Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 01:15 PM EDT

PDB ID	:	1N0H
Title	:	Crystal Structure of Yeast Acetohydroxyacid Synthase in Complex with a Sulfonylurea Herbicide, Chlorimuron Ethyl
Authors	:	Pang, S.S.; Guddat, L.W.; Duggleby, R.G.
Deposited on	:	2002-10-14
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 (i)) were used in the production of this report:

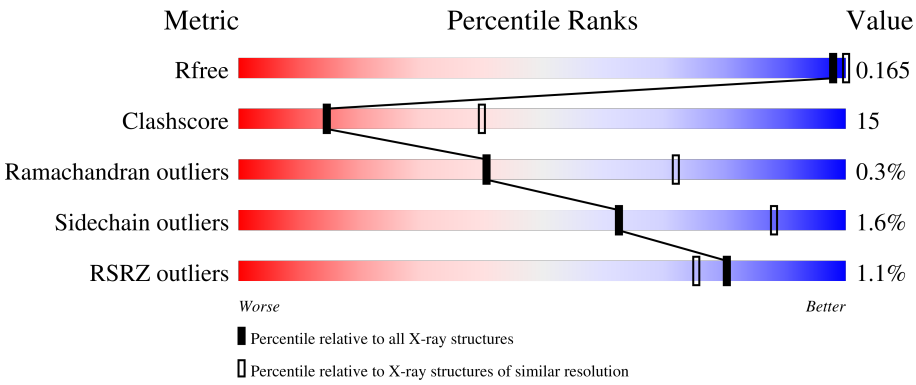
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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	677	% 68% 20% • 12%
1	B	677	% 62% 26% • 12%

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	CIE	A	695	-	X	-	-
4	CIE	B	1695	-	X	-	-
6	AYD	A	700	-	X	-	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 10196 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 Acetolactate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	599	4571	2894	791	864	22	0	2	0
1	B	598	4563	2891	788	862	22	0	2	0

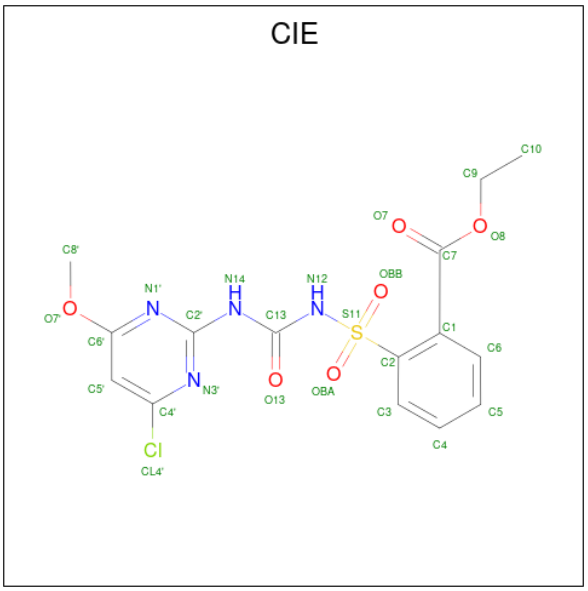
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	K		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

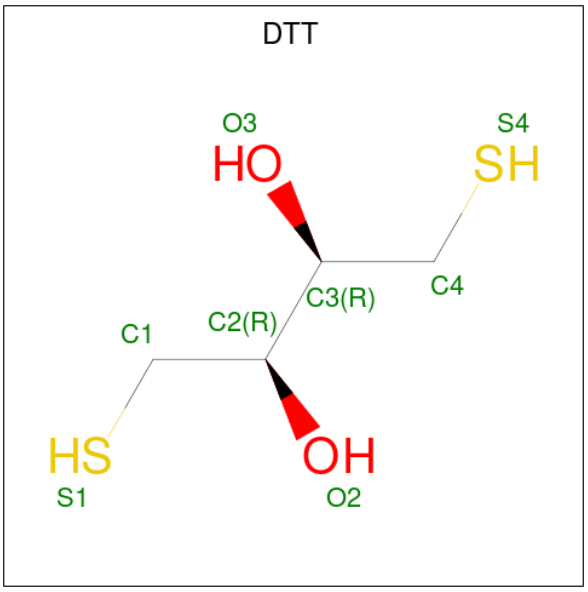
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	A	1	1	1	0	0
3	B	1	1	1	0	0

- Molecule 4 is 2-[[[[(4-CHLORO-6-METHOXY-2-PYRIMIDINYL)AMINO]CARBONYL]AMINO]SULFONYL]BENZOIC ACID ETHYL ESTER (three-letter code: CIE) (formula: $C_{15}H_{15}ClN_4O_6S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
4	A	1	27	15	1	4	6	1	0	0
			Total	C	Cl	N	O	S		
4	B	1	27	15	1	4	6	1	0	0

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	A	1	8	4	2	2	0	0

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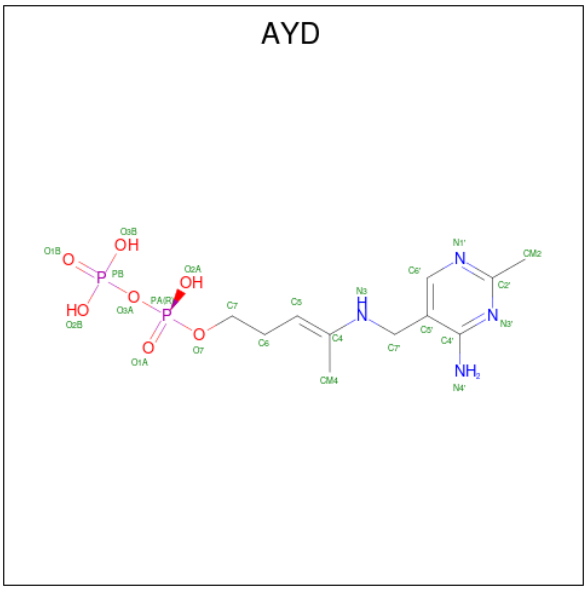
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
5	B	1	8	4	2	2	0	0

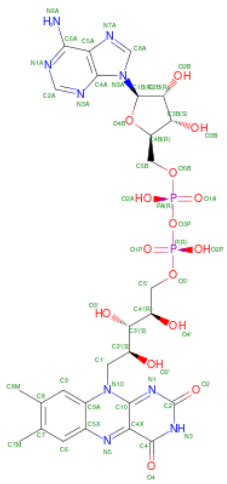
- Molecule 6 is 4-{[(4'-AMINO-2'-METHYLPYRIMIDIN-5'-YL)METHYL]AMINO}PENT-3-ENYL DIPHOSPHATE (three-letter code: AYD) (formula: $C_{11}H_{20}N_4O_7P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	24	11	4	7	2	0	0

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

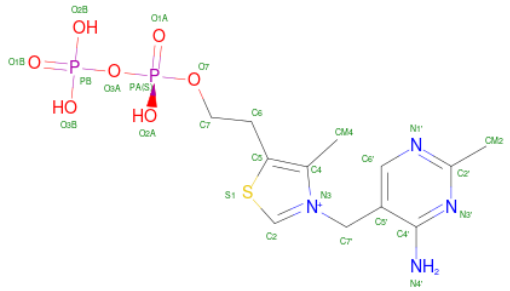
FAD



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
7	B	1	53	27	9	15	2	0	0

- Molecule 8 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).

TPP



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
8	B	1	26	12	4	7	2	1	0	0

- Molecule 9 is water.

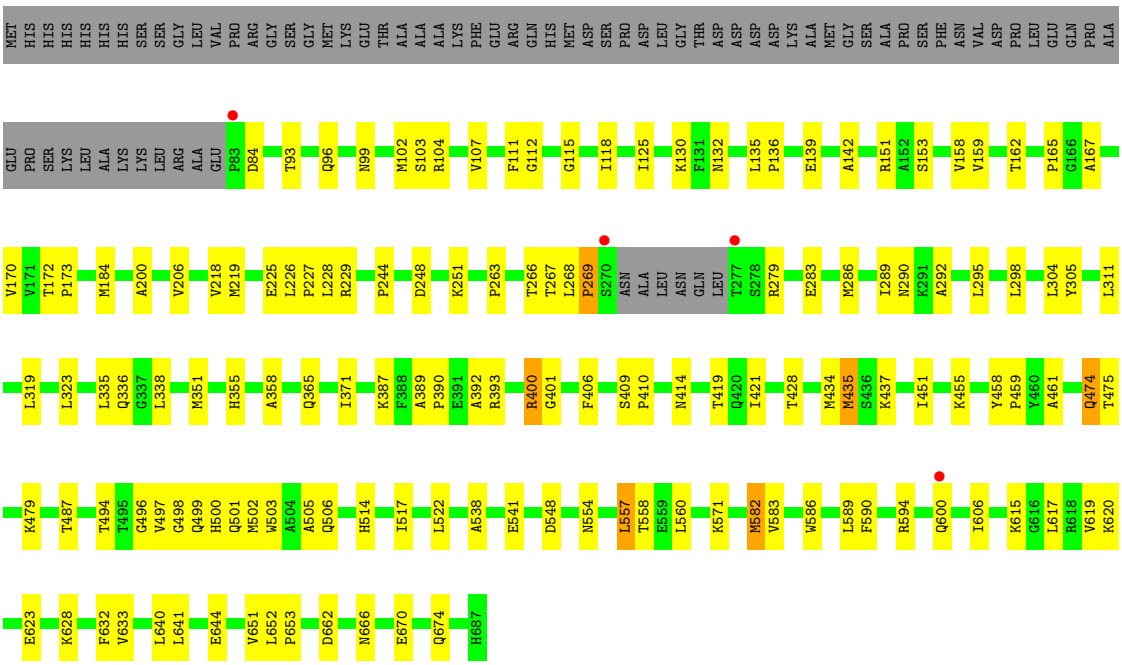
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	A	505	505	505	0	0
			Total	O		
9	B	327	327	327	0	0

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.

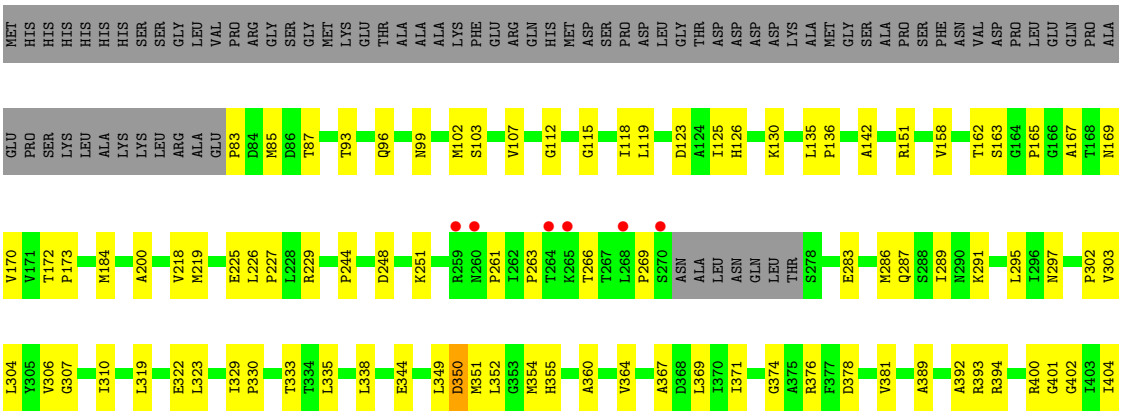
• Molecule 1: Acetolactate synthase

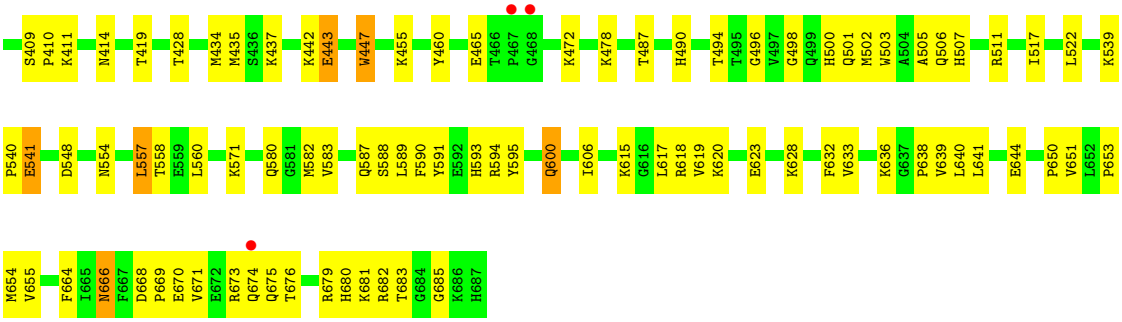
Chain A:



• Molecule 1: Acetolactate synthase

Chain B:




S409
P410
K411
N414
T419
T428
M434
M435
S436
K437
K442
E443
W447
K455
Y460
E465
T466
P467
G468
K472
K478
T487
H490
T494
T495
G496
V497
G498
Q499
H500
Q501
M502
W503
A504
A505
Q506
H507
R511
I517
L522
K539
P540
E541
D548
N554
L557
T558
E559
L560
K571
Q580
G581
M582
V583
Q587
S588
L589
F590
Y591
E592
H593
R594
Y595
Q600
I606
K615
G616
L617
R618
V619
K620
E623
K628
F632
V633
K636
G637
P638
V639
L640
L641
E644
P650
V651
L652
P653
M654
V655
F664
I665
N666
F667
D668
P669
E670
V671
E672
R673
Q674
Q675
T676
R679
H680
K681
R682
T683
G684
G685
K686
H687

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 2 2	Depositor
Cell constants a, b, c, α, β, γ	153.98Å 153.98Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.80 92.92 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.3 (48.70-2.80) 89.0 (92.92-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.163 , 0.205 0.163 , 0.165	Depositor DCC
R_{free} test set	5303 reflections (9.70%)	wwPDB-VP
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 64.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10196	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 2.79% 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: DTT, MG, CIE, AYD, FAD, K, TPP

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	0.33	0/4676	0.60	0/6345
1	B	0.30	0/4668	0.57	0/6334
All	All	0.32	0/9344	0.58	0/12679

There are no bond length outliers.

There are no bond angle outliers.

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	4571	0	4557	133	0
1	B	4563	0	4552	159	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	14	4	0
4	B	27	0	14	5	0
5	A	8	0	9	2	0
5	B	8	0	9	3	0
6	A	24	0	17	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	53	0	31	1	0
7	B	53	0	31	3	0
8	B	26	0	16	8	0
9	A	505	0	0	10	0
9	B	327	0	0	14	0
All	All	10196	0	9250	286	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 15.

All (286) 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:B:498:GLY:HA2	1:B:582[A]:MET:HE3	1.48	0.96
1:B:498:GLY:HA2	1:B:582[A]:MET:CE	1.98	0.93
1:A:474:GLN:H	1:A:474:GLN:HE21	1.25	0.84
4:A:695:CIE:H8'2	7:A:701:FAD:HM72	1.66	0.77
9:A:1038:HOH:O	1:B:600:GLN:HB3	1.87	0.75
1:B:414:ASN:OD1	1:B:419:THR:HG22	1.87	0.74
1:B:619:VAL:HG22	1:B:628:LYS:HG3	1.70	0.74
1:B:591:TYR:O	1:B:594:ARG:HG3	1.88	0.73
1:B:619:VAL:HG23	1:B:641:LEU:HD11	1.70	0.73
1:B:289:ILE:HG23	1:B:434:MET:HB2	1.71	0.72
1:A:474:GLN:H	1:A:474:GLN:NE2	1.86	0.72
1:A:619:VAL:HG22	1:A:628:LYS:HG3	1.72	0.72
1:B:335:LEU:HA	1:B:351:MET:HE2	1.70	0.71
1:B:295:LEU:HD11	1:B:401:GLY:HA2	1.73	0.70
1:B:351:MET:HE1	1:B:505:ALA:HB1	1.74	0.69
1:A:335:LEU:HA	1:A:351:MET:HE2	1.73	0.68
1:B:354:MET:HA	1:B:655:VAL:HB	1.74	0.68
1:A:499:GLN:HG2	1:A:582[A]:MET:HE3	1.76	0.68
1:B:355:HIS:HB2	1:B:502:MET:HE2	1.75	0.68
1:A:600:GLN:HE21	1:B:135:LEU:HB3	1.58	0.66
1:A:582[B]:MET:HE3	6:A:700:AYD:H5	1.79	0.65
1:B:355:HIS:HB2	1:B:502:MET:CE	2.26	0.65
1:B:226:LEU:HB3	1:B:227:PRO:HD3	1.79	0.65
1:A:619:VAL:HG23	1:A:641:LEU:HD11	1.79	0.64
1:B:410:PRO:HG2	1:B:411:LYS:HD2	1.80	0.64
1:A:226:LEU:HB3	1:A:227:PRO:HD3	1.78	0.64
1:B:323:LEU:HA	1:B:435:MET:HE1	1.81	0.62
1:B:490:HIS:CE1	9:B:1259:HOH:O	2.52	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1695:CIE:H8'2	7:B:1701:FAD:HM72	1.81	0.62
1:A:289:ILE:HG23	1:A:434:MET:HB2	1.82	0.61
1:A:338:LEU:HD11	1:A:351:MET:HE3	1.81	0.61
1:A:600:GLN:HG2	1:B:135:LEU:HD13	1.83	0.61
1:B:668:ASP:HB3	1:B:671:VAL:HB	1.82	0.60
1:A:498:GLY:HA2	1:A:582[B]:MET:HE2	1.84	0.60
1:A:136:PRO:HG3	1:A:142:ALA:HB2	1.84	0.59
1:B:304:LEU:HD23	1:B:371:ILE:HB	1.84	0.59
1:B:381:VAL:HG22	7:B:1701:FAD:O2	2.03	0.59
1:A:292:ALA:HB3	1:A:434:MET:HE2	1.85	0.59
1:A:414:ASN:ND2	1:A:419:THR:H	2.01	0.59
1:B:638:PRO:HD3	9:B:1082:HOH:O	2.03	0.58
1:B:539:LYS:HG3	9:B:1259:HOH:O	2.02	0.58
1:A:286:MET:HE2	1:A:437:LYS:HE2	1.86	0.58
1:B:582[A]:MET:CE	8:B:1702:TPP:S1	2.92	0.57
1:B:286:MET:HE1	1:B:437:LYS:NZ	2.19	0.57
1:A:620:LYS:HE2	1:A:644:GLU:OE2	2.03	0.57
1:A:251:LYS:NZ	4:B:1695:CIE:H12	2.02	0.57
1:B:593:HIS:HD1	1:B:682:ARG:HH11	1.53	0.57
1:A:338:LEU:HD11	1:A:351:MET:CE	2.35	0.57
1:A:165:PRO:HD3	1:B:522:LEU:HG	1.86	0.56
1:B:669:PRO:O	1:B:673:ARG:HG3	2.04	0.56
1:B:286:MET:HE1	1:B:437:LYS:HZ2	1.70	0.56
1:B:442:LYS:HG2	1:B:443:GLU:HG3	1.86	0.56
1:A:135:LEU:HD13	9:A:1038:HOH:O	2.04	0.56
1:B:360:ALA:O	1:B:364:VAL:HG23	2.06	0.56
1:A:582[A]:MET:CE	9:A:964:HOH:O	2.54	0.56
1:A:102:MET:CE	1:A:158:VAL:HG11	2.36	0.55
1:A:200:ALA:HB1	4:B:1695:CIE:H5	1.88	0.55
4:A:695:CIE:H5	1:B:200:ALA:HB1	1.89	0.55
1:B:580:GLN:HA	8:B:1702:TPP:H72	1.88	0.55
1:A:102:MET:HE2	1:A:158:VAL:HG11	1.89	0.55
1:A:522:LEU:HG	1:B:165:PRO:HD3	1.88	0.55
5:A:698:DTT:S1	5:A:698:DTT:S4	3.05	0.55
1:B:102:MET:CE	1:B:158:VAL:HG11	2.36	0.55
1:B:172:THR:HB	1:B:173:PRO:HD3	1.89	0.55
1:B:619:VAL:CG2	1:B:641:LEU:HD11	2.35	0.55
1:A:151:ARG:HG3	1:A:517:ILE:HG23	1.88	0.55
1:B:620:LYS:HE2	1:B:644:GLU:OE2	2.07	0.55
1:A:319:LEU:HD12	1:A:428:THR:HG23	1.88	0.54
1:B:411:LYS:HD2	1:B:411:LYS:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:PRO:HG3	1:B:142:ALA:HB2	1.90	0.54
1:A:135:LEU:HD12	9:B:1041:HOH:O	2.07	0.54
1:A:172:THR:HB	1:A:173:PRO:HD3	1.90	0.54
1:B:371:ILE:HD12	1:B:371:ILE:N	2.24	0.53
1:B:163:SER:HB2	9:B:987:HOH:O	2.08	0.53
1:B:434:MET:O	1:B:434:MET:HG2	2.08	0.53
1:A:172:THR:OG1	1:B:169:ASN:ND2	2.42	0.53
1:A:251:LYS:HZ3	4:B:1695:CIE:H12	1.54	0.53
1:B:306:VAL:HB	1:B:333:THR:HG22	1.88	0.53
1:A:474:GLN:HE21	1:A:474:GLN:N	1.99	0.53
1:B:589:LEU:HD23	1:B:590:PHE:CE1	2.44	0.53
1:B:295:LEU:HD11	1:B:401:GLY:CA	2.38	0.53
1:A:102:MET:HE3	1:A:107:VAL:HG11	1.89	0.53
1:A:279:ARG:O	1:A:283:GLU:HB2	2.08	0.53
1:A:498:GLY:HA2	1:A:582[B]:MET:CE	2.39	0.53
1:B:102:MET:HE2	1:B:158:VAL:HG11	1.91	0.53
1:B:582[A]:MET:SD	4:B:1695:CIE:H5'	2.49	0.53
1:A:571:LYS:HB3	1:A:632:PHE:CZ	2.44	0.53
1:A:594:ARG:HD3	9:B:947:HOH:O	2.08	0.53
1:B:302:PRO:O	1:B:330:PRO:HD2	2.09	0.52
1:B:478:LYS:HE2	1:B:507:HIS:ND1	2.24	0.52
1:B:322:GLU:OE2	1:B:435:MET:HG2	2.09	0.52
1:B:557:LEU:HD23	1:B:558:THR:N	2.24	0.52
1:B:582[A]:MET:HE3	8:B:1702:TPP:S1	2.49	0.52
5:B:1698:DTT:H2	9:B:1018:HOH:O	2.08	0.52
1:A:323:LEU:HB2	1:A:435:MET:HE1	1.91	0.52
5:B:1698:DTT:S1	5:B:1698:DTT:S4	3.08	0.52
1:B:571:LYS:HB3	1:B:632:PHE:CZ	2.46	0.51
1:A:103:SER:HB2	1:A:130:LYS:HD3	1.92	0.51
1:A:319:LEU:HD12	1:A:428:THR:CG2	2.40	0.51
1:B:102:MET:HE3	1:B:107:VAL:HG11	1.92	0.51
1:A:292:ALA:HB3	1:A:434:MET:CE	2.41	0.51
1:B:263:PRO:HB2	1:B:266:THR:HG23	1.92	0.51
1:B:455:LYS:HA	5:B:1698:DTT:S4	2.50	0.51
1:A:640:LEU:C	1:A:640:LEU:HD23	2.31	0.51
1:B:498:GLY:HA2	1:B:582[A]:MET:HE2	1.89	0.51
1:B:496:GLY:H	1:B:500:HIS:HE1	1.58	0.51
1:A:583:VAL:HG21	6:A:700:AYD:HM43	1.93	0.50
1:A:496:GLY:H	1:A:500:HIS:HE1	1.59	0.50
1:B:297:ASN:HA	9:B:1214:HOH:O	2.11	0.50
1:A:557:LEU:HD23	1:A:558:THR:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:LEU:HD23	1:A:590:PHE:CE1	2.46	0.50
1:B:307:GLY:O	1:B:310:ILE:HG22	2.11	0.50
1:B:319:LEU:HD12	1:B:428:THR:HG23	1.93	0.50
1:A:311:LEU:O	1:A:514:HIS:HE1	1.92	0.50
1:A:99:ASN:ND2	1:A:125:ILE:HG22	2.27	0.50
1:A:497:VAL:O	6:A:700:AYD:H62	2.11	0.50
1:B:670:GLU:HA	1:B:673:ARG:NH1	2.26	0.50
1:A:335:LEU:CD1	1:A:351:MET:HE1	2.41	0.49
1:B:354:MET:O	1:B:654:MET:HA	2.12	0.49
1:B:653:PRO:HG2	9:B:1066:HOH:O	2.11	0.49
1:B:283:GLU:O	1:B:287:GLN:HG3	2.12	0.49
1:A:118:ILE:HG13	1:A:118:ILE:O	2.13	0.49
1:A:600:GLN:HG3	9:A:870:HOH:O	2.12	0.49
1:B:103:SER:HB2	1:B:130:LYS:HD3	1.95	0.48
1:B:623:GLU:CD	1:B:623:GLU:H	2.16	0.48
1:B:389:ALA:HB1	1:B:392:ALA:HB3	1.95	0.48
1:B:554:ASN:HA	1:B:557:LEU:HD13	1.95	0.48
1:A:170:VAL:C	1:A:173:PRO:HD2	2.33	0.48
1:A:623:GLU:CD	1:A:623:GLU:H	2.16	0.48
1:A:290:ASN:OD1	1:A:437:LYS:HE2	2.13	0.48
1:B:636:LYS:HA	9:B:1418:HOH:O	2.14	0.48
1:B:378:ASP:HB2	9:B:1409:HOH:O	2.13	0.48
1:A:554:ASN:HA	1:A:557:LEU:HD13	1.96	0.48
1:B:170:VAL:C	1:B:173:PRO:HD2	2.34	0.48
1:A:497:VAL:HG12	1:A:582[B]:MET:CE	2.44	0.48
1:A:351:MET:HE3	1:A:505:ALA:HB1	1.96	0.48
1:B:184:MET:O	1:B:244:PRO:HA	2.14	0.48
1:B:83:PRO:HG2	1:B:85:MET:O	2.14	0.47
1:A:557:LEU:O	1:A:560:LEU:HB2	2.14	0.47
1:B:587:GLN:NE2	1:B:595:TYR:HA	2.28	0.47
1:B:394:ARG:HH12	1:B:400:ARG:NH2	2.12	0.47
1:A:228:LEU:HD13	1:A:266:THR:HG22	1.95	0.47
1:A:335:LEU:HD13	1:A:351:MET:HE1	1.96	0.47
1:B:593:HIS:NE2	1:B:675:GLN:NE2	2.63	0.47
1:B:303:VAL:HG23	1:B:367:ALA:HB2	1.96	0.47
1:A:304:LEU:HD23	1:A:371:ILE:HB	1.96	0.47
1:A:93:THR:OG1	1:A:96:GLN:HG3	2.15	0.46
1:A:582[B]:MET:CE	6:A:700:AYD:H5	2.43	0.46
1:A:600:GLN:NE2	1:B:135:LEU:HD22	2.31	0.46
1:B:557:LEU:HD23	1:B:557:LEU:C	2.36	0.46
1:B:600:GLN:H	1:B:600:GLN:NE2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:MET:O	1:B:506:GLN:HG3	2.15	0.46
8:B:1702:TPP:HN42	8:B:1702:TPP:H2	1.78	0.46
1:A:497:VAL:HG12	1:A:582[B]:MET:HE1	1.96	0.46
1:A:502:MET:O	1:A:506:GLN:HG3	2.15	0.46
1:B:349:LEU:O	1:B:350:ASP:CB	2.63	0.46
1:B:557:LEU:O	1:B:560:LEU:HB2	2.15	0.46
1:A:132:ASN:HB3	9:A:1551:HOH:O	2.15	0.46
1:B:118:ILE:HG13	1:B:118:ILE:O	2.15	0.46
1:A:355:HIS:HB2	1:A:502:MET:CE	2.45	0.46
1:B:460:TYR:HB3	1:B:507:HIS:CE1	2.51	0.46
1:A:582[A]:MET:HE2	9:A:964:HOH:O	2.13	0.46
1:A:295:LEU:HD12	1:A:421:ILE:CD1	2.46	0.46
1:A:455:LYS:HA	5:A:698:DTT:S4	2.56	0.46
1:B:472:LYS:HD2	9:B:1257:HOH:O	2.14	0.46
1:A:400:ARG:NH2	9:A:912:HOH:O	2.47	0.46
1:B:93:THR:OG1	1:B:96:GLN:HG3	2.16	0.46
1:B:291:LYS:HE2	9:B:1408:HOH:O	2.16	0.46
1:A:619:VAL:CG2	1:A:641:LEU:HD11	2.44	0.45
4:A:695:CIE:H12	1:B:251:LYS:HZ3	1.65	0.45
1:B:335:LEU:HA	1:B:351:MET:CE	2.43	0.45
1:B:487:THR:HG21	1:B:633:VAL:HG11	1.96	0.45
1:B:115:GLY:HA3	1:B:162:THR:CB	2.47	0.45
1:A:351:MET:CE	1:A:505:ALA:HB1	2.47	0.45
1:A:494:THR:HG22	1:A:517:ILE:HB	1.99	0.45
1:A:557:LEU:HD23	1:A:557:LEU:C	2.37	0.45
1:B:151:ARG:HG3	1:B:517:ILE:HG23	1.97	0.45
8:B:1702:TPP:HN42	8:B:1702:TPP:C2	2.30	0.45
1:A:184:MET:O	1:A:244:PRO:HA	2.16	0.45
1:A:652:LEU:HA	1:A:653:PRO:C	2.37	0.45
1:B:286:MET:CE	1:B:437:LYS:NZ	2.79	0.45
1:B:681:LYS:NZ	1:B:681:LYS:HB3	2.32	0.45
1:B:225:GLU:HG2	1:B:229:ARG:HG2	1.97	0.45
1:A:225:GLU:HG2	1:A:229:ARG:HG2	1.99	0.45
1:B:115:GLY:HA3	1:B:162:THR:HB	1.99	0.45
1:B:494:THR:HG22	1:B:517:ILE:HB	1.99	0.45
1:B:392:ALA:O	1:B:402:GLY:HA2	2.17	0.44
1:B:496:GLY:N	1:B:500:HIS:HE1	2.15	0.44
1:B:615:LYS:HE2	1:B:617:LEU:HD21	1.99	0.44
1:B:670:GLU:O	1:B:674:GLN:HG3	2.18	0.44
1:A:153:SER:HB3	1:A:538:ALA:HB1	2.00	0.44
1:B:503:TRP:CE2	1:B:651:VAL:HG22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ALA:HB3	1:A:458:TYR:CB	2.48	0.44
1:B:447:TRP:HE3	1:B:447:TRP:HA	1.82	0.44
1:B:465:GLU:HG3	1:B:472:LYS:HG2	1.98	0.44
1:B:593:HIS:CE1	1:B:675:GLN:NE2	2.86	0.44
1:A:219:MET:HA	1:A:248:ASP:HB3	2.00	0.44
1:B:498:GLY:O	1:B:501:GLN:HB3	2.18	0.44
1:B:540:PRO:HB2	1:B:541:GLU:OE2	2.17	0.44
1:A:406:PHE:HZ	1:A:434:MET:CE	2.31	0.44
1:A:498:GLY:O	1:A:501:GLN:HB3	2.17	0.44
1:B:389:ALA:O	1:B:393:ARG:HG3	2.18	0.44
1:A:115:GLY:HA3	1:A:162:THR:HB	2.00	0.44
1:A:167:ALA:O	1:A:170:VAL:HG22	2.17	0.44
1:A:409:SER:HA	1:A:410:PRO:HD3	1.85	0.43
1:B:219:MET:HA	1:B:248:ASP:HB3	2.00	0.43
1:A:139:GLU:OE2	8:B:1702:TPP:N1'	2.51	0.43
1:A:414:ASN:HD21	1:A:419:THR:H	1.65	0.43
1:B:286:MET:CE	1:B:437:LYS:HZ2	2.30	0.43
1:B:411:LYS:HD2	1:B:411:LYS:H	1.83	0.43
1:B:447:TRP:HA	1:B:447:TRP:CE3	2.52	0.43
1:B:588:SER:HG	1:B:595:TYR:HH	1.61	0.43
1:B:666:ASN:HD22	1:B:666:ASN:HA	1.62	0.43
1:A:393:ARG:HD2	9:A:1559:HOH:O	2.19	0.43
1:B:650:PRO:HG3	9:B:1206:HOH:O	2.18	0.43
1:B:676:THR:HG22	1:B:680:HIS:CD2	2.54	0.43
1:A:84:ASP:O	1:A:263:PRO:HA	2.19	0.43
1:A:387:LYS:O	1:A:390:PRO:HD3	2.19	0.43
1:A:496:GLY:N	1:A:500:HIS:HE1	2.17	0.43
1:A:451:ILE:O	1:A:455:LYS:HG3	2.19	0.43
1:A:594:ARG:HB3	1:B:126:HIS:ND1	2.34	0.43
1:B:369:LEU:HD11	1:B:404:ILE:HG13	2.00	0.43
1:B:640:LEU:C	1:B:640:LEU:HD23	2.39	0.43
1:A:365:GLN:HG3	1:A:662:ASP:HB3	2.01	0.42
1:A:582[B]:MET:HE3	6:A:700:AYD:C5	2.47	0.42
1:B:580:GLN:CA	8:B:1702:TPP:H72	2.49	0.42
1:A:586[B]:TRP:CD1	1:B:119:LEU:HD12	2.55	0.42
1:B:87:THR:HG22	1:B:261:PRO:HB3	2.01	0.42
1:B:303:VAL:CG2	1:B:367:ALA:HB2	2.48	0.42
1:A:115:GLY:HA3	1:A:162:THR:CB	2.48	0.42
1:A:206:VAL:HG21	9:A:732:HOH:O	2.18	0.42
1:A:459:PRO:O	1:A:461:ALA:N	2.50	0.42
1:B:218:VAL:HG22	1:B:219:MET:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:GLY:HA3	1:B:374:GLY:O	2.18	0.42
1:A:135:LEU:HD22	9:A:1038:HOH:O	2.19	0.42
1:A:295:LEU:HD12	1:A:421:ILE:HD12	2.01	0.42
1:A:268:LEU:HA	1:A:269:PRO:HD3	1.93	0.42
1:A:311:LEU:O	1:A:514:HIS:CE1	2.72	0.42
1:A:336:GLN:HA	1:A:336:GLN:OE1	2.20	0.42
1:B:414:ASN:CG	1:B:419:THR:HG22	2.39	0.42
1:B:99:ASN:ND2	1:B:125:ILE:HG22	2.35	0.42
1:B:352:LEU:HG	1:B:381:VAL:HG13	2.01	0.42
1:A:487:THR:HG21	1:A:633:VAL:HG11	2.02	0.42
1:A:290:ASN:OD1	1:A:437:LYS:CE	2.68	0.41
1:B:394:ARG:HH12	1:B:400:ARG:HH21	1.67	0.41
1:A:218:VAL:HG22	1:A:219:MET:N	2.34	0.41
1:A:503:TRP:CE2	1:A:651:VAL:HG22	2.54	0.41
1:A:594:ARG:HD2	1:B:123:ASP:OD2	2.19	0.41
1:A:600:GLN:NE2	1:B:136:PRO:O	2.47	0.41
1:B:394:ARG:HB3	1:B:394:ARG:CZ	2.50	0.41
4:A:695:CIE:H12	1:B:251:LYS:NZ	2.18	0.41
1:A:475:THR:O	1:A:479:LYS:HG3	2.21	0.41
1:A:615:LYS:HE2	1:A:617:LEU:HD21	2.02	0.41
1:B:435:MET:HA	1:B:435:MET:CE	2.51	0.41
1:B:167:ALA:O	1:B:170:VAL:HG22	2.21	0.41
1:B:606:ILE:HD13	1:B:618:ARG:NH2	2.35	0.41
1:A:498:GLY:HA2	1:A:582[B]:MET:HB2	2.03	0.41
1:B:102:MET:HE1	1:B:158:VAL:HG11	2.03	0.41
1:B:683:THR:C	1:B:685:GLY:H	2.24	0.41
1:A:112:GLY:O	1:A:136:PRO:HD2	2.21	0.41
1:A:670:GLU:HG2	1:A:674:GLN:NE2	2.36	0.41
1:B:329:ILE:HA	1:B:330:PRO:HD3	1.88	0.41
1:B:338:LEU:HD11	1:B:351:MET:CE	2.51	0.41
1:A:358:ALA:HB3	1:A:458:TYR:HB3	2.03	0.41
1:A:389:ALA:HB1	1:A:392:ALA:HB3	2.03	0.41
1:A:406:PHE:HZ	1:A:434:MET:HE1	1.84	0.41
1:A:594:ARG:NH1	1:B:123:ASP:OD1	2.54	0.41
1:B:112:GLY:O	1:B:136:PRO:HD2	2.20	0.41
1:A:355:HIS:HB2	1:A:502:MET:HE3	2.03	0.41
1:A:104:ARG:NH1	1:A:267:THR:O	2.54	0.40
1:A:111:PHE:O	1:A:159:VAL:HA	2.21	0.40
1:A:295:LEU:HD22	1:A:401:GLY:HA2	2.03	0.40
1:A:600:GLN:NE2	1:B:135:LEU:HB3	2.32	0.40
1:B:344:GLU:HG3	1:B:511:ARG:CZ	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:MET:HB2	1:B:655:VAL:O	2.21	0.40
1:B:676:THR:HG23	1:B:679:ARG:NH2	2.36	0.40
1:A:606:ILE:N	1:A:606:ILE:HD12	2.35	0.40
1:B:571:LYS:HD2	1:B:639:VAL:CG1	2.51	0.40
1:A:298:LEU:HD21	1:A:400:ARG:HA	2.04	0.40
1:B:376:ARG:HB3	7:B:1701:FAD:O3B	2.22	0.40
1:B:409:SER:HA	1:B:410:PRO:HD2	1.96	0.40
1:B:655:VAL:HG22	1:B:664:PHE:HB3	2.03	0.40
1:A:594:ARG:HH11	1:B:123:ASP:CG	2.24	0.40
1:B:335:LEU:CA	1:B:351:MET:HE2	2.45	0.40
1:B:583:VAL:HG23	8:B:1702:TPP:H61	2.04	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	597/677 (88%)	580 (97%)	16 (3%)	1 (0%)	47 78
1	B	596/677 (88%)	575 (96%)	19 (3%)	2 (0%)	41 72
All	All	1193/1354 (88%)	1155 (97%)	35 (3%)	3 (0%)	41 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	350	ASP
1	B	269	PRO
1	A	269	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	490/556 (88%)	480 (98%)	10 (2%)	55	84
1	B	489/556 (88%)	482 (99%)	7 (1%)	67	90
All	All	979/1112 (88%)	962 (98%)	17 (2%)	62	87

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	TYR
1	A	400	ARG
1	A	435	MET
1	A	474	GLN
1	A	541	GLU
1	A	548	ASP
1	A	557	LEU
1	A	582[A]	MET
1	A	582[B]	MET
1	A	666	ASN
1	B	443	GLU
1	B	447	TRP
1	B	541	GLU
1	B	548	ASP
1	B	557	LEU
1	B	600	GLN
1	B	666	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	106	ASN
1	A	126	HIS
1	A	127	ASN
1	A	132	ASN

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Mol	Chain	Res	Type
1	A	169	ASN
1	A	312	ASN
1	A	355	HIS
1	A	414	ASN
1	A	450	GLN
1	A	474	GLN
1	A	500	HIS
1	A	554	ASN
1	A	587	GLN
1	A	602	ASN
1	A	666	ASN
1	A	674	GLN
1	A	675	GLN
1	B	99	ASN
1	B	106	ASN
1	B	132	ASN
1	B	169	ASN
1	B	312	ASN
1	B	452	ASN
1	B	500	HIS
1	B	512	ASN
1	B	514	HIS
1	B	554	ASN
1	B	587	GLN
1	B	600	GLN
1	B	602	ASN
1	B	666	ASN
1	B	675	GLN

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)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	CIE	B	1695	-	28,28,28	4.53	16 (57%)	38,39,39	4.32	15 (39%)
5	DTT	A	698	1	7,7,7	1.27	1 (14%)	4,8,8	5.28	4 (100%)
7	FAD	A	701	-	53,58,58	2.18	18 (33%)	68,89,89	1.14	3 (4%)
4	CIE	A	695	-	28,28,28	4.57	16 (57%)	38,39,39	4.29	14 (36%)
7	FAD	B	1701	-	53,58,58	2.24	19 (35%)	68,89,89	1.14	2 (2%)
8	TPP	B	1702	3	22,27,27	3.10	11 (50%)	29,40,40	2.14	7 (24%)
6	AYD	A	700	3	21,24,24	3.60	14 (66%)	31,34,34	3.14	10 (32%)
5	DTT	B	1698	1	7,7,7	1.28	1 (14%)	4,8,8	5.31	4 (100%)

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	CIE	B	1695	-	-	9/24/24/24	0/2/2/2
5	DTT	A	698	1	-	2/8/8/8	-
7	FAD	A	701	-	-	1/30/50/50	0/6/6/6
4	CIE	A	695	-	-	9/24/24/24	0/2/2/2
7	FAD	B	1701	-	-	1/30/50/50	0/6/6/6
8	TPP	B	1702	3	-	1/16/17/17	0/2/2/2
6	AYD	A	700	3	-	8/19/19/19	0/1/1/1
5	DTT	B	1698	1	-	2/8/8/8	-

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	695	CIE	OBA-S11	15.25	1.60	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1695	CIE	OBA-S11	14.70	1.60	1.43
4	B	1695	CIE	C1-C2	7.79	1.48	1.40
6	A	700	AYD	C4'-N3'	7.62	1.45	1.35
8	B	1702	TPP	C4'-N3'	6.74	1.44	1.35
4	A	695	CIE	C3-C2	6.74	1.47	1.39
4	A	695	CIE	C1-C2	6.63	1.47	1.40
4	A	695	CIE	OBB-S11	6.57	1.51	1.43
4	B	1695	CIE	OBB-S11	6.56	1.51	1.43
4	B	1695	CIE	C3-C2	6.45	1.46	1.39
4	A	695	CIE	C5'-C6'	6.11	1.48	1.38
4	A	695	CIE	C6-C1	5.67	1.48	1.39
4	B	1695	CIE	C6-C1	5.67	1.48	1.39
7	B	1701	FAD	C9A-C5X	5.65	1.50	1.41
4	B	1695	CIE	C5'-C6'	5.65	1.47	1.38
4	A	695	CIE	C2'-N14	-5.55	1.31	1.38
7	A	701	FAD	C9A-C5X	5.41	1.50	1.41
6	A	700	AYD	C6'-C5'	5.36	1.48	1.37
6	A	700	AYD	C5'-C4'	5.36	1.52	1.42
8	B	1702	TPP	C6'-C5'	5.06	1.48	1.37
6	A	700	AYD	C6'-N1'	5.00	1.45	1.34
7	B	1701	FAD	C9-C9A	4.99	1.47	1.39
4	B	1695	CIE	C5'-C4'	4.92	1.46	1.38
7	B	1701	FAD	C9-C8	4.92	1.46	1.39
6	A	700	AYD	C2'-N1'	4.88	1.42	1.34
8	B	1702	TPP	C6'-N1'	4.87	1.44	1.34
6	A	700	AYD	C7'-N3	4.85	1.55	1.46
8	B	1702	TPP	C2'-N1'	4.79	1.42	1.34
7	A	701	FAD	C9-C9A	4.60	1.47	1.39
4	A	695	CIE	C5'-C4'	4.59	1.45	1.38
8	B	1702	TPP	C5'-C4'	4.57	1.50	1.42
7	B	1701	FAD	C6-C7	4.55	1.46	1.39
7	A	701	FAD	C6-C7	4.50	1.46	1.39
4	B	1695	CIE	S11-N12	4.47	1.73	1.64
4	B	1695	CIE	C4'-N3'	4.46	1.41	1.33
7	A	701	FAD	C9-C8	4.43	1.46	1.39
7	A	701	FAD	C8-C7	4.29	1.51	1.40
4	B	1695	CIE	O8-C7	4.20	1.44	1.33
7	B	1701	FAD	C8-C7	4.17	1.51	1.40
4	B	1695	CIE	C2'-N14	-4.16	1.33	1.38
8	B	1702	TPP	C6-C5	4.04	1.52	1.50
4	A	695	CIE	C4'-N3'	3.96	1.40	1.33
4	A	695	CIE	S11-N12	3.94	1.72	1.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1701	FAD	C4X-N5	3.89	1.38	1.30
7	A	701	FAD	C4X-N5	3.88	1.38	1.30
4	A	695	CIE	O8-C7	3.87	1.43	1.33
7	A	701	FAD	C2A-N3A	3.84	1.38	1.32
7	B	1701	FAD	C2A-N3A	3.80	1.38	1.32
6	A	700	AYD	O7-C7	3.79	1.60	1.44
6	A	700	AYD	PA-O2A	-3.69	1.38	1.55
8	B	1702	TPP	O7-C7	3.63	1.59	1.44
4	A	695	CIE	C5-C6	3.39	1.46	1.38
4	B	1695	CIE	C5-C6	3.28	1.45	1.38
7	B	1701	FAD	C4A-N3A	3.21	1.40	1.35
7	B	1701	FAD	C10-N1	3.19	1.39	1.33
6	A	700	AYD	C4-N3	3.18	1.43	1.33
7	B	1701	FAD	C6-C5X	3.17	1.44	1.40
7	A	701	FAD	C6-C5X	3.15	1.44	1.40
7	A	701	FAD	C4A-N3A	3.15	1.40	1.35
4	A	695	CIE	C4-C3	3.13	1.45	1.38
7	A	701	FAD	C10-N1	3.09	1.39	1.33
4	B	1695	CIE	C4-C3	3.06	1.45	1.38
7	A	701	FAD	C7M-C7	2.91	1.56	1.51
6	A	700	AYD	PB-O2B	-2.87	1.43	1.54
7	B	1701	FAD	C2A-N1A	2.87	1.39	1.33
7	A	701	FAD	C2A-N1A	2.80	1.39	1.33
6	A	700	AYD	C2'-N3'	2.78	1.39	1.34
4	A	695	CIE	C5-C4	2.75	1.45	1.38
7	B	1701	FAD	C10-N10	2.73	1.43	1.37
6	A	700	AYD	C6-C7	2.71	1.58	1.51
4	B	1695	CIE	C5-C4	2.69	1.45	1.38
8	B	1702	TPP	PA-O2A	-2.68	1.42	1.55
7	B	1701	FAD	C9A-N10	2.67	1.45	1.41
8	B	1702	TPP	PB-O2B	-2.62	1.44	1.54
7	B	1701	FAD	O4'-C4'	2.62	1.48	1.43
7	A	701	FAD	O4B-C1B	2.60	1.44	1.41
4	A	695	CIE	C13-N12	-2.51	1.33	1.39
8	B	1702	TPP	CM4-C4	2.47	1.54	1.49
7	A	701	FAD	O4'-C4'	2.46	1.48	1.43
6	A	700	AYD	PA-O1A	-2.44	1.42	1.50
5	A	698	DTT	C1-S1	2.39	1.86	1.81
4	B	1695	CIE	C2-S11	2.37	1.81	1.77
7	A	701	FAD	C10-N10	2.29	1.42	1.37
7	B	1701	FAD	O4B-C1B	2.29	1.44	1.41
7	A	701	FAD	C9A-N10	2.26	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	695	CIE	C13-N14	-2.23	1.32	1.37
4	B	1695	CIE	C13-N12	-2.18	1.34	1.39
7	A	701	FAD	C4-N3	2.18	1.42	1.38
5	B	1698	DTT	C1-S1	2.16	1.86	1.81
6	A	700	AYD	PA-O7	-2.14	1.50	1.59
7	A	701	FAD	C1'-C2'	2.09	1.55	1.52
7	B	1701	FAD	C7M-C7	2.06	1.55	1.51
7	B	1701	FAD	C4-N3	2.06	1.42	1.38
8	B	1702	TPP	PA-O7	-2.05	1.51	1.59
7	B	1701	FAD	C1'-C2'	2.05	1.55	1.52
7	B	1701	FAD	C5'-C4'	-2.05	1.48	1.51

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1695	CIE	C8'-O7'-C6'	18.52	146.40	117.36
4	A	695	CIE	C8'-O7'-C6'	18.05	145.66	117.36
6	A	700	AYD	O7-C7-C6	10.62	148.48	109.00
4	A	695	CIE	C2'-N14-C13	10.40	141.48	130.40
4	B	1695	CIE	C2'-N14-C13	9.67	140.70	130.40
5	B	1698	DTT	C3-C4-S4	9.22	141.29	114.47
5	A	698	DTT	C3-C4-S4	9.06	140.83	114.47
6	A	700	AYD	C7-C6-C5	8.26	143.76	112.36
4	B	1695	CIE	C3-C2-S11	-7.64	107.04	117.42
4	A	695	CIE	C3-C2-S11	-7.13	107.73	117.42
4	A	695	CIE	C2-C1-C7	-6.49	115.28	124.25
4	B	1695	CIE	C2-C1-C7	-5.82	116.21	124.25
8	B	1702	TPP	CM2-C2'-N1'	5.77	123.49	117.14
4	B	1695	CIE	C2'-N1'-C6'	4.98	120.85	114.99
4	B	1695	CIE	O8-C7-O7	-4.94	113.65	123.67
6	A	700	AYD	CM2-C2'-N1'	4.91	122.53	117.14
4	A	695	CIE	O8-C7-O7	-4.88	113.77	123.67
4	A	695	CIE	OBB-S11-OBA	4.86	125.52	119.55
4	B	1695	CIE	OBB-S11-OBA	4.76	125.40	119.55
4	A	695	CIE	C2'-N1'-C6'	4.54	120.33	114.99
4	A	695	CIE	C6-C1-C7	4.48	127.86	118.66
6	A	700	AYD	PA-O7-C7	4.44	143.43	121.59
8	B	1702	TPP	C7'-N3-C2	-4.38	117.44	125.35
8	B	1702	TPP	C6'-N1'-C2'	4.20	123.11	115.96
4	A	695	CIE	C4'-N3'-C2'	4.15	118.08	114.69
8	B	1702	TPP	PA-O7-C7	4.15	142.01	121.59
4	B	1695	CIE	C6-C1-C7	4.09	127.06	118.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1698	DTT	O3-C3-C2	-4.09	101.33	109.72
5	A	698	DTT	O3-C3-C2	-3.95	101.61	109.72
6	A	700	AYD	C6'-N1'-C2'	3.80	122.43	115.96
6	A	700	AYD	C5'-C7'-N3	3.72	120.89	113.03
4	B	1695	CIE	O8-C7-C1	-3.68	104.92	112.21
4	B	1695	CIE	C4'-N3'-C2'	3.65	117.67	114.69
8	B	1702	TPP	N1'-C2'-N3'	-3.62	119.31	125.54
4	B	1695	CIE	N12-C13-N14	3.59	119.68	114.93
4	A	695	CIE	C5'-C4'-N3'	-3.58	121.57	125.50
4	B	1695	CIE	C5'-C4'-N3'	-3.50	121.66	125.50
6	A	700	AYD	C7'-N3-C4	-3.45	118.63	125.39
4	A	695	CIE	O8-C7-C1	-3.30	105.68	112.21
6	A	700	AYD	N1'-C2'-N3'	-3.18	120.06	125.54
5	A	698	DTT	C2-C1-S1	3.02	123.24	114.47
4	A	695	CIE	OBB-S11-N12	-2.99	98.33	106.74
4	B	1695	CIE	OBB-S11-N12	-2.92	98.54	106.74
7	B	1701	FAD	C9-C9A-N10	2.82	125.65	121.84
8	B	1702	TPP	C2'-N3'-C4'	2.73	122.33	118.08
4	A	695	CIE	N12-C13-N14	2.71	118.52	114.93
8	B	1702	TPP	C5'-C6'-N1'	-2.71	119.31	123.82
7	A	701	FAD	O2-C2-N1	-2.68	117.39	121.83
7	A	701	FAD	C9-C9A-N10	2.66	125.43	121.84
5	B	1698	DTT	C2-C1-S1	2.61	122.06	114.47
6	A	700	AYD	C2'-N3'-C4'	2.54	122.04	118.08
7	B	1701	FAD	O2-C2-N1	-2.48	117.71	121.83
6	A	700	AYD	C5'-C6'-N1'	-2.37	119.87	123.82
4	B	1695	CIE	N14-C2'-N3'	2.30	123.20	116.46
5	A	698	DTT	O2-C2-C3	-2.15	105.31	109.72
5	B	1698	DTT	O2-C2-C3	-2.11	105.39	109.72
4	B	1695	CIE	C5'-C6'-N1'	-2.06	121.67	124.08
7	A	701	FAD	C5'-C4'-C3'	-2.06	108.22	112.20
4	A	695	CIE	N14-C2'-N3'	2.06	122.49	116.46

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	695	CIE	N12-C13-N14-C2'
4	B	1695	CIE	C1-C2-S11-OBA
4	B	1695	CIE	N12-C13-N14-C2'
5	A	698	DTT	S1-C1-C2-C3
5	B	1698	DTT	S1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
6	A	700	AYD	C4'-C5'-C7'-N3
6	A	700	AYD	C5-C4-N3-C7'
6	A	700	AYD	CM4-C4-N3-C7'
6	A	700	AYD	N3-C4-C5-C6
6	A	700	AYD	C4-C5-C6-C7
6	A	700	AYD	C6-C7-O7-PA
8	B	1702	TPP	C4'-C5'-C7'-N3
4	B	1695	CIE	O7-C7-O8-C9
4	A	695	CIE	O7-C7-O8-C9
4	A	695	CIE	C1-C2-S11-OBA
4	A	695	CIE	C3-C2-S11-N12
4	B	1695	CIE	C3-C2-S11-N12
4	A	695	CIE	C1-C2-S11-OBB
4	B	1695	CIE	C1-C2-S11-OBB
4	A	695	CIE	C1-C2-S11-N12
4	B	1695	CIE	C1-C2-S11-N12
6	A	700	AYD	C5-C6-C7-O7
6	A	700	AYD	PB-O3A-PA-O7
4	B	1695	CIE	C3-C2-S11-OBA
4	A	695	CIE	C3-C2-S11-OBA
5	A	698	DTT	S1-C1-C2-O2
5	B	1698	DTT	S1-C1-C2-O2
4	A	695	CIE	O13-C13-N14-C2'
4	B	1695	CIE	O13-C13-N14-C2'
4	B	1695	CIE	C3-C2-S11-OBB
4	A	695	CIE	C3-C2-S11-OBB
7	A	701	FAD	O4B-C4B-C5B-O5B
7	B	1701	FAD	O4B-C4B-C5B-O5B

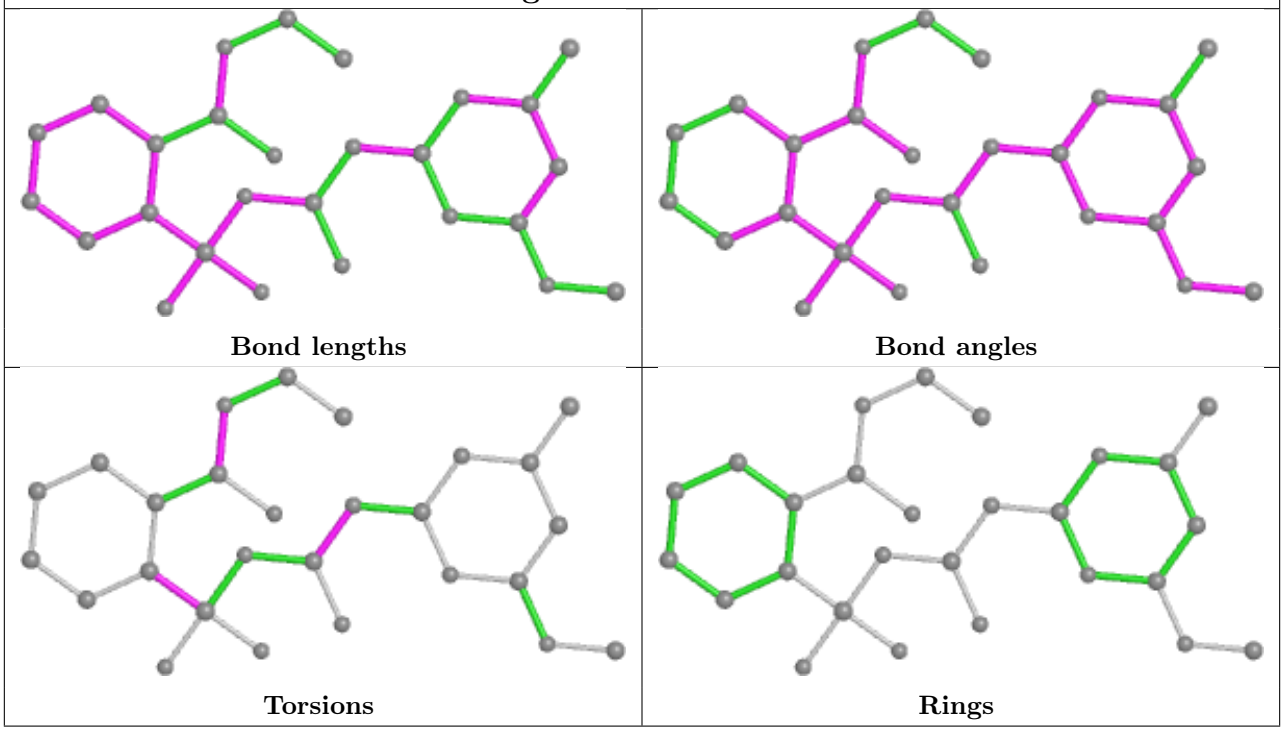
There are no ring outliers.

8 monomers are involved in 29 short contacts:

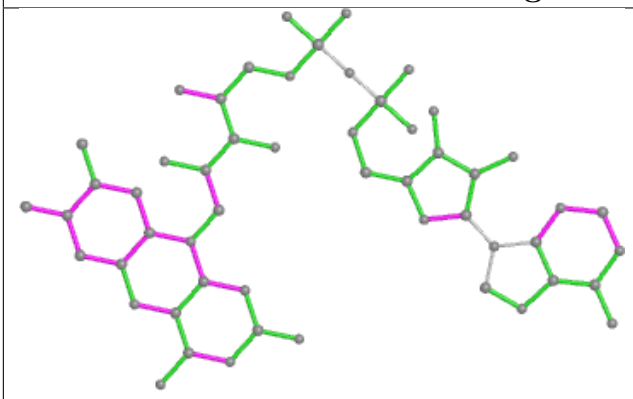
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1695	CIE	5	0
5	A	698	DTT	2	0
7	A	701	FAD	1	0
4	A	695	CIE	4	0
7	B	1701	FAD	3	0
8	B	1702	TPP	8	0
6	A	700	AYD	5	0
5	B	1698	DTT	3	0

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.

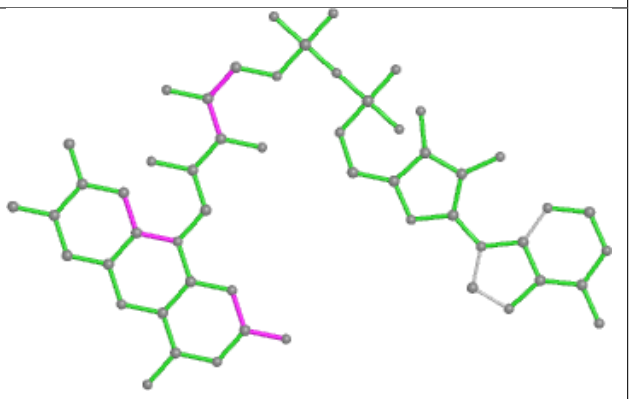
Ligand CIE B 1695



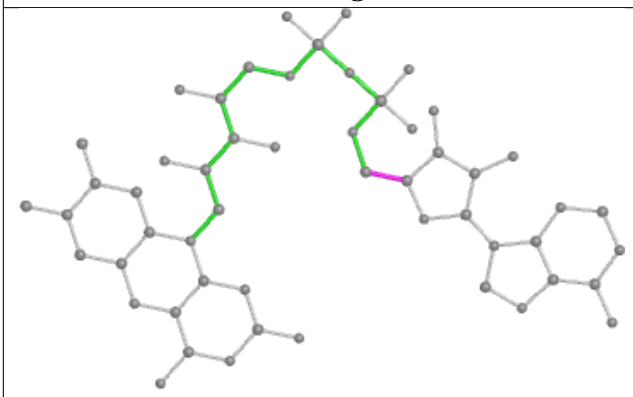
Ligand FAD A 701



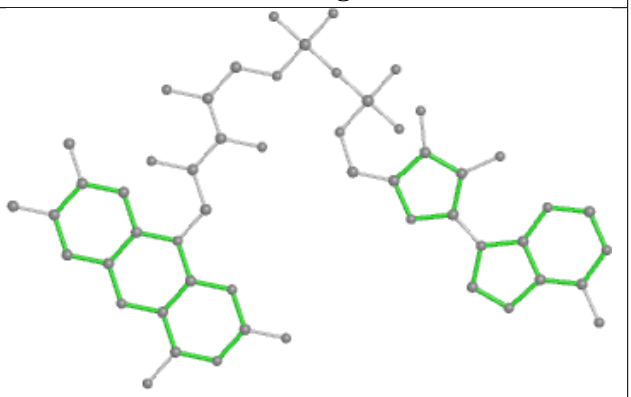
Bond lengths



Bond angles

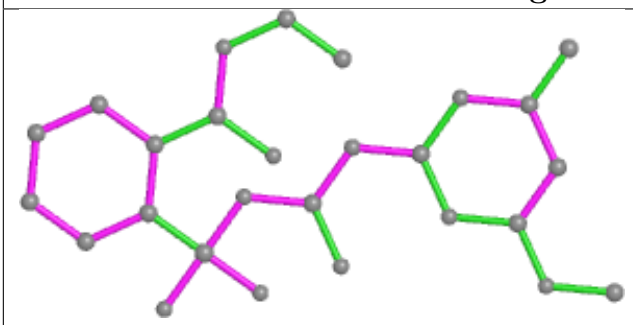


Torsions

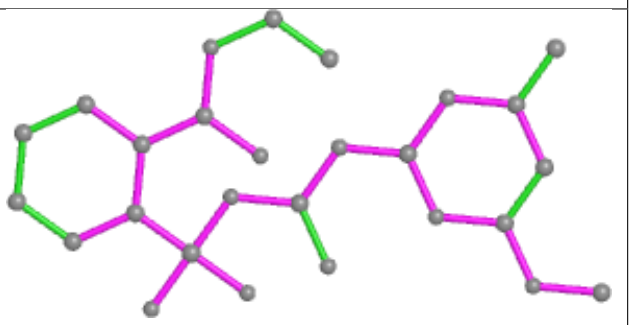


Rings

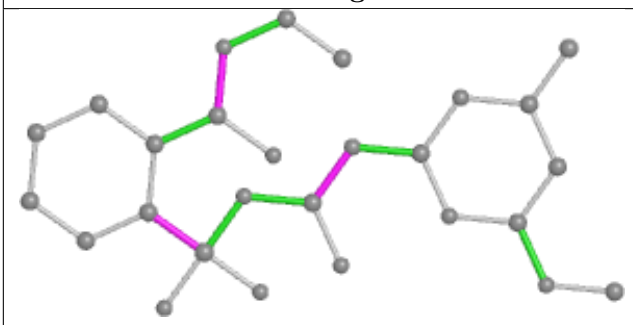
Ligand CIE A 695



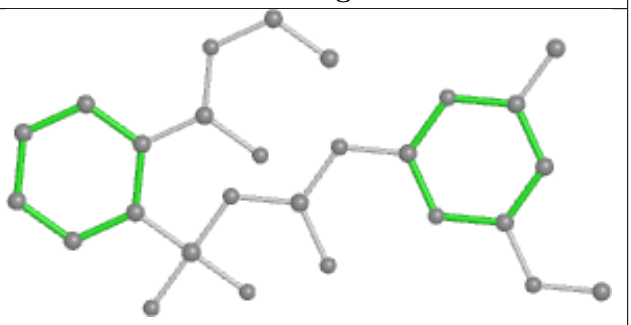
Bond lengths



Bond angles

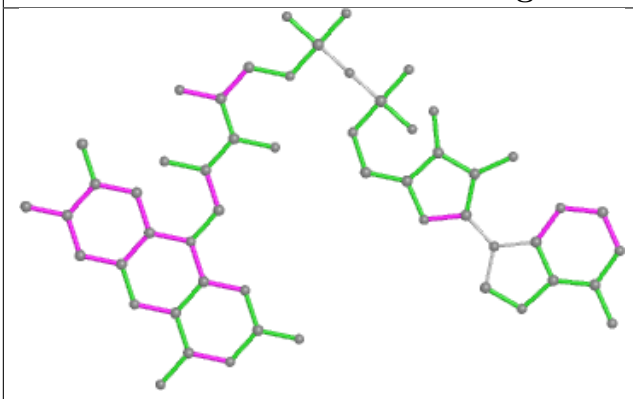


Torsions

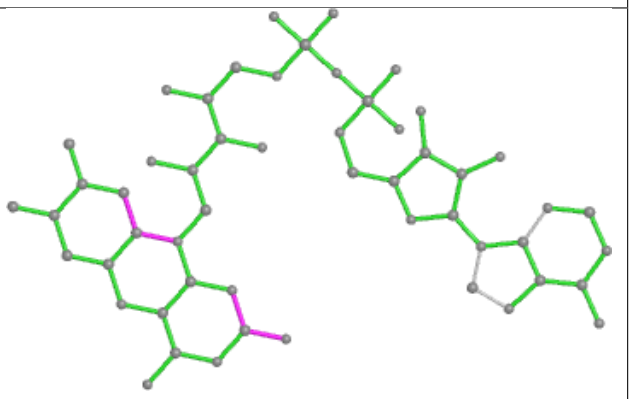


Rings

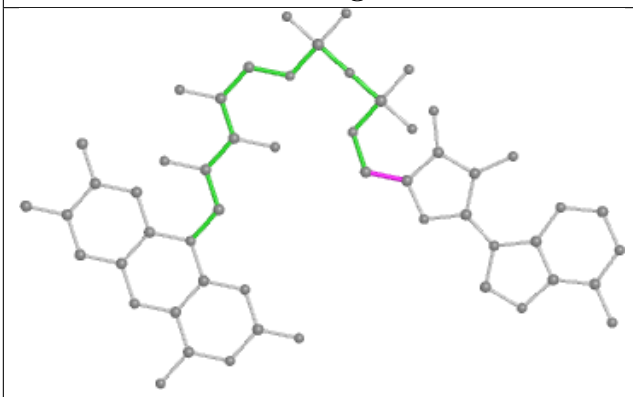
Ligand FAD B 1701



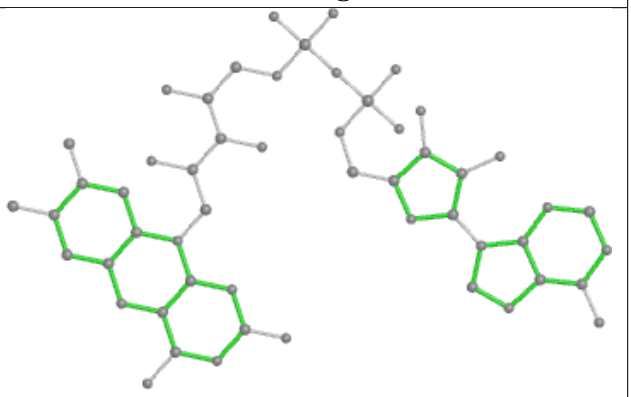
Bond lengths



Bond angles

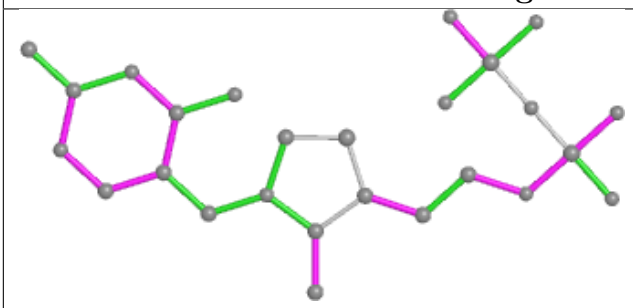


Torsions

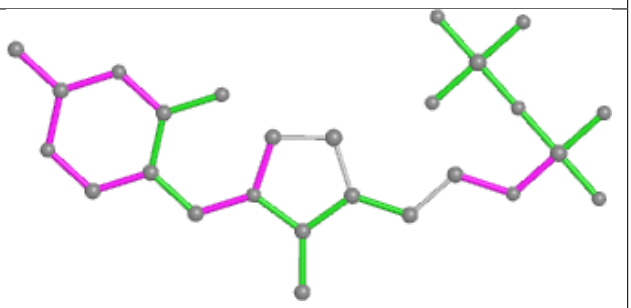


Rings

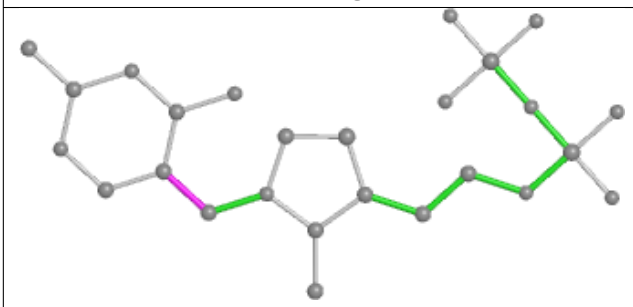
Ligand TPP B 1702



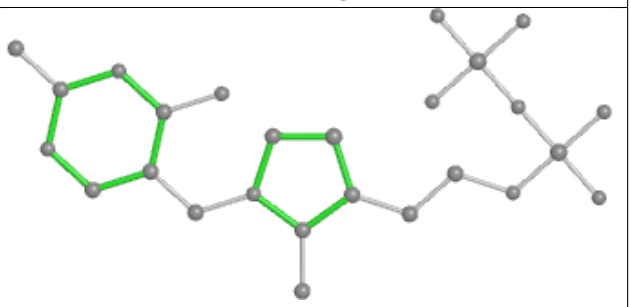
Bond lengths



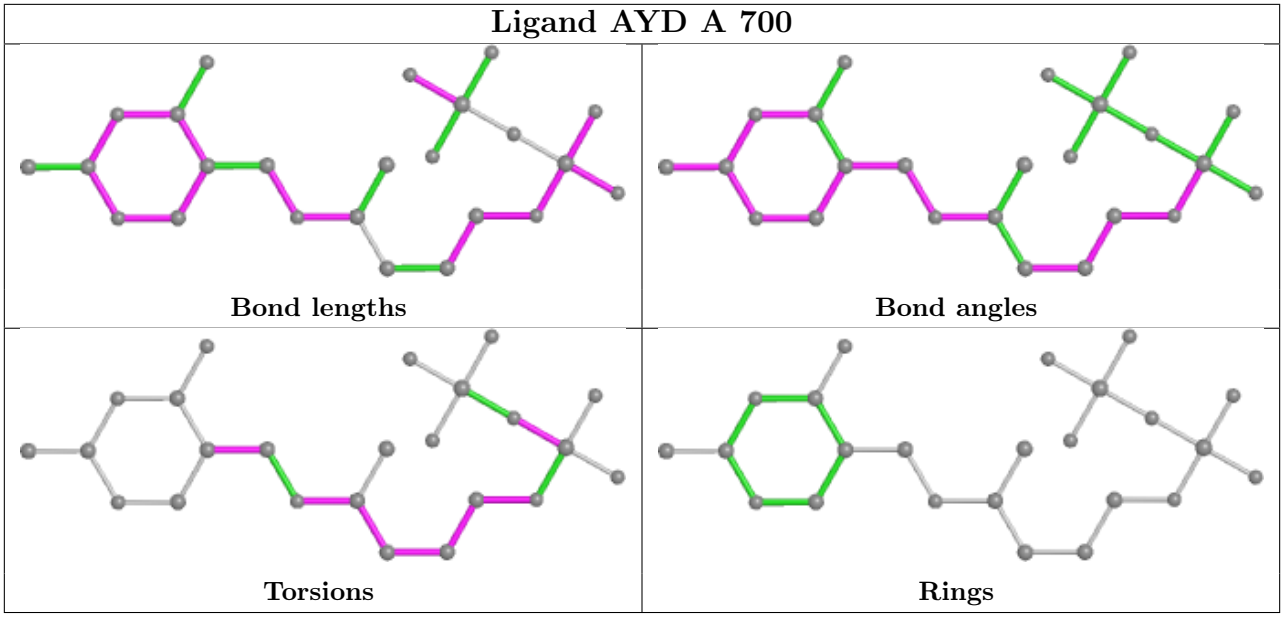
Bond angles



Torsions



Rings



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	599/677 (88%)	-0.39	4 (0%)	87	84	7, 20, 42, 85	0
1	B	598/677 (88%)	0.14	9 (1%)	73	68	14, 35, 70, 101	0
All	All	1197/1354 (88%)	-0.13	13 (1%)	80	75	7, 25, 64, 101	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	260	ASN	3.6
1	A	83	PRO	3.4
1	B	270	SER	3.1
1	A	270	SER	2.9
1	A	277	THR	2.6
1	B	259	ARG	2.6
1	B	268	LEU	2.5
1	B	264	THR	2.4
1	B	265	LYS	2.2
1	B	467	PRO	2.2
1	B	468	GLY	2.1
1	A	600	GLN	2.1
1	B	674	GLN	2.0

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)

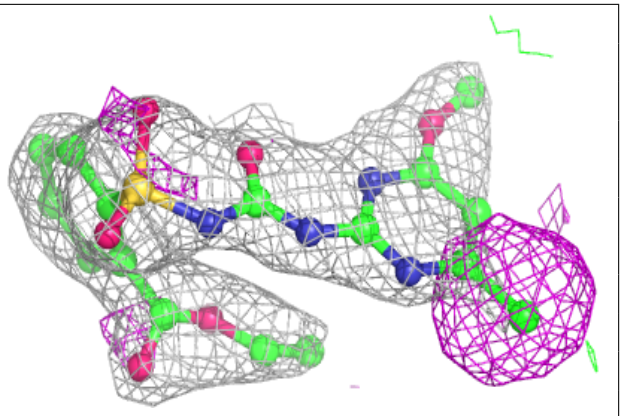
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

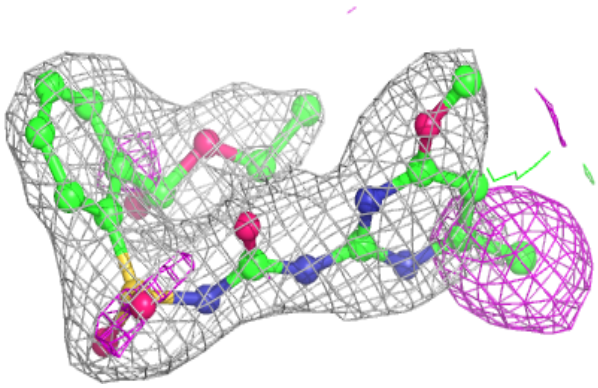
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DTT	B	1698	8/8	0.82	0.40	76,86,89,93	5
5	DTT	A	698	8/8	0.86	0.30	48,57,59,65	2
4	CIE	B	1695	27/27	0.90	0.27	41,46,51,51	0
4	CIE	A	695	27/27	0.92	0.20	19,24,27,31	0
8	TPP	B	1702	26/26	0.96	0.24	32,39,46,46	2
3	MG	B	1699	1/1	0.97	0.07	25,25,25,25	0
7	FAD	B	1701	53/53	0.97	0.19	29,32,40,41	0
2	K	B	1696	1/1	0.97	0.07	42,42,42,42	0
6	AYD	A	700	24/24	0.98	0.20	16,41,47,47	0
7	FAD	A	701	53/53	0.99	0.16	5,11,14,15	0
2	K	A	696	1/1	0.99	0.08	18,18,18,18	0
3	MG	A	699	1/1	0.99	0.07	2,2,2,2	0

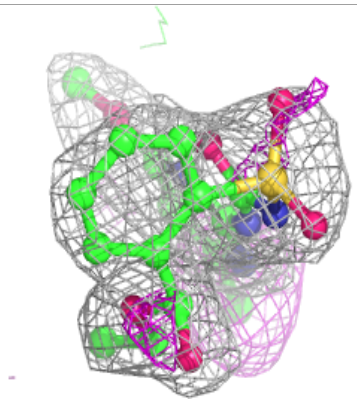
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CIE B 1695:

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

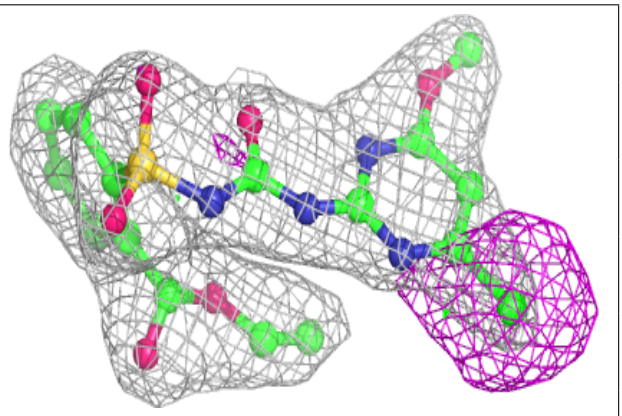


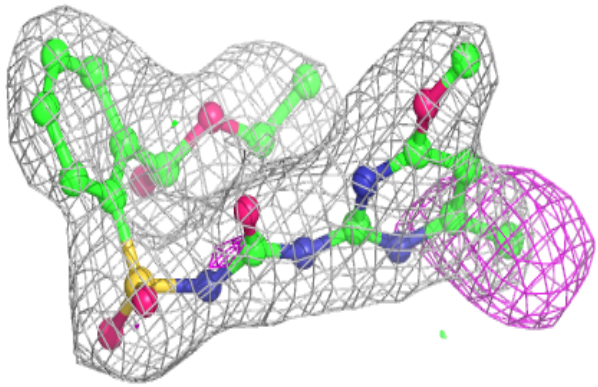


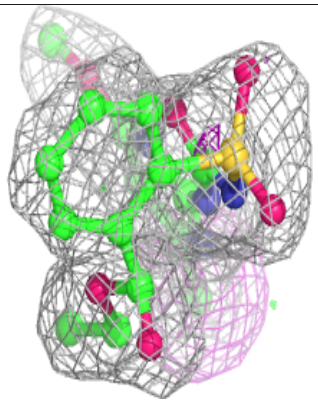


Electron density around CIE A 695:

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

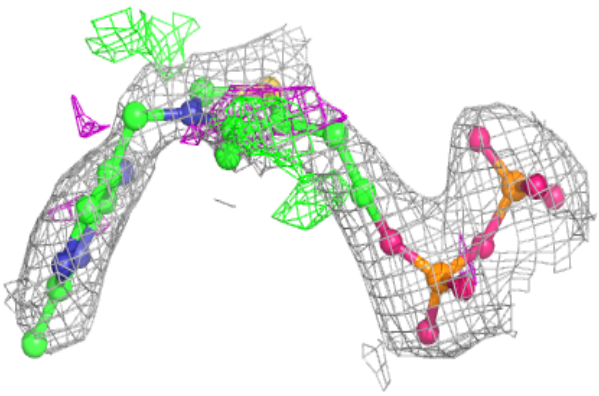


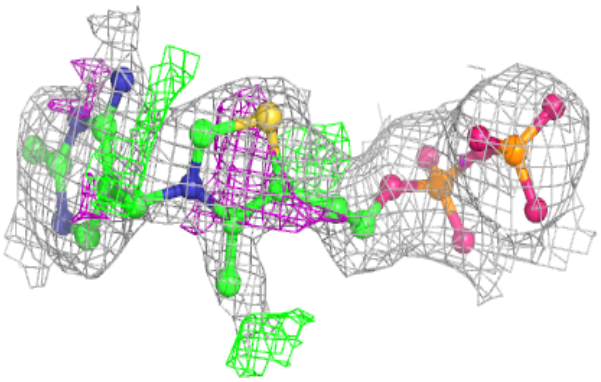


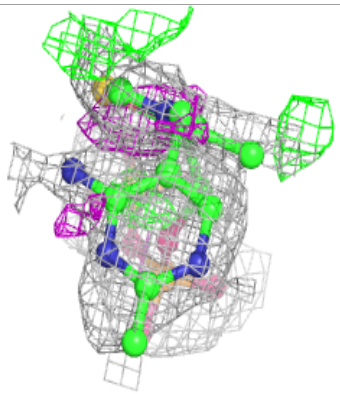


Electron density around TPP B 1702:

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

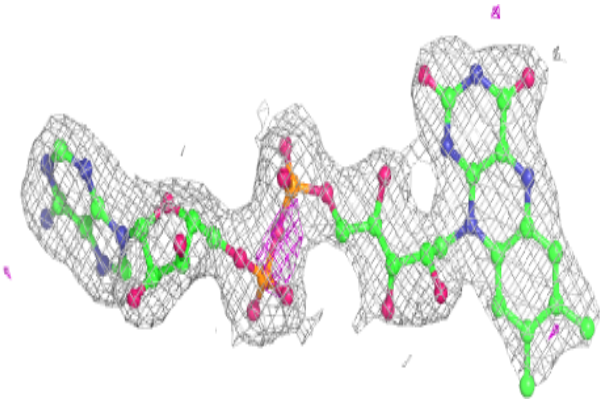


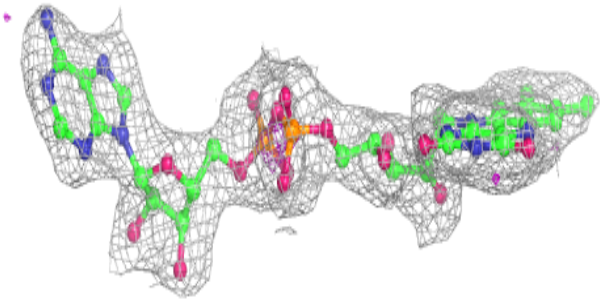


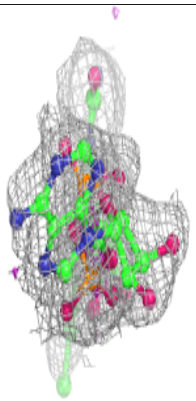


Electron density around FAD B 1701:

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

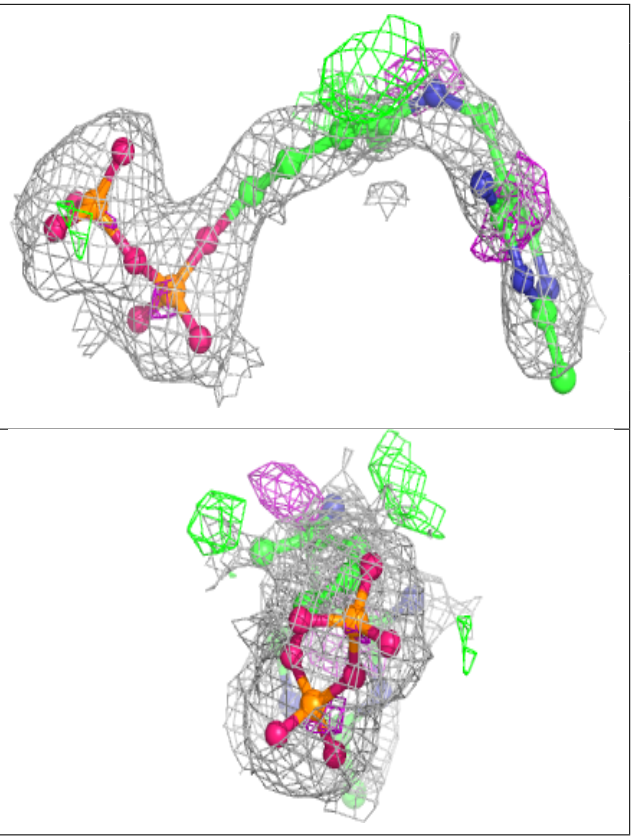


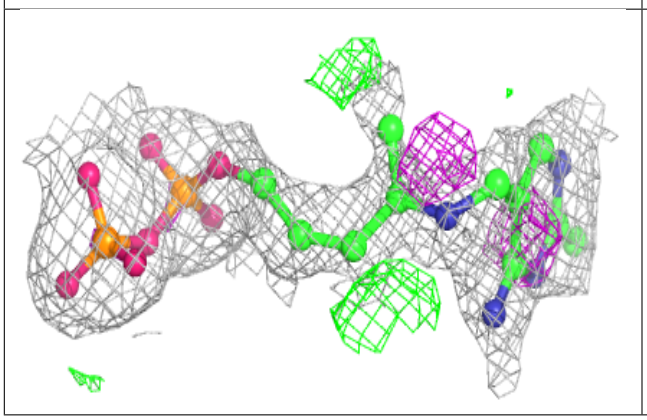




Electron density around AYD A 700:

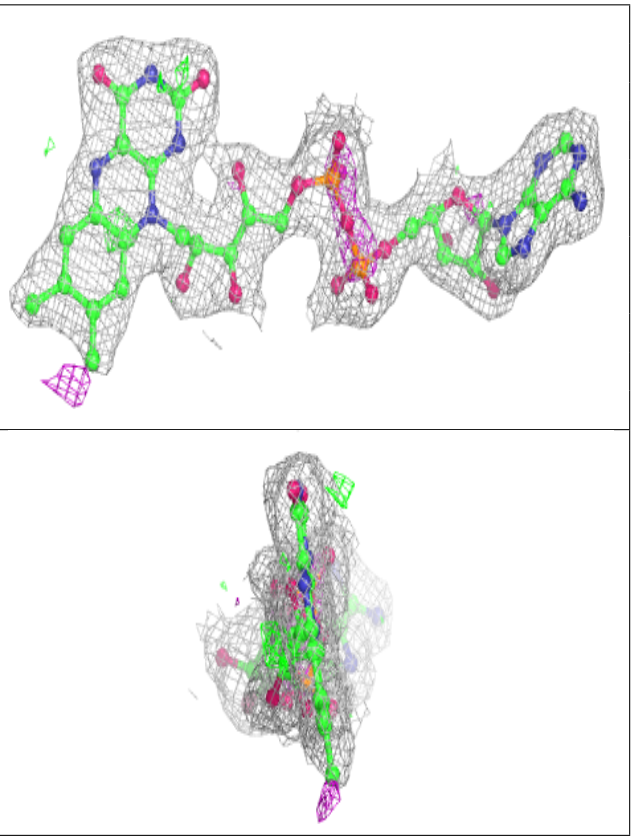
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

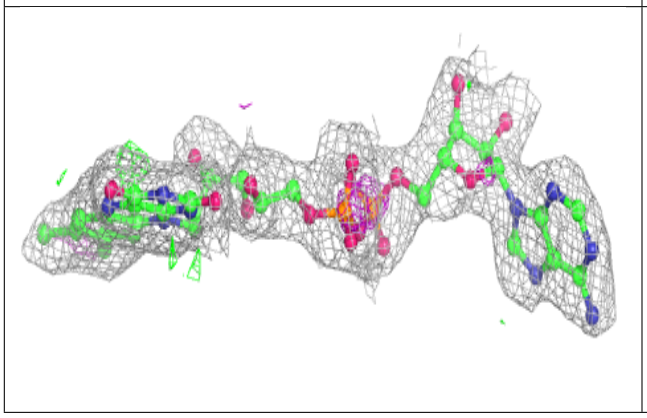




Electron density around FAD A 701:

$2mF_o$-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.