wwPDB X-ray Structure Validation Summary Report (i)

Sep 9, 2026 – 03:14 pm BST

PDB ID	:	2VPW / pdb_00002vpw
Title	:	Polysulfide reductase with bound menaquinone
Authors	:	Jormakka, M.; Yokoyama, K.; Yano, T.; Tamakoshi, M.; Akimoto, S.; Shimamura, T.; Curmi, P.; Iwata, S.
Deposited on	:	2008-03-09
Resolution	:	3.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i)) were used in the production of this report:

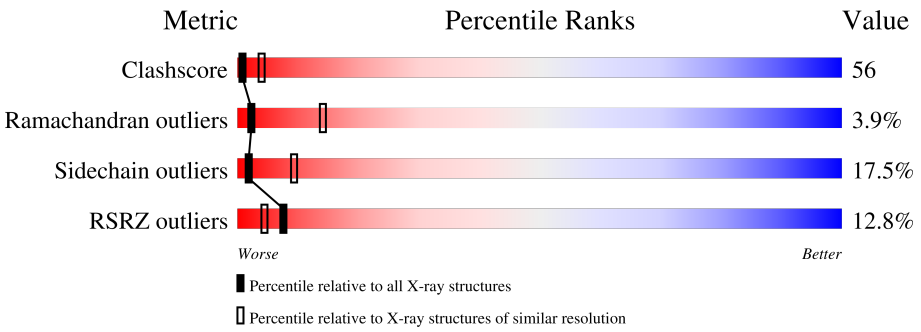
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	765	12%; 31%, 43%, 17%, 5%, •
1	E	765	10%; 32%, 41%, 17%, 6%, •
2	B	195	8%; 38%, 44%, 13%, • •
2	F	195	14%; 36%, 47%, 13%, • •
3	C	253	9%; 49%, 38%, 11%, • •
3	G	253	28%; 43%, 40%, 13%, • •

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
4	SF4	B	1194	-	-	X	-
4	SF4	B	1195	-	-	X	-
4	SF4	B	1196	-	-	X	-
4	SF4	F	1194	-	-	X	-
4	SF4	F	1195	-	-	X	-
7	MQ7	C	1252	-	-	-	X
7	MQ7	G	1251	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 20223 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 THIOSULFATE REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	735	5896	3802	1032	1043	19	0	0	1
1	E	735	5896	3802	1032	1043	19	0	0	1

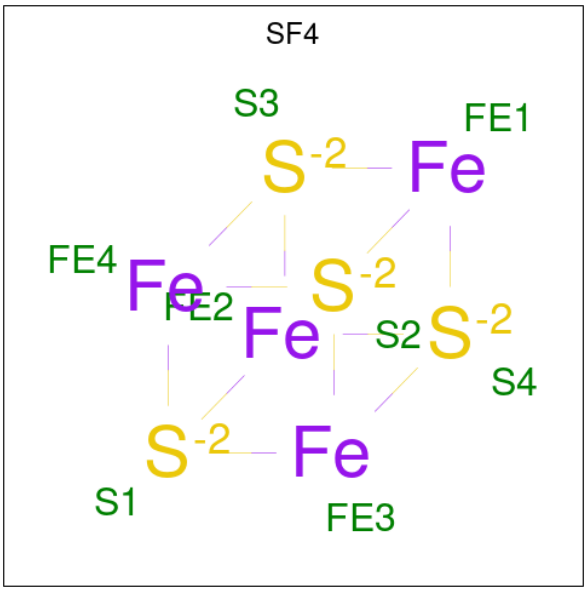
- Molecule 2 is a protein called NRFC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	194	1475	930	256	269	20	0	0	1
2	F	194	1475	930	256	269	20	0	0	1

- Molecule 3 is a protein called HYPOTHETICAL MEMBRANE SPANNING PROTEIN.

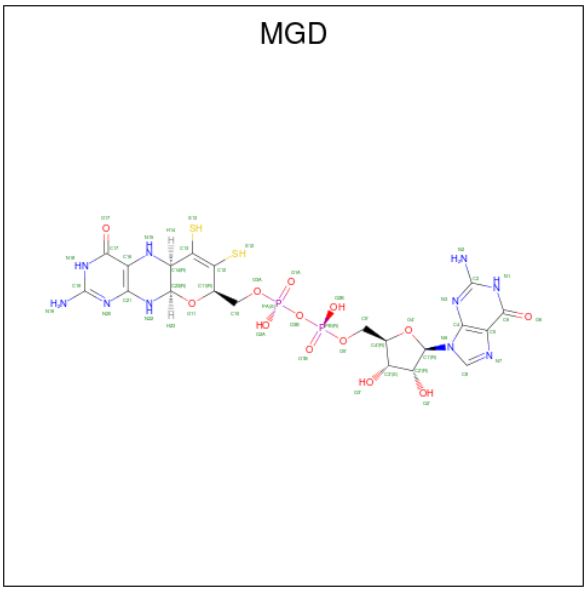
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	251	1948	1323	320	303	2	0	0	1
3	G	251	1948	1323	320	303	2	0	0	1

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	A	1	8	4	4	0	0
4	B	1	8	4	4	0	0
4	B	1	8	4	4	0	0
4	B	1	8	4	4	0	0
4	B	1	8	4	4	0	0
4	E	1	8	4	4	0	0
4	F	1	8	4	4	0	0
4	F	1	8	4	4	0	0
4	F	1	8	4	4	0	0
4	F	1	8	4	4	0	0

- Molecule 5 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: $C_{20}H_{26}N_{10}O_{13}P_2S_2$).

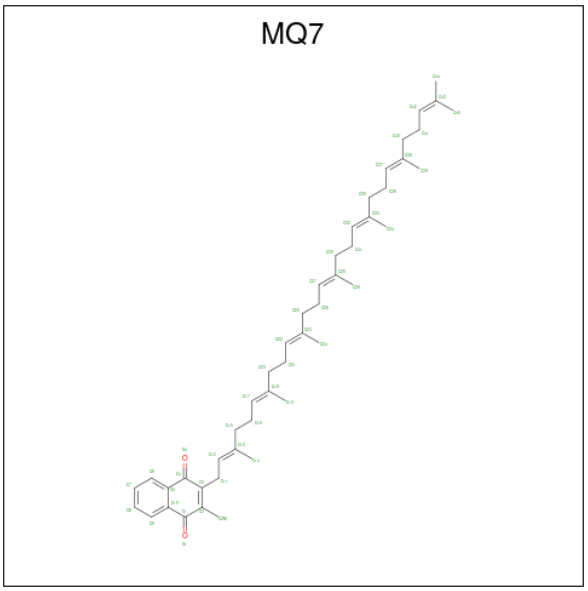


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
5	A	1	47	20	10	13	2	2	0	0
			Total	C	N	O	P	S		
5	A	1	47	20	10	13	2	2	0	0
			Total	C	N	O	P	S		
5	E	1	47	20	10	13	2	2	0	0
			Total	C	N	O	P	S		
5	E	1	47	20	10	13	2	2	0	0

- Molecule 6 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mo		
6	A	1	1	1	0	0
			Total	Mo		
6	E	1	1	1	0	0

- Molecule 7 is MENAQUINONE-7 (CCD ID: MQ7) (formula: $C_{46}H_{64}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	C	1	15	13	2	0	0
			Total	C	O		
7	G	1	15	13	2	0	0

- Molecule 8 is water.

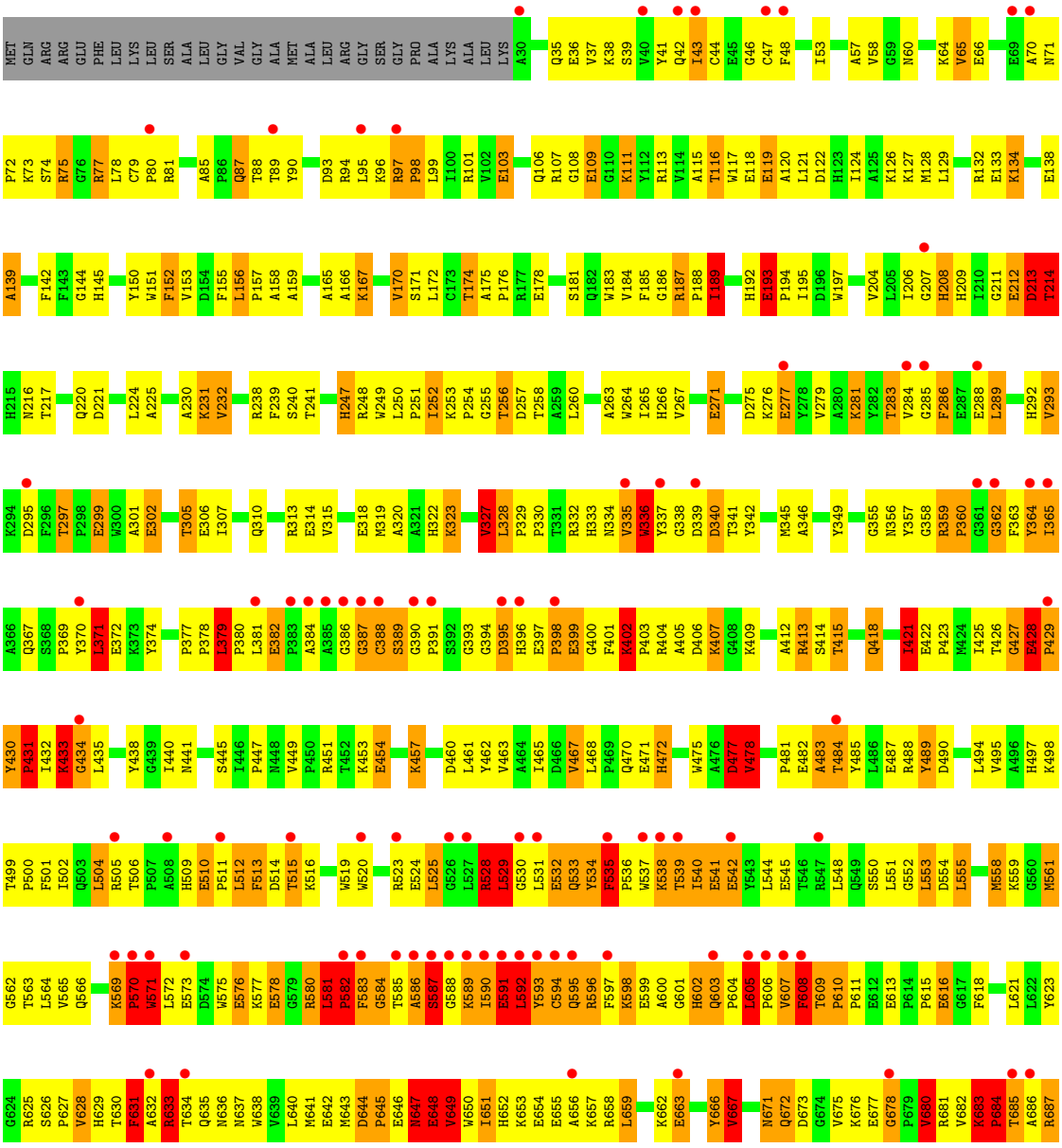
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	386	386	386	0	0
			Total	O		
8	B	149	149	149	0	0
			Total	O		
8	C	90	90	90	0	0
			Total	O		
8	E	453	453	453	0	0
			Total	O		
8	F	129	129	129	0	0
			Total	O		
8	G	78	78	78	0	0

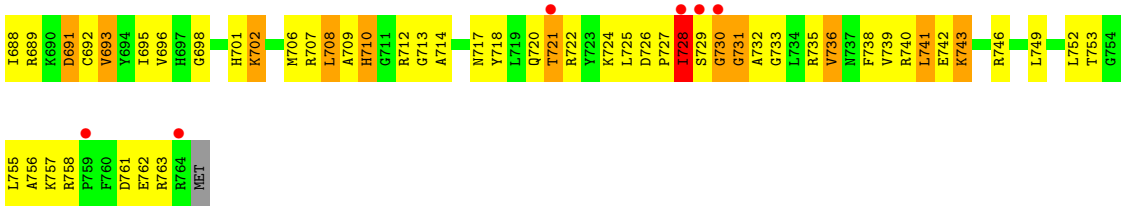
3 Residue-property plots (i)

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: THIOSULFATE REDUCTASE

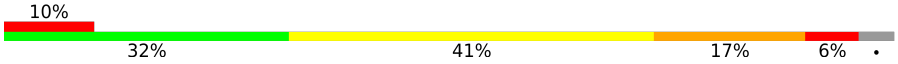
Chain A: 12% 31% 43% 17% 5%

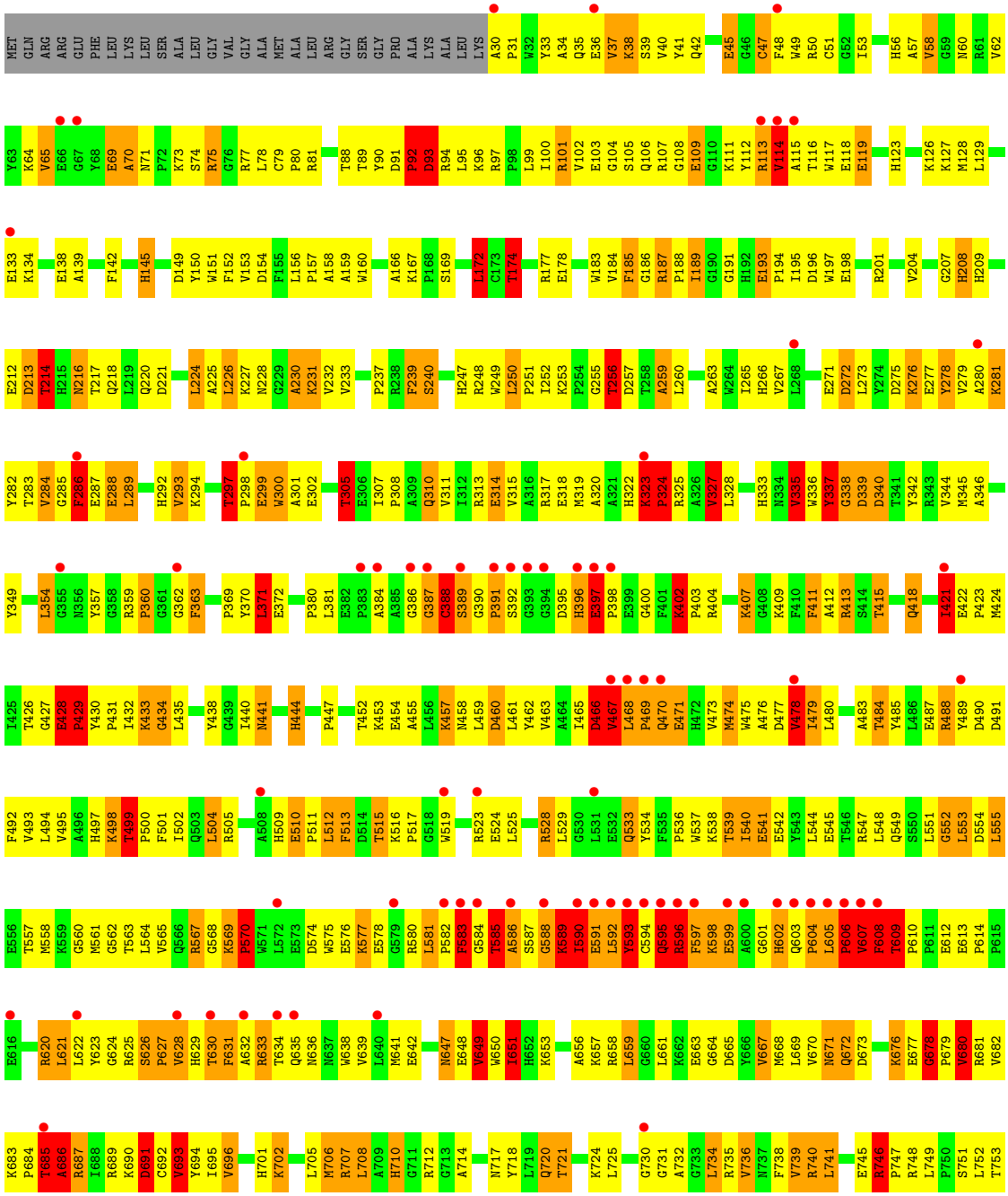




- Molecule 1: THIOSULFATE REDUCTASE

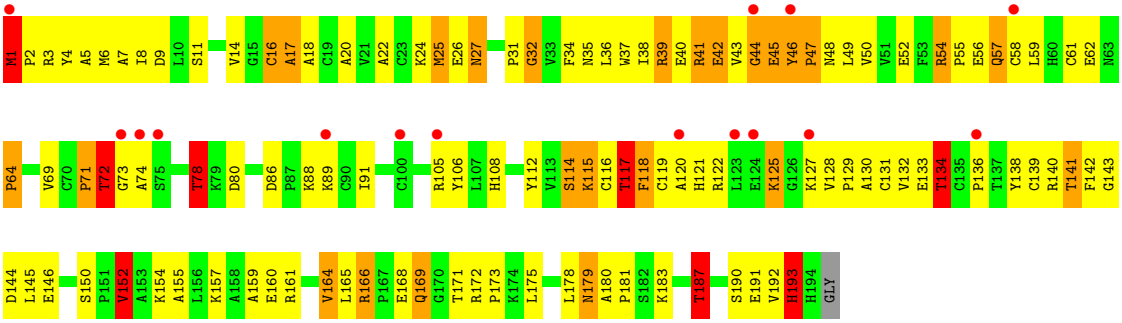
Chain E:





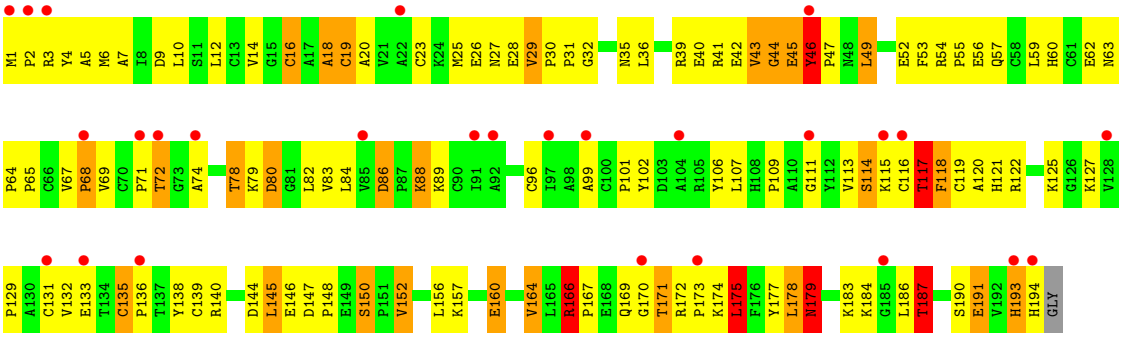
• Molecule 2: NRFC PROTEIN

Chain B:



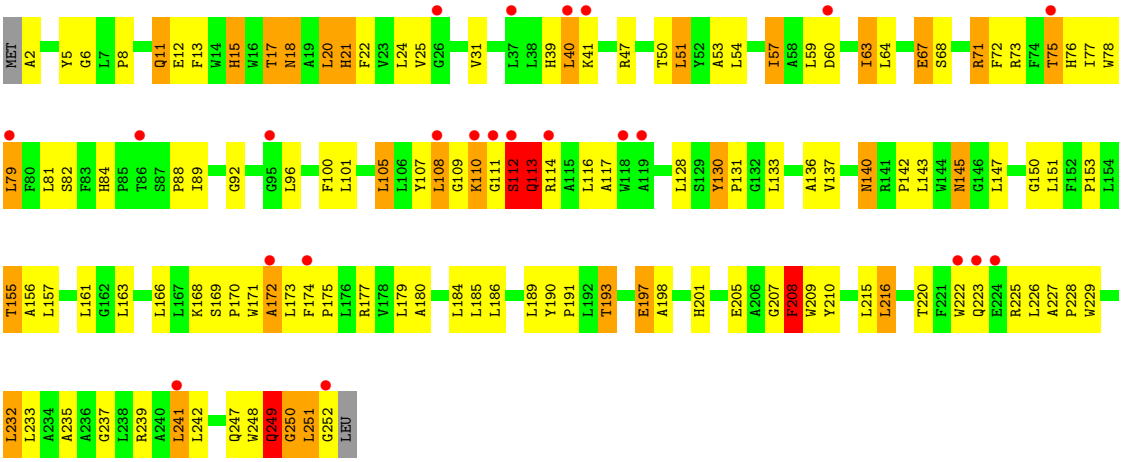
• Molecule 2: NRFC PROTEIN

Chain F:



• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN

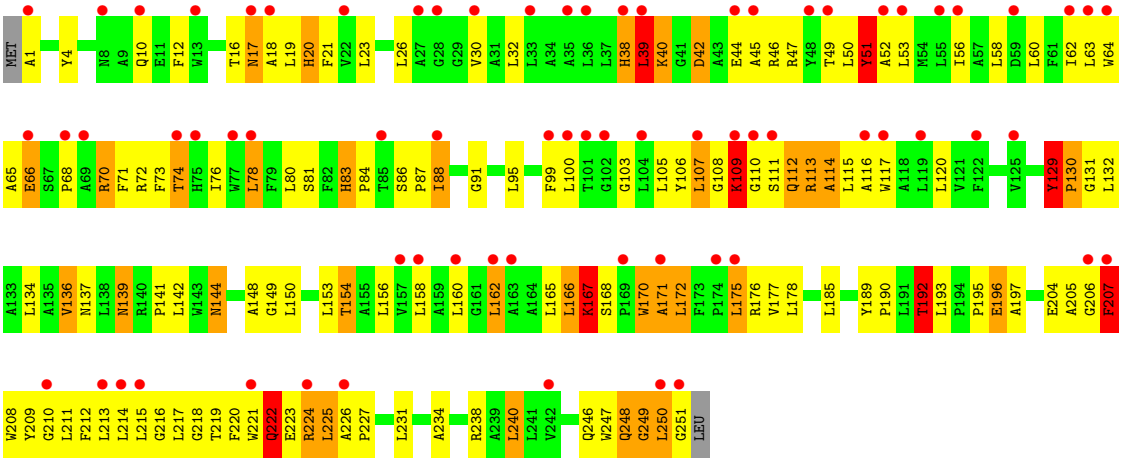
Chain C:



• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN

Chain G:

28%
43%
40%
13%


MET A1 Y4 N8 A9 Q10 E11 F12 W13 T16 N17 A18 L19 H20 F21 V22 L23 L26 A27 G28 G29 V30 A31 L32 L33 A34 A35 L36 L37 H38 L39 K40 G41 D42 A43 E44 A45 R46 R47 Y48 T49 L50 Y51 A52 L53 M54 L55 I56 A57 L58 D59 L60 F61 I62 L63 W64
A65 E66 S67 P68 A69 R70 F71 R72 F73 T74 H75 I76 W77 L78 F79 L80 S81 F82 H83 P84 T85 S86 P87 I88 G91 L95 F99 L100 T101 G102 G103 L104 L105 Y106 L107 G108 K109 G110 S111 Q112 R113 A114 L115 A116 W117 A118 L119 L120 V121 F122 V125 Y129 P130 G131 L132
A133 L134 A135 V136 N137 L138 N139 R140 P141 L142 W143 N144 A148 G149 L150 L153 T154 A155 L156 V157 L158 A159 L160 G161 L162 A163 A164 L165 L166 K167 S168 P169 W170 A171 L172 F173 P174 L175 R176 V177 L178 L185 Y189 P190 L191 T192 L193 P194 P195 E196 A197 E204 A205 G206 F207
W208 Y209 G210 L211 F212 L213 L214 L215 G216 L217 G218 T219 F220 W221 Q222 E223 R224 L225 A226 P227 L231 A234 R238 A239 L240 L241 V242 Q246 W247 Q248 G249 L250 G251 LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	115.38Å 163.58Å 238.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.82 – 3.10 39.82 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.82-3.10) 95.9 (39.82-3.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.271 , 0.275 0.263 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	77.7	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 73.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	20223	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MQ7, MGD, MO, SF4

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	1.15	16/6079 (0.3%)	1.64	120/8267 (1.5%)
1	E	1.32	18/6079 (0.3%)	1.95	193/8267 (2.3%)
2	B	1.17	3/1512 (0.2%)	1.68	33/2058 (1.6%)
2	F	1.19	5/1512 (0.3%)	1.77	40/2058 (1.9%)
3	C	0.96	3/2016 (0.1%)	1.38	23/2764 (0.8%)
3	G	1.08	4/2016 (0.2%)	1.59	37/2764 (1.3%)
All	All	1.19	49/19214 (0.3%)	1.73	446/26178 (1.7%)

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	1	2
1	E	1	5
3	G	0	1
All	All	2	8

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	387	GLY	C-N	-48.15	0.66	1.33
1	A	583	PHE	C-N	25.89	1.71	1.33
3	G	109	LYS	C-N	-19.12	1.05	1.33
1	E	323	LYS	C-N	14.06	1.66	1.33
1	E	388	CYS	C-N	11.30	1.49	1.33

The worst 5 of 446 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	240	SER	N-CA-CB	-26.20	62.28	109.18
1	E	595	GLN	N-CA-CB	-25.15	74.10	110.57
1	E	594	CYS	N-CA-C	25.02	137.84	111.07
1	E	387	GLY	O-C-N	-24.26	91.16	122.70
1	E	421	ILE	N-CA-CB	-23.23	81.38	112.28

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	401	PHE	CA
1	E	585	THR	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	402	LYS	Mainchain
1	A	571	TRP	Mainchain
1	E	185	PHE	Mainchain
1	E	387	GLY	Mainchain
1	E	388	CYS	Mainchain

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	5896	0	5813	788	3
1	E	5896	0	5814	716	3
2	B	1475	0	1453	171	0
2	F	1475	0	1454	147	0
3	C	1948	0	2001	167	0
3	G	1948	0	2003	187	0
4	A	8	0	0	0	0
4	B	32	0	0	7	0
4	E	8	0	0	1	0
4	F	32	0	0	6	0
5	A	94	0	44	11	0
5	E	94	0	43	18	0
6	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1	0	0	0	0
7	C	15	0	9	19	0
7	G	15	0	9	20	0
8	A	386	0	0	97	0
8	B	149	0	0	44	0
8	C	90	0	0	11	0
8	E	453	0	0	138	0
8	F	129	0	0	33	0
8	G	78	0	0	34	0
All	All	20223	0	18643	2122	3

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 56.

The worst 5 of 2122 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:602:HIS:CE1	1:A:606:PRO:HG3	1.28	1.63
1:A:186:GLY:HA3	1:A:583:PHE:C	1.15	1.49
1:A:583:PHE:C	1:A:584:GLY:N	1.71	1.48
1:A:184:VAL:CG2	1:A:592:LEU:HD23	1.45	1.45
2:F:135:CYS:SG	2:F:135:CYS:CB	2.06	1.43

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:GLU:OE2	1:E:133:GLU:C[2_674]	1.32	0.88
1:A:399:GLU:OE2	1:E:134:LYS:N[2_674]	1.51	0.69
1:A:399:GLU:OE2	1:E:133:GLU:O[2_674]	1.91	0.29

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	733/765 (96%)	651 (89%)	46 (6%)	36 (5%)	1	11
1	E	733/765 (96%)	634 (86%)	65 (9%)	34 (5%)	2	12
2	B	192/195 (98%)	176 (92%)	12 (6%)	4 (2%)	5	25
2	F	192/195 (98%)	181 (94%)	7 (4%)	4 (2%)	5	25
3	C	249/253 (98%)	232 (93%)	12 (5%)	5 (2%)	6	25
3	G	249/253 (98%)	220 (88%)	20 (8%)	9 (4%)	2	16
All	All	2348/2426 (97%)	2094 (89%)	162 (7%)	92 (4%)	2	14

5 of 92 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	TRP
1	A	340	ASP
1	A	428	GLU
1	A	429	PRO
1	A	430	TYR

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	610/632 (96%)	489 (80%)	121 (20%)	1	6
1	E	610/632 (96%)	491 (80%)	119 (20%)	1	6
2	B	162/163 (99%)	139 (86%)	23 (14%)	3	14
2	F	162/163 (99%)	142 (88%)	20 (12%)	4	20
3	C	185/187 (99%)	159 (86%)	26 (14%)	3	15
3	G	185/187 (99%)	160 (86%)	25 (14%)	4	16
All	All	1914/1964 (98%)	1580 (82%)	334 (18%)	2	9

5 of 334 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	515	THR
1	E	748	ARG
1	E	554	ASP
1	E	626	SER
2	F	145	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 73 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	647	ASN
3	G	139	ASN
1	E	672	GLN
2	F	169	GLN
2	B	27	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 18 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
4	SF4	F	1195	2	0,12,12	-	-	-		
5	MGD	A	1766	6	45,52,52	2.59	18 (40%)	54,81,81	2.83	17 (31%)
4	SF4	B	1194	2	0,12,12	-	-	-		
4	SF4	F	1194	2	0,12,12	-	-	-		
4	SF4	F	1196	2	0,12,12	-	-	-		
5	MGD	E	1766	6	45,52,52	2.73	17 (37%)	54,81,81	2.52	17 (31%)
4	SF4	B	1197	2	0,12,12	-	-	-		
4	SF4	A	1764	1	0,12,12	-	-	-		
4	SF4	F	1197	2	0,12,12	-	-	-		
4	SF4	B	1195	2	0,12,12	-	-	-		
7	MQ7	G	1251	-	16,16,49	0.33	0	21,23,63	1.46	3 (14%)
5	MGD	E	1765	6	45,52,52	2.59	20 (44%)	54,81,81	2.81	18 (33%)
4	SF4	B	1196	2	0,12,12	-	-	-		
5	MGD	A	1765	6	45,52,52	2.56	19 (42%)	54,81,81	2.80	17 (31%)
7	MQ7	C	1252	-	16,16,49	0.28	0	21,23,63	1.43	4 (19%)
4	SF4	E	1764	1	0,12,12	-	-	-		

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
4	SF4	F	1195	2	-	-	0/6/5/5
5	MGD	A	1766	6	-	1/22/66/66	0/6/6/6
4	SF4	B	1194	2	-	-	0/6/5/5
4	SF4	F	1194	2	-	-	0/6/5/5
4	SF4	F	1196	2	-	-	0/6/5/5
4	SF4	E	1764	1	-	-	0/6/5/5
4	SF4	B	1197	2	-	-	0/6/5/5
4	SF4	A	1764	1	-	-	0/6/5/5
4	SF4	F	1197	2	-	-	0/6/5/5
4	SF4	B	1195	2	-	-	0/6/5/5
7	MQ7	G	1251	-	-	0/2/22/61	0/2/2/2
5	MGD	E	1765	6	-	2/22/66/66	0/6/6/6
4	SF4	B	1196	2	-	-	0/6/5/5
5	MGD	A	1765	6	-	6/22/66/66	0/6/6/6
7	MQ7	C	1252	-	-	2/2/22/61	0/2/2/2
5	MGD	E	1766	6	-	1/22/66/66	0/6/6/6

The worst 5 of 74 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1765	MGD	C23-C14	-9.69	1.45	1.53
5	E	1766	MGD	C21-N22	-9.03	1.25	1.35
5	A	1766	MGD	C23-C14	-7.61	1.47	1.53
5	E	1765	MGD	C23-C14	-7.15	1.48	1.53
5	E	1766	MGD	C23-C14	-6.91	1.48	1.53

The worst 5 of 76 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1766	MGD	O11-C23-C14	13.19	117.76	108.96
5	A	1765	MGD	O11-C23-C14	11.86	116.88	108.96
5	E	1766	MGD	O11-C23-C14	9.67	115.42	108.96
5	E	1765	MGD	O11-C23-N22	-9.22	99.10	108.57
5	E	1765	MGD	O11-C23-C14	-8.05	103.60	108.96

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1765	MGD	C5'-O5'-PB-O2B
7	C	1252	MQ7	C12-C11-C3-C2
7	C	1252	MQ7	C12-C11-C3-C4
5	E	1765	MGD	O4'-C4'-C5'-O5'
5	A	1765	MGD	PA-O3B-PB-O5'

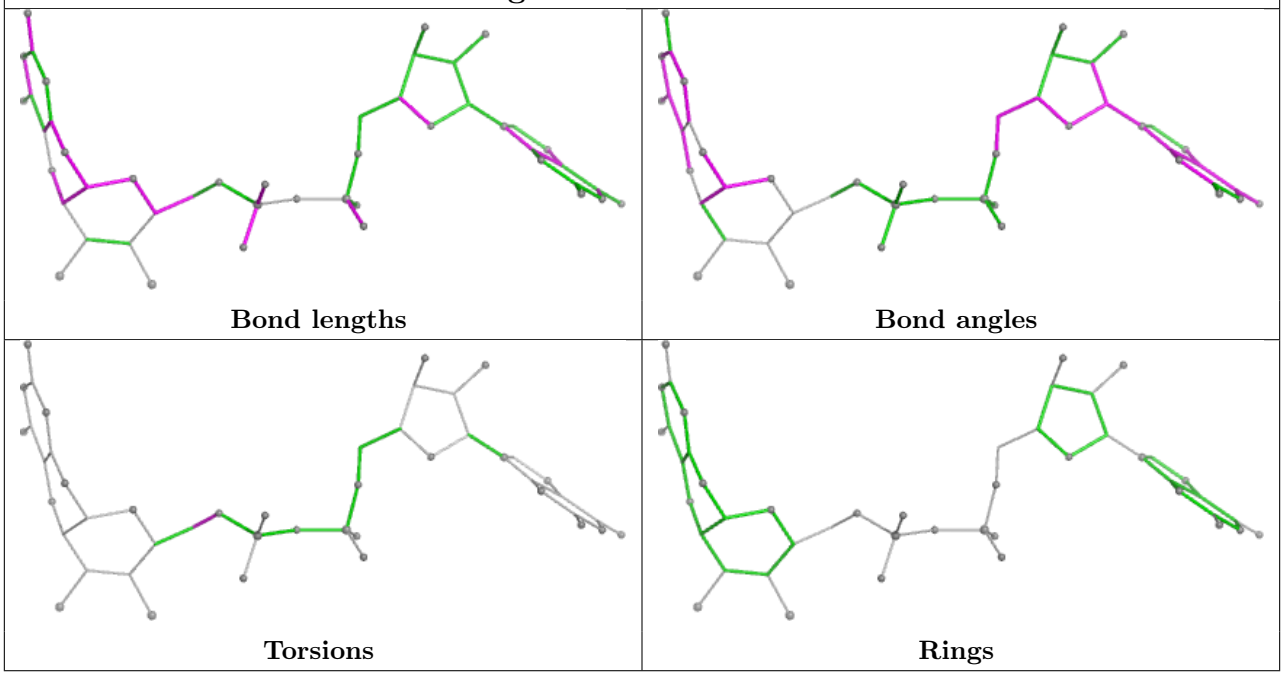
There are no ring outliers.

13 monomers are involved in 82 short contacts:

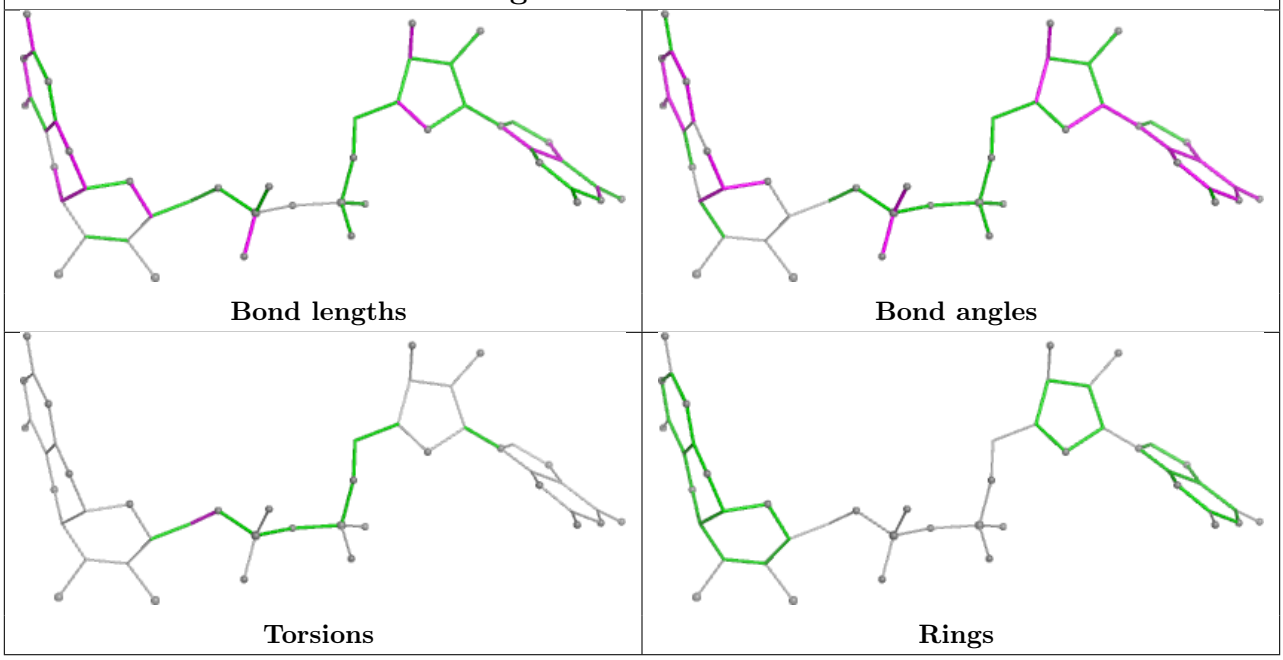
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	1195	SF4	2	0
5	A	1766	MGD	5	0
4	B	1194	SF4	3	0
4	F	1194	SF4	3	0
4	F	1196	SF4	1	0
5	E	1766	MGD	11	0
4	B	1195	SF4	2	0
7	G	1251	MQ7	20	0
5	E	1765	MGD	7	0
4	B	1196	SF4	2	0
5	A	1765	MGD	6	0
7	C	1252	MQ7	19	0
4	E	1764	SF4	1	0

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 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.

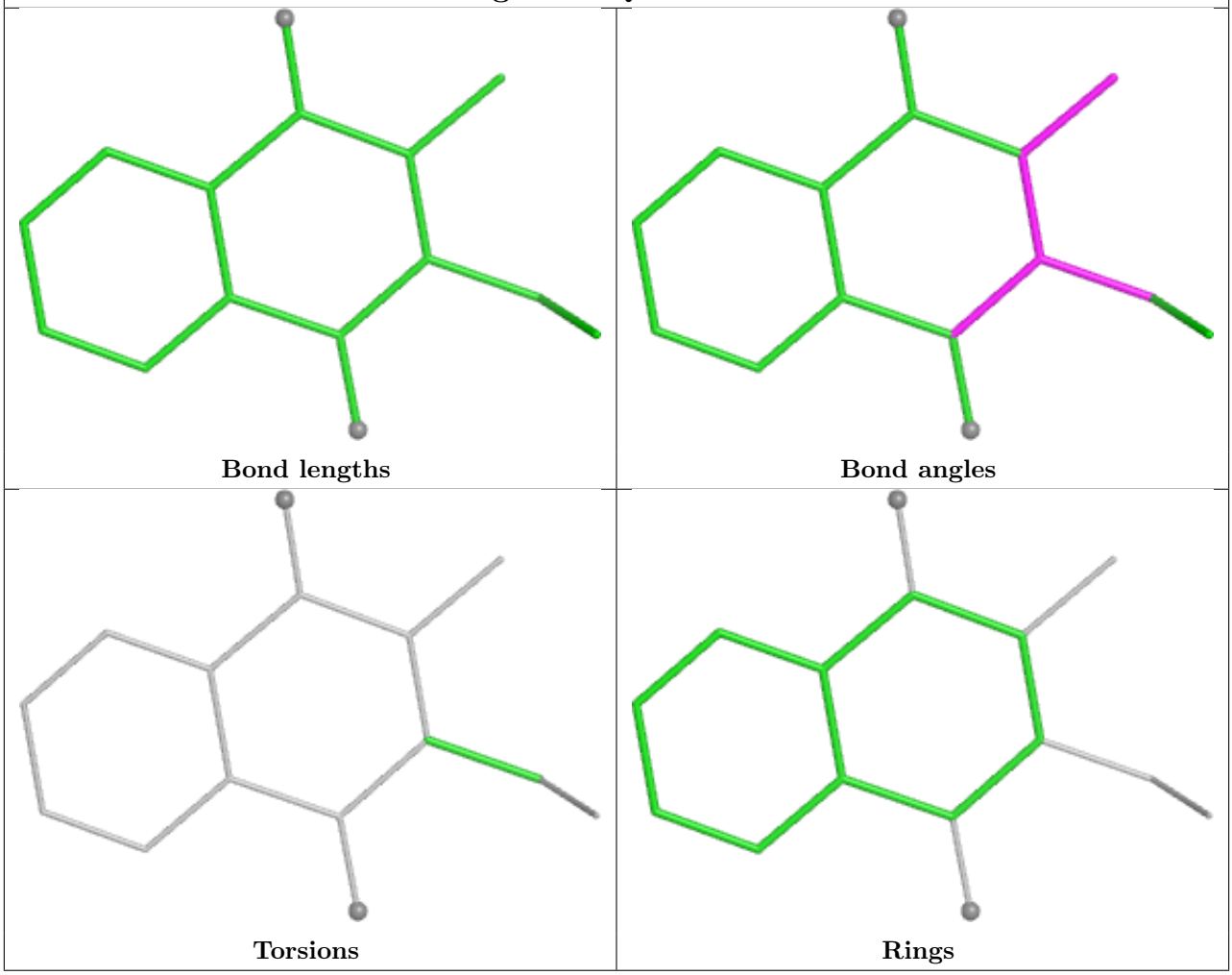
Ligand MGD A 1766



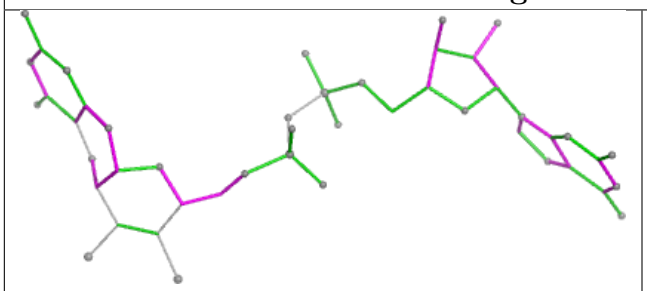
Ligand MGD E 1766



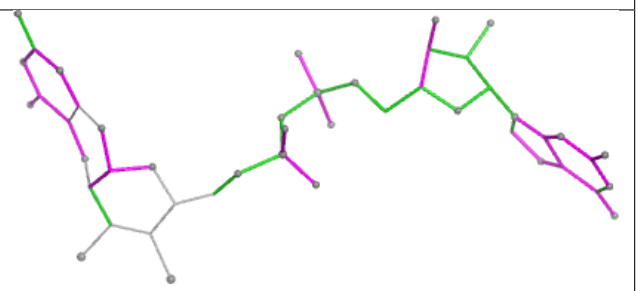
Ligand MQ7 G 1251



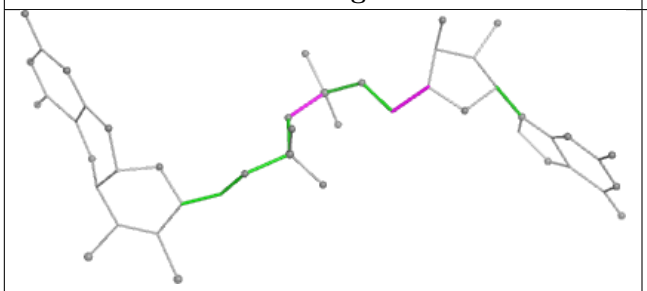
Ligand MGD E 1765



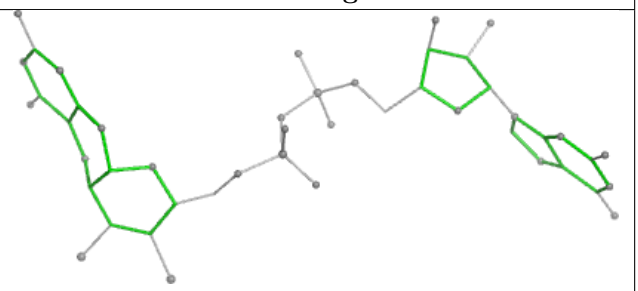
Bond lengths



Bond angles

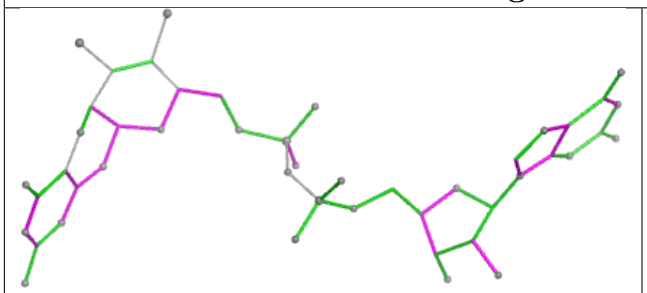


Torsions

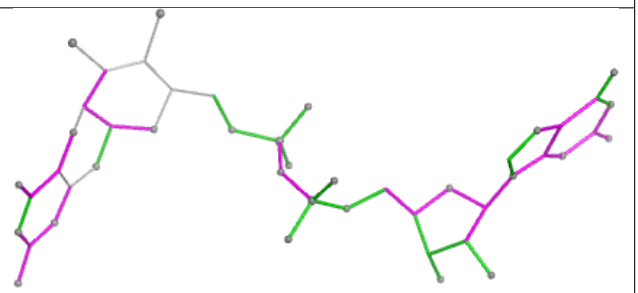


Rings

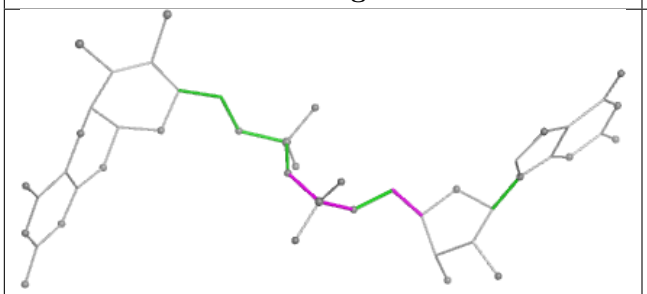
Ligand MGD A 1765



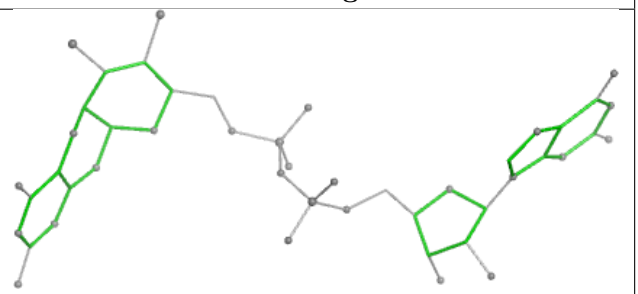
Bond lengths



Bond angles

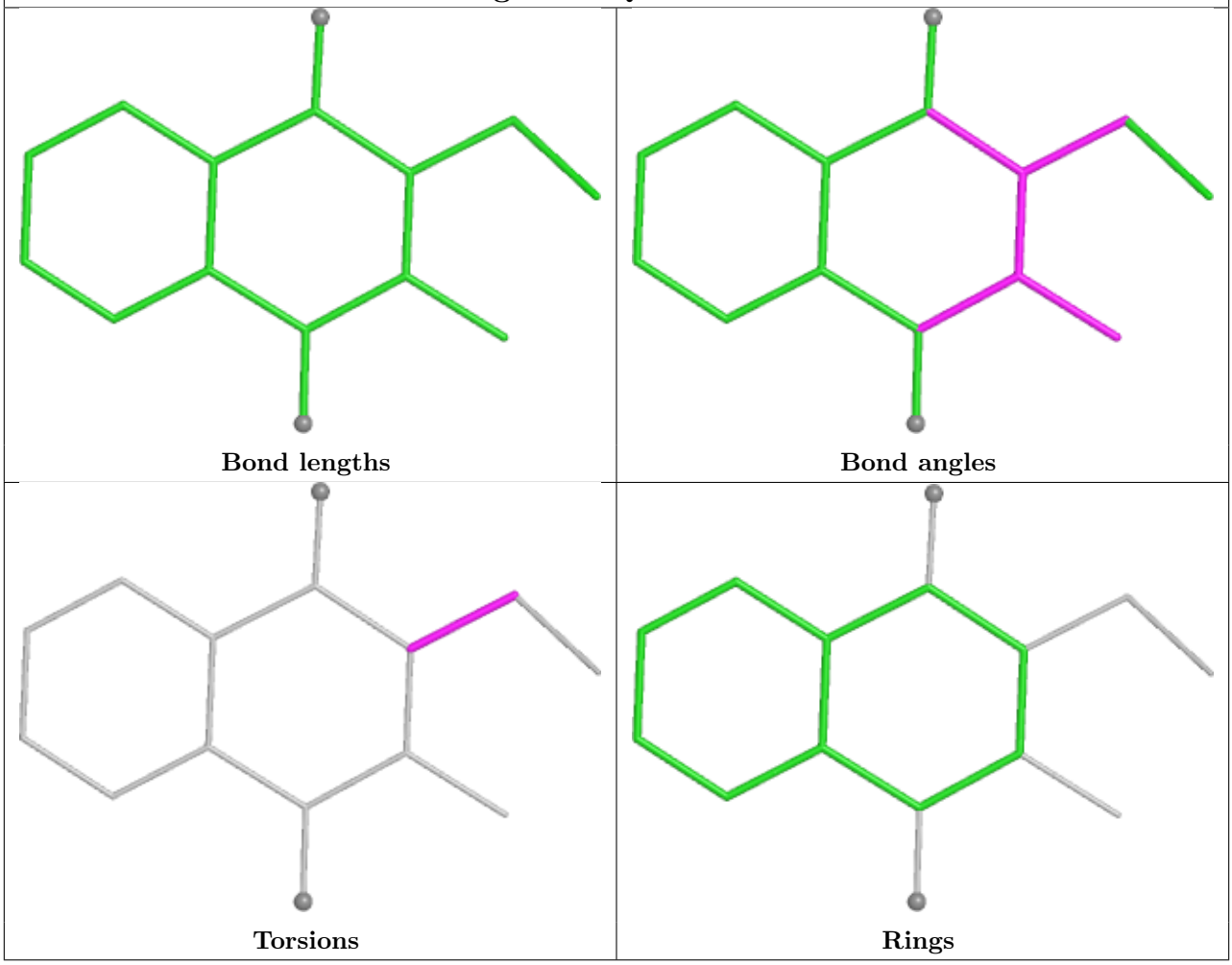


Torsions



Rings

Ligand MQ7 C 1252



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	E	2
1	A	1
3	G	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	583:PHE	C	584:GLY	N	1.71
1	E	323:LYS	C	324:PRO	N	1.66
1	G	109:LYS	C	110:GLY	N	1.05
1	E	387:GLY	C	388:CYS	N	0.66

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	735/765 (96%)	0.96	93 (12%)	8	4	48, 71, 103, 158	0
1	E	735/765 (96%)	0.90	74 (10%)	12	6	46, 70, 101, 161	0
2	B	194/195 (99%)	0.75	15 (7%)	19	10	50, 66, 88, 115	0
2	F	194/195 (99%)	1.08	27 (13%)	6	4	53, 71, 91, 114	0
3	C	251/253 (99%)	1.03	23 (9%)	14	8	55, 78, 105, 123	0
3	G	251/253 (99%)	1.54	71 (28%)	1	1	57, 86, 116, 131	0
All	All	2360/2426 (97%)	1.00	303 (12%)	7	4	46, 72, 105, 161	0

The worst 5 of 303 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	252	GLY	10.1
3	G	251	GLY	9.0
1	E	607	VAL	6.1
1	A	607	VAL	5.9
2	F	194	HIS	5.9

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)

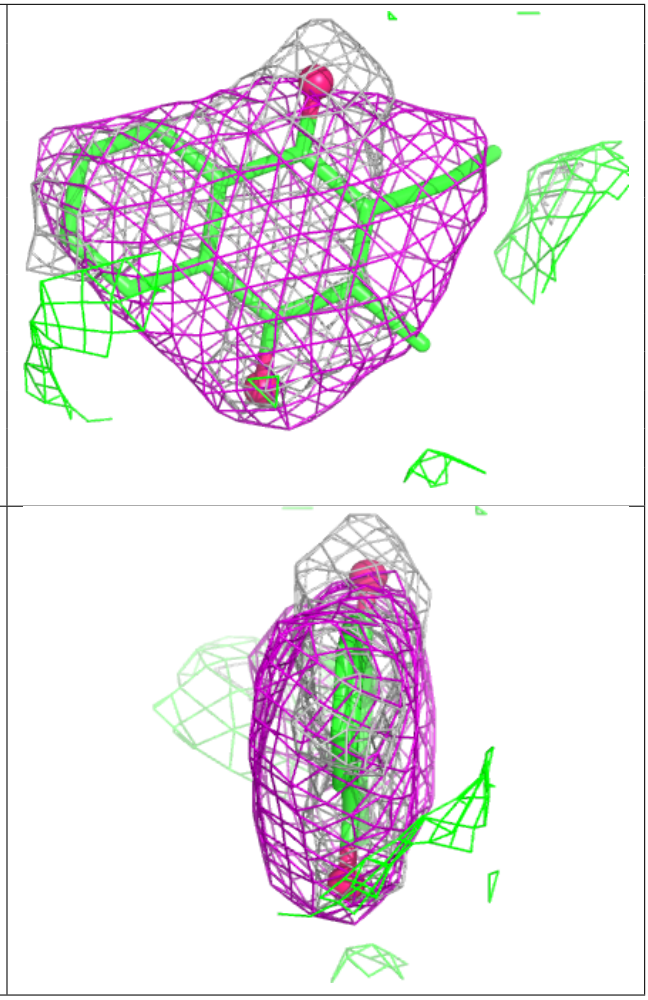
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MQ7	G	1251	15/48	0.74	0.43	27,31,36,42	0
7	MQ7	C	1252	15/48	0.75	0.41	26,27,28,29	0
4	SF4	B	1196	8/8	0.91	0.11	55,59,62,65	0
4	SF4	F	1197	8/8	0.93	0.09	68,72,73,75	0
5	MGD	E	1766	47/47	0.93	0.10	41,46,48,50	0
4	SF4	F	1195	8/8	0.93	0.09	70,71,74,75	0
4	SF4	F	1196	8/8	0.93	0.11	60,65,67,68	0
5	MGD	A	1765	47/47	0.94	0.11	48,52,55,58	0
4	SF4	F	1194	8/8	0.94	0.12	81,83,84,87	0
5	MGD	E	1765	47/47	0.95	0.11	46,53,56,56	0
4	SF4	B	1194	8/8	0.95	0.10	78,79,80,81	0
5	MGD	A	1766	47/47	0.96	0.09	37,46,48,52	0
6	MO	A	1767	1/1	0.98	0.04	54,54,54,54	0
4	SF4	B	1195	8/8	0.98	0.05	65,66,68,68	0
4	SF4	B	1197	8/8	0.98	0.05	57,60,61,63	0
4	SF4	E	1764	8/8	0.99	0.03	45,49,52,52	0
4	SF4	A	1764	8/8	0.99	0.03	44,46,48,49	0
6	MO	E	1767	1/1	1.00	0.03	60,60,60,60	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.

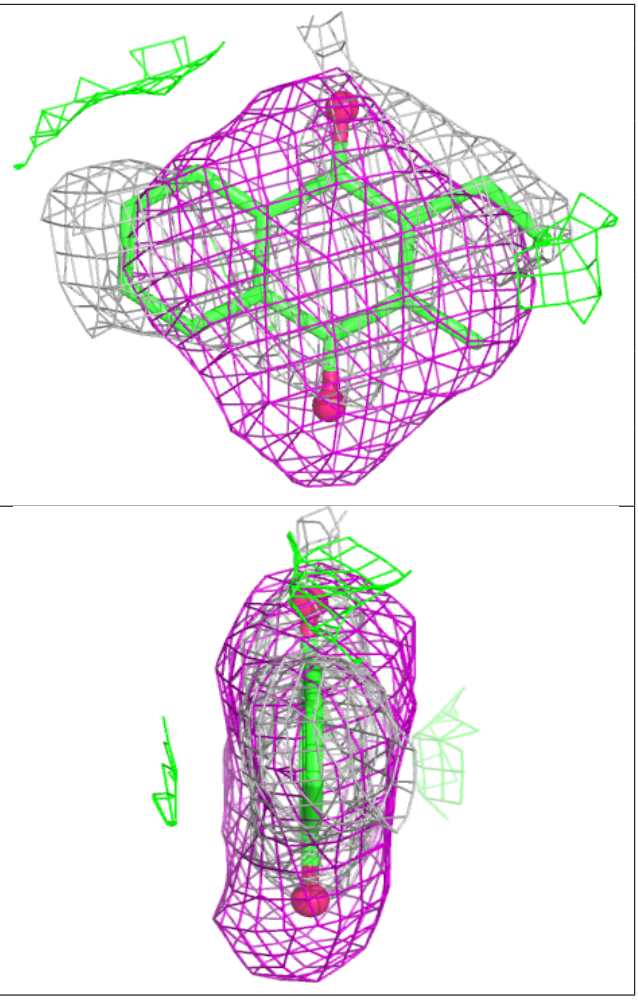
Electron density around MQ7 G 1251:

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



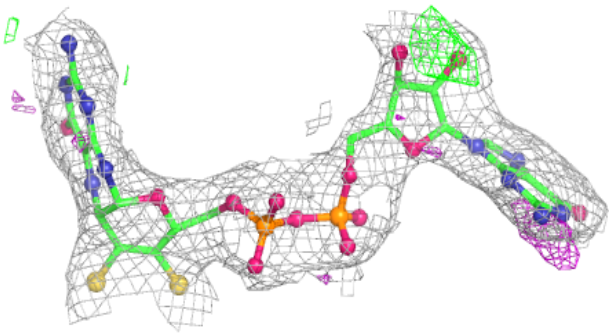
Electron density around MQ7 C 1252:

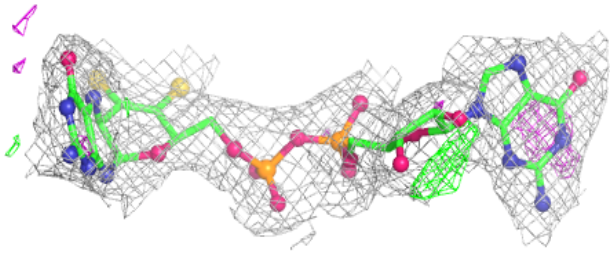
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

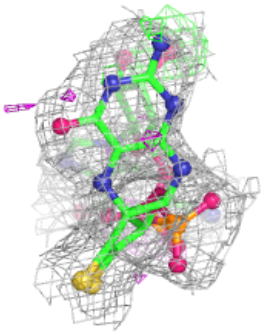


Electron density around MGD E 1766:

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

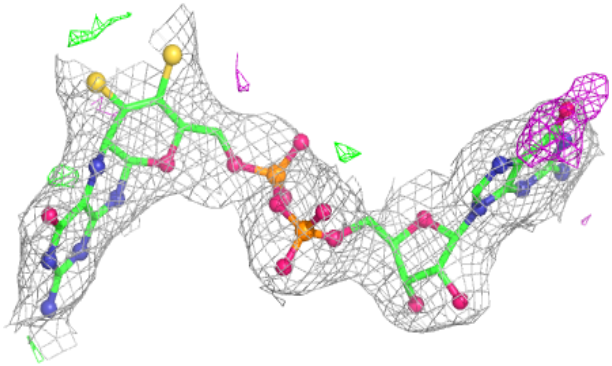


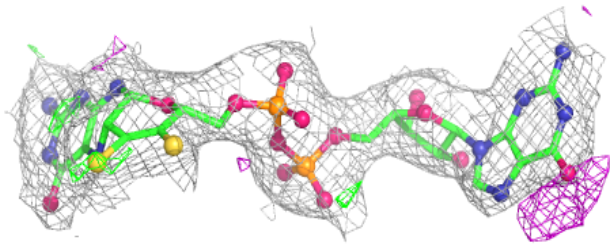


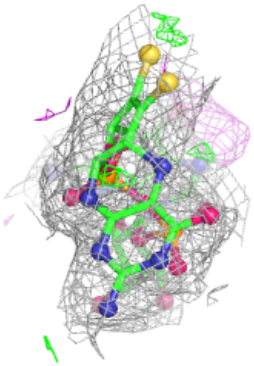


Electron density around MGD A 1765:

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

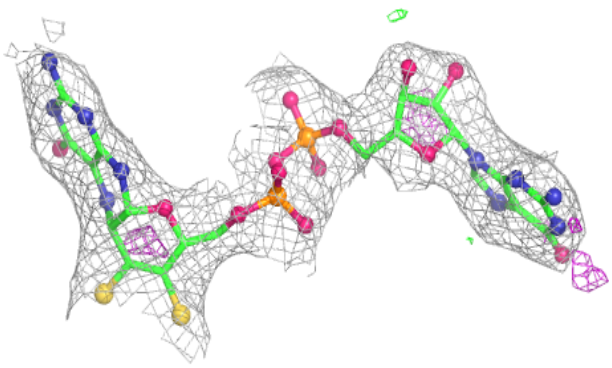


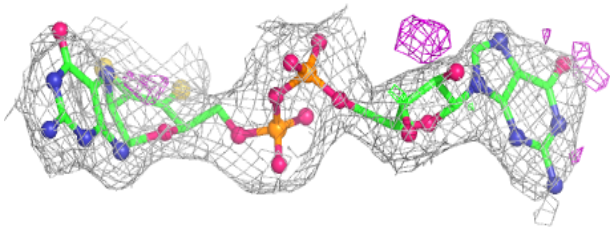


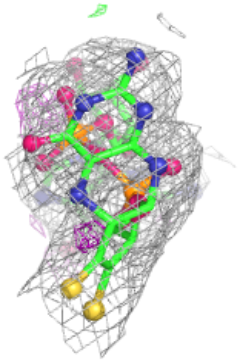


Electron density around MGD E 1765:

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

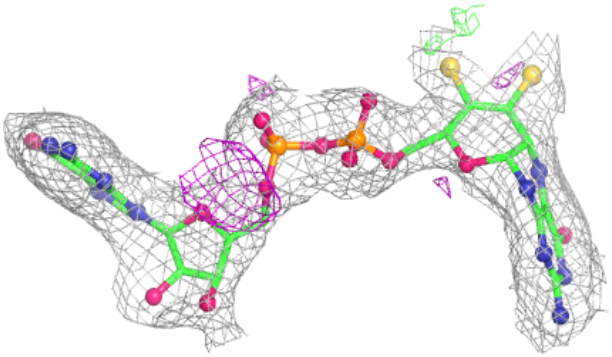


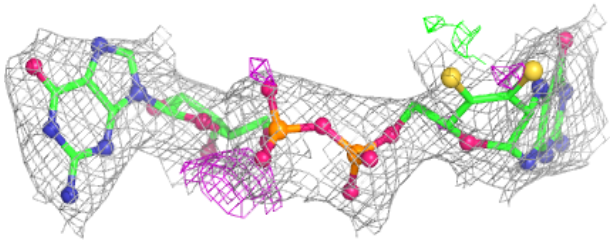


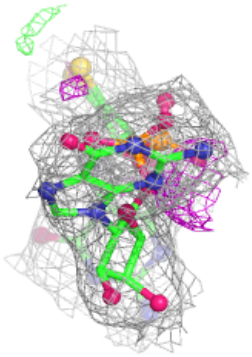


Electron density around MGD A 1766:

$2mF_o$-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.