wwPDB X-ray Structure Validation Summary Report (i)

Aug 24, 2026 – 01:49 am BST

PDB ID	:	2VPZ / pdb_00002vpz
Title	:	Polysulfide reductase native structure
Authors	:	Jormakka, M.; Yokoyama, K.; Yano, T.; Tamakoshi, M.; Akimoto, S.; Shimamura, T.; Curmi, P.; Iwata, S.
Deposited on	:	2008-03-09
Resolution	:	2.40 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:

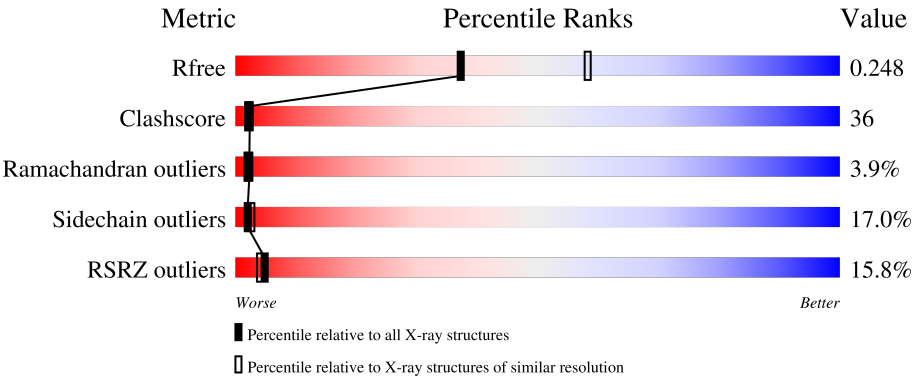
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	18% 41% 34% 16% 6% ·
1	E	765	15% 41% 35% 14% 6% ·
2	B	195	8% 51% 34% 12% · ·
2	F	195	6% 52% 34% 11% · ·
3	C	253	14% 63% 24% 9% · ·

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	253	

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	F	1194	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 20193 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
1	A	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			
1	E	735	Total	C	N	O	S	0	0	1
			5896	3802	1032	1043	19			

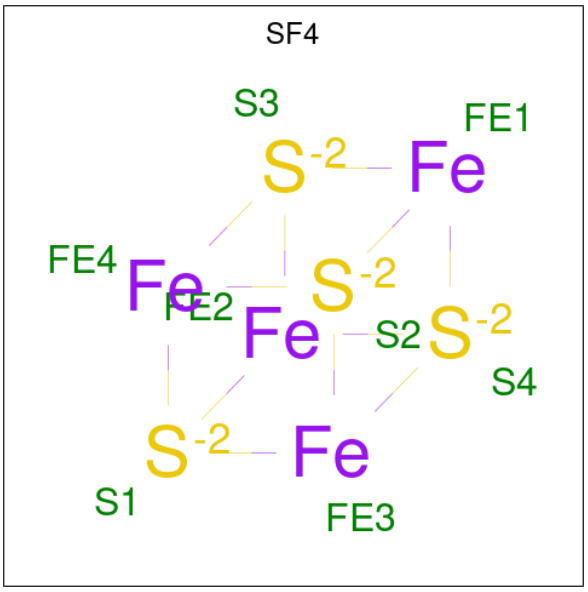
- Molecule 2 is a protein called NRFC PROTEIN.

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

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

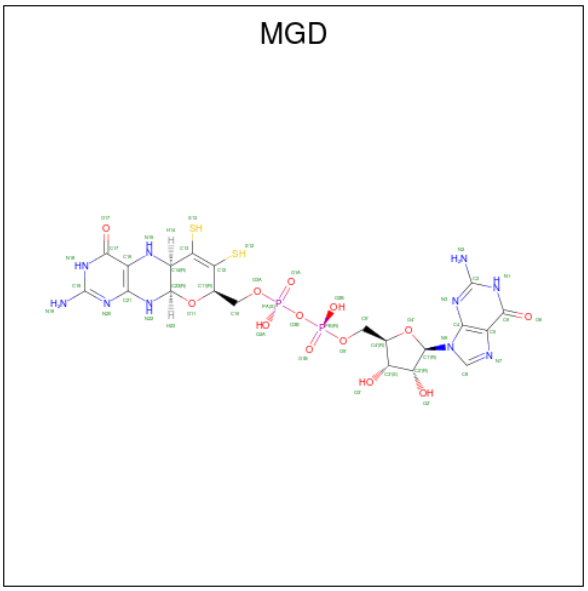
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			
3	G	251	Total	C	N	O	S	0	0	1
			1948	1323	320	303	2			

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0
4	E	1	Total Fe S 8 4 4	0	0
4	F	1	Total Fe S 8 4 4	0	0
4	F	1	Total Fe S 8 4 4	0	0
4	F	1	Total Fe S 8 4 4	0	0
4	F	1	Total Fe S 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
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		
5	E	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	386	Total	O	0	0
			386	386		
7	B	150	Total	O	0	0
			150	150		
7	C	88	Total	O	0	0
			88	88		

Continued on next page...

Continued from previous page...

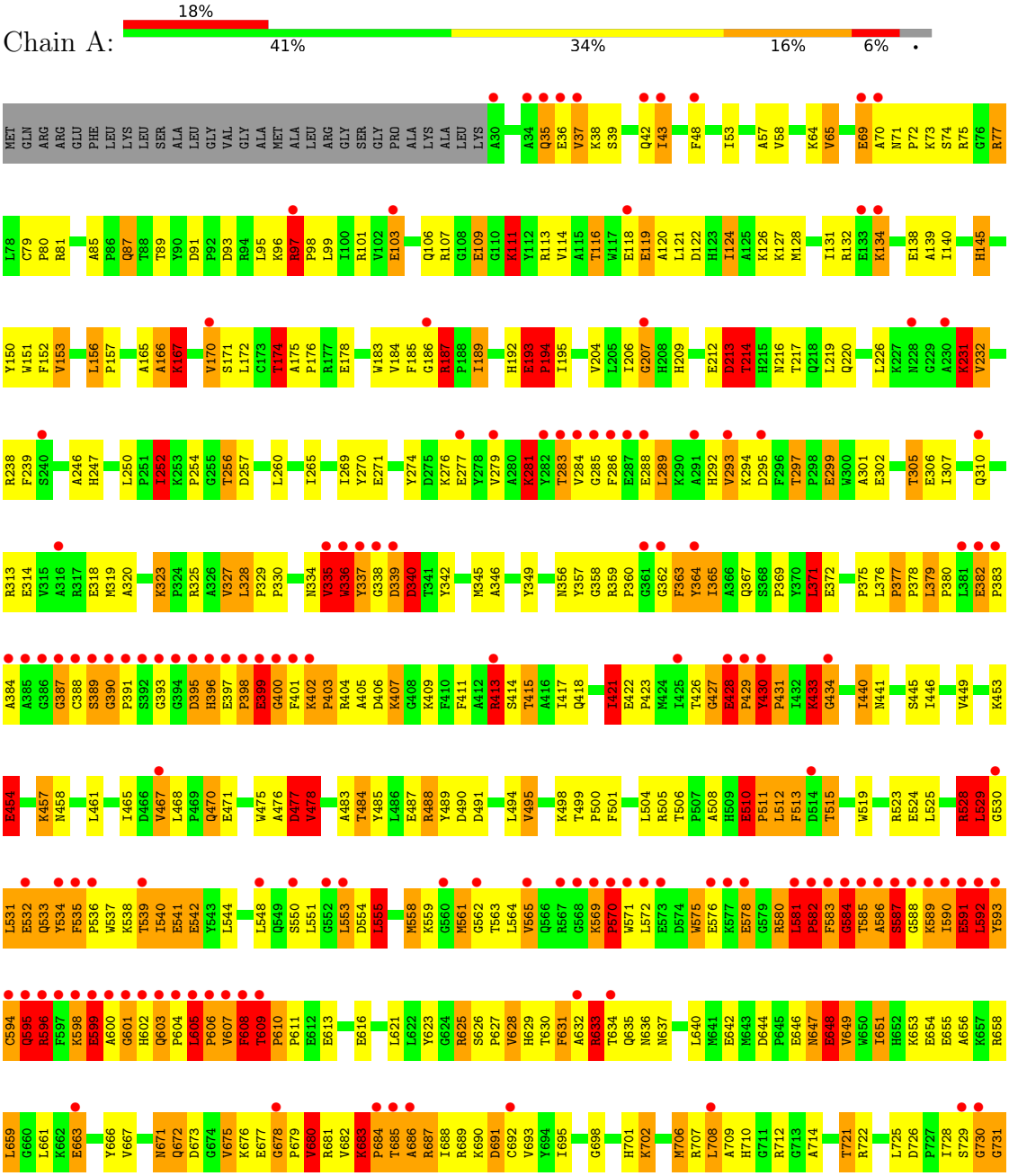
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	452	Total O 452 452	0	0
7	F	130	Total O 130 130	0	0
7	G	79	Total O 79 79	0	0

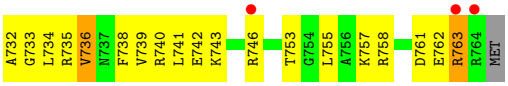
3 Residue-property plots (i)

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:

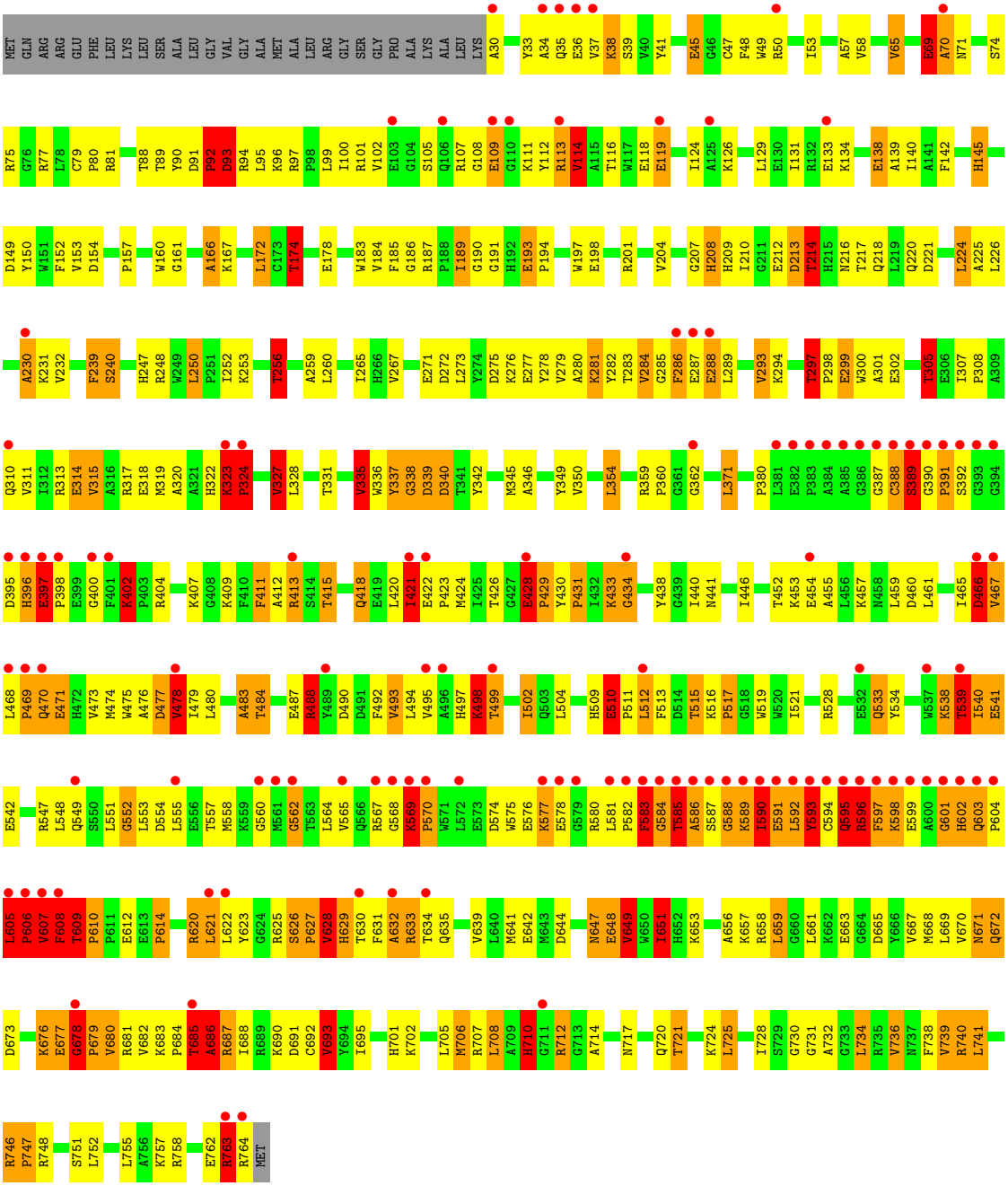




• Molecule 1: THIOSULFATE REDUCTASE

Chain E:

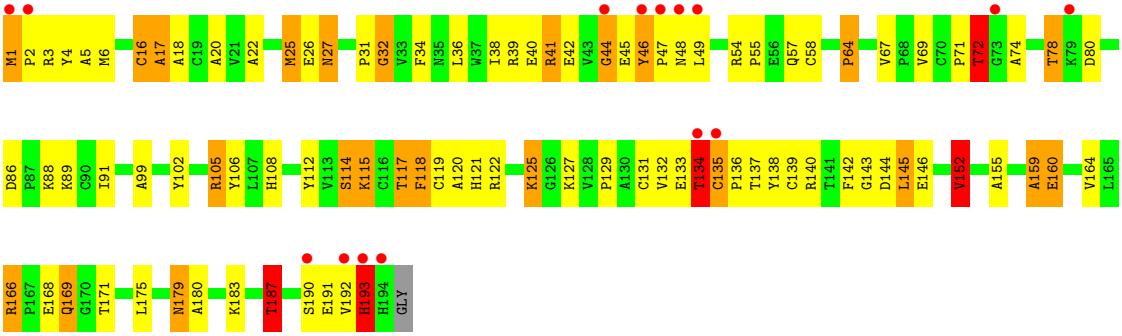




• Molecule 2: NRFC PROTEIN

Chain B:

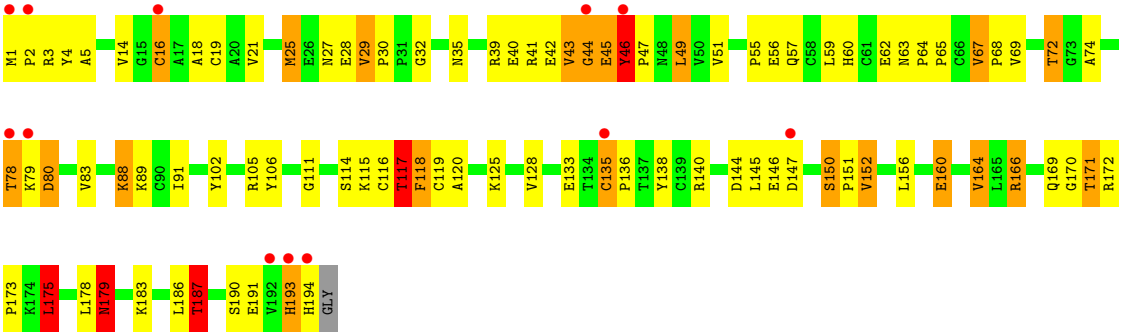




• Molecule 2: NRFC PROTEIN

Chain F:

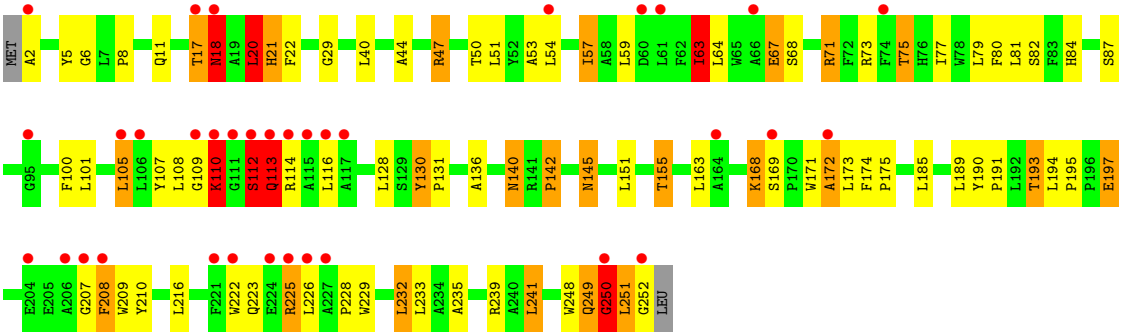




• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN

Chain C:

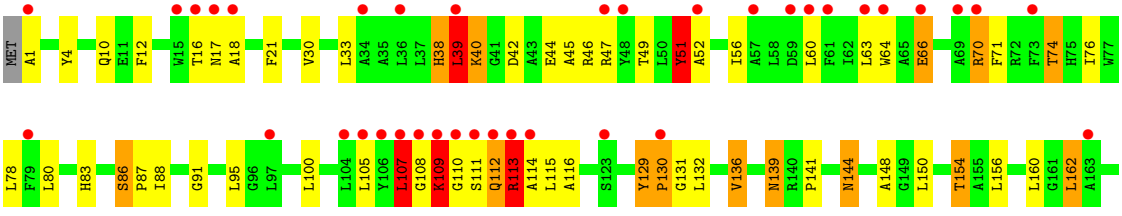


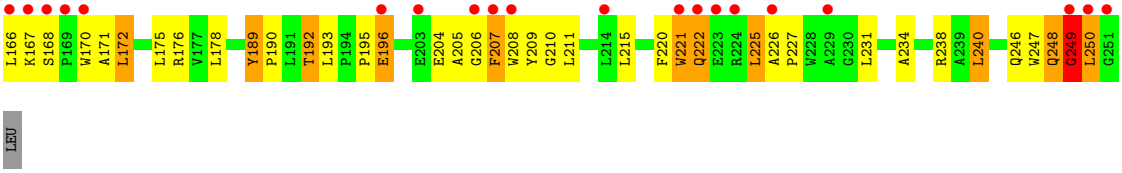


• Molecule 3: HYPOTHETICAL MEMBRANE SPANNING PROTEIN

Chain G:






L166
K167
S168
P169
W170
A171
L172
L175
R176
V177
L178
Y189
P190
L191
T192
L193
P194
P195
E196
E203
E204
A205
G206
F207
W208
Y209
G210
L211
L214
L215
F220
W221
Q222
E223
R224
L225
A226
P227
W228
A229
G230
L231
A234
R238
A239
L240
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	118.41Å 166.26Å 246.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.83 – 2.40 29.83 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.2 (29.83-2.40) 93.2 (29.83-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.24Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.253 0.241 , 0.248	Depositor DCC
R_{free} test set	4206 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å^2)	45.9	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 69.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20193	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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: MO, MGD, 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	1.40	54/6079 (0.9%)	1.65	149/8267 (1.8%)
1	E	1.52	69/6079 (1.1%)	1.83	200/8267 (2.4%)
2	B	1.25	10/1512 (0.7%)	1.69	33/2058 (1.6%)
2	F	1.27	10/1512 (0.7%)	1.79	41/2058 (2.0%)
3	C	1.35	11/2016 (0.5%)	1.40	26/2764 (0.9%)
3	G	1.18	6/2016 (0.3%)	1.56	31/2764 (1.1%)
All	All	1.39	160/19214 (0.8%)	1.69	480/26178 (1.8%)

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	E	0	3

The worst 5 of 160 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	324	PRO	N-CD	17.31	1.72	1.47
1	E	592	LEU	CG-CD1	17.10	2.08	1.52
1	E	323	LYS	C-O	16.69	1.45	1.24
1	E	324	PRO	CA-C	14.88	1.73	1.52
3	C	114	ARG	NE-CZ	14.58	1.49	1.33

The worst 5 of 480 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	171	THR	N-CA-C	23.93	139.58	111.82
1	E	324	PRO	CA-N-CD	-23.05	79.73	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	467	VAL	N-CA-C	18.56	129.85	110.36
2	F	44	GLY	N-CA-C	18.38	138.18	112.81
1	E	323	LYS	O-C-N	-18.18	100.42	121.32

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	323	LYS	Mainchain,Peptide
1	E	428	GLU	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	5814	515	3
1	E	5896	0	5815	459	3
2	B	1475	0	1453	115	0
2	F	1475	0	1454	87	0
3	C	1948	0	2001	92	0
3	G	1948	0	2004	99	0
4	A	8	0	0	0	0
4	B	32	0	0	3	0
4	E	8	0	0	1	0
4	F	32	0	0	3	0
5	A	94	0	44	7	0
5	E	94	0	44	7	0
6	A	1	0	0	0	0
6	E	1	0	0	0	0
7	A	386	0	0	68	0
7	B	150	0	0	35	0
7	C	88	0	0	5	0
7	E	452	0	0	105	0
7	F	130	0	0	20	0
7	G	79	0	0	21	0
All	All	20193	0	18629	1335	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 36.

The worst 5 of 1335 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:E:324:PRO:CD	1:E:324:PRO:CG	1.80	1.60
2:B:135:CYS:SG	2:B:135:CYS:CB	2.02	1.47
1:A:602:HIS:CE1	1:A:606:PRO:HG3	1.52	1.43
1:E:592:LEU:HA	1:E:603:GLN:NE2	1.27	1.41
2:F:135:CYS:CB	2:F:135:CYS:SG	2.10	1.40

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:134:LYS:N[2_674]	1.60	0.60
1:A:399:GLU:OE2	1:E:133:GLU:C[2_674]	1.61	0.59
1:A:399:GLU:OE2	1:E:133:GLU:O[2_674]	2.10	0.10

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 1
1	E	733/765 (96%)	634 (86%)	63 (9%)	36 (5%)	1 1
2	B	192/195 (98%)	176 (92%)	13 (7%)	3 (2%)	7 11
2	F	192/195 (98%)	179 (93%)	9 (5%)	4 (2%)	5 7
3	C	249/253 (98%)	231 (93%)	13 (5%)	5 (2%)	6 7
3	G	249/253 (98%)	220 (88%)	22 (9%)	7 (3%)	4 3
All	All	2348/2426 (97%)	2091 (89%)	166 (7%)	91 (4%)	2 2

5 of 91 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	431	PRO

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%)	490 (80%)	120 (20%)	1 2
1	E	610/632 (96%)	495 (81%)	115 (19%)	1 2
2	B	162/163 (99%)	140 (86%)	22 (14%)	3 5
2	F	162/163 (99%)	143 (88%)	19 (12%)	5 7
3	C	185/187 (99%)	159 (86%)	26 (14%)	3 4
3	G	185/187 (99%)	162 (88%)	23 (12%)	4 6
All	All	1914/1964 (98%)	1589 (83%)	325 (17%)	2 2

5 of 325 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	540	ILE
2	F	78	THR
1	E	577	LYS
1	E	651	ILE
2	F	187	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	717	ASN
2	F	35	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	38	HIS
2	B	48	ASN
2	B	35	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 16 ligands modelled in this entry, 2 are 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	$\#\|Z\| > 2$
5	MGD	A	1766	6	45,52,52	1.83	11 (24%)	54,81,81	2.92	17 (31%)
4	SF4	F	1196	2	0,12,12	-	-	-		
5	MGD	A	1765	6	45,52,52	1.74	7 (15%)	54,81,81	2.86	16 (29%)
4	SF4	E	1764	1	0,12,12	-	-	-		
4	SF4	A	1764	1	0,12,12	-	-	-		
4	SF4	B	1194	2	0,12,12	-	-	-		
4	SF4	F	1194	2	0,12,12	-	-	-		
5	MGD	E	1765	6	45,52,52	1.73	7 (15%)	54,81,81	2.82	18 (33%)
4	SF4	F	1197	2	0,12,12	-	-	-		
4	SF4	B	1195	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SF4	B	1197	2	0,12,12	-	-	-		
4	SF4	B	1196	2	0,12,12	-	-	-		
4	SF4	F	1195	2	0,12,12	-	-	-		
5	MGD	E	1766	6	45,52,52	1.98	10 (22%)	54,81,81	2.63	18 (33%)

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
5	MGD	A	1766	6	-	1/22/66/66	0/6/6/6
4	SF4	F	1196	2	-	-	0/6/5/5
5	MGD	A	1765	6	-	6/22/66/66	0/6/6/6
4	SF4	E	1764	1	-	-	0/6/5/5
4	SF4	B	1194	2	-	-	0/6/5/5
4	SF4	F	1194	2	-	-	0/6/5/5
5	MGD	E	1765	6	-	2/22/66/66	0/6/6/6
4	SF4	F	1197	2	-	-	0/6/5/5
4	SF4	A	1764	1	-	-	0/6/5/5
4	SF4	B	1195	2	-	-	0/6/5/5
4	SF4	B	1197	2	-	-	0/6/5/5
4	SF4	B	1196	2	-	-	0/6/5/5
4	SF4	F	1195	2	-	-	0/6/5/5
5	MGD	E	1766	6	-	1/22/66/66	0/6/6/6

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1765	MGD	C16-C21	6.61	1.49	1.38
5	E	1766	MGD	C21-N22	-5.84	1.29	1.35
5	E	1766	MGD	C16-C21	5.49	1.48	1.38
5	A	1765	MGD	C16-C21	5.45	1.47	1.38
5	A	1766	MGD	C16-C21	5.05	1.47	1.38

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1766	MGD	O11-C23-C14	14.07	118.35	108.96
5	A	1765	MGD	O11-C23-C14	12.57	117.35	108.96
5	E	1766	MGD	O11-C23-C14	10.62	116.05	108.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	1765	MGD	O11-C23-N22	-9.81	98.49	108.57
5	E	1766	MGD	C5-C4-N3	-7.08	116.97	128.46

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1765	MGD	C5'-O5'-PB-O2B
5	E	1765	MGD	O4'-C4'-C5'-O5'
5	A	1765	MGD	PA-O3B-PB-O5'
5	E	1765	MGD	PA-O3B-PB-O5'
5	A	1766	MGD	C11-C10-O3A-PA

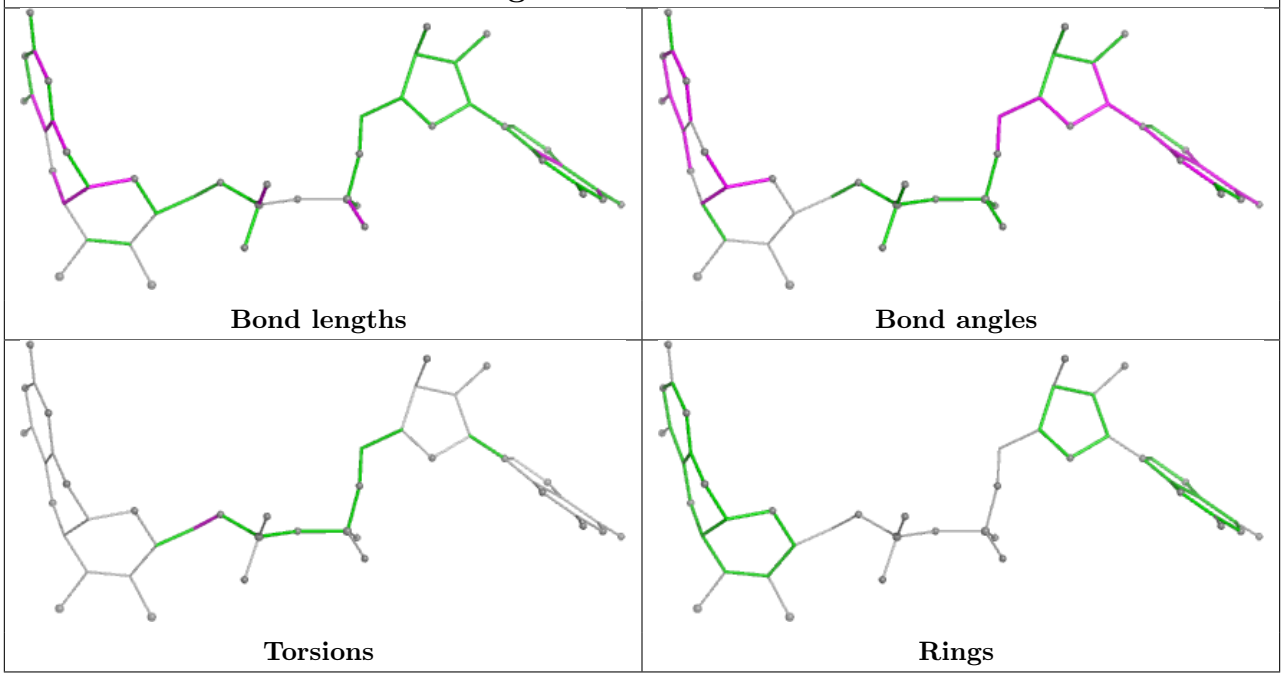
There are no ring outliers.

10 monomers are involved in 21 short contacts:

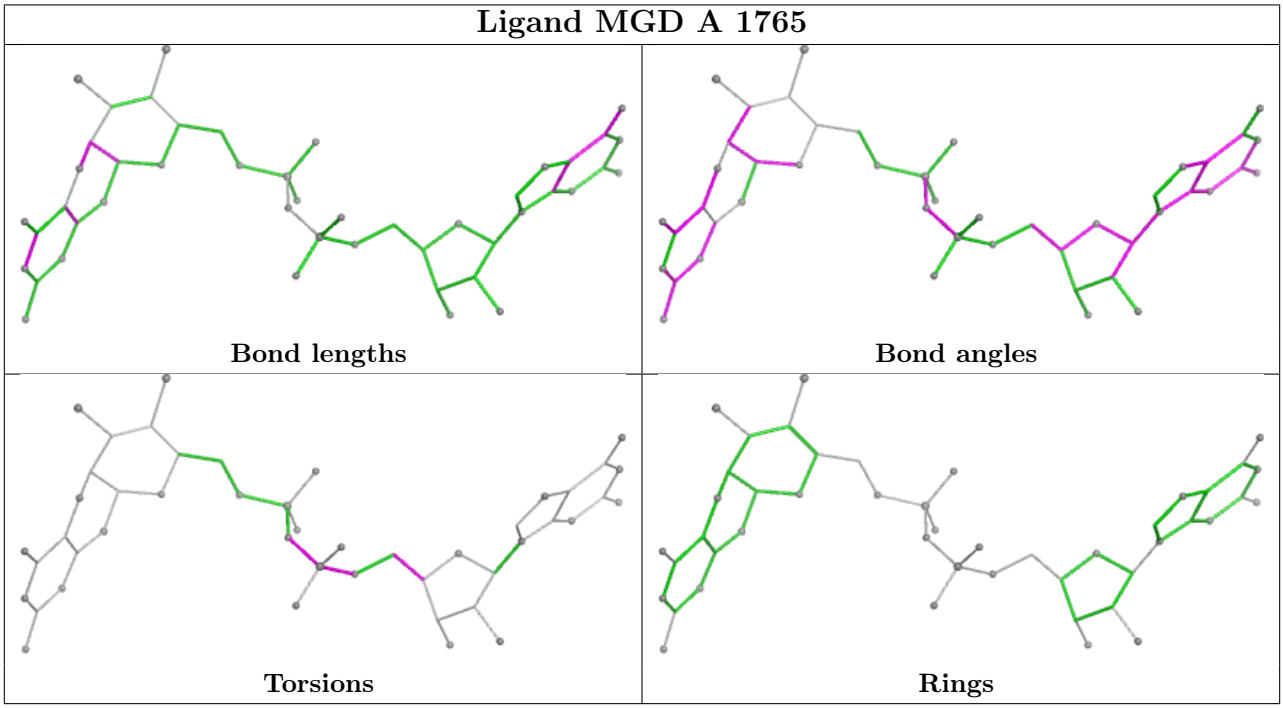
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1766	MGD	3	0
4	F	1196	SF4	1	0
5	A	1765	MGD	4	0
4	E	1764	SF4	1	0
4	B	1194	SF4	1	0
4	F	1194	SF4	2	0
5	E	1765	MGD	4	0
4	B	1195	SF4	1	0
4	B	1196	SF4	1	0
5	E	1766	MGD	3	0

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.

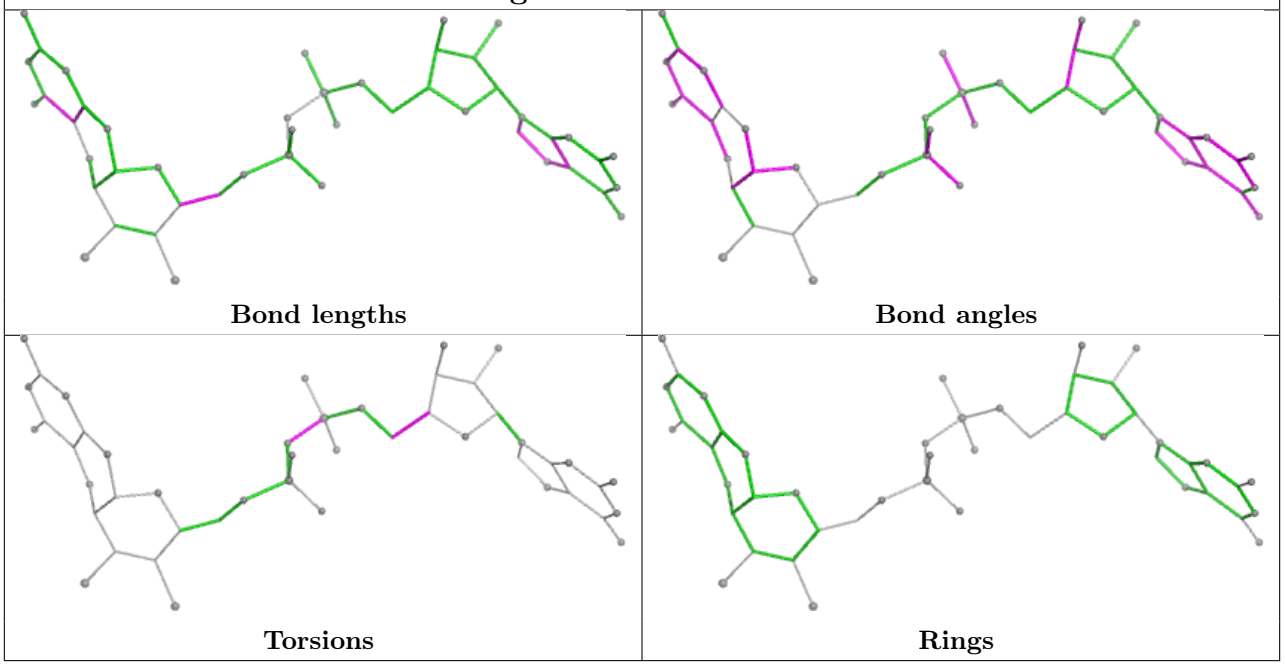
Ligand MGD A 1766



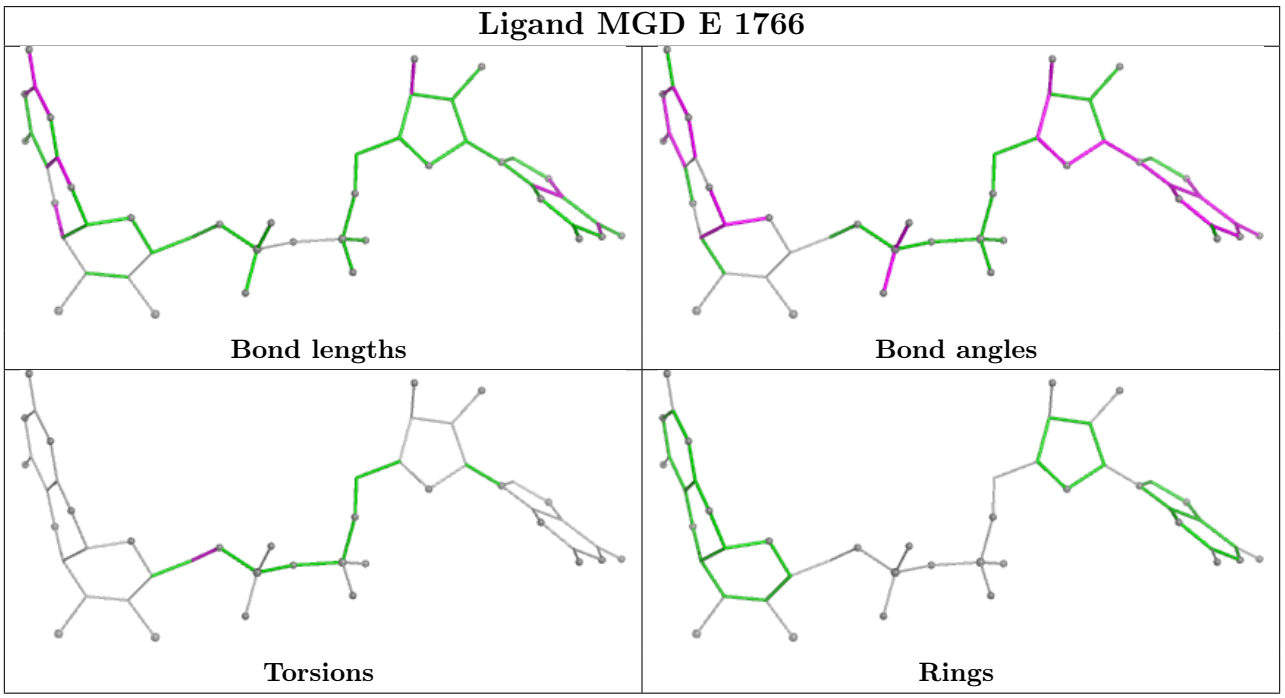
Ligand MGD A 1765



Ligand MGD E 1765



Ligand MGD E 1766



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	735/765 (96%)	1.05	139 (18%) 3 2	25, 48, 80, 134	0
1	E	735/765 (96%)	1.01	115 (15%) 5 4	25, 46, 78, 136	0
2	B	194/195 (99%)	0.57	15 (7%) 19 16	29, 42, 63, 90	0
2	F	194/195 (99%)	0.59	12 (6%) 26 23	31, 46, 67, 90	0
3	C	251/253 (99%)	1.12	35 (13%) 6 5	32, 54, 81, 99	0
3	G	251/253 (99%)	1.34	57 (22%) 2 2	34, 62, 91, 107	0
All	All	2360/2426 (97%)	1.00	373 (15%) 5 4	25, 48, 80, 136	0

The worst 5 of 373 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	251	GLY	17.6
1	A	583	PHE	13.2
1	E	592	LEU	10.7
1	E	607	VAL	10.4
1	A	586	ALA	10.2

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 (i)

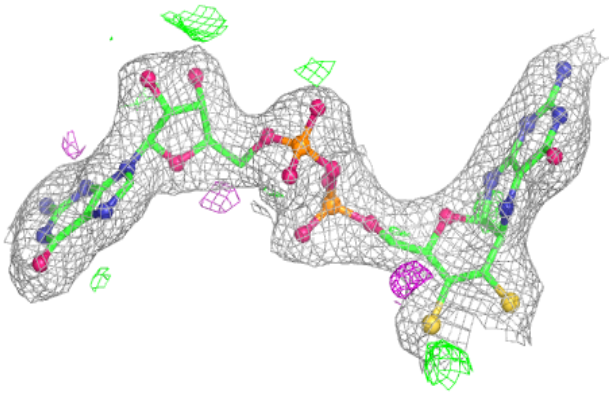
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

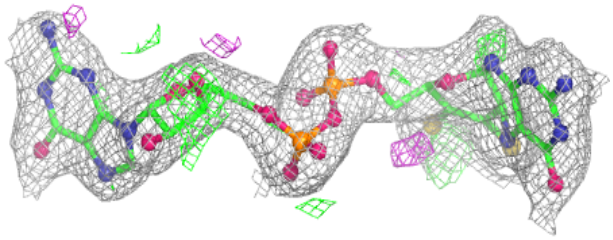
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SF4	F	1194	8/8	0.87	0.16	59,63,70,71	0
4	SF4	B	1196	8/8	0.89	0.17	43,45,50,51	0
4	SF4	B	1194	8/8	0.90	0.15	49,52,53,54	0
4	SF4	B	1195	8/8	0.93	0.11	46,48,52,55	0
4	SF4	F	1196	8/8	0.96	0.08	40,42,43,43	0
4	SF4	B	1197	8/8	0.97	0.07	36,39,43,43	0
4	SF4	F	1195	8/8	0.97	0.07	42,43,43,44	0
4	SF4	E	1764	8/8	0.97	0.08	33,38,40,42	0
5	MGD	E	1765	47/47	0.97	0.07	31,38,40,41	0
5	MGD	E	1766	47/47	0.97	0.08	25,32,36,39	0
5	MGD	A	1765	47/47	0.98	0.07	28,39,42,45	0
5	MGD	A	1766	47/47	0.98	0.07	23,33,40,40	0
4	SF4	A	1764	8/8	0.98	0.07	32,37,40,41	0
4	SF4	F	1197	8/8	0.98	0.06	44,46,48,49	0
6	MO	A	1767	1/1	0.99	0.04	35,35,35,35	0
6	MO	E	1767	1/1	0.99	0.03	31,31,31,31	0

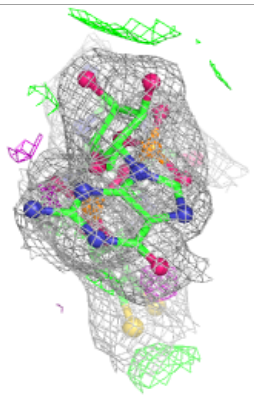
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

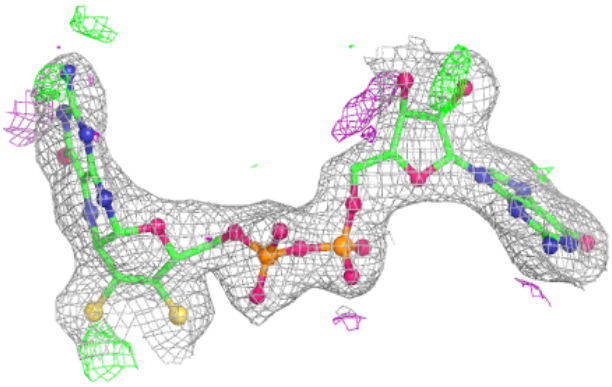


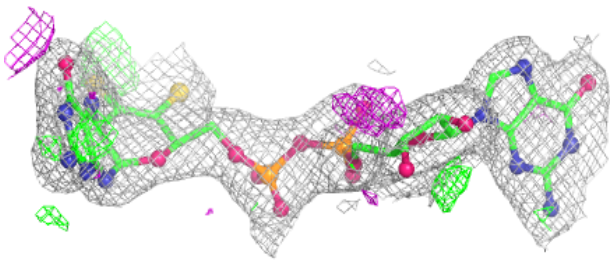


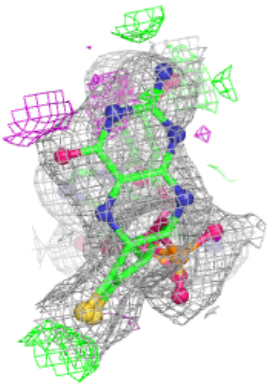


Electron density around MGD E 1766:

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

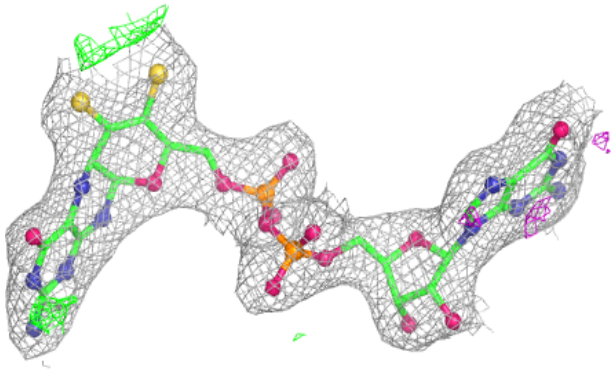


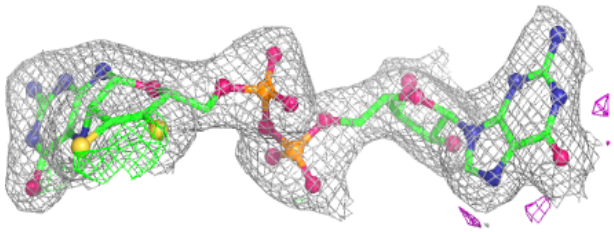


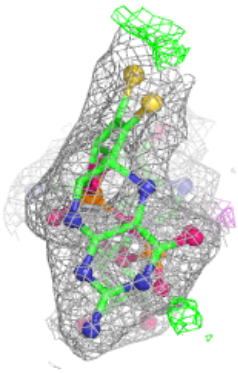


Electron density around MGD A 1765:

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

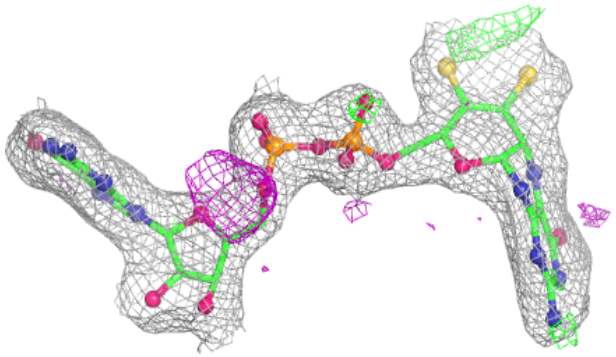


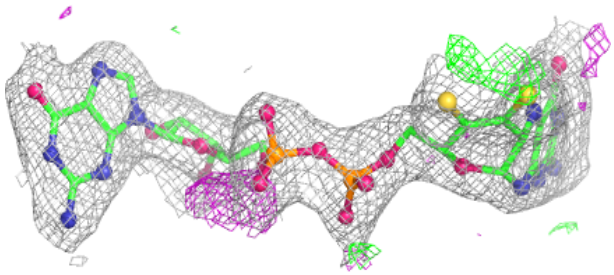


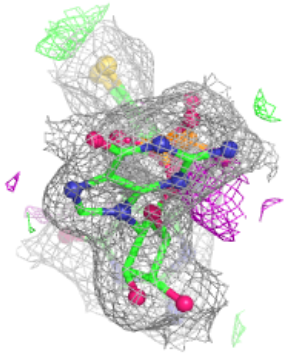


Electron density around MGD A 1766:

$2mF_o$-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.