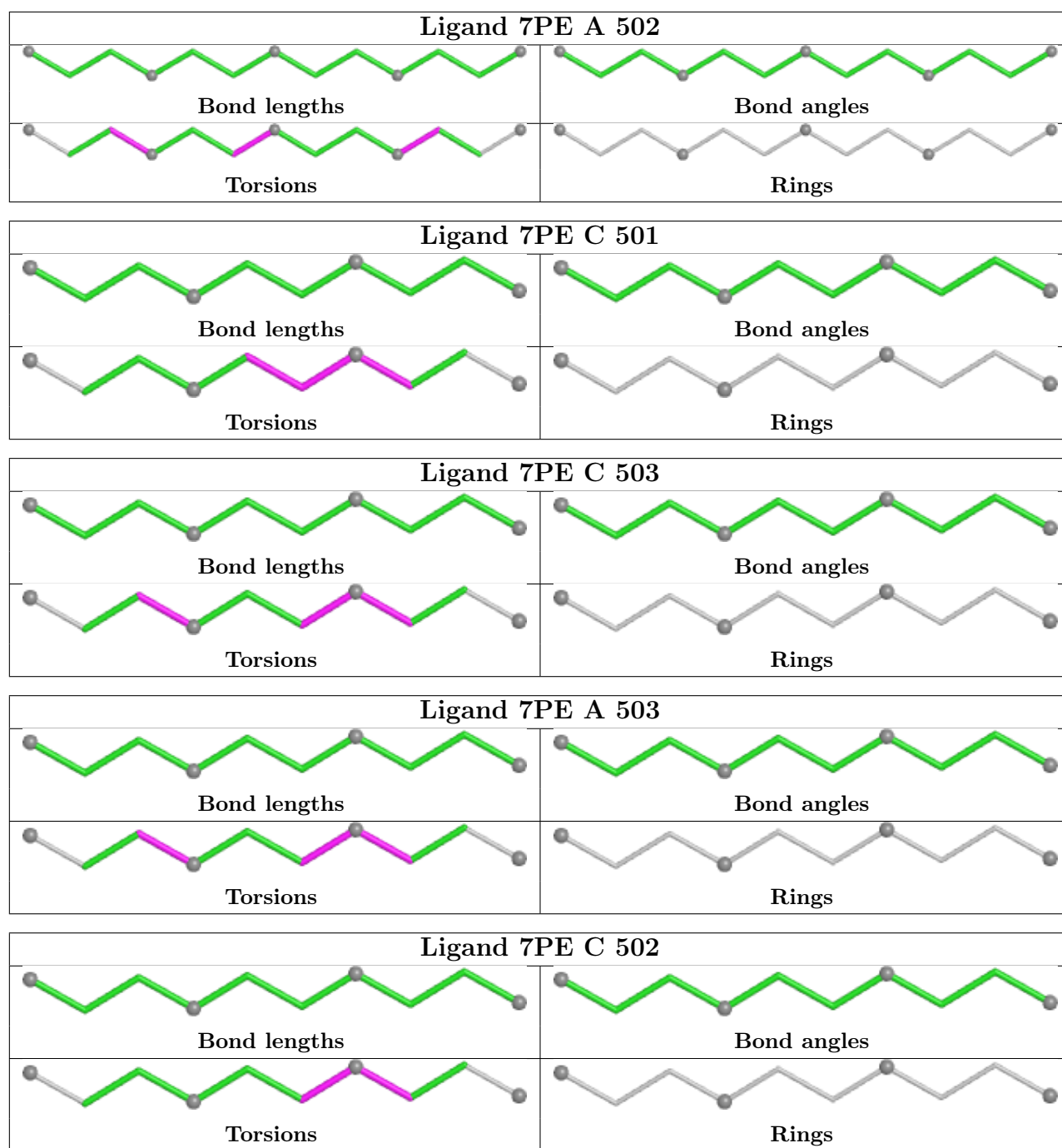
7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	505	7PE	1	0
3	B	507	ACT	2	0
2	C	501	7PE	3	0
2	C	503	7PE	1	0
2	B	503	7PE	1	0
2	A	503	7PE	4	0
2	C	502	7PE	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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	424/427 (99%)	-1.62	0 100 100	19, 53, 85, 113	3 (0%)
1	B	414/427 (96%)	-1.68	0 100 100	31, 49, 79, 99	0
1	C	414/427 (96%)	-1.58	0 100 100	26, 55, 81, 102	3 (0%)
1	D	423/427 (99%)	-1.45	0 100 100	47, 66, 101, 123	0
All	All	1675/1708 (98%)	-1.58	0 100 100	19, 56, 89, 123	6 (0%)

There are no RSRZ outliers to report.

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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	7PE	A	501	10/21	0.97	0.07	76,81,84,84	0
2	7PE	C	503	10/21	0.97	0.10	90,92,93,93	0
3	ACT	A	504	4/4	0.97	0.08	73,75,75,80	0
2	7PE	D	501	7/21	0.98	0.06	63,63,65,66	0

Continued on next page...

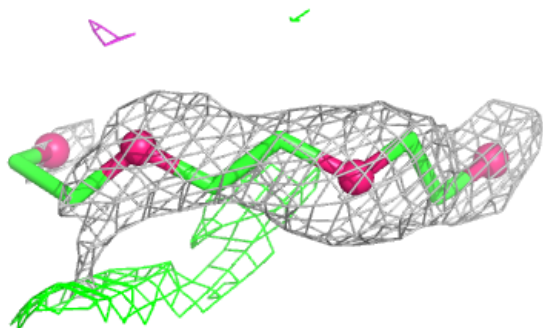
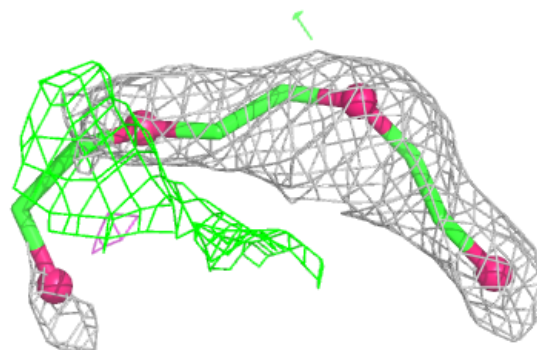
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	7PE	B	502	13/21	0.98	0.09	71,85,94,94	0
2	7PE	B	503	7/21	0.99	0.07	58,61,64,65	0
2	7PE	B	504	7/21	0.99	0.04	56,56,62,63	0
2	7PE	B	505	7/21	0.99	0.04	58,61,65,66	0
2	7PE	C	501	10/21	0.99	0.04	62,66,73,75	0
2	7PE	C	502	10/21	0.99	0.05	74,78,82,82	0
2	7PE	A	503	10/21	0.99	0.08	72,88,93,95	0
2	7PE	B	501	11/21	0.99	0.05	49,54,59,60	0
2	7PE	A	502	13/21	0.99	0.04	56,60,74,77	0
3	ACT	A	505	4/4	0.99	0.06	69,72,73,74	0
3	ACT	B	506	4/4	0.99	0.06	73,76,77,77	0
3	ACT	B	507	4/4	0.99	0.06	64,70,72,75	0
4	CA	A	508	1/1	0.99	0.04	99,99,99,99	0
4	CA	B	508	1/1	0.99	0.05	91,91,91,91	0
5	CL	A	510	1/1	0.99	0.04	72,72,72,72	0
4	CA	A	509	1/1	1.00	0.03	79,79,79,79	0
4	CA	A	507	1/1	1.00	0.02	90,90,90,90	0
4	CA	A	506	1/1	1.00	0.02	81,81,81,81	0
5	CL	C	504	1/1	1.00	0.06	78,78,78,78	0

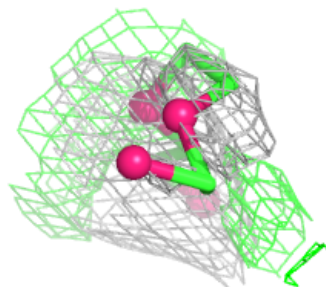
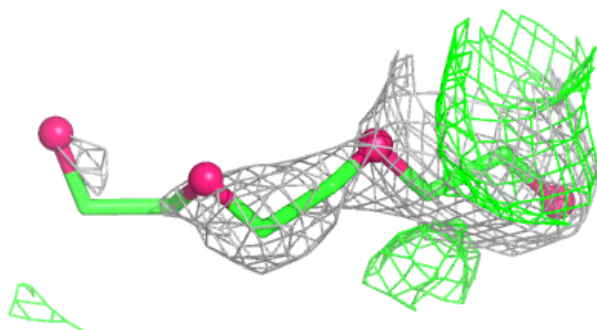
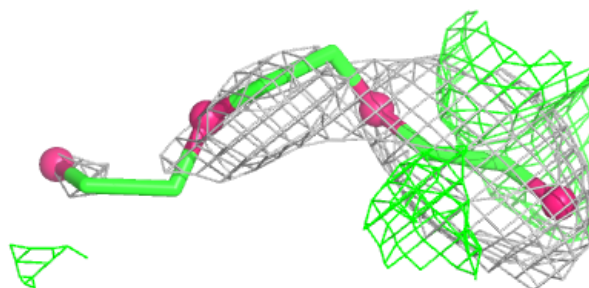
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 7PE A 501:

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

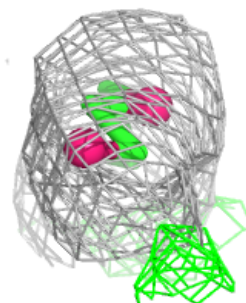
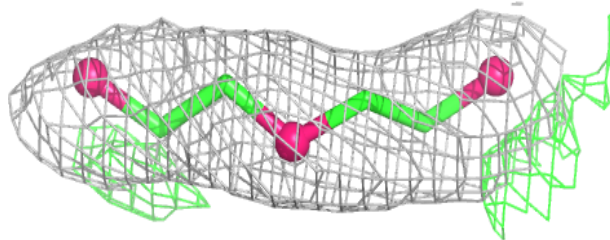
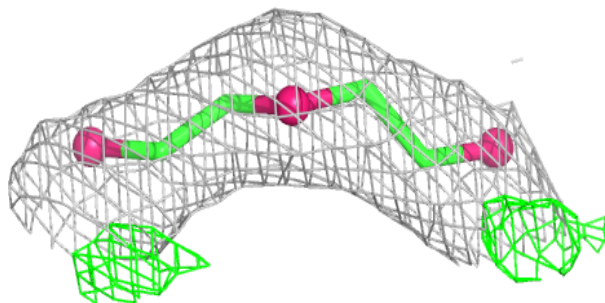
**Electron density around 7PE C 503:**

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

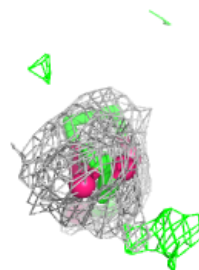
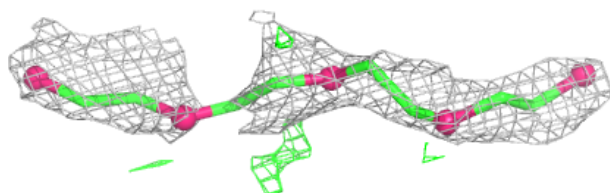
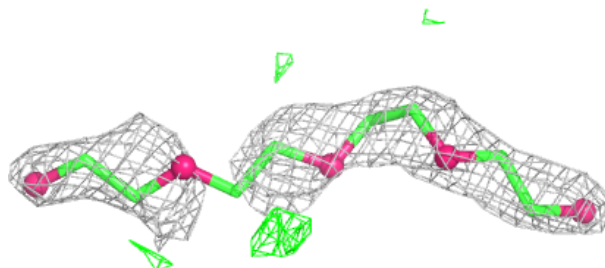


Electron density around 7PE D 501:

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

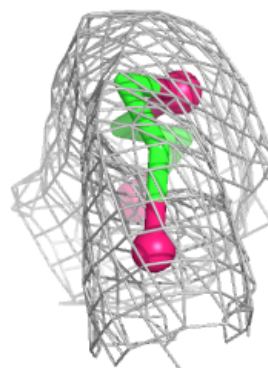
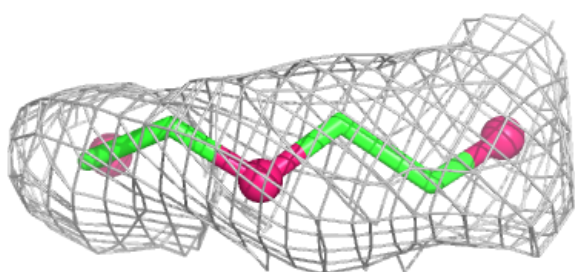
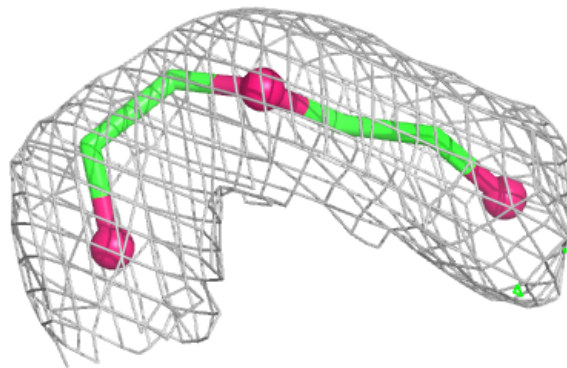
**Electron density around 7PE B 502:**

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

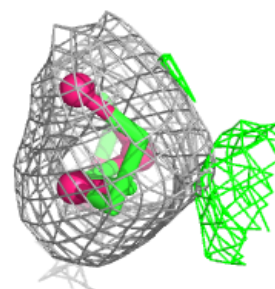
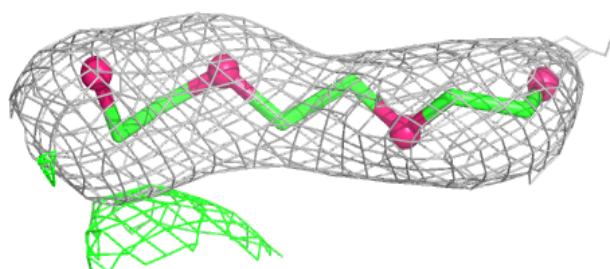
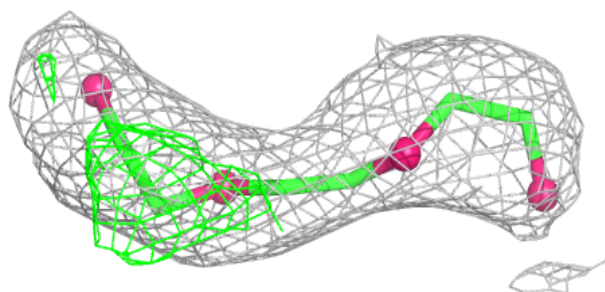


Electron density around 7PE B 505:

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

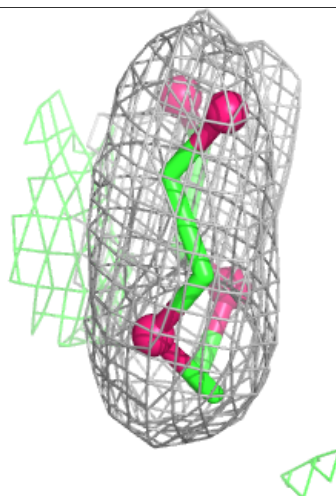
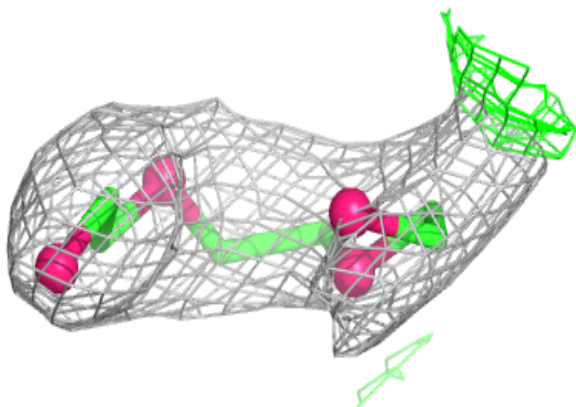
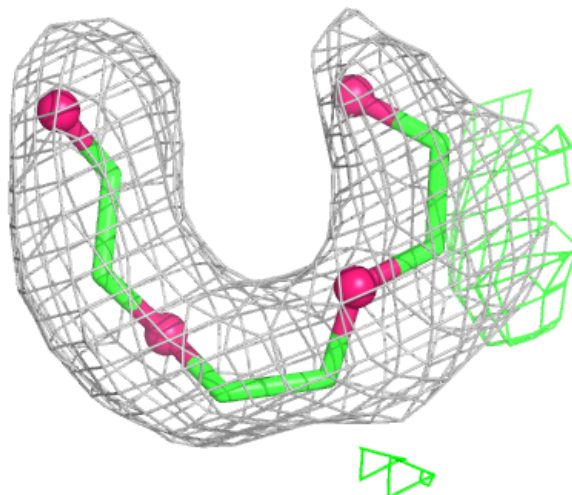
**Electron density around 7PE C 501:**

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



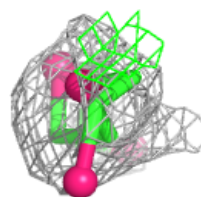
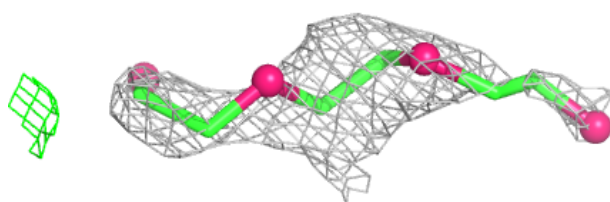
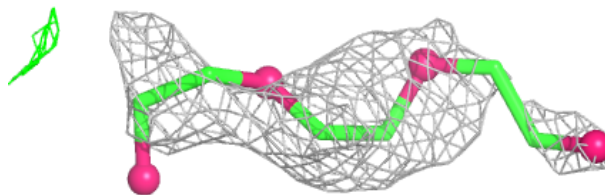
Electron density around 7PE C 502:

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

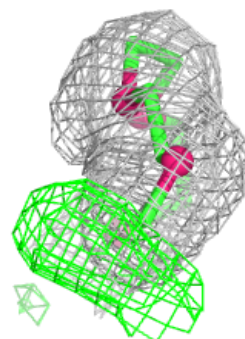
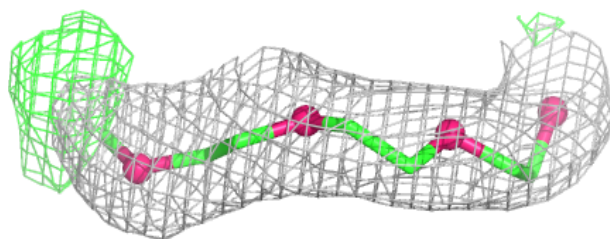
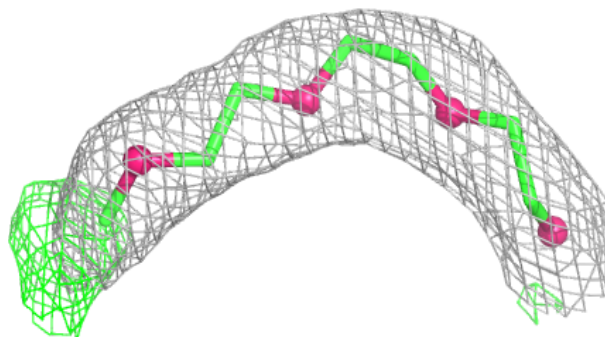


Electron density around 7PE A 503:

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

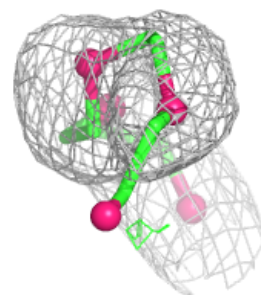
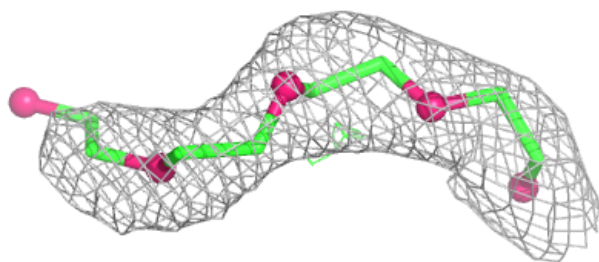
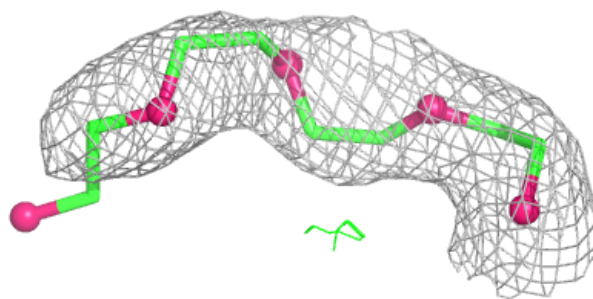
**Electron density around 7PE B 501:**

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



Electron density around 7PE A 502:

$2mF_o-DF_c$ (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.