



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 05:19 pm BST

PDB ID : 2W16
Title : Structures of FpvA bound to heterologous pyoverdines
Authors : Greenwald, J.; Nader, M.; Celia, H.; Gruffaz, C.; Meyer, J.-M.; Schalk, I.J.; Pattus, F.
Deposited on : 2008-10-14
Resolution : 2.71 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 : 2.11
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) : 2.11

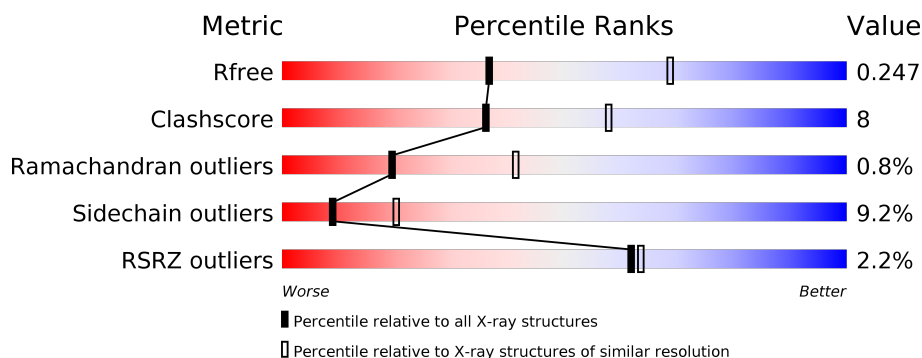
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	772	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 18%, green 78%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> % 78% 18% . </div> </div>
1	B	772	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 19%, green 76%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 3% 76% 19% .. </div> </div>
2	C	8	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 63%, yellow 38%);"></div> <div style="display: flex; justify-content: space-between; margin-top: 2px;"> 63% 38% </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12325 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.

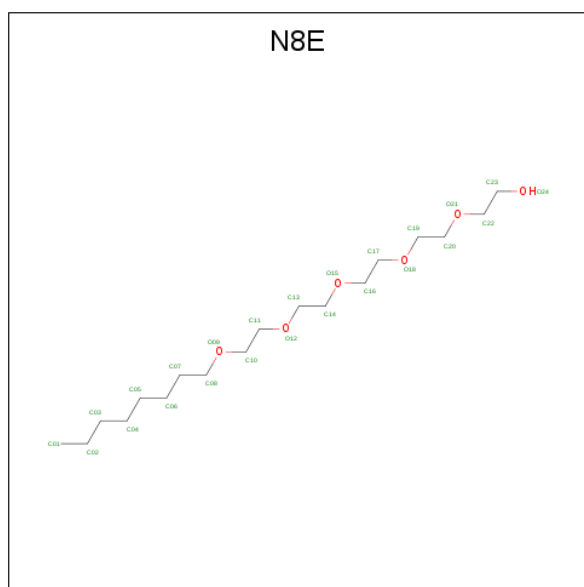
- Molecule 1 is a protein called FERRIPYOVERDINE RECEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	772	Total	C	N	O	S	0	0	0
			6114	3845	1046	1211	12			
1	B	754	Total	C	N	O	S	0	0	0
			5994	3775	1027	1181	11			

- Molecule 2 is a protein called DSN-ARG-DSN-FHO-LYS-FHO-THR-THR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			68	38	14	16			

- Molecule 3 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (three-letter code: N8E) (formula: $C_{18}H_{38}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			24	18	6		

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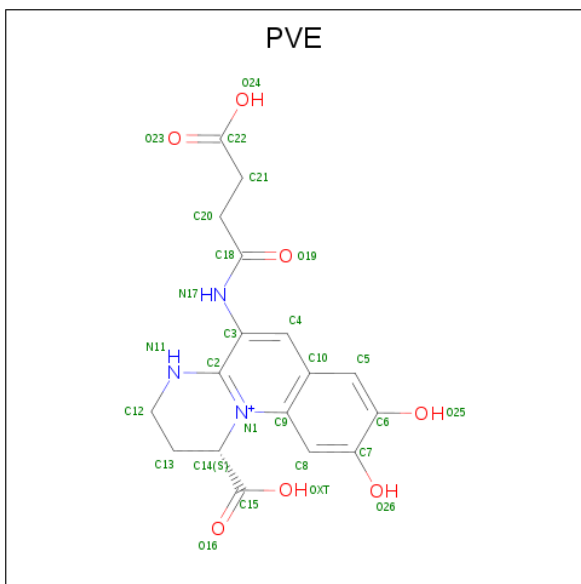
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			48	36	12		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 5 is (1S)-1-CARBOXY-5-[(3-CARBOXYPROANOYL)AMINO]-8,9-DIHYDROXY-1,2,3,4-TETRAHYDROPYRIMIDO[1,2-A]QUINOLIN-11-IUM (three-letter code: PVE) (formula: C₁₇H₁₈N₃O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			26	17	3	6		

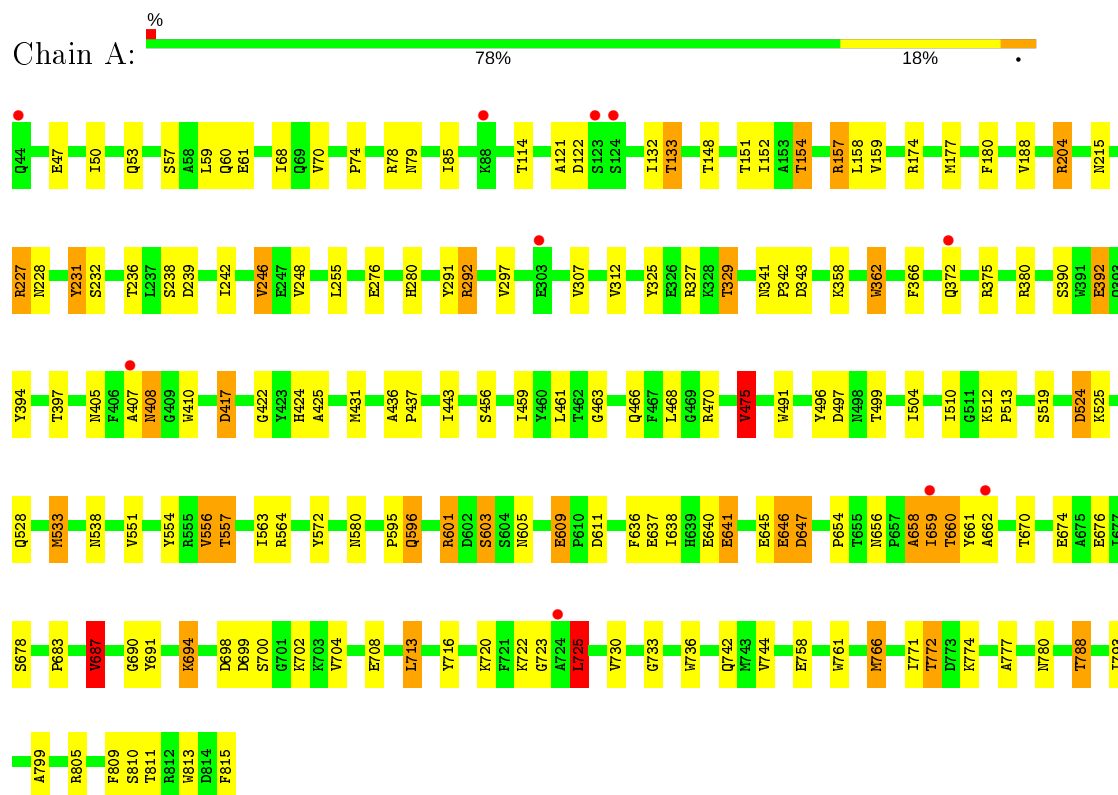
- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Fe	0	0
			1	1		

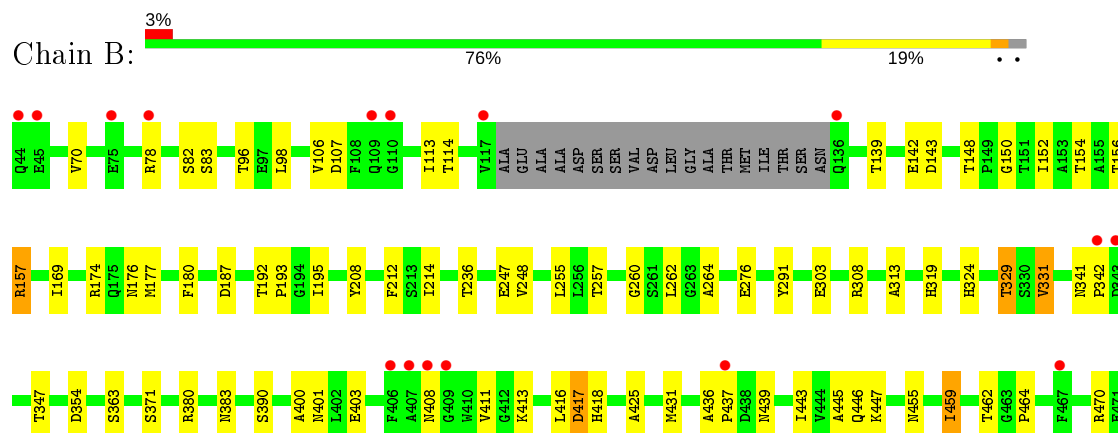
3 Residue-property plots

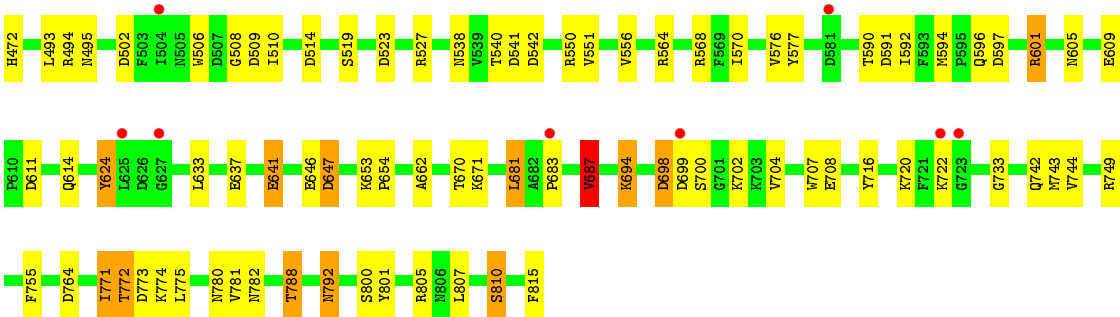
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: FERRIPYOVERDINE RECEPTOR



• Molecule 1: FERRIPYOVERDINE RECEPTOR





● Molecule 2: DSN-ARG-DSN-FHO-LYS-FHO-THR-THR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	195.22Å 130.08Å 141.78Å 90.00° 130.67° 90.00°	Depositor
Resolution (Å)	107.83 – 2.71 29.53 – 2.71	Depositor EDS
% Data completeness (in resolution range)	95.2 (107.83-2.71) 95.3 (29.53-2.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.4.0054	Depositor
R, R_{free}	0.217 , 0.253 0.214 , 0.247	Depositor DCC
R_{free} test set	3512 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 64.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12325	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DSN, FHO, PO4, N8E, PVE, FE

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	0.91	2/6266 (0.0%)	0.96	12/8514 (0.1%)
1	B	0.77	1/6145 (0.0%)	0.84	6/8347 (0.1%)
2	C	0.79	0/31	1.27	0/36
All	All	0.85	3/12442 (0.0%)	0.90	18/16897 (0.1%)

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	A	0	1
1	B	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	61	GLU	CG-CD	5.94	1.60	1.51
1	B	810	SER	CB-OG	-5.39	1.35	1.42
1	A	758	GLU	CB-CG	5.04	1.61	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	292	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	A	292	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	A	713	LEU	CA-CB-CG	7.93	133.55	115.30
1	A	687	VAL	CB-CA-C	-7.77	96.64	111.40
1	B	687	VAL	CB-CA-C	-6.65	98.76	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	725	LEU	CA-CB-CG	6.52	130.30	115.30
1	B	187	ASP	CB-CG-OD1	6.47	124.12	118.30
1	A	647	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	683	PRO	C-N-CA	-5.75	110.22	122.30
1	A	766	MET	CG-SD-CE	-5.69	91.10	100.20
1	A	475	VAL	CB-CA-C	-5.68	100.61	111.40
1	B	633	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	681	LEU	CA-CB-CG	5.61	128.20	115.30
1	B	308	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	362	TRP	CA-CB-CG	5.25	123.68	113.70
1	A	641	GLU	CB-CA-C	5.14	120.69	110.40
1	B	523	ASP	CB-CG-OD1	5.14	122.92	118.30
1	A	204	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	TYR	Peptide
1	B	698	ASP	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	6114	0	5788	92	0
1	B	5994	0	5675	102	0
2	C	68	0	62	2	0
3	A	72	0	114	5	0
4	A	30	0	0	1	0
4	B	20	0	0	1	0
5	C	26	0	14	0	0
6	C	1	0	0	0	0
All	All	12325	0	11653	191	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 8.

All (191) 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:722:LYS:HG3	1:A:723:GLY:H	1.24	1.01
1:A:772:THR:HG21	1:B:291:TYR:OH	1.63	0.98
1:B:694:LYS:HE3	1:B:708:GLU:OE1	1.67	0.94
1:A:772:THR:HG22	1:A:774:LYS:H	1.32	0.92
1:A:470:ARG:NH1	1:A:538:ASN:OD1	2.04	0.90
1:B:472:HIS:HD2	1:B:538:ASN:H	1.18	0.84
1:A:700:SER:OG	1:A:702:LYS:HG2	1.78	0.84
1:A:151:THR:O	1:A:152:ILE:HD13	1.77	0.83
1:A:777:ALA:HB1	3:A:1817[B]:N8E:H192	1.59	0.82
1:A:694:LYS:HE2	1:A:708:GLU:OE1	1.80	0.82
1:A:722:LYS:HG3	1:A:723:GLY:N	1.97	0.79
1:A:291:TYR:OH	1:B:772:THR:HG21	1.83	0.78
1:B:418:HIS:HD2	1:B:455:ASN:HD21	1.28	0.78
1:B:772:THR:HG22	1:B:775:LEU:H	1.50	0.74
1:B:154:THR:OG1	1:B:247:GLU:OE1	2.04	0.73
1:A:525:LYS:HB2	1:A:557:THR:HG22	1.70	0.72
1:B:347:THR:HB	1:B:401:ASN:HB2	1.72	0.72
1:A:809:PHE:CD1	1:B:771:ILE:HG12	2.23	0.72
1:B:472:HIS:CD2	1:B:538:ASN:H	2.05	0.71
1:A:50:ILE:HD12	1:A:85:ILE:HD11	1.71	0.71
1:A:656:ASN:HB3	1:A:659:ILE:HD12	1.71	0.71
1:A:554:TYR:CD2	1:A:595:PRO:HG2	2.25	0.71
1:B:772:THR:HG22	1:B:774:LYS:H	1.56	0.71
1:B:341:ASN:HB2	1:B:342:PRO:HD2	1.73	0.70
1:A:343:ASP:HB2	1:A:405:ASN:HB2	1.74	0.70
1:A:341:ASN:HB2	1:A:342:PRO:HD2	1.73	0.69
1:B:472:HIS:HD2	1:B:538:ASN:N	1.91	0.69
1:A:53:GLN:OE1	1:A:57:SER:HB3	1.95	0.67
1:B:772:THR:CG2	1:B:774:LYS:H	2.07	0.67
1:B:764:ASP:HB3	1:B:782:ASN:HA	1.77	0.67
1:B:152:ILE:CD1	1:B:169:ILE:HG12	2.26	0.65
1:B:418:HIS:CD2	1:B:455:ASN:HD21	2.12	0.64
1:A:188:VAL:HG11	1:A:246:VAL:CG1	2.28	0.64
1:B:380:ARG:HD3	1:B:788:THR:HB	1.81	0.63
1:B:156:THR:O	1:B:157:ARG:HB2	1.99	0.63
1:B:152:ILE:HD12	1:B:169:ILE:HG12	1.79	0.62
1:B:540:THR:HG22	1:B:541:ASP:H	1.64	0.62
1:A:152:ILE:HG22	1:A:154:THR:H	1.64	0.62
1:A:133:THR:HG21	1:A:159:VAL:HG21	1.81	0.61
1:B:646:GLU:O	1:B:647:ASP:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:ARG:HD2	1:B:514:ASP:OD2	2.01	0.61
1:B:418:HIS:HE1	4:B:1820:PO4:O1	1.84	0.61
1:B:694:LYS:HE3	1:B:708:GLU:CD	2.22	0.61
1:B:646:GLU:O	1:B:662:ALA:O	2.19	0.60
1:B:540:THR:HG22	1:B:541:ASP:N	2.16	0.60
1:B:744:VAL:HG21	1:B:755:PHE:CE1	2.37	0.60
1:A:239:ASP:OD2	1:A:292:ARG:NH2	2.33	0.60
1:B:744:VAL:CG2	1:B:755:PHE:CD1	2.85	0.60
1:B:698:ASP:HB3	1:B:700:SER:H	1.68	0.59
1:B:276:GLU:H	1:B:276:GLU:CD	2.06	0.59
1:B:772:THR:HG22	1:B:774:LYS:N	2.17	0.58
1:A:325:TYR:OH	1:A:327:ARG:NH1	2.35	0.58
1:B:601:ARG:NH1	1:B:605:ASN:O	2.37	0.58
1:B:772:THR:HG22	1:B:775:LEU:N	2.18	0.58
1:B:764:ASP:HB2	1:B:781:VAL:O	2.03	0.58
1:A:188:VAL:HG11	1:A:246:VAL:HG11	1.85	0.58
1:A:152:ILE:CG2	1:A:154:THR:OG1	2.51	0.57
1:A:408:ASN:HB3	1:A:410:TRP:HD1	1.70	0.57
1:A:556:VAL:HG13	1:A:563:ILE:HB	1.87	0.57
1:A:611:ASP:OD1	1:A:640:GLU:OE2	2.23	0.57
1:A:742:GLN:HG3	1:A:793:ILE:O	2.04	0.56
3:A:1817[B]:N8E:H051	1:B:805:ARG:HD3	1.86	0.56
1:A:174:ARG:CZ	1:A:177:MET:HE3	2.36	0.56
1:B:744:VAL:HG22	1:B:755:PHE:HD1	1.69	0.56
1:A:601:ARG:NH1	1:A:605:ASN:O	2.39	0.56
1:B:443:ILE:HD11	1:B:506:TRP:CH2	2.41	0.56
1:A:174:ARG:CZ	1:A:177:MET:CE	2.83	0.55
1:A:656:ASN:ND2	1:A:658:ALA:HB3	2.21	0.55
1:B:403:GLU:HB3	1:B:413:LYS:HG3	1.88	0.55
1:B:716:TYR:CD1	1:B:733:GLY:HA3	2.42	0.55
1:A:656:ASN:O	1:A:659:ILE:O	2.24	0.54
1:A:394:TYR:CE1	1:A:422:GLY:HA3	2.43	0.54
1:B:744:VAL:HG21	1:B:755:PHE:CD1	2.42	0.54
1:A:408:ASN:HB3	1:A:410:TRP:CD1	2.42	0.54
1:A:736:TRP:HB2	1:A:761:TRP:CE3	2.42	0.54
1:B:324:HIS:CE1	1:B:383:ASN:HB3	2.43	0.53
1:B:792:ASN:HB3	1:B:800:SER:HB2	1.90	0.53
1:B:694:LYS:CE	1:B:708:GLU:OE1	2.50	0.53
1:B:436:ALA:HB1	1:B:437:PRO:HD2	1.90	0.53
1:A:443:ILE:N	1:A:443:ILE:HD13	2.23	0.53
1:A:74:PRO:HG3	1:A:132:ILE:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:ASP:O	1:B:577:TYR:HA	2.09	0.53
1:B:624:TYR:N	1:B:624:TYR:CD1	2.78	0.52
1:B:694:LYS:NZ	1:B:708:GLU:O	2.42	0.52
1:B:276:GLU:N	1:B:276:GLU:OE1	2.42	0.52
1:B:195:ILE:HD11	1:B:248:VAL:HG11	1.91	0.52
1:B:506:TRP:CZ2	1:B:508:GLY:HA2	2.45	0.52
1:B:417:ASP:O	1:B:455:ASN:HA	2.10	0.51
1:A:410:TRP:CD2	1:A:463:GLY:HA3	2.45	0.51
1:B:681:LEU:HD13	1:B:687:VAL:CG2	2.40	0.51
3:A:1817[B]:N8E:H052	1:B:807:LEU:HD11	1.92	0.51
1:A:603:SER:O	1:A:659:ILE:HD11	2.12	0.50
1:A:470:ARG:HD3	1:A:538:ASN:O	2.11	0.50
1:A:188:VAL:HG11	1:A:246:VAL:HG13	1.93	0.50
1:A:242:ILE:HG22	1:A:312:VAL:HG22	1.94	0.49
1:A:805:ARG:HD2	3:A:1817[A]:N8E:H031	1.93	0.49
1:A:638:ILE:HB	1:A:670:THR:HB	1.94	0.49
1:A:392:GLU:HG3	1:A:424:HIS:HB3	1.95	0.49
1:A:496:TYR:CG	1:A:513:PRO:HB3	2.48	0.49
1:B:744:VAL:CG2	1:B:755:PHE:CE1	2.96	0.49
1:B:744:VAL:HG22	1:B:755:PHE:CD1	2.45	0.49
1:B:255:LEU:O	1:B:550:ARG:HD2	2.13	0.49
1:B:425:ALA:O	1:B:447:LYS:HA	2.12	0.48
1:A:512:LYS:HG3	1:A:513:PRO:HD2	1.95	0.48
1:A:716:TYR:CD1	1:A:733:GLY:HA3	2.48	0.48
1:B:156:THR:O	1:B:157:ARG:CB	2.59	0.48
1:B:363:SER:HB2	2:C:8:FHO:HZ	1.93	0.48
1:B:506:TRP:CE2	1:B:508:GLY:HA2	2.49	0.47
1:A:656:ASN:CB	1:A:659:ILE:HD12	2.42	0.47
1:A:646:GLU:O	1:A:662:ALA:O	2.32	0.47
1:B:371:SER:OG	1:B:436:ALA:HA	2.14	0.47
1:A:394:TYR:CZ	1:A:422:GLY:HA3	2.48	0.47
1:A:596:GLN:NE2	1:A:609:GLU:O	2.48	0.47
1:B:413:LYS:O	1:B:459:ILE:HA	2.14	0.47
1:A:79:ASN:OD1	1:A:79:ASN:N	2.47	0.47
1:B:707:TRP:HB2	1:B:742:GLN:HE21	1.79	0.47
1:A:725:LEU:N	1:A:725:LEU:HD23	2.30	0.47
1:B:142:GLU:O	1:B:143:ASP:HB2	2.16	0.46
1:B:180:PHE:HA	1:B:780:ASN:HD21	1.80	0.46
1:B:260:GLY:O	1:B:594:MET:HB2	2.14	0.46
1:A:805:ARG:HD2	3:A:1817[A]:N8E:C03	2.46	0.46
1:A:380:ARG:HD3	1:A:788:THR:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:GLU:O	1:B:647:ASP:CB	2.63	0.46
1:A:59:LEU:HD22	1:A:70:VAL:HG11	1.98	0.45
1:B:347:THR:O	1:B:400:ALA:HA	2.16	0.45
1:A:694:LYS:CE	1:A:708:GLU:OE1	2.58	0.45
1:B:614:GLN:NE2	1:B:641:GLU:OE2	2.41	0.45
1:B:653:LYS:HA	1:B:654:PRO:HD2	1.67	0.45
1:B:208:TYR:HA	1:B:212:PHE:O	2.16	0.45
1:B:470:ARG:HH12	1:B:540:THR:CA	2.30	0.45
1:A:157:ARG:HB3	1:A:475:VAL:HG11	1.99	0.45
1:B:597:ASP:OD2	2:C:4:ARG:NH2	2.50	0.44
1:A:280:HIS:HA	1:A:813:TRP:O	2.17	0.44
1:A:174:ARG:CZ	4:A:1823:PO4:O2	2.65	0.44
1:A:436:ALA:HB1	1:A:437:PRO:HD2	1.99	0.44
1:B:681:LEU:HD13	1:B:687:VAL:HG21	1.98	0.44
1:B:174:ARG:NH1	1:B:177:MET:HE3	2.33	0.43
1:B:464:PRO:HA	1:B:472:HIS:O	2.18	0.43
1:B:540:THR:CG2	1:B:541:ASP:H	2.31	0.43
1:A:637:GLU:HA	1:A:670:THR:O	2.18	0.43
1:B:439:ASN:ND2	1:B:502:ASP:HA	2.33	0.43
1:A:417:ASP:HB2	1:A:456:SER:HB2	2.00	0.43
1:A:158:LEU:CD2	1:A:475:VAL:HG22	2.49	0.43
1:B:82:SER:HB2	1:B:98:LEU:HG	2.00	0.43
1:B:262:LEU:HD23	1:B:592:ILE:HG22	2.01	0.43
1:B:380:ARG:HA	1:B:801:TYR:CD2	2.52	0.43
1:B:807:LEU:N	1:B:807:LEU:HD12	2.34	0.43
1:B:139:THR:OG1	1:B:150:GLY:HA3	2.19	0.43
1:A:228:ASN:O	1:A:232:SER:HB3	2.19	0.43
1:B:443:ILE:HG13	1:B:510:ILE:HD13	2.01	0.42
1:B:313:ALA:HA	1:B:331:VAL:O	2.18	0.42
1:A:390:SER:O	1:A:425:ALA:HA	2.19	0.42
1:A:443:ILE:HG13	1:A:510:ILE:CD1	2.50	0.42
1:B:445:ALA:O	1:B:446:GLN:HG2	2.19	0.42
1:B:470:ARG:O	1:B:472:HIS:CE1	2.72	0.42
1:A:174:ARG:NH1	1:A:177:MET:CE	2.82	0.42
1:B:590:THR:O	1:B:614:GLN:HA	2.18	0.42
1:A:659:ILE:HG22	1:A:660:THR:H	1.84	0.42
1:B:174:ARG:CZ	1:B:177:MET:CE	2.98	0.42
1:B:257:THR:HG22	1:B:257:THR:O	2.20	0.42
1:B:540:THR:CG2	1:B:541:ASP:N	2.83	0.42
1:A:698:ASP:OD1	1:A:698:ASP:C	2.57	0.42
1:A:646:GLU:HG3	1:A:661:TYR:OH	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ILE:HG12	1:B:264:ALA:HB3	2.02	0.42
1:A:636:PHE:CD1	1:A:636:PHE:O	2.72	0.42
1:B:390:SER:O	1:B:425:ALA:HA	2.19	0.42
1:A:366:PHE:CZ	1:A:799:ALA:HB3	2.54	0.42
1:B:276:GLU:N	1:B:276:GLU:CD	2.72	0.41
1:B:329:THR:HA	1:B:354:ASP:O	2.20	0.41
1:A:227:ARG:HG2	1:A:227:ARG:NH1	2.36	0.41
1:A:327:ARG:HG2	1:A:329:THR:HG22	2.02	0.41
1:A:678:SER:HA	1:A:687:VAL:O	2.20	0.41
1:A:491:TRP:CE2	1:A:519:SER:HB3	2.56	0.41
1:A:231:TYR:OH	1:A:524:ASP:HB3	2.21	0.41
1:A:690:GLY:O	1:A:713:LEU:HA	2.21	0.41
1:A:443:ILE:HG13	1:A:510:ILE:HD12	2.03	0.41
1:A:533:MET:HB2	1:A:533:MET:HE2	1.99	0.41
1:A:255:LEU:HD22	1:A:572:TYR:CD2	2.56	0.41
1:A:227:ARG:HG2	1:A:227:ARG:HH11	1.85	0.40
1:A:410:TRP:CE2	1:A:463:GLY:HA3	2.56	0.40
1:A:636:PHE:C	1:A:636:PHE:CD1	2.94	0.40
1:B:594:MET:N	1:B:611:ASP:O	2.53	0.40
1:A:497:ASP:OD1	1:A:497:ASP:C	2.60	0.40
1:B:174:ARG:NH2	1:B:177:MET:HB3	2.37	0.40
1:B:637:GLU:HA	1:B:670:THR:O	2.21	0.40
1:B:70:VAL:HG22	1:B:113:ILE:HG12	2.04	0.40
1:A:443:ILE:CG1	1:A:510:ILE:HD12	2.51	0.40
1:B:192:THR:HA	1:B:193:PRO:HD2	1.95	0.40
1:B:570:ILE:HG23	1:B:591:ASP:HB3	2.03	0.40
1:A:674:GLU:HA	1:A:691:TYR:O	2.21	0.40
1:A:180:PHE:HA	1:A:780:ASN:HD21	1.86	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	770/772 (100%)	728 (94%)	33 (4%)	9 (1%)	13	30
1	B	750/772 (97%)	710 (95%)	37 (5%)	3 (0%)	34	58
2	C	3/8 (38%)	2 (67%)	1 (33%)	0	100	100
All	All	1523/1552 (98%)	1440 (95%)	71 (5%)	12 (1%)	19	41

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	ALA
1	A	603	SER
1	A	646	GLU
1	A	227	ARG
1	B	408	ASN
1	A	658	ALA
1	B	647	ASP
1	A	647	ASP
1	A	407	ALA
1	A	122	ASP
1	A	699	ASP
1	B	683	PRO

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	650/650 (100%)	584 (90%)	66 (10%)	7	16
1	B	637/650 (98%)	585 (92%)	52 (8%)	11	25
2	C	4/4 (100%)	3 (75%)	1 (25%)	0	1
All	All	1291/1304 (99%)	1172 (91%)	119 (9%)	9	20

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLU

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Mol	Chain	Res	Type
1	A	60	GLN
1	A	68	ILE
1	A	78	ARG
1	A	114	THR
1	A	133	THR
1	A	148	THR
1	A	154	THR
1	A	157	ARG
1	A	204	ARG
1	A	215	ASN
1	A	236	THR
1	A	238	SER
1	A	246	VAL
1	A	248	VAL
1	A	276	GLU
1	A	297	VAL
1	A	307	VAL
1	A	329	THR
1	A	358	LYS
1	A	362	TRP
1	A	372	GLN
1	A	375	ARG
1	A	392	GLU
1	A	397	THR
1	A	408	ASN
1	A	417	ASP
1	A	431	MET
1	A	459	ILE
1	A	461	LEU
1	A	466	GLN
1	A	468	LEU
1	A	475	VAL
1	A	499	THR
1	A	504	ILE
1	A	524	ASP
1	A	528	GLN
1	A	533	MET
1	A	551	VAL
1	A	556	VAL
1	A	557	THR
1	A	564	ARG
1	A	580	ASN

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Mol	Chain	Res	Type
1	A	596	GLN
1	A	601	ARG
1	A	609	GLU
1	A	641	GLU
1	A	645	GLU
1	A	654	PRO
1	A	659	ILE
1	A	660	THR
1	A	676	GLU
1	A	687	VAL
1	A	694	LYS
1	A	704	VAL
1	A	720	LYS
1	A	725	LEU
1	A	730	VAL
1	A	744	VAL
1	A	766	MET
1	A	771	ILE
1	A	772	THR
1	A	788	THR
1	A	810	SER
1	A	811	THR
1	A	815	PHE
1	B	78	ARG
1	B	83	SER
1	B	96	THR
1	B	106	VAL
1	B	107	ASP
1	B	114	THR
1	B	148	THR
1	B	157	ARG
1	B	176	ASN
1	B	236	THR
1	B	303	GLU
1	B	319	HIS
1	B	329	THR
1	B	331	VAL
1	B	411	VAL
1	B	416	LEU
1	B	417	ASP
1	B	431	MET
1	B	459	ILE

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Mol	Chain	Res	Type
1	B	462	THR
1	B	493	LEU
1	B	495	ASN
1	B	509	ASP
1	B	519	SER
1	B	527	ARG
1	B	551	VAL
1	B	556	VAL
1	B	564	ARG
1	B	568	ARG
1	B	576	VAL
1	B	596	GLN
1	B	601	ARG
1	B	609	GLU
1	B	624	TYR
1	B	641	GLU
1	B	671	LYS
1	B	687	VAL
1	B	694	LYS
1	B	699	ASP
1	B	702	LYS
1	B	704	VAL
1	B	720	LYS
1	B	722	LYS
1	B	743	MET
1	B	749	ARG
1	B	771	ILE
1	B	772	THR
1	B	773	ASP
1	B	788	THR
1	B	792	ASN
1	B	810	SER
1	B	815	PHE
2	C	10	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	205	ASN
1	A	218	GLN
1	A	401	ASN

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Mol	Chain	Res	Type
1	A	408	ASN
1	A	455	ASN
1	A	492	ASN
1	A	580	ASN
1	A	596	GLN
1	A	780	ASN
1	B	109	GLN
1	B	176	ASN
1	B	205	ASN
1	B	418	HIS
1	B	472	HIS
1	B	495	ASN
1	B	538	ASN
1	B	596	GLN
1	B	688	GLN
1	B	742	GLN
1	B	780	ASN

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	$\# Z > 2$
2	FHO	C	6	2,6	8,10,11	1.81	1 (12%)	4,11,13	1.74	2 (50%)
2	FHO	C	8	2,6	8,10,11	1.91	1 (12%)	4,11,13	2.58	3 (75%)

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	FHO	C	6	2,6	-	4/7/10/12	-
2	FHO	C	8	2,6	-	4/7/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	8	FHO	CZ-NE	-5.29	1.26	1.34
2	C	6	FHO	CZ-NE	-4.83	1.27	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	8	FHO	CG-CD-NE	-3.40	104.06	111.07
2	C	8	FHO	OZ-NE-CD	2.77	120.49	113.67
2	C	8	FHO	OH-CZ-NE	-2.63	118.22	125.80
2	C	6	FHO	OZ-NE-CD	2.26	119.24	113.67
2	C	6	FHO	OH-CZ-NE	-2.20	119.46	125.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6	FHO	N-CA-CB-CG
2	C	6	FHO	C-CA-CB-CG
2	C	6	FHO	CG-CD-NE-OZ
2	C	8	FHO	O-C-CA-CB
2	C	8	FHO	CG-CD-NE-OZ
2	C	8	FHO	CG-CD-NE-CZ
2	C	8	FHO	CA-CB-CG-CD
2	C	6	FHO	CA-CB-CG-CD

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	8	FHO	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 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
4	PO4	A	1820	-	4,4,4	1.41	0	6,6,6	0.91	0
4	PO4	B	1819	-	4,4,4	0.81	0	6,6,6	0.59	0
4	PO4	A	1821	-	4,4,4	0.79	0	6,6,6	0.57	0
4	PO4	B	1818	-	4,4,4	0.96	0	6,6,6	1.31	1 (16%)
4	PO4	A	1823	-	4,4,4	1.21	0	6,6,6	0.93	0
3	N8E	A	1816	-	23,23,23	0.52	0	22,22,22	0.49	0
4	PO4	A	1822	-	4,4,4	0.95	0	6,6,6	0.60	0
3	N8E	A	1817[B]	-	23,23,23	0.63	0	22,22,22	0.52	0
5	PVE	C	1	2,6	23,28,29	1.44	2 (8%)	25,40,42	1.72	3 (12%)
3	N8E	A	1817[A]	-	23,23,23	0.64	0	22,22,22	0.49	0
4	PO4	A	1818	-	4,4,4	0.88	0	6,6,6	1.26	1 (16%)
4	PO4	A	1819	-	4,4,4	0.99	0	6,6,6	1.03	0
4	PO4	B	1820	-	4,4,4	0.82	0	6,6,6	0.66	0
4	PO4	B	1817	-	4,4,4	0.67	0	6,6,6	1.16	1 (16%)

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
3	N8E	A	1817[B]	-	-	12/21/21/21	-
5	PVE	C	1	2,6	-	3/8/21/23	0/2/3/3
3	N8E	A	1817[A]	-	-	13/21/21/21	-
3	N8E	A	1816	-	-	11/21/21/21	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1	PVE	C8-C7	5.36	1.42	1.37
5	C	1	PVE	C5-C6	2.20	1.39	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	PVE	C15-C14-N1	-6.05	104.26	111.97
4	B	1818	PO4	O3-P-O2	2.80	116.95	107.97
4	A	1818	PO4	O4-P-O1	-2.44	101.97	110.89
5	C	1	PVE	C8-C9-C10	-2.11	116.94	119.66
5	C	1	PVE	O26-C7-C8	2.09	126.51	120.85
4	B	1817	PO4	O3-P-O1	-2.09	103.26	110.89

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	1	PVE	C13-C14-C15-O16
3	A	1817[A]	N8E	O15-C16-C17-O18
3	A	1817[B]	N8E	O18-C19-C20-O21
3	A	1817[A]	N8E	O18-C19-C20-O21
3	A	1817[B]	N8E	O09-C10-C11-O12
3	A	1817[A]	N8E	O12-C13-C14-O15
3	A	1817[A]	N8E	O09-C10-C11-O12
3	A	1816	N8E	O12-C13-C14-O15
3	A	1817[B]	N8E	C03-C04-C05-C06
3	A	1817[B]	N8E	O21-C22-C23-O24
3	A	1817[A]	N8E	O21-C22-C23-O24
3	A	1817[B]	N8E	C01-C02-C03-C04
3	A	1817[A]	N8E	C03-C04-C05-C06
3	A	1817[A]	N8E	C05-C06-C07-C08
3	A	1817[A]	N8E	C06-C07-C08-O09
3	A	1816	N8E	O09-C10-C11-O12
5	C	1	PVE	C4-C3-N17-C18
5	C	1	PVE	C2-C3-N17-C18
3	A	1816	N8E	C19-C20-O21-C22
3	A	1817[B]	N8E	C19-C20-O21-C22
3	A	1817[A]	N8E	C10-C11-O12-C13
3	A	1816	N8E	C16-C17-O18-C19
3	A	1816	N8E	C17-C16-O15-C14
3	A	1817[B]	N8E	O12-C13-C14-O15

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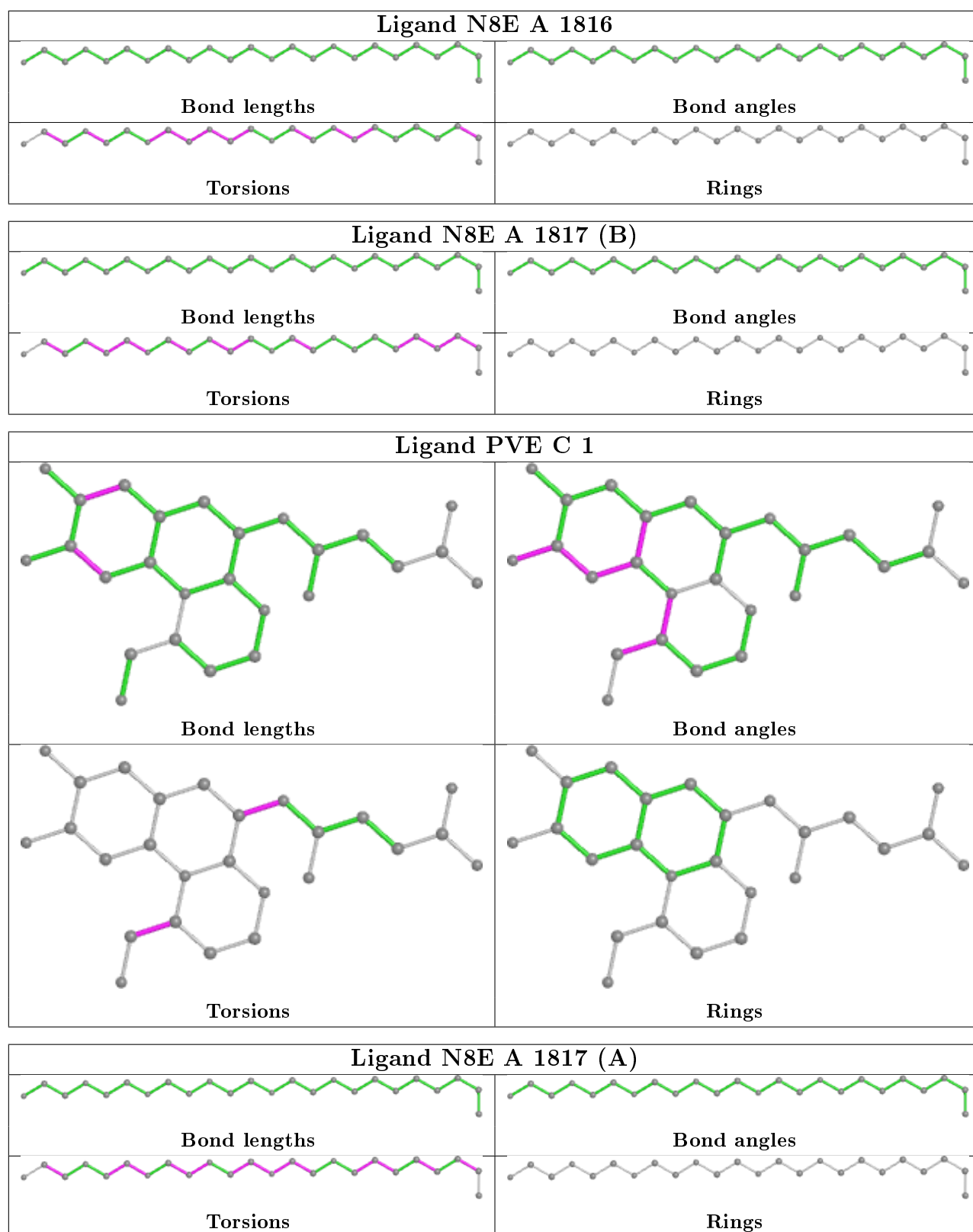
Mol	Chain	Res	Type	Atoms
3	A	1817[A]	N8E	C20-C19-O18-C17
3	A	1816	N8E	O21-C22-C23-O24
3	A	1817[A]	N8E	C01-C02-C03-C04
3	A	1816	N8E	C13-C14-O15-C16
3	A	1816	N8E	O15-C16-C17-O18
3	A	1817[A]	N8E	C14-C13-O12-C11
3	A	1817[A]	N8E	C17-C16-O15-C14
3	A	1816	N8E	C01-C02-C03-C04
3	A	1817[B]	N8E	C20-C19-O18-C17
3	A	1816	N8E	C07-C08-O09-C10
3	A	1816	N8E	C06-C07-C08-O09
3	A	1817[B]	N8E	C02-C03-C04-C05
3	A	1817[B]	N8E	C04-C05-C06-C07
3	A	1817[B]	N8E	O15-C16-C17-O18
3	A	1817[B]	N8E	C13-C14-O15-C16

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1823	PO4	1	0
3	A	1817[B]	N8E	3	0
3	A	1817[A]	N8E	2	0
4	B	1820	PO4	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 ⓘ

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	772/772 (100%)	-0.26	10 (1%) 77 78	15, 29, 42, 54	0
1	B	754/772 (97%)	-0.10	24 (3%) 47 48	17, 29, 40, 58	0
2	C	4/8 (50%)	0.18	0 100 100	44, 46, 47, 48	0
All	All	1530/1552 (98%)	-0.18	34 (2%) 62 63	15, 29, 41, 58	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	407	ALA	8.5
1	A	44	GLN	7.5
1	B	78	ARG	5.1
1	B	44	GLN	5.0
1	A	123	SER	4.4
1	A	407	ALA	4.3
1	B	109	GLN	3.8
1	B	406	PHE	3.5
1	B	117	VAL	3.4
1	B	581	ASP	3.4
1	A	662	ALA	3.4
1	B	342	PRO	3.3
1	B	409	GLY	3.2
1	A	303	GLU	2.8
1	B	136	GLN	2.7
1	B	683	PRO	2.7
1	B	437	PRO	2.6
1	B	723	GLY	2.5
1	B	625	LEU	2.4
1	A	724	ALA	2.3
1	B	408	ASN	2.3
1	B	45	GLU	2.3
1	B	504	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	467	PHE	2.3
1	B	627	GLY	2.3
1	B	343	ASP	2.2
1	A	659	ILE	2.2
1	B	110	GLY	2.2
1	B	699	ASP	2.2
1	B	75	GLU	2.1
1	A	88	LYS	2.1
1	A	372	GLN	2.1
1	A	124	SER	2.0
1	B	722	LYS	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
2	DSN	C	5	6/7	0.91	0.23	46,47,47,48	0
2	DSN	C	3	6/7	0.91	0.27	43,44,44,45	0
2	FHO	C	6	11/12	0.95	0.14	36,42,47,47	0
2	FHO	C	8	11/12	0.98	0.11	34,38,45,45	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.

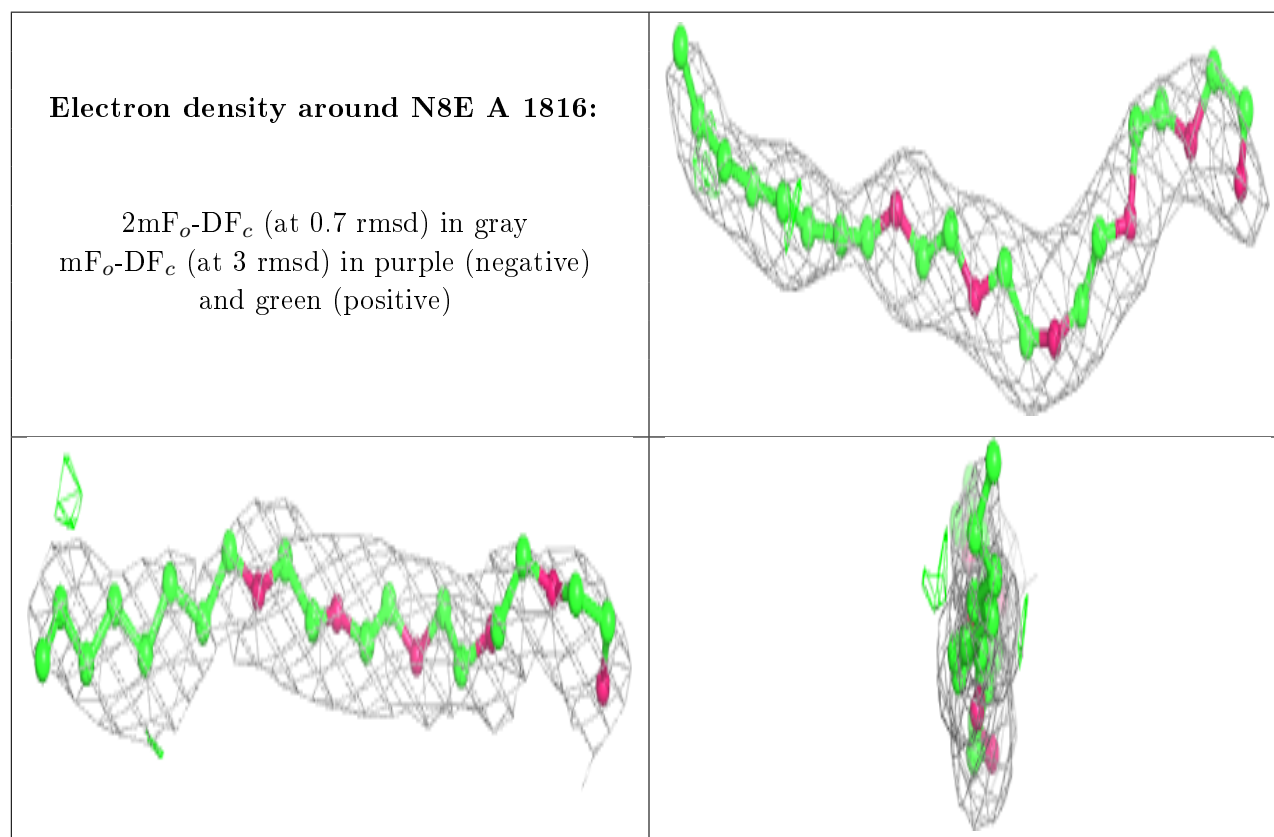
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	N8E	A	1816	24/24	0.84	0.32	48,59,78,80	0
3	N8E	A	1817[B]	24/24	0.84	0.28	2,16,22,24	24
3	N8E	A	1817[A]	24/24	0.84	0.28	12,21,29,30	24

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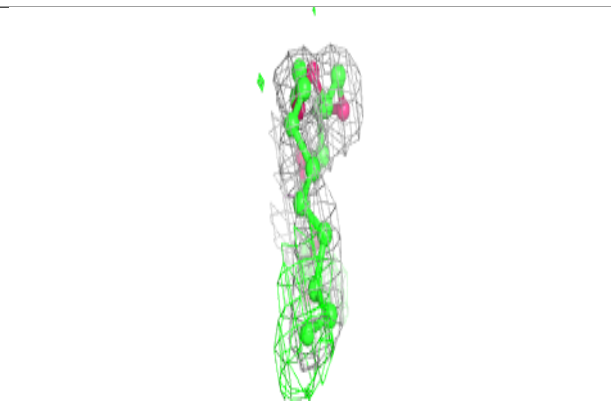
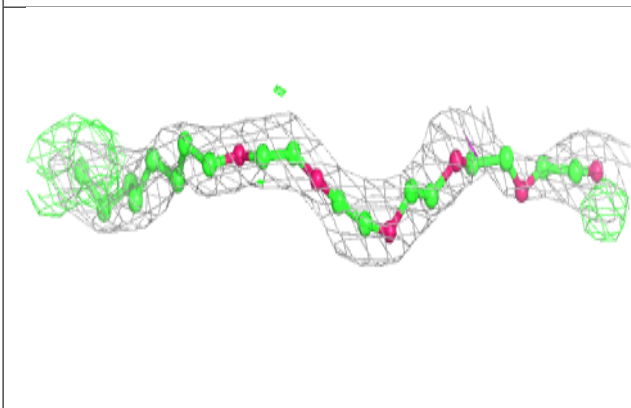
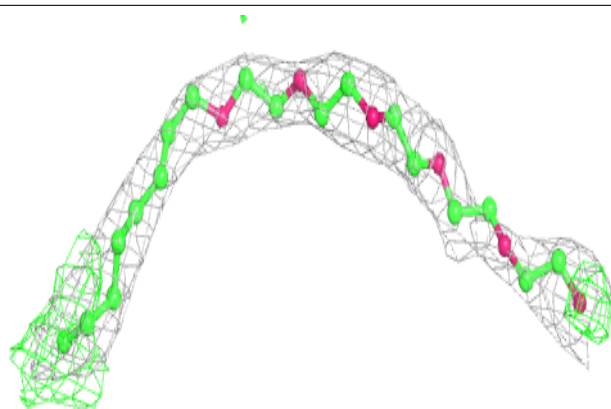
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	PO4	B	1817	5/5	0.93	0.26	65,66,66,67	0
4	PO4	B	1819	5/5	0.94	0.15	71,72,73,73	0
4	PO4	A	1823	5/5	0.94	0.17	54,57,57,57	0
4	PO4	A	1822	5/5	0.95	0.20	68,68,69,70	0
5	PVE	C	1	26/27	0.95	0.18	33,40,48,49	0
4	PO4	A	1821	5/5	0.96	0.21	57,58,59,59	0
4	PO4	B	1818	5/5	0.98	0.09	29,34,36,37	0
4	PO4	A	1818	5/5	0.98	0.14	32,32,33,36	0
4	PO4	B	1820	5/5	0.98	0.21	49,50,50,51	0
4	PO4	A	1819	5/5	0.98	0.07	29,30,33,35	0
6	FE	C	2	1/1	0.98	0.03	34,34,34,34	0
4	PO4	A	1820	5/5	0.99	0.11	40,42,45,45	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.

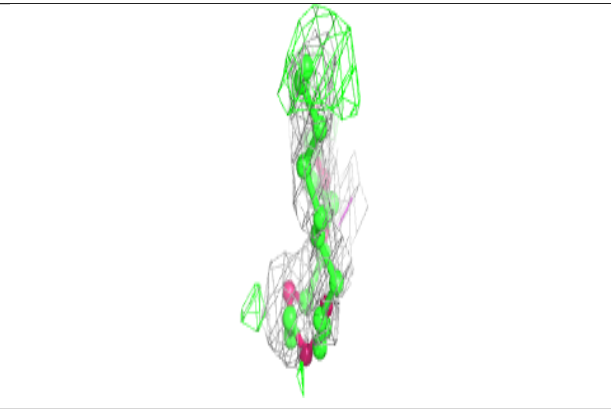
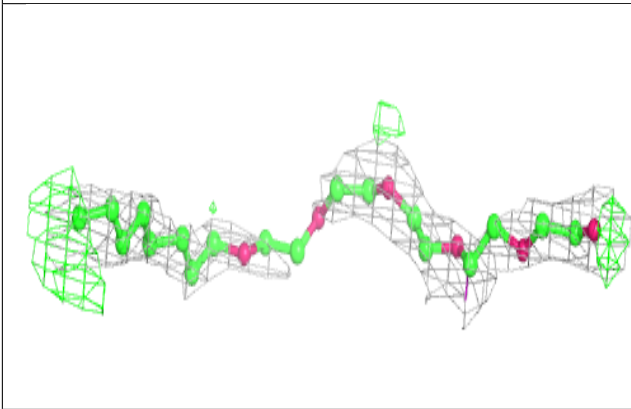
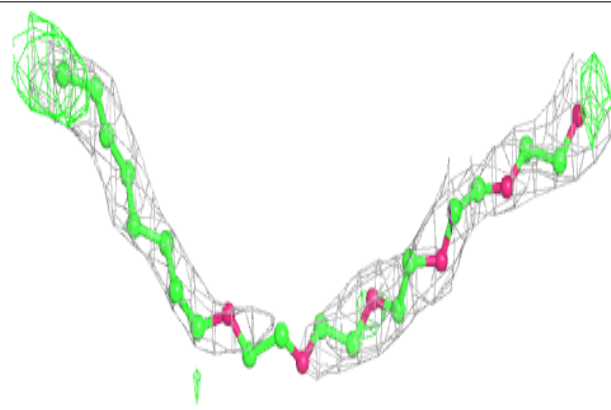


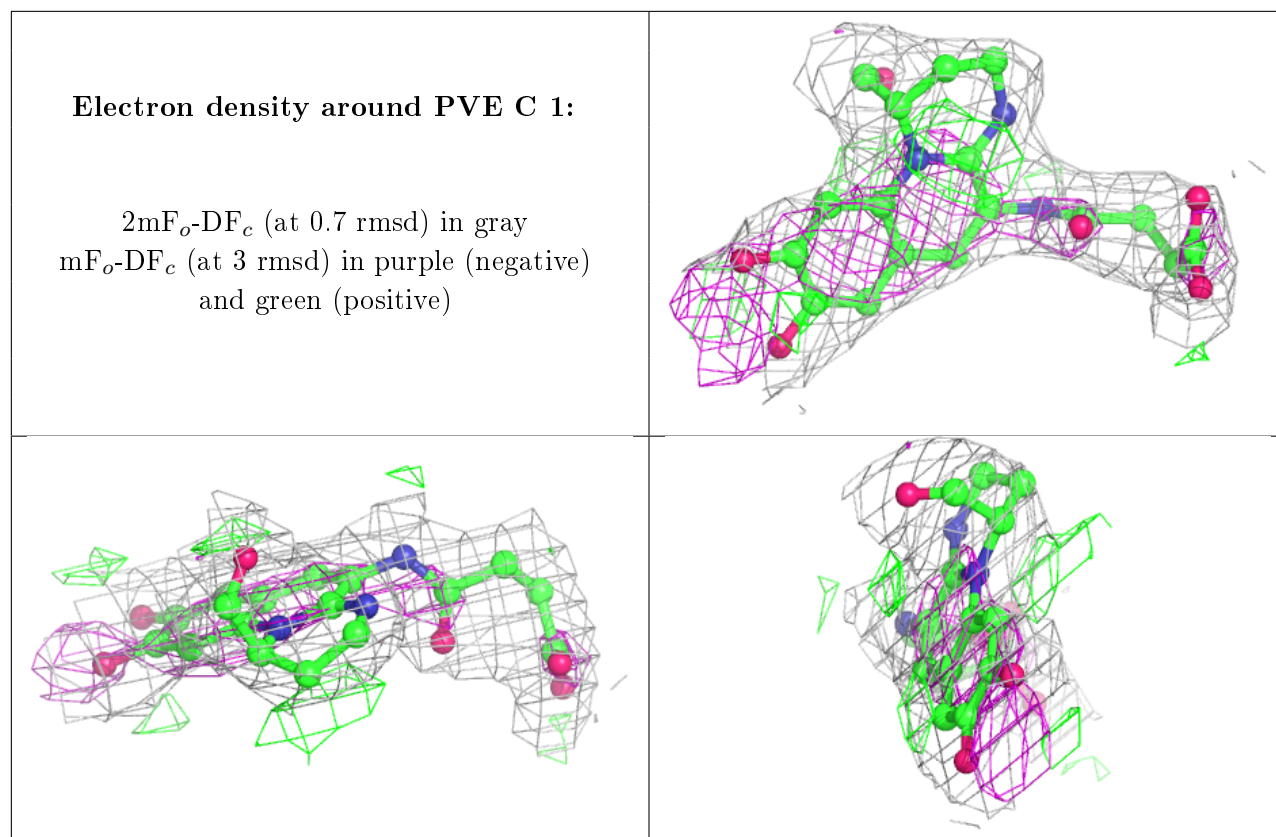
Electron density around N8E A 1817 (B):

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

**Electron density around N8E A 1817 (A):**

$2mF_o-DF_c$ (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.