Full wwPDB X-ray Structure Validation Report (i)

Mar 4, 2026 – 08:38 PM UTC

PDB ID	:	1C72 / pdb_00001c72
Title	:	TYR115, GLN165 AND TRP209 CONTRIBUTE TO THE 1,2-EPOXY-3-(P-NITROPHENOXY)PROPANE CONJUGATING ACTIVITIES OF GLUTATHIONE S-TRANSFERASE CGSTM1-1
Authors	:	Chern, M.K.; Wu, T.C.; Hsieh, C.H.; Chou, C.C.; Liu, L.F.; Kuan, I.C.; Yeh, Y.H.; Hsiao, C.D.; Tam, M.F.
Deposited on	:	2000-02-02
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

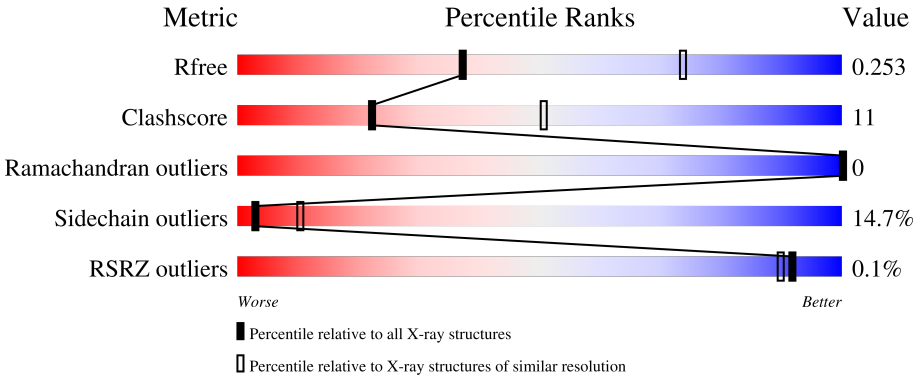
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 <=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	219	70% 22% 7%
1	B	219	69% 27%
1	C	219	73% 22%
1	D	219	69% 25% 5%

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
2	EPY	A	220	X	-	-	-
2	EPY	B	221	X	-	-	-
2	EPY	C	222	X	-	-	-

2 Entry composition

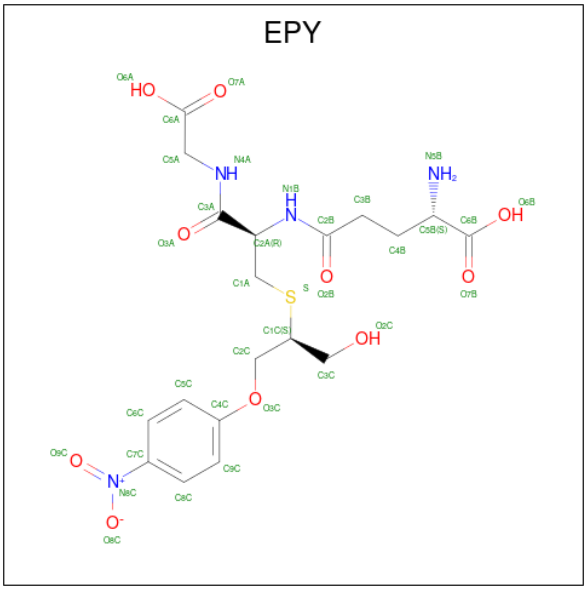
There are 3 unique types of molecules in this entry. The entry contains 7490 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (GLUTATHIONE S-TRANSFERASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1799	1164	306	320	9			
1	B	217	Total	C	N	O	S	0	0	0
			1799	1164	306	320	9			
1	C	217	Total	C	N	O	S	0	0	0
			1799	1164	306	320	9			
1	D	217	Total	C	N	O	S	0	0	0
			1799	1164	306	320	9			

- Molecule 2 is 1-HYDROXY-2-S-GLUTATHIONYL-3-PARA-NITROPHENOXY-PROPANE (CCD ID: EPY) (formula: $C_{19}H_{26}N_4O_{10}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			34	19	4	10	1		
2	B	1	Total	C	N	O	S	0	0
			34	19	4	10	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			34	19	4	10	1		
2	D	1	Total	C	N	O	S	0	0
			34	19	4	10	1		

- Molecule 3 is water.

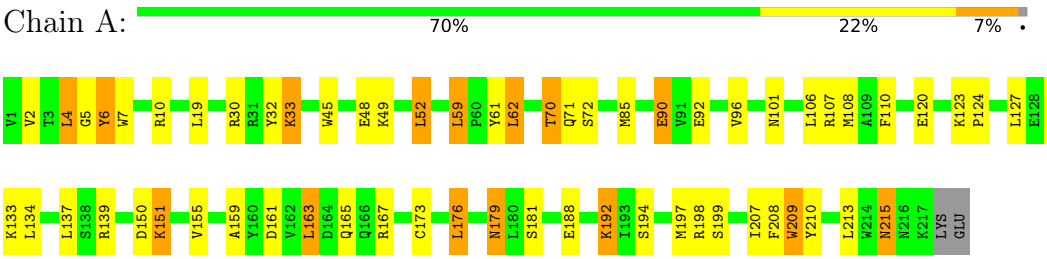
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	42	Total	O	0	0
			42	42		
3	C	50	Total	O	0	0
			50	50		
3	D	36	Total	O	0	0
			36	36		

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.

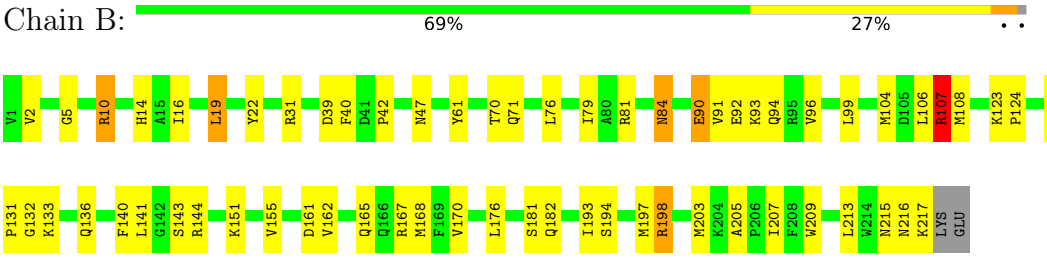
• Molecule 1: PROTEIN (GLUTATHIONE S-TRANSFERASE)

Chain A:



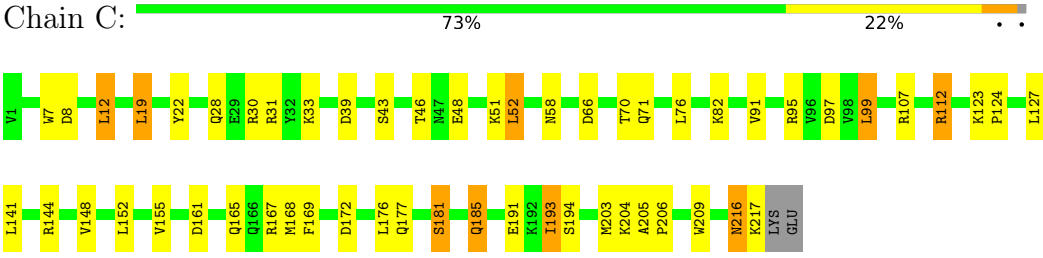
• Molecule 1: PROTEIN (GLUTATHIONE S-TRANSFERASE)

Chain B:



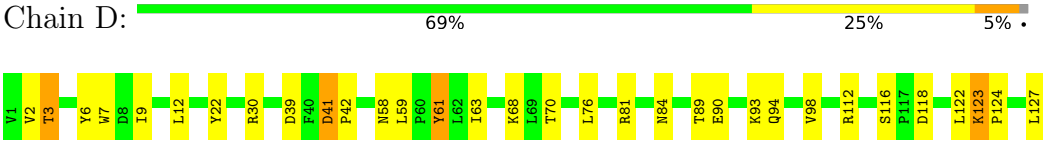
• Molecule 1: PROTEIN (GLUTATHIONE S-TRANSFERASE)

Chain C:



• Molecule 1: PROTEIN (GLUTATHIONE S-TRANSFERASE)

Chain D:



K133
L134
R135
Q136
L137
S138
R139
R144
S145
W146
G149
T153
F154
V155
L158
Q166
V170
S181
E191
K192
I193
S194
M197
R198
A205
P206
I207
F208
W209
Y210
T211
N215
M216
K217
LYS
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	125.60Å 136.65Å 125.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.00 – 2.80 31.00 – 2.81	Depositor EDS
% Data completeness (in resolution range)	86.6 (31.00-2.80) 81.7 (31.00-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.08 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.190 , 0.280 0.171 , 0.253	Depositor DCC
R_{free} test set	2306 reflections (9.87%)	wwPDB-VP
Wilson B-factor (Å^2)	42.1	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 60.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7490	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: EPY

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	0.52	2/1847 (0.1%)	0.81	1/2499 (0.0%)
1	B	0.47	1/1847 (0.1%)	0.83	2/2499 (0.1%)
1	C	0.44	0/1847	0.77	0/2499
1	D	0.45	0/1847	0.78	2/2499 (0.1%)
All	All	0.47	3/7388 (0.0%)	0.80	5/9996 (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	2
1	B	0	2
1	D	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	165	GLN	CD-OE1	7.88	1.38	1.23
1	B	107	ARG	CD-NE	-6.78	1.36	1.46
1	A	209	TRP	C-N	-5.92	1.25	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	107	ARG	CD-NE-CZ	-10.80	109.28	124.40
1	B	107	ARG	CG-CD-NE	5.66	124.45	112.00
1	D	41	ASP	CA-C-N	5.22	126.25	120.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	41	ASP	C-N-CA	5.22	126.25	120.45
1	A	209	TRP	O-C-N	-5.13	116.50	122.81

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	32	TYR	Sidechain
1	A	6	TYR	Sidechain
1	B	107	ARG	Sidechain
1	B	198	ARG	Sidechain
1	D	61	TYR	Sidechain

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	1799	0	1784	41	0
1	B	1799	0	1784	33	0
1	C	1799	0	1784	32	0
1	D	1799	0	1784	45	0
2	A	34	0	23	6	0
2	B	34	0	23	6	0
2	C	34	0	22	4	0
2	D	34	0	24	13	0
3	A	30	0	0	0	0
3	B	42	0	0	0	0
3	C	50	0	0	0	0
3	D	36	0	0	0	0
All	All	7490	0	7228	154	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 11.

All (154) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:TRP:CZ2	2:C:222:EPY:H6C1	2.04	0.93
1:B:107:ARG:HD2	2:B:221:EPY:O8C	1.69	0.92
1:A:19:LEU:HD11	1:A:85:MET:HE1	1.55	0.89
1:D:7:TRP:CZ2	2:D:223:EPY:H6C1	2.11	0.84
1:D:216:ASN:H	1:D:216:ASN:HD22	1.28	0.80
2:D:223:EPY:C2A	2:D:223:EPY:C2C	2.56	0.79
2:D:223:EPY:H3A1	2:D:223:EPY:H2C1	1.64	0.78
1:B:107:ARG:HG3	2:B:221:EPY:O8C	1.86	0.75
1:D:216:ASN:H	1:D:216:ASN:ND2	1.82	0.74
2:D:223:EPY:C2C	2:D:223:EPY:H3A1	2.19	0.73
1:A:208:PHE:H	1:A:215:ASN:HD21	1.38	0.69
2:A:220:EPY:C2B	2:A:220:EPY:S	2.80	0.69
1:A:192:LYS:HD2	1:A:192:LYS:H	1.57	0.69
2:D:223:EPY:C2A	2:D:223:EPY:H2C2	2.07	0.69
2:D:223:EPY:S	2:D:223:EPY:O2B	2.50	0.69
1:C:216:ASN:HD22	1:C:216:ASN:H	1.41	0.69
1:A:134:LEU:HD13	1:A:176:LEU:HD13	1.74	0.67
1:B:22:TYR:HB2	1:B:193:ILE:HD11	1.77	0.67
1:C:205:ALA:HB1	1:C:217:LYS:HB2	1.76	0.67
1:C:19:LEU:HD12	1:C:76:LEU:HD23	1.77	0.66
1:C:216:ASN:H	1:C:216:ASN:ND2	1.92	0.66
1:B:107:ARG:CD	2:B:221:EPY:O8C	2.42	0.66
1:A:107:ARG:HG2	2:A:220:EPY:O8C	1.97	0.65
1:D:206:PRO:HA	1:D:216:ASN:HD21	1.63	0.64
1:D:208:PHE:H	1:D:215:ASN:HD21	1.45	0.64
1:B:31:ARG:HH12	1:B:203:MET:HG3	1.63	0.64
1:A:107:ARG:CG	2:A:220:EPY:O8C	2.46	0.64
1:C:112:ARG:HH21	1:D:112:ARG:HE	1.46	0.63
1:A:4:LEU:HD23	1:A:62:LEU:HD12	1.80	0.63
1:C:58:ASN:OD1	2:C:222:EPY:H3B1	1.98	0.62
1:A:151:LYS:HD2	1:A:151:LYS:H	1.64	0.62
1:C:205:ALA:CB	1:C:217:LYS:HB2	2.30	0.62
1:D:94:GLN:O	1:D:98:VAL:HG23	2.01	0.61
1:C:7:TRP:HZ2	2:C:222:EPY:H6C1	1.60	0.61
1:A:159:ALA:O	1:A:163:LEU:HD22	2.00	0.60
1:B:107:ARG:CG	2:B:221:EPY:O8C	2.49	0.60
1:C:12:LEU:HD11	1:C:107:ARG:HD3	1.83	0.60
1:D:118:ASP:O	1:D:122:LEU:HG	2.01	0.60
1:C:112:ARG:HH21	1:D:112:ARG:NE	1.99	0.60
1:B:132:GLY:O	1:B:136:GLN:HG3	2.02	0.59
1:D:7:TRP:HZ2	2:D:223:EPY:H6C1	1.67	0.59
1:D:3:THR:HG23	1:D:63:ILE:HB	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ASN:HD22	1:D:216:ASN:N	1.97	0.58
1:C:141:LEU:O	1:C:144:ARG:HB2	2.04	0.58
1:D:7:TRP:HE1	2:D:223:EPY:H5C1	1.68	0.58
1:A:188:GLU:HG2	1:A:197:MET:SD	2.44	0.57
1:A:150:ASP:HB2	1:A:151:LYS:HE3	1.86	0.56
1:A:48:GLU:O	1:A:52:LEU:HD12	2.06	0.56
1:B:84:ASN:HD22	1:B:84:ASN:N	2.05	0.55
1:C:8:ASP:HB2	1:C:33:LYS:HE3	1.88	0.55
1:D:216:ASN:ND2	1:D:216:ASN:N	2.52	0.55
1:B:10:ARG:HG2	1:B:14:HIS:HB2	1.89	0.54
1:A:179:ASN:HD22	1:A:179:ASN:N	2.05	0.54
1:A:6:TYR:HA	1:A:59:LEU:HG	1.89	0.54
1:B:70:THR:O	1:B:71:GLN:HB2	2.08	0.54
1:D:7:TRP:NE1	2:D:223:EPY:H5C1	2.22	0.54
2:A:220:EPY:S	2:A:220:EPY:O2B	2.66	0.54
1:A:179:ASN:HD22	1:A:179:ASN:H	1.56	0.53
1:B:193:ILE:HG22	1:B:197:MET:HE3	1.89	0.53
1:C:22:TYR:HB2	1:C:193:ILE:HD11	1.91	0.53
1:C:70:THR:O	1:C:71:GLN:HB2	2.07	0.53
1:D:216:ASN:O	1:D:217:LYS:HG3	2.09	0.53
1:A:10:ARG:HB3	1:A:207:ILE:HA	1.92	0.52
1:A:209:TRP:HD1	1:A:210:TYR:H	1.56	0.52
1:C:48:GLU:O	1:C:52:LEU:HD22	2.10	0.52
1:D:76:LEU:CD1	1:D:158:LEU:HD21	2.40	0.52
1:D:206:PRO:HA	1:D:216:ASN:ND2	2.25	0.52
1:A:101:ASN:HB3	1:B:71:GLN:OE1	2.09	0.51
1:D:123:LYS:N	1:D:124:PRO:HD2	2.26	0.51
1:D:145:SER:HG	1:D:146:TRP:CD1	2.27	0.51
1:C:31:ARG:NH1	1:C:203:MET:SD	2.83	0.51
1:A:45:TRP:CZ2	1:A:49:LYS:HG3	2.46	0.51
1:B:124:PRO:HA	1:B:127:LEU:HD12	1.92	0.51
1:D:89:THR:O	1:D:93:LYS:HG3	2.10	0.51
1:B:107:ARG:HD2	2:B:221:EPY:N8C	2.26	0.51
1:D:193:ILE:O	1:D:197:MET:HG3	2.12	0.50
1:B:40:PHE:O	1:B:42:PRO:HD3	2.12	0.50
1:B:141:LEU:O	1:B:144:ARG:HB2	2.12	0.50
1:D:144:ARG:HD3	1:D:149:GLY:HA2	1.94	0.49
1:B:205:ALA:HB2	1:B:216:ASN:ND2	2.27	0.49
1:B:123:LYS:HG2	1:B:127:LEU:HD11	1.93	0.49
1:C:43:SER:HA	1:C:46:THR:OG1	2.12	0.49
1:B:5:GLY:HA3	1:B:61:TYR:CE2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ASP:O	1:B:165:GLN:HG3	2.12	0.49
1:D:30:ARG:HD2	1:D:30:ARG:HA	1.78	0.48
1:A:72:SER:H	2:A:220:EPY:C6B	2.27	0.48
1:C:95:ARG:HB2	1:C:148:VAL:HG23	1.95	0.48
1:C:123:LYS:HB3	1:C:124:PRO:HD3	1.96	0.48
1:C:216:ASN:HD22	1:C:216:ASN:N	2.06	0.48
1:A:90:GLU:OE2	1:B:81:ARG:HD2	2.14	0.48
1:B:193:ILE:HG22	1:B:197:MET:CE	2.44	0.48
1:B:130:LEU:N	1:B:131:PRO:HD2	2.28	0.47
1:D:205:ALA:HB1	1:D:217:LYS:HB2	1.96	0.47
1:B:209:TRP:HB2	2:B:221:EPY:O2C	2.15	0.47
1:D:76:LEU:HD13	1:D:158:LEU:HD21	1.96	0.47
1:A:107:ARG:NH2	1:A:161:ASP:OD2	2.47	0.47
1:D:22:TYR:HA	1:D:192:LYS:HG3	1.97	0.47
1:B:123:LYS:N	1:B:124:PRO:HD2	2.29	0.47
1:D:90:GLU:HG3	1:D:94:GLN:NE2	2.30	0.47
1:B:129:LEU:HB3	1:B:133:LYS:NZ	2.30	0.46
1:D:130:LEU:HD22	1:D:134:LEU:HG	1.97	0.46
1:A:130:LEU:HB3	1:A:131:PRO:HD3	1.98	0.46
1:B:104:MET:O	1:B:107:ARG:HB3	2.16	0.46
1:B:99:LEU:HD22	1:B:140:PHE:HE2	1.81	0.46
1:C:7:TRP:NE1	2:C:222:EPY:H5C1	2.31	0.46
1:D:170:VAL:O	1:D:170:VAL:HG13	2.15	0.46
1:C:33:LYS:HA	1:C:33:LYS:HE2	1.98	0.45
1:C:216:ASN:ND2	1:C:216:ASN:N	2.57	0.45
2:D:223:EPY:H2C2	2:D:223:EPY:H1A2	1.30	0.45
1:A:123:LYS:N	1:A:124:PRO:HD2	2.32	0.45
1:A:33:LYS:HE3	1:A:33:LYS:HB3	1.76	0.45
1:D:130:LEU:N	1:D:131:PRO:HD2	2.32	0.45
1:B:10:ARG:HB3	1:B:207:ILE:HA	1.99	0.44
1:A:209:TRP:CD1	1:A:210:TYR:H	2.34	0.44
1:C:161:ASP:O	1:C:165:GLN:HG3	2.18	0.43
1:A:96:VAL:HG13	1:A:155:VAL:CG2	2.47	0.43
1:D:7:TRP:HB2	1:D:9:ILE:HG12	1.99	0.43
1:C:99:LEU:HD23	1:C:99:LEU:HA	1.76	0.43
1:A:110:PHE:CE2	1:A:208:PHE:HZ	2.36	0.43
1:D:6:TYR:HA	1:D:59:LEU:HD22	2.00	0.43
1:D:7:TRP:NE1	2:D:223:EPY:O3A	2.51	0.43
1:D:42:PRO:HB3	2:D:223:EPY:O9C	2.19	0.43
1:D:90:GLU:HG3	1:D:94:GLN:HE21	1.84	0.43
1:A:151:LYS:H	1:A:151:LYS:CD	2.31	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LEU:HD21	1:C:169:PHE:HE2	1.83	0.42
1:D:7:TRP:CZ2	2:D:223:EPY:C6C	2.95	0.42
1:A:19:LEU:CD1	1:A:85:MET:HE1	2.38	0.42
1:C:97:ASP:OD2	1:D:81:ARG:NH2	2.53	0.42
1:D:41:ASP:HA	1:D:42:PRO:HD3	1.74	0.42
1:D:61:TYR:C	1:D:61:TYR:CD1	2.97	0.42
1:A:209:TRP:HD1	1:A:210:TYR:N	2.17	0.42
1:B:19:LEU:HD13	1:B:79:ILE:HG21	2.01	0.42
1:A:48:GLU:HG2	1:A:52:LEU:HD11	2.00	0.42
1:A:173:CYS:HB3	1:A:176:LEU:HD22	2.02	0.42
1:C:181:SER:O	1:C:185:GLN:HG2	2.20	0.42
1:D:153:THR:OG1	1:D:155:VAL:HG23	2.20	0.42
1:D:205:ALA:CB	1:D:217:LYS:HB2	2.49	0.41
1:B:92:GLU:O	1:B:96:VAL:HG23	2.20	0.41
1:C:206:PRO:HA	1:C:216:ASN:HD21	1.86	0.41
1:D:207:ILE:H	1:D:216:ASN:HD21	1.68	0.41
1:A:5:GLY:HA3	1:A:61:TYR:CZ	2.55	0.41
1:B:16:ILE:HA	1:B:76:LEU:HD21	2.03	0.41
1:A:19:LEU:HD11	1:A:85:MET:CE	2.38	0.41
1:A:192:LYS:H	1:A:192:LYS:CD	2.24	0.41
1:C:12:LEU:HD12	1:C:12:LEU:HA	1.73	0.41
1:D:209:TRP:CD1	1:D:211:THR:HG23	2.55	0.41
1:A:7:TRP:NE1	2:A:220:EPY:O3A	2.53	0.41
1:A:70:THR:O	1:A:71:GLN:HB2	2.21	0.40
1:A:208:PHE:N	1:A:215:ASN:HD21	2.11	0.40
1:D:133:LYS:O	1:D:136:GLN:HB2	2.21	0.40
1:A:92:GLU:O	1:A:96:VAL:HG23	2.21	0.40
1:B:90:GLU:O	1:B:94:GLN:HG3	2.22	0.40
1:A:123:LYS:HE2	1:A:127:LEU:HD11	2.02	0.40
1:C:124:PRO:O	1:C:128:GLU:HG2	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	215/219 (98%)	209 (97%)	6 (3%)	0	100	100
1	B	215/219 (98%)	205 (95%)	10 (5%)	0	100	100
1	C	215/219 (98%)	208 (97%)	7 (3%)	0	100	100
1	D	215/219 (98%)	205 (95%)	10 (5%)	0	100	100
All	All	860/876 (98%)	827 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	192/194 (99%)	163 (85%)	29 (15%)	3	10
1	B	192/194 (99%)	164 (85%)	28 (15%)	3	11
1	C	192/194 (99%)	163 (85%)	29 (15%)	3	10
1	D	192/194 (99%)	165 (86%)	27 (14%)	3	12
All	All	768/776 (99%)	655 (85%)	113 (15%)	3	10

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	4	LEU
1	A	30	ARG
1	A	33	LYS
1	A	52	LEU
1	A	59	LEU
1	A	62	LEU
1	A	70	THR
1	A	90	GLU
1	A	106	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	108	MET
1	A	120	GLU
1	A	129	LEU
1	A	130	LEU
1	A	133	LYS
1	A	137	LEU
1	A	139	ARG
1	A	151	LYS
1	A	163	LEU
1	A	167	ARG
1	A	176	LEU
1	A	179	ASN
1	A	181	SER
1	A	192	LYS
1	A	194	SER
1	A	198	ARG
1	A	199	SER
1	A	213	LEU
1	A	215	ASN
1	B	2	VAL
1	B	10	ARG
1	B	19	LEU
1	B	39	ASP
1	B	47	ASN
1	B	84	ASN
1	B	90	GLU
1	B	91	VAL
1	B	93	LYS
1	B	106	LEU
1	B	107	ARG
1	B	108	MET
1	B	130	LEU
1	B	143	SER
1	B	151	LYS
1	B	155	VAL
1	B	162	VAL
1	B	167	ARG
1	B	168	MET
1	B	170	VAL
1	B	176	LEU
1	B	181	SER
1	B	182	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	194	SER
1	B	198	ARG
1	B	213	LEU
1	B	215	ASN
1	B	217	LYS
1	C	12	LEU
1	C	19	LEU
1	C	28	GLN
1	C	30	ARG
1	C	39	ASP
1	C	51	LYS
1	C	52	LEU
1	C	66	ASP
1	C	82	LYS
1	C	91	VAL
1	C	99	LEU
1	C	112	ARG
1	C	129	LEU
1	C	130	LEU
1	C	152	LEU
1	C	155	VAL
1	C	167	ARG
1	C	168	MET
1	C	172	ASP
1	C	176	LEU
1	C	177	GLN
1	C	181	SER
1	C	185	GLN
1	C	191	GLU
1	C	193	ILE
1	C	194	SER
1	C	204	LYS
1	C	209	TRP
1	C	216	ASN
1	D	2	VAL
1	D	3	THR
1	D	12	LEU
1	D	39	ASP
1	D	58	ASN
1	D	68	LYS
1	D	70	THR
1	D	84	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	116	SER
1	D	123	LYS
1	D	127	LEU
1	D	130	LEU
1	D	135	ARG
1	D	136	GLN
1	D	137	LEU
1	D	138	SER
1	D	139	ARG
1	D	145	SER
1	D	155	VAL
1	D	166	GLN
1	D	181	SER
1	D	191	GLU
1	D	192	LYS
1	D	194	SER
1	D	198	ARG
1	D	215	ASN
1	D	216	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	71	GLN
1	A	102	HIS
1	A	136	GLN
1	A	179	ASN
1	A	215	ASN
1	B	28	GLN
1	B	73	ASN
1	B	83	HIS
1	B	84	ASN
1	B	101	ASN
1	B	102	HIS
1	B	165	GLN
1	B	215	ASN
1	C	28	GLN
1	C	47	ASN
1	C	71	GLN
1	C	94	GLN
1	C	102	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	185	GLN
1	C	215	ASN
1	C	216	ASN
1	D	47	ASN
1	D	58	ASN
1	D	71	GLN
1	D	94	GLN
1	D	136	GLN
1	D	165	GLN
1	D	166	GLN
1	D	215	ASN
1	D	216	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	EPY	C	222	-	32,34,34	7.80	9 (28%)	34,44,44	2.01	9 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EPY	B	221	-	32,34,34	5.22	6 (18%)	34,44,44	3.52	11 (32%)
2	EPY	D	223	-	32,34,34	7.08	10 (31%)	34,44,44	2.12	12 (35%)
2	EPY	A	220	-	32,34,34	7.16	10 (31%)	34,44,44	3.65	7 (20%)

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	EPY	C	222	-	1/1/8/10	8/36/38/38	0/1/1/1
2	EPY	B	221	-	1/1/8/10	13/36/38/38	0/1/1/1
2	EPY	D	223	-	-	13/36/38/38	0/1/1/1
2	EPY	A	220	-	1/1/8/10	9/36/38/38	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	222	EPY	C1A-S	-40.10	1.42	1.82
2	A	220	EPY	C1A-S	-35.98	1.46	1.82
2	D	223	EPY	C1A-S	-34.01	1.48	1.82
2	B	221	EPY	C1A-S	-25.80	1.56	1.82
2	D	223	EPY	C1C-S	-16.61	1.50	1.83
2	C	222	EPY	C1C-S	-14.85	1.54	1.83
2	A	220	EPY	C1C-S	-14.53	1.54	1.83
2	B	221	EPY	C1C-S	-11.94	1.59	1.83
2	A	220	EPY	C2B-N1B	6.29	1.47	1.34
2	D	223	EPY	C1A-C2A	-6.18	1.37	1.53
2	C	222	EPY	C5C-C6C	5.85	1.48	1.38
2	D	223	EPY	O2B-C2B	-5.66	1.12	1.23
2	A	220	EPY	C7C-N8C	-5.53	1.32	1.45
2	D	223	EPY	C9C-C4C	5.53	1.49	1.38
2	C	222	EPY	C1A-C2A	-4.57	1.41	1.53
2	D	223	EPY	C8C-C9C	-4.14	1.32	1.38
2	B	221	EPY	C7C-N8C	-3.56	1.36	1.45
2	D	223	EPY	C7C-N8C	-3.56	1.36	1.45
2	A	220	EPY	C2A-C3A	2.94	1.60	1.52
2	C	222	EPY	O3C-C4C	-2.88	1.31	1.37
2	C	222	EPY	C7C-N8C	-2.41	1.39	1.45
2	A	220	EPY	C2C-C1C	-2.30	1.44	1.52
2	C	222	EPY	C8C-C9C	2.26	1.42	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	221	EPY	C8C-C9C	2.24	1.42	1.38
2	D	223	EPY	C2A-N1B	-2.22	1.41	1.45
2	B	221	EPY	O6A-C6A	-2.21	1.23	1.30
2	A	220	EPY	C8C-C9C	2.21	1.42	1.38
2	A	220	EPY	C2A-N1B	-2.19	1.41	1.45
2	C	222	EPY	O6A-C6A	-2.19	1.23	1.30
2	A	220	EPY	O6A-C6A	-2.18	1.23	1.30
2	D	223	EPY	O6A-C6A	-2.18	1.23	1.30
2	C	222	EPY	C3B-C2B	2.12	1.55	1.51
2	B	221	EPY	C3B-C2B	2.11	1.55	1.51
2	A	220	EPY	C3B-C2B	2.10	1.55	1.51
2	D	223	EPY	C8C-C7C	2.08	1.42	1.38

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	220	EPY	O3C-C2C-C1C	17.58	137.39	107.05
2	B	221	EPY	C1A-C2A-C3A	11.58	135.57	109.46
2	A	220	EPY	C2C-O3C-C4C	-9.68	96.54	117.85
2	B	221	EPY	O3C-C2C-C1C	9.20	122.93	107.05
2	B	221	EPY	C1A-C2A-N1B	-6.62	93.75	111.06
2	B	221	EPY	C2A-C1A-S	6.58	137.61	113.66
2	C	222	EPY	O3C-C2C-C1C	5.56	116.64	107.05
2	B	221	EPY	O3A-C3A-C2A	-5.32	109.35	120.48
2	D	223	EPY	O3C-C2C-C1C	5.22	116.06	107.05
2	C	222	EPY	C2A-C1A-S	4.98	131.78	113.66
2	D	223	EPY	C1A-C2A-N1B	-4.85	98.39	111.06
2	B	221	EPY	C2A-N1B-C2B	4.73	133.55	121.68
2	B	221	EPY	C2A-C3A-N4A	4.71	126.65	116.54
2	C	222	EPY	C2A-N1B-C2B	4.54	133.07	121.68
2	D	223	EPY	C2A-C1A-S	4.15	128.76	113.66
2	B	221	EPY	C2C-O3C-C4C	-3.80	109.48	117.85
2	C	222	EPY	C1A-C2A-N1B	-3.58	101.70	111.06
2	D	223	EPY	O2B-C2B-N1B	-3.48	117.06	122.95
2	D	223	EPY	C2A-N1B-C2B	3.12	129.50	121.68
2	C	222	EPY	O3A-C3A-C2A	-3.08	114.02	120.48
2	C	222	EPY	C2A-C3A-N4A	3.02	123.02	116.54
2	C	222	EPY	C3A-C2A-N1B	2.80	118.70	111.11
2	D	223	EPY	C5C-C4C-C9C	-2.77	116.12	120.16
2	A	220	EPY	C3A-C2A-N1B	-2.75	103.67	111.11
2	D	223	EPY	C8C-C9C-C4C	2.74	122.86	119.73
2	B	221	EPY	C8C-C7C-N8C	2.67	121.67	119.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	223	EPY	O2B-C2B-C3B	2.66	126.83	122.02
2	A	220	EPY	O9C-N8C-C7C	-2.63	115.20	118.82
2	D	223	EPY	O3A-C3A-C2A	-2.33	115.61	120.48
2	D	223	EPY	C3B-C4B-C5B	2.28	119.11	113.86
2	A	220	EPY	O6A-C6A-O7A	-2.18	117.71	123.33
2	C	222	EPY	O6A-C6A-O7A	-2.16	117.78	123.33
2	A	220	EPY	O6A-C6A-C5A	2.14	120.96	112.81
2	C	222	EPY	O6A-C6A-C5A	2.13	120.92	112.81
2	D	223	EPY	O6A-C6A-C5A	2.13	120.91	112.81
2	B	221	EPY	O6A-C6A-O7A	-2.13	117.86	123.33
2	D	223	EPY	O6A-C6A-O7A	-2.13	117.86	123.33
2	B	221	EPY	O6A-C6A-C5A	2.13	120.89	112.81
2	A	220	EPY	C8C-C7C-N8C	2.00	121.09	119.34

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	220	EPY	C1C
2	B	221	EPY	C1C
2	C	222	EPY	C1C

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	220	EPY	C2A-C3A-N4A-C5A
2	A	220	EPY	O3A-C3A-N4A-C5A
2	B	221	EPY	C2A-C1A-S-C1C
2	B	221	EPY	S-C1A-C2A-N1B
2	B	221	EPY	C2A-C3A-N4A-C5A
2	B	221	EPY	O3A-C3A-N4A-C5A
2	B	221	EPY	S-C1C-C3C-O2C
2	B	221	EPY	S-C1C-C2C-O3C
2	C	222	EPY	C2A-C3A-N4A-C5A
2	C	222	EPY	O3A-C3A-N4A-C5A
2	C	222	EPY	S-C1C-C2C-O3C
2	D	223	EPY	C2C-C1C-S-C1A
2	D	223	EPY	C2A-C3A-N4A-C5A
2	D	223	EPY	O3A-C3A-N4A-C5A
2	D	223	EPY	C2C-C1C-C3C-O2C
2	D	223	EPY	S-C1C-C2C-O3C
2	B	221	EPY	C5C-C4C-O3C-C2C
2	B	221	EPY	C9C-C4C-O3C-C2C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	222	EPY	C9C-C4C-O3C-C2C
2	C	222	EPY	C5C-C4C-O3C-C2C
2	A	220	EPY	C9C-C4C-O3C-C2C
2	A	220	EPY	C5C-C4C-O3C-C2C
2	A	220	EPY	S-C1A-C2A-C3A
2	D	223	EPY	C9C-C4C-O3C-C2C
2	D	223	EPY	C5C-C4C-O3C-C2C
2	C	222	EPY	C3C-C1C-C2C-O3C
2	D	223	EPY	O2B-C2B-N1B-C2A
2	A	220	EPY	C2C-C1C-C3C-O2C
2	C	222	EPY	C1C-C2C-O3C-C4C
2	A	220	EPY	N1B-C2A-C3A-O3A
2	A	220	EPY	S-C1A-C2A-N1B
2	B	221	EPY	C1A-C2A-N1B-C2B
2	A	220	EPY	C3A-C2A-N1B-C2B
2	D	223	EPY	N1B-C2A-C3A-O3A
2	D	223	EPY	C3B-C4B-C5B-N5B
2	D	223	EPY	C3A-C2A-N1B-C2B
2	B	221	EPY	O2B-C2B-N1B-C2A
2	B	221	EPY	C2C-C1C-C3C-O2C
2	D	223	EPY	S-C1C-C3C-O2C
2	B	221	EPY	C3C-C1C-C2C-O3C
2	D	223	EPY	C3B-C4B-C5B-C6B
2	C	222	EPY	C3A-C2A-N1B-C2B
2	B	221	EPY	S-C1A-C2A-C3A

There are no ring outliers.

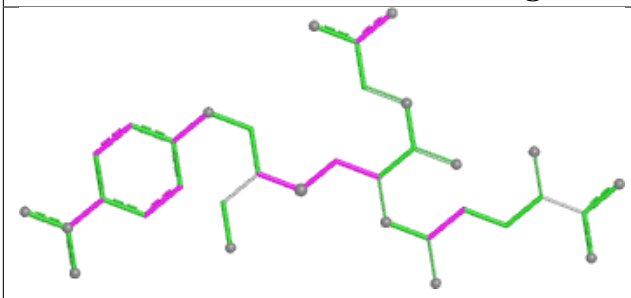
4 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	222	EPY	4	0
2	B	221	EPY	6	0
2	D	223	EPY	13	0
2	A	220	EPY	6	0

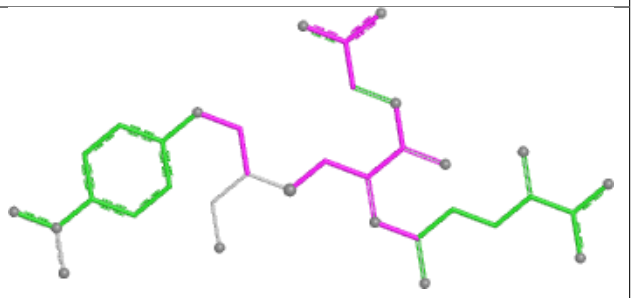
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

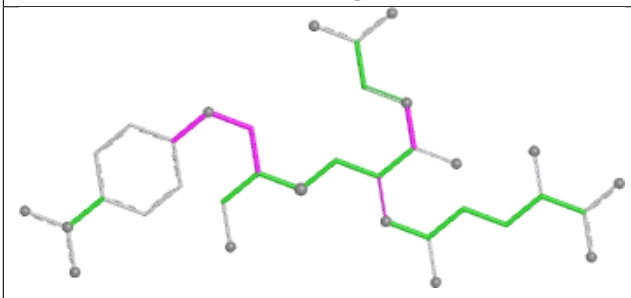
Ligand EPY C 222



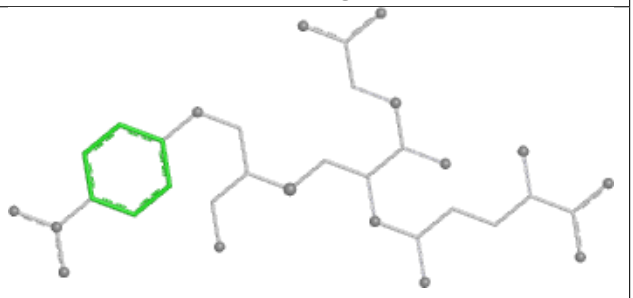
Bond lengths



Bond angles

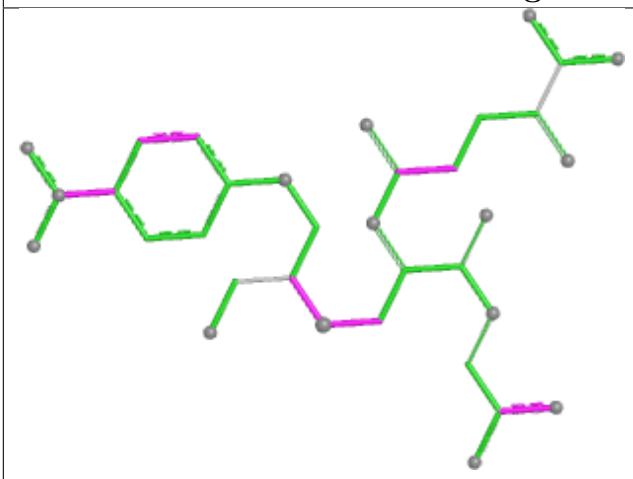


Torsions

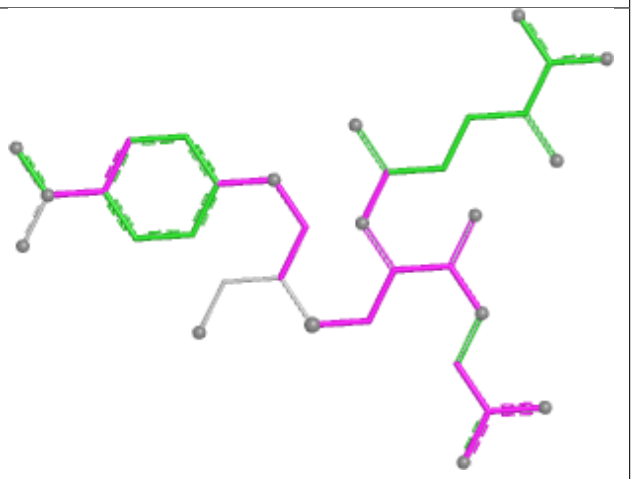


Rings

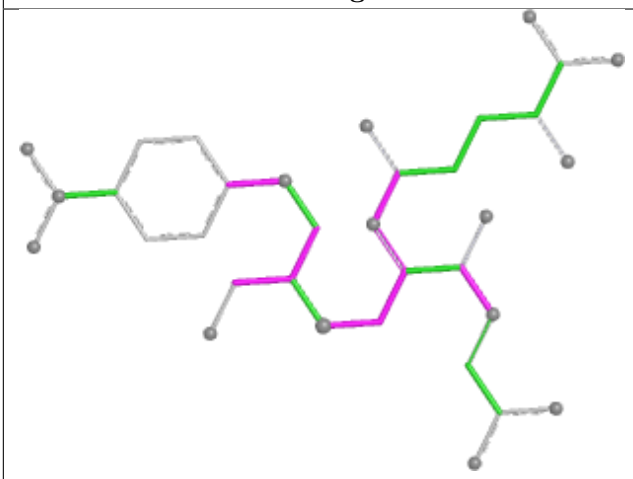
Ligand EPY B 221



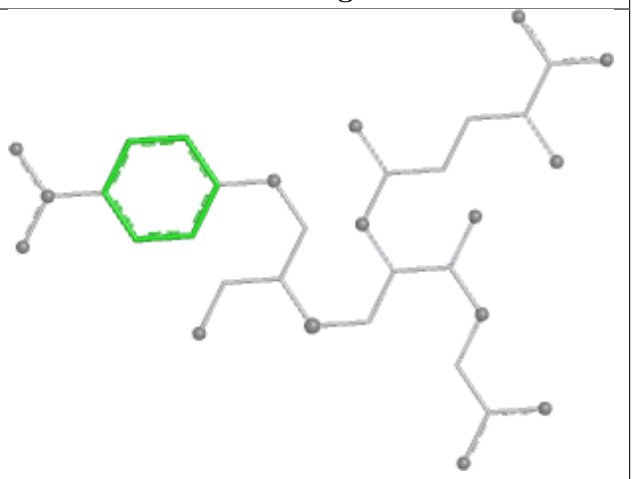
Bond lengths



Bond angles

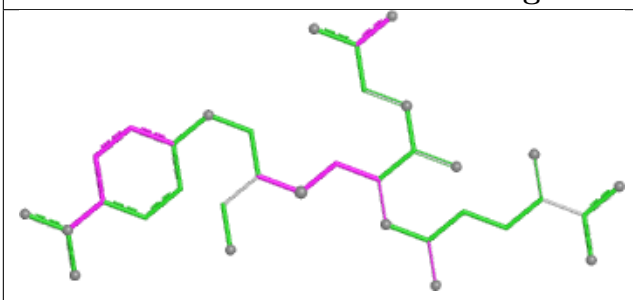


Torsions

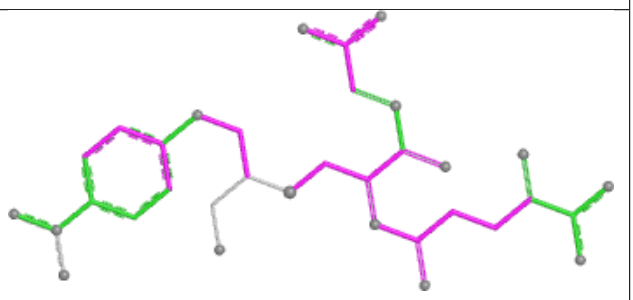


Rings

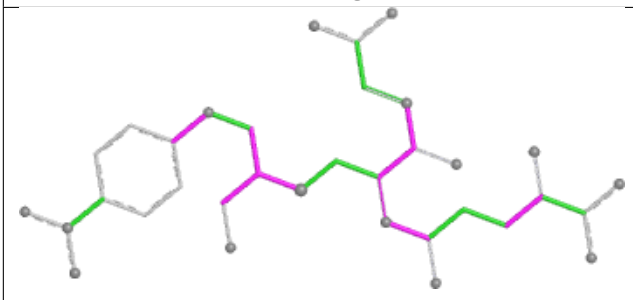
Ligand EPY D 223



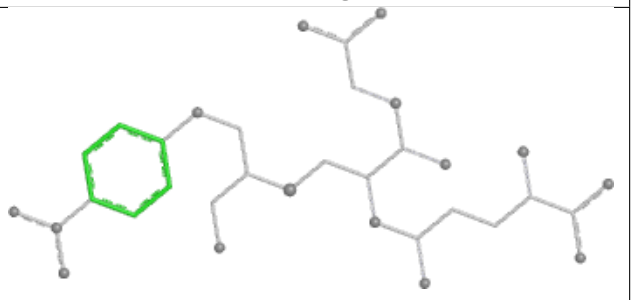
Bond lengths



Bond angles

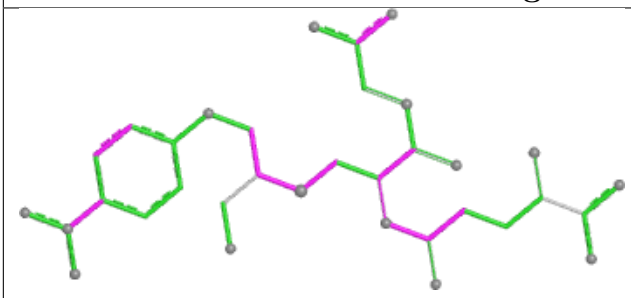


Torsions

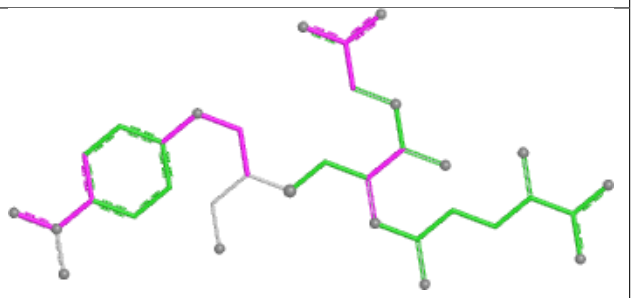


Rings

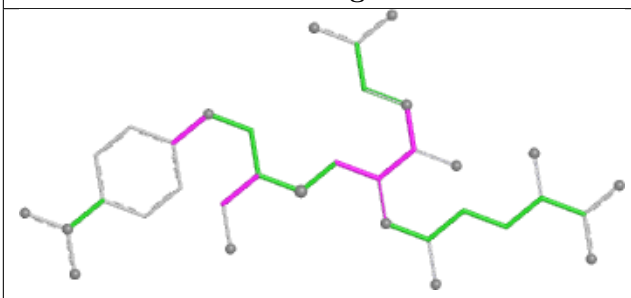
Ligand EPY A 220



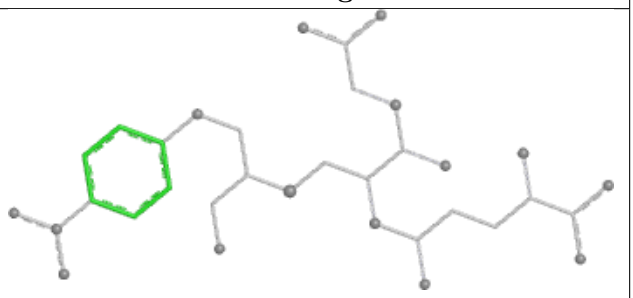
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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	217/219 (99%)	-0.47	0	100	100	9, 29, 54, 67	0
1	B	217/219 (99%)	-0.50	0	100	100	10, 31, 52, 68	0
1	C	217/219 (99%)	-0.55	0	100	100	9, 29, 51, 70	0
1	D	217/219 (99%)	-0.50	1 (0%)	87	82	8, 28, 54, 74	0
All	All	868/876 (99%)	-0.50	1 (0%)	92	90	8, 30, 53, 74	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	217	LYS	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	EPY	D	223	34/34	0.82	0.12	28,39,51,54	0

Continued on next page...

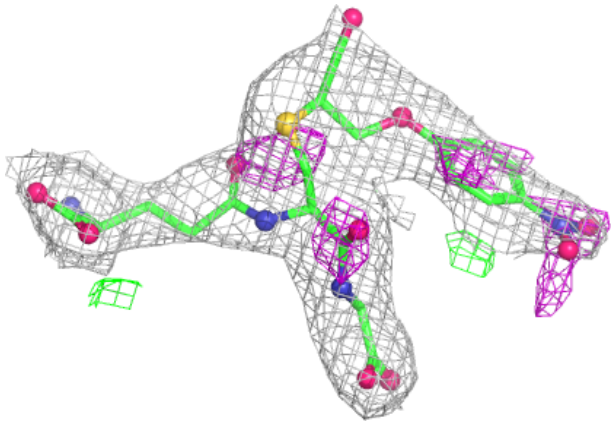
Continued from previous page...

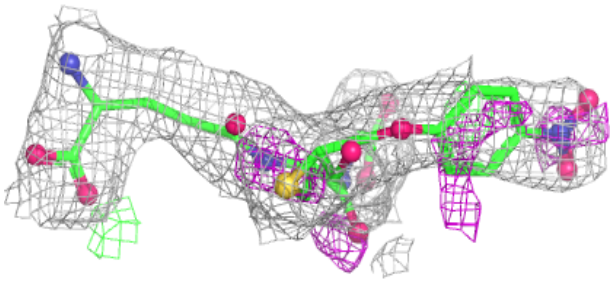
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EPY	B	221	34/34	0.86	0.13	21,36,51,59	0
2	EPY	A	220	34/34	0.86	0.14	25,33,51,55	0
2	EPY	C	222	34/34	0.87	0.12	14,35,53,56	0

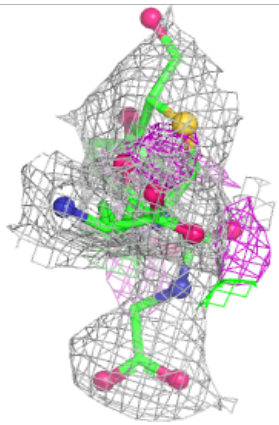
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EPY D 223:

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

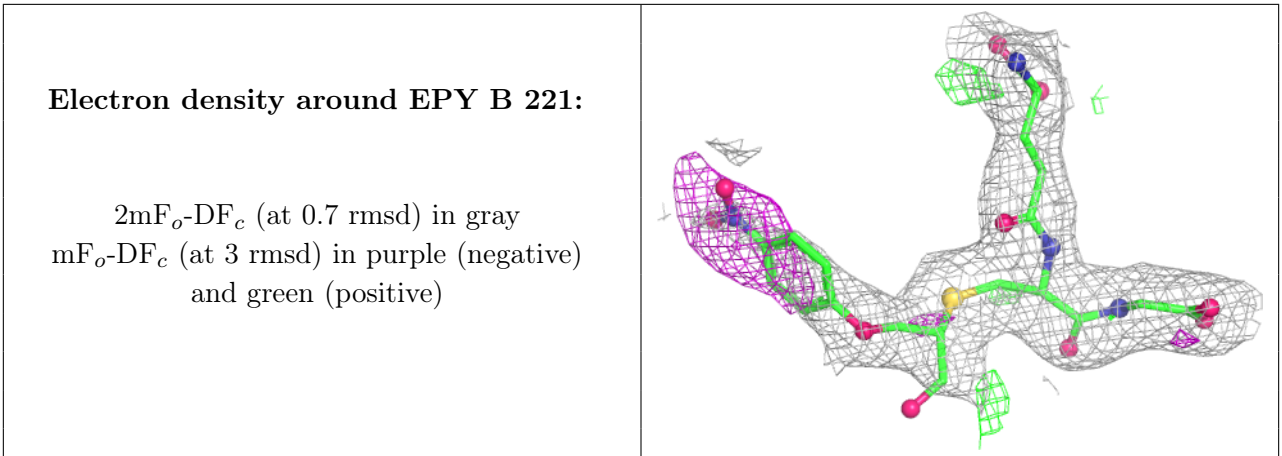


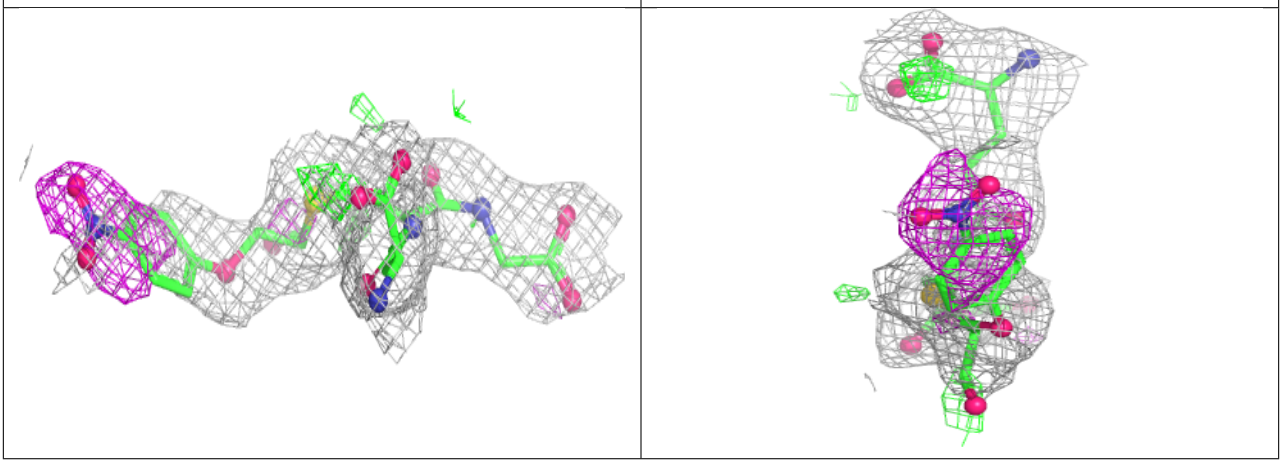




Electron density around EPY B 221:

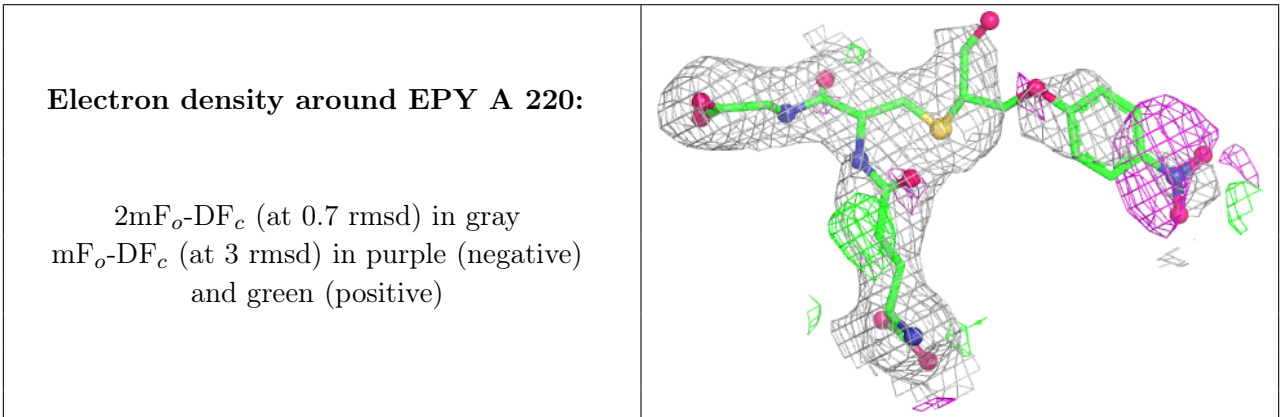
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

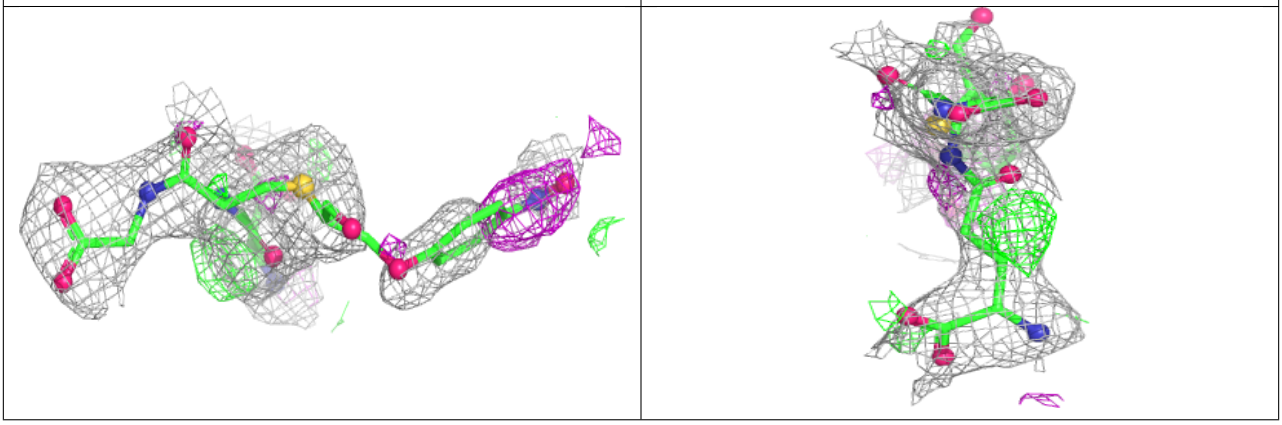




Electron density around EPY A 220:

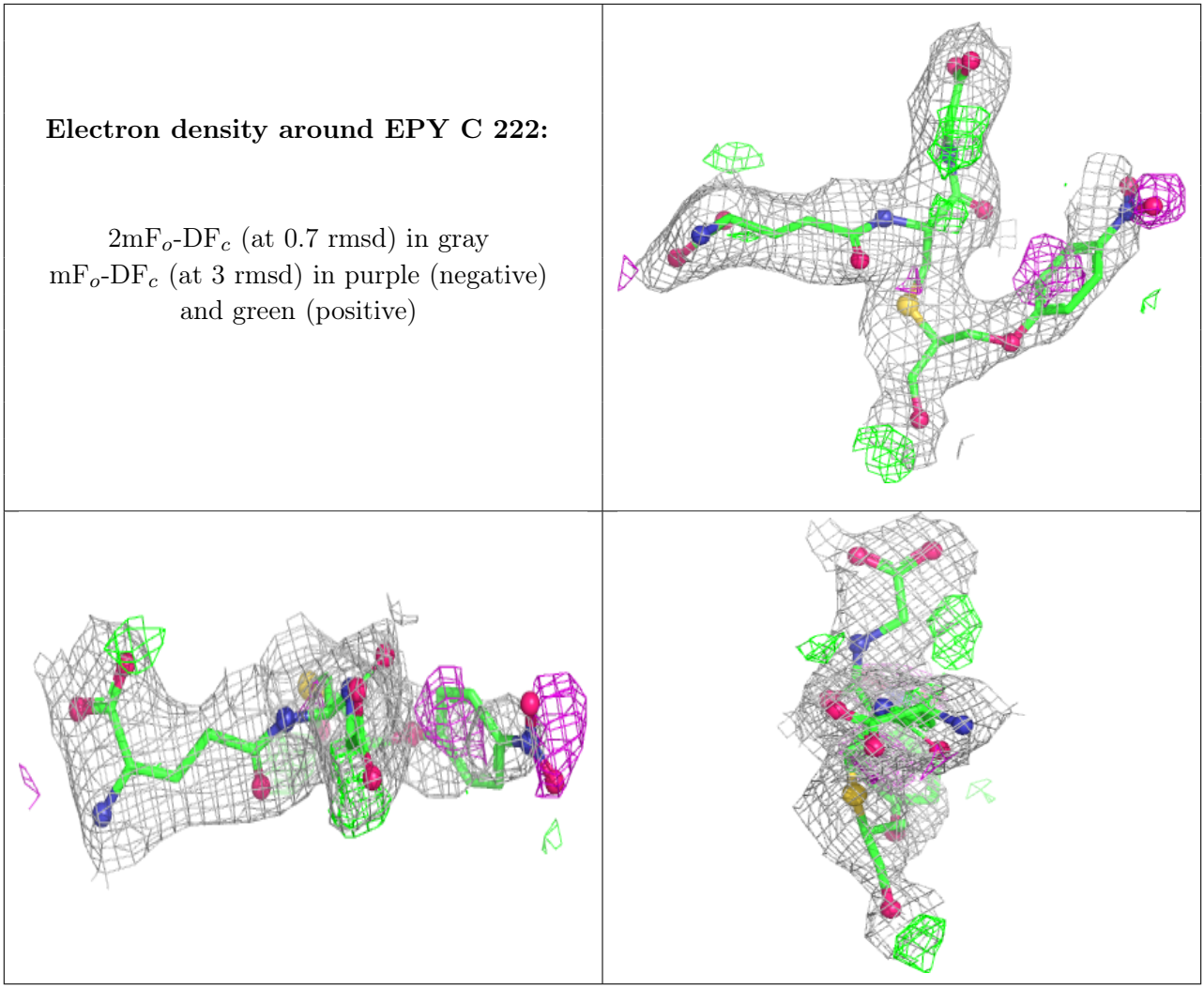
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around EPY C 222:

$2mF_o$-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.