wwPDB X-ray Structure Validation Summary Report (i)

Oct 26, 2023 – 10:28 PM EDT

PDB ID	:	3Q9T
Title	:	Crystal structure analysis of formate oxidase
Authors	:	Doubayashi, D.; Ootake, T.; Maeda, Y.; Oki, M.; Tokunaga, Y.; Sakurai, A.; Nagaosa, Y.; Mikami, B.; Uchida, H.
Deposited on	:	2011-01-09
Resolution	:	2.24 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:

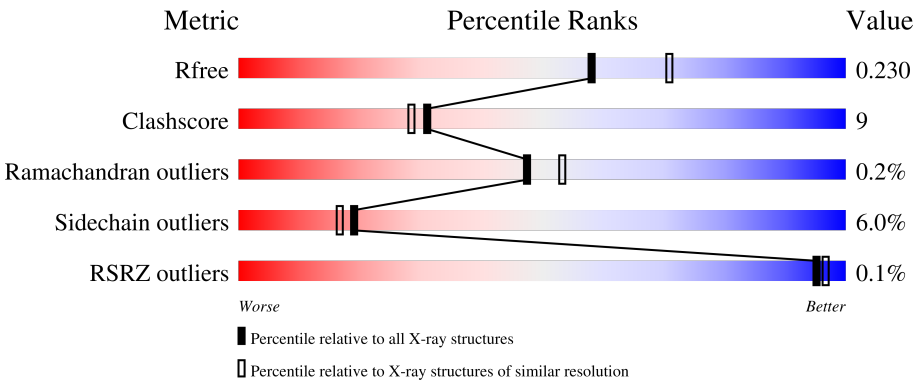
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.24 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	577	82% 16% ·
1	B	577	80% 17% ·
1	C	577	80% 18% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MRD	A	581	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 14820 atoms, of which 0 are hydrogens and 0 are deuteriums.

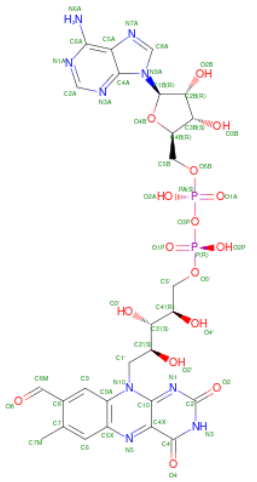
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Choline dehydrogenase and related flavoproteins.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	577	4590	2910	800	860	20	8	9	0
1	B	577	4571	2899	793	858	21	8	7	0
1	C	577	4562	2893	791	858	20	0	5	0

- Molecule 2 is [(2R,3S,4R,5R)-5-(6-amino-9H-purin-9-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methyl (2R,3S,4S)-5-(8-formyl-7-methyl-2,4-dioxo-3,4-dihydrobenzo[g]pteridin-10(2H)-yl)-2,3,4-trihydroxypentyl dihydrogen diphosphate (three-letter code: FAY) (formula: $C_{27}H_{31}N_9O_{16}P_2$).

FAY



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	54	27	9	16	2	0	0
2	B	1	54	27	9	16	2	0	0

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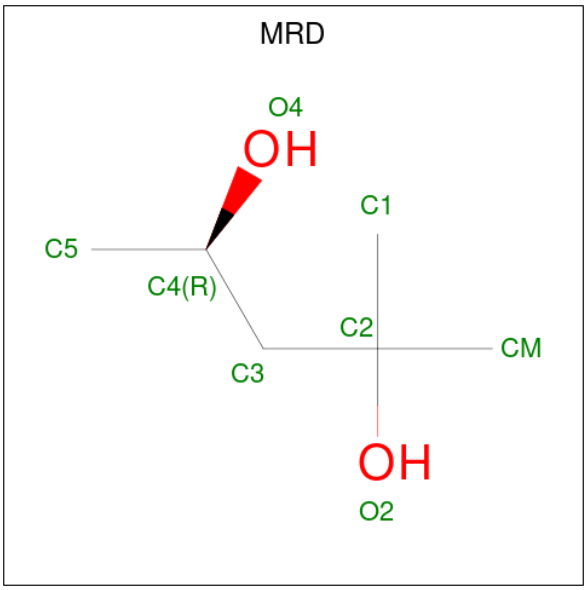
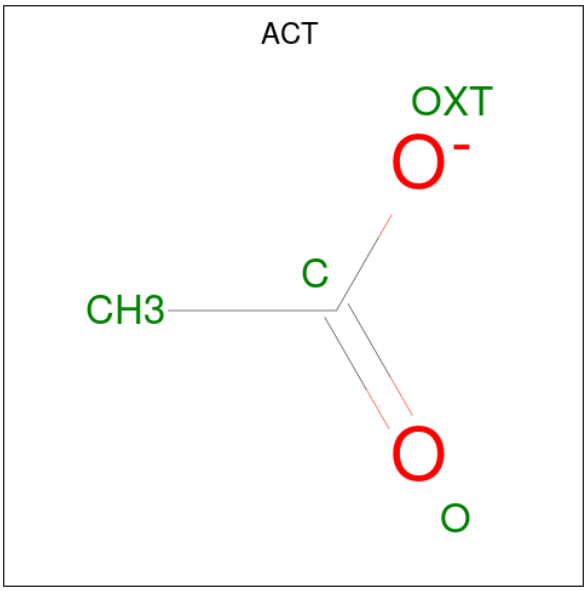
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	54	27	9	16	2	0	0

- Molecule 3 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: $C_6H_{14}O_2$).



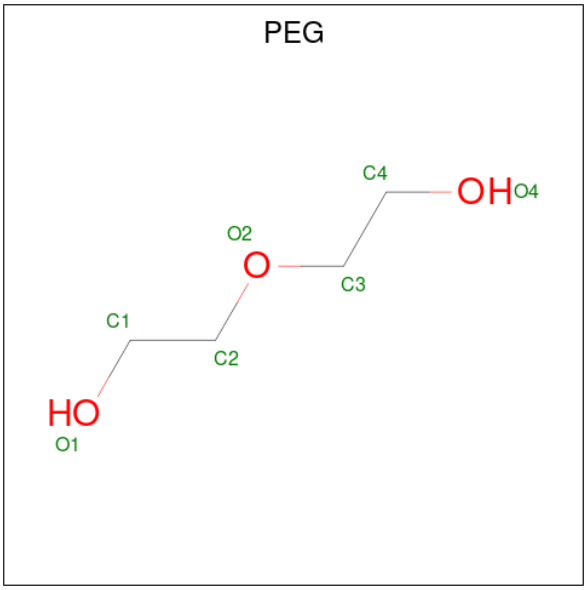
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	8	6	2	0	0
			Total	C	O		
3	A	1	8	6	2	0	0

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



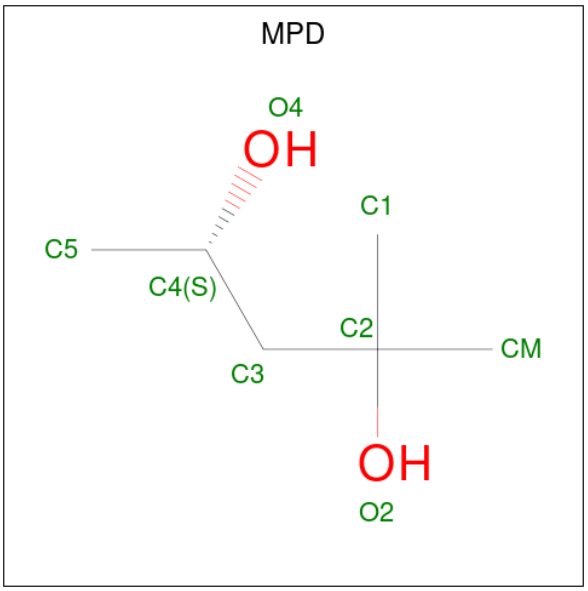
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	4	2	2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	B	1	7	4	3	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	C	1	8	6	2	0	0

- Molecule 7 is water.

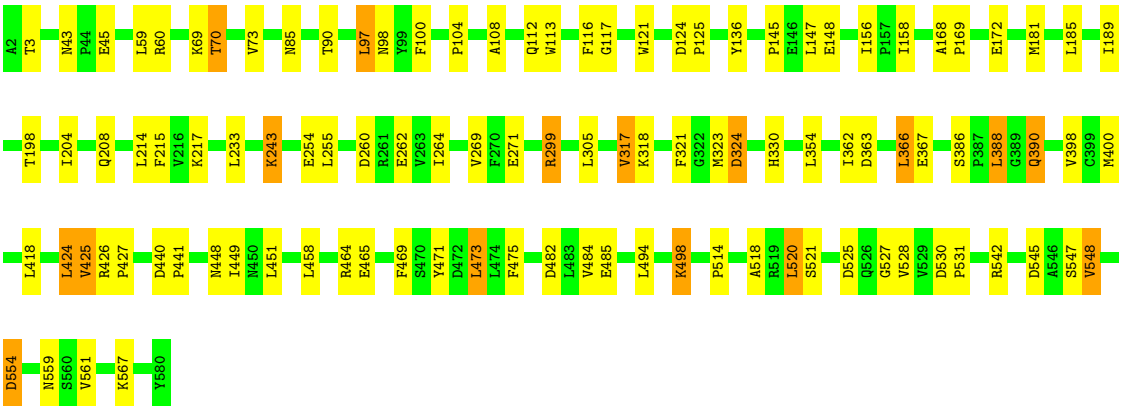
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	406	406	406	0	0
			Total	O		
7	B	265	265	265	0	0
			Total	O		
7	C	229	229	229	0	0

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.

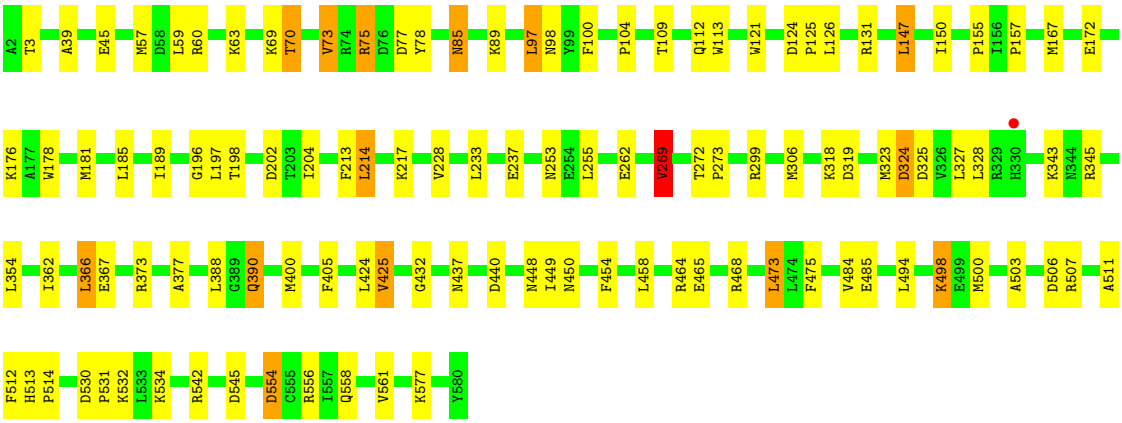
• Molecule 1: Choline dehydrogenase and related flavoproteins

Chain A: 82% 16% •



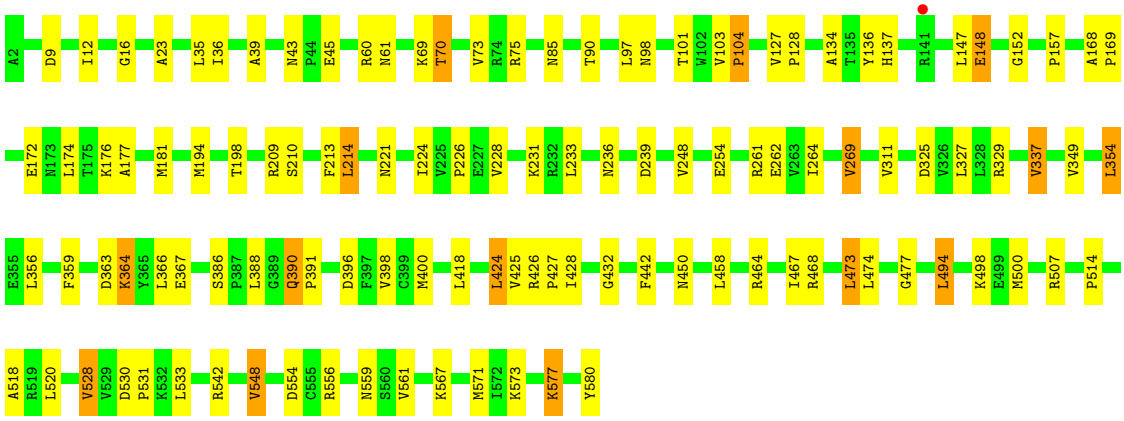
• Molecule 1: Choline dehydrogenase and related flavoproteins

Chain B: 80% 17% •



• Molecule 1: Choline dehydrogenase and related flavoproteins

Chain C: 80% 18% •


A2
D9
I12
G16
A23
L35
I36
A39
N43
P44
E45
R60
N61
K69
T70
V73
R74
R75
N85
T90
L97
N98
T101
W102
V103
P104
V127
P128
A134
T135
Y136
H137
R141
L147
E148
G152
P157
A168
P169
E172
N173
L174
T175
K176
A177
M181
M194
T198
R209
S210
F213
L214
N221
I224
V225
P226
E227
V228
K231
R232
L233
N236
D239
V248
E254
R261
E262
V263
I264
V269
V311
D325
V326
L327
L328
R329
V337
V349
L354
E355
L356
F359
D363
K364
Y365
L366
E367
S386
P387
L388
G389
Q390
P391
D396
F397
V398
C399
M400
L418
L424
V425
R426
P427
I428
G432
F442
N450
L458
R464
I467
R468
L473
L474
G477
L494
K498
E499
M500
R507
P514
A518
R519
L520
V528
V529
D530
P531
K532
L533
R542
V548
D554
C555
R556
N559
S560
V561
K567
M571
I572
K573
K577
Y580

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	156.68Å 156.02Å 184.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.52 – 2.24 49.53 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.52-2.24) 98.4 (49.53-2.24)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.26 (at 2.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.184 , 0.236 0.179 , 0.230	Depositor DCC
R_{free} test set	5334 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 39.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.016 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14820	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: PEG, FAY, ACT, MPD, MRD

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	0.41	0/4724	0.61	1/6405 (0.0%)
1	B	0.37	0/4702	0.56	1/6375 (0.0%)
1	C	0.34	0/4687	0.54	0/6355
All	All	0.38	0/14113	0.57	2/19135 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	269	VAL	CB-CA-C	-6.31	99.41	111.40
1	A	473	LEU	CA-CB-CG	5.67	128.33	115.30

There are no chirality outliers.

There are no planarity outliers.

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	4590	0	4525	84	0
1	B	4571	0	4503	77	0
1	C	4562	0	4488	80	0
2	A	54	0	29	3	0
2	B	54	0	29	7	0
2	C	54	0	29	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	16	0	28	12	0
4	A	4	0	3	1	0
5	B	7	0	10	1	0
6	C	8	0	14	3	0
7	A	406	0	0	11	0
7	B	265	0	0	12	0
7	C	229	0	0	5	0
All	All	14820	0	13658	251	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 9.

The worst 5 of 251 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:325:ASP:HB3	1:C:329:ARG:HH21	1.20	1.00
3:A:581:MRD:H5C3	3:A:581:MRD:H1C2	1.43	0.99
1:A:299[A]:ARG:HB2	1:A:299[A]:ARG:HH11	1.29	0.96
1:B:390[B]:GLN:H	1:B:390[B]:GLN:HE21	1.14	0.95
1:B:327:LEU:HB2	1:B:400:MET:HE3	1.53	0.88

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	584/577 (101%)	560 (96%)	22 (4%)	2 (0%)	41	44
1	B	582/577 (101%)	551 (95%)	30 (5%)	1 (0%)	47	53
1	C	580/577 (100%)	543 (94%)	36 (6%)	1 (0%)	47	53
All	All	1746/1731 (101%)	1654 (95%)	88 (5%)	4 (0%)	47	53

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	THR
1	C	104	PRO
1	B	104	PRO
1	A	104	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	501/492 (102%)	469 (94%)	32 (6%)	17	14
1	B	499/492 (101%)	468 (94%)	31 (6%)	18	15
1	C	497/492 (101%)	463 (93%)	34 (7%)	16	13
All	All	1497/1476 (101%)	1400 (94%)	97 (6%)	19	14

5 of 97 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	458	LEU
1	C	148	GLU
1	B	494	LEU
1	C	75[A]	ARG
1	C	214	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	183	GLN
1	B	253	ASN
1	B	559	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	FAY	A	600	-	54,59,59	1.26	7 (12%)	68,90,90	1.69	11 (16%)
3	MRD	A	581	-	7,7,7	0.30	0	9,10,10	0.79	0
4	ACT	A	1	-	3,3,3	0.83	0	3,3,3	1.54	0
5	PEG	B	1	-	6,6,6	0.59	0	5,5,5	1.04	1 (20%)
3	MRD	A	582	-	7,7,7	0.43	0	9,10,10	0.51	0
6	MPD	C	1	-	7,7,7	0.28	0	9,10,10	0.43	0
2	FAY	B	600	-	54,59,59	1.29	6 (11%)	68,90,90	1.70	15 (22%)
2	FAY	C	600	-	54,59,59	1.21	5 (9%)	68,90,90	1.59	11 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAY	A	600	-	-	9/32/52/52	0/6/6/6
3	MRD	A	581	-	-	2/5/5/5	-
5	PEG	B	1	-	-	1/4/4/4	-
3	MRD	A	582	-	-	2/5/5/5	-
6	MPD	C	1	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAY	B	600	-	-	9/32/52/52	0/6/6/6
2	FAY	C	600	-	-	12/32/52/52	0/6/6/6

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	FAY	C2A-N3A	4.32	1.39	1.32
2	A	600	FAY	C2A-N3A	4.28	1.39	1.32
2	B	600	FAY	C2A-N3A	4.02	1.38	1.32
2	C	600	FAY	C4X-N5	3.91	1.38	1.30
2	B	600	FAY	C4X-N5	3.67	1.37	1.30

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	FAY	N3A-C2A-N1A	-5.25	120.47	128.68
2	C	600	FAY	N3A-C2A-N1A	-5.07	120.75	128.68
2	B	600	FAY	N3A-C2A-N1A	-4.89	121.04	128.68
2	B	600	FAY	C1'-C2'-C3'	4.84	123.31	109.79
2	A	600	FAY	O5'-C5'-C4'	4.63	121.72	109.36

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAY	C5'-O5'-P-O2P
2	A	600	FAY	C1'-C2'-C3'-O3'
2	A	600	FAY	C1'-C2'-C3'-C4'
2	A	600	FAY	O2'-C2'-C3'-O3'
2	A	600	FAY	O2'-C2'-C3'-C4'

There are no ring outliers.

8 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAY	3	0
3	A	581	MRD	10	0
4	A	1	ACT	1	0
5	B	1	PEG	1	0
3	A	582	MRD	2	0

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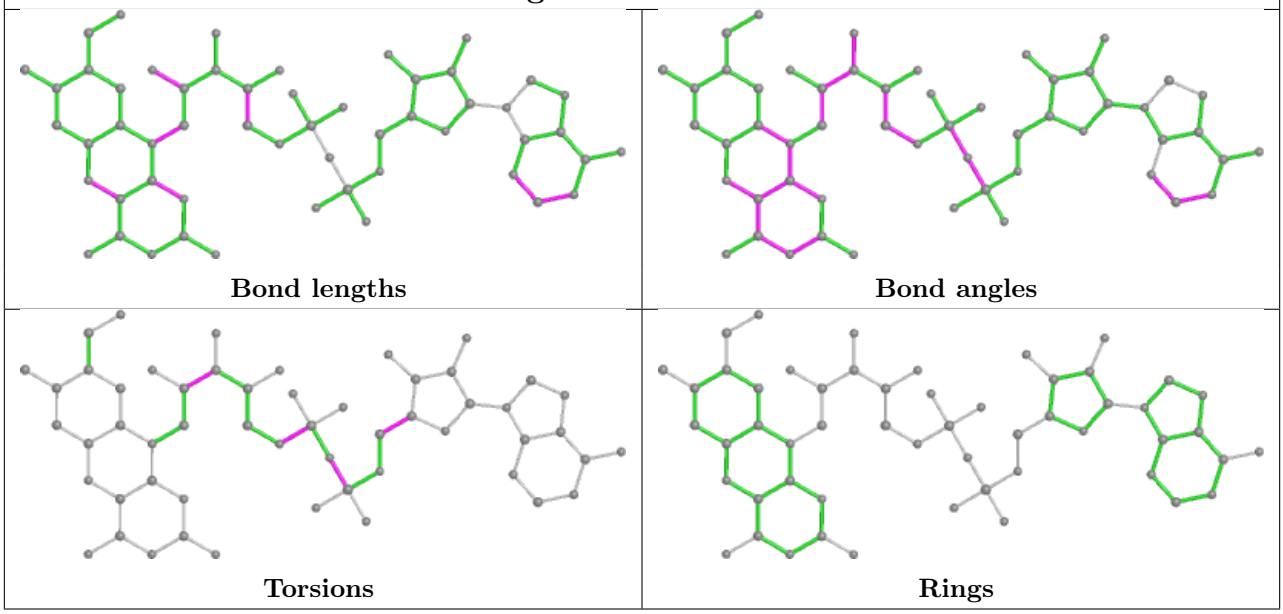
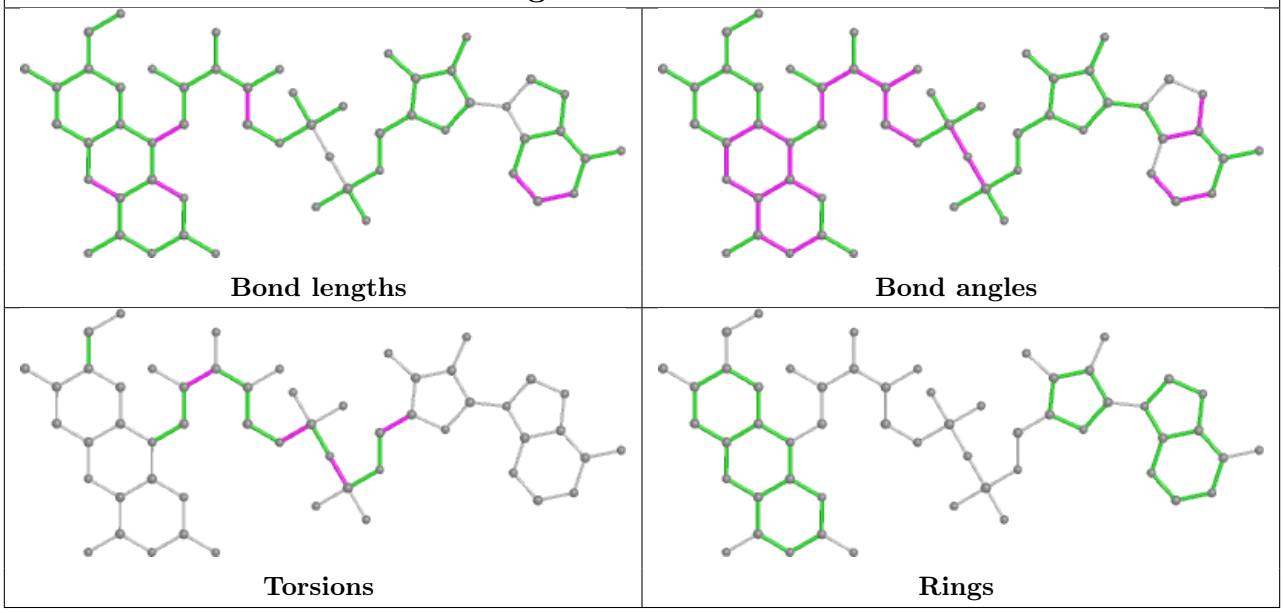
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1	MPD	3	0
2	B	600	FAY	7	0
2	C	600	FAY	5	0

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.

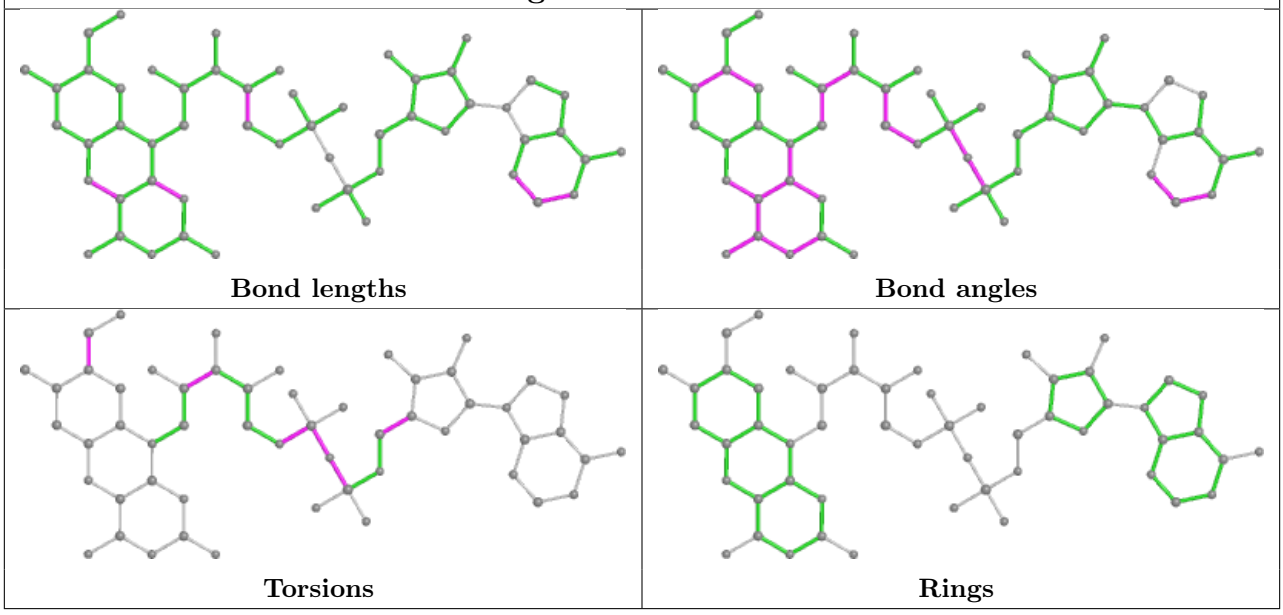
Ligand FAY A 600



Ligand FAY B 600



Ligand FAY C 600



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	577/577 (100%)	-0.73	0	100	100	15, 22, 36, 57	0
1	B	577/577 (100%)	-0.49	1 (0%)	95	96	16, 29, 49, 79	0
1	C	577/577 (100%)	-0.33	1 (0%)	95	96	19, 36, 54, 81	0
All	All	1731/1731 (100%)	-0.52	2 (0%)	95	97	15, 28, 50, 81	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	330	HIS	2.8
1	C	141	ARG	2.5

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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MRD	A	582	8/8	0.72	0.28	24,49,56,57	0

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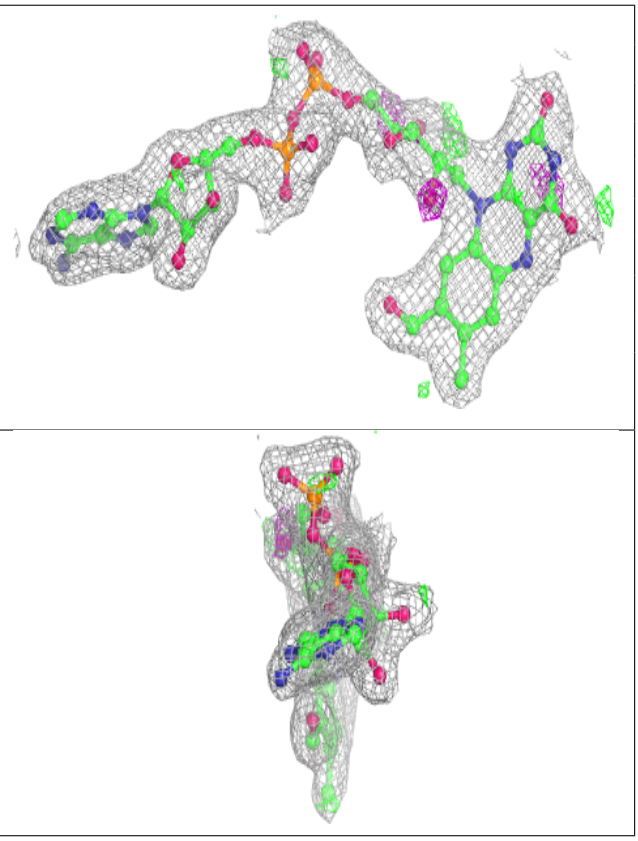
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PEG	B	1	7/7	0.90	0.17	41,45,55,57	0
3	MRD	A	581	8/8	0.93	0.14	27,37,46,46	0
4	ACT	A	1	4/4	0.95	0.25	28,29,30,36	0
2	FAY	C	600	54/54	0.95	0.12	21,31,40,42	0
6	MPD	C	1	8/8	0.96	0.18	29,35,40,42	0
2	FAY	B	600	54/54	0.97	0.12	15,22,31,35	0
2	FAY	A	600	54/54	0.98	0.10	14,19,26,28	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.

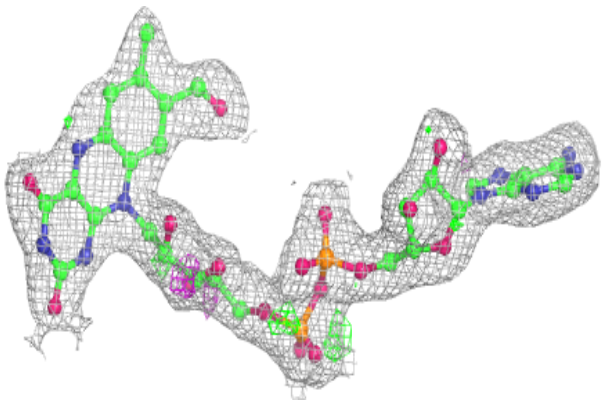
Electron density around FAY C 600:

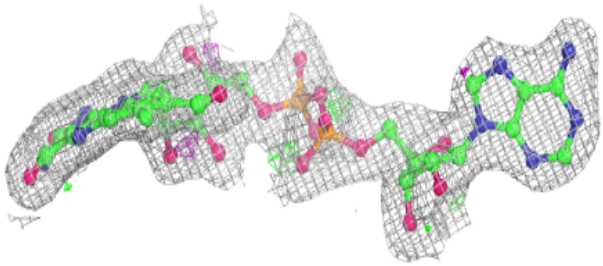
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

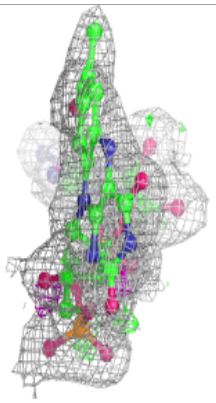


Electron density around FAY B 600:

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

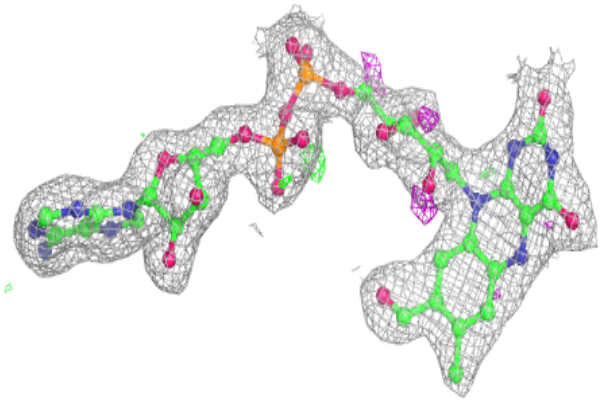


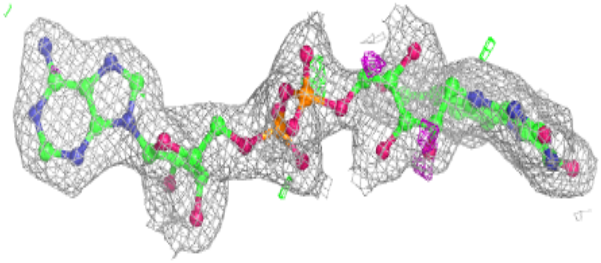


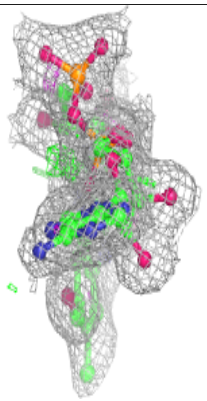


Electron density around FAY A 600:

$2mF_o$-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.