Full wwPDB X-ray Structure Validation Report (i)

Jul 26, 2023 – 05:01 AM EDT

PDB ID	:	1A4L
Title	:	ADA STRUCTURE COMPLEXED WITH DEOXYCOFORMYCIN AT PH 7.0
Authors	:	Wang, Z.; Quiocho, F.A.
Deposited on	:	1998-01-31
Resolution	:	2.60 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:

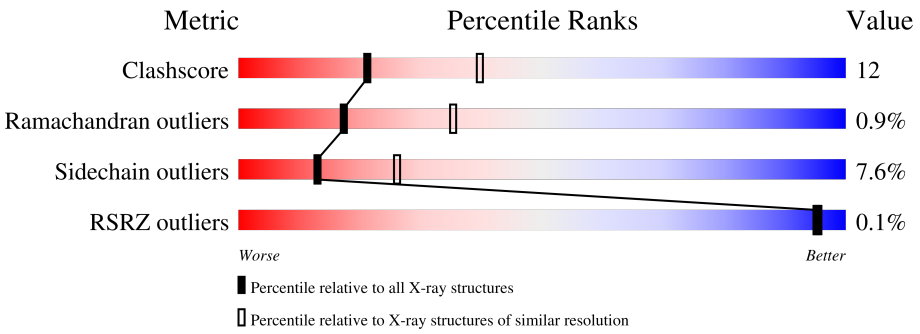
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	349	70% 25% •
1	B	349	69% 27% •
1	C	349	68% 28% •
1	D	349	67% 31% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11473 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.

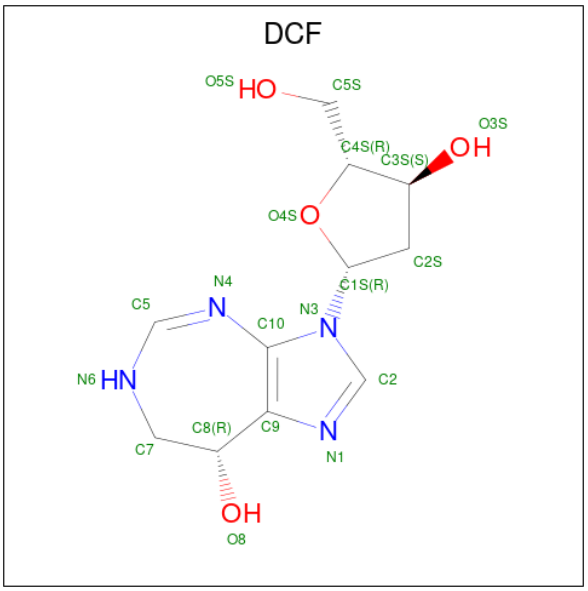
- Molecule 1 is a protein called ADENOSINE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	349	2790	1778	470	528	14	0	0	0
1	B	349	2790	1778	470	528	14	0	0	0
1	C	349	2790	1778	470	528	14	0	0	0
1	D	349	2790	1778	470	528	14	0	0	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 is 2'-DEOXYCOFORMYCIN (three-letter code: DCF) (formula: $C_{11}H_{16}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	19	11	4	4	0	0
3	B	1	19	11	4	4	0	0
3	C	1	19	11	4	4	0	0
3	D	1	19	11	4	4	0	0

- Molecule 4 is water.

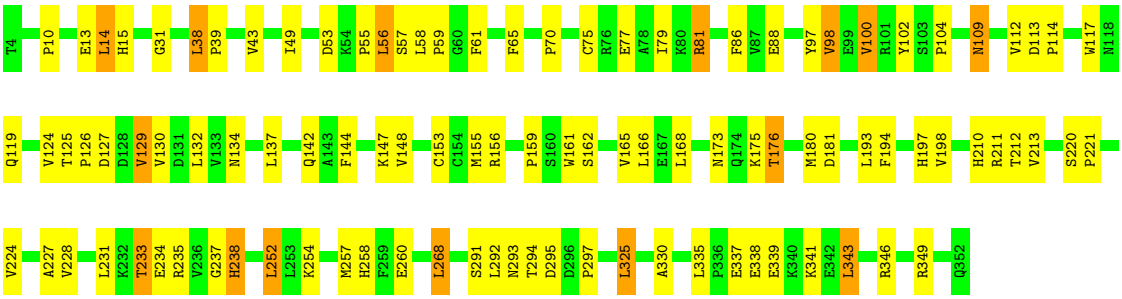
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	54	54	54	0	0
4	B	53	53	53	0	0
4	C	46	46	46	0	0
4	D	80	80	80	0	0

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.

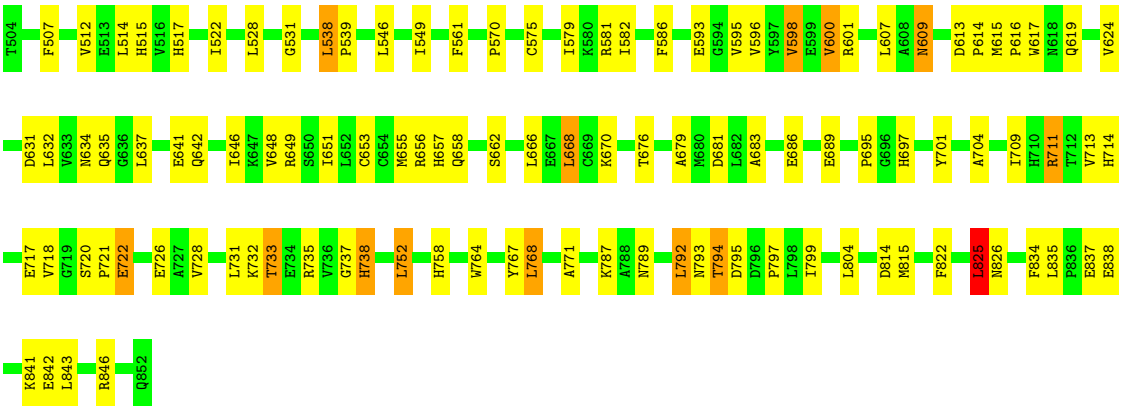
• Molecule 1: ADENOSINE DEAMINASE

Chain A: 70% 25% •



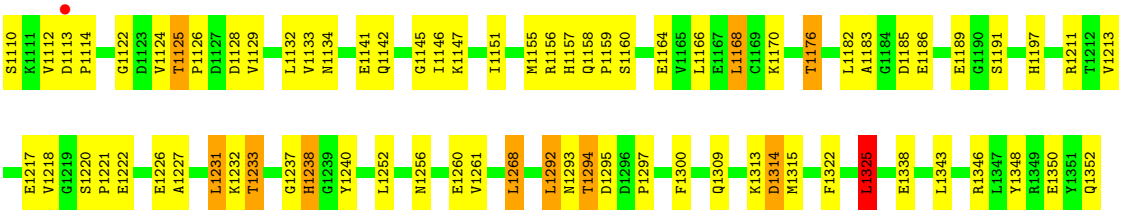
• Molecule 1: ADENOSINE DEAMINASE

Chain B: 69% 27% •



• Molecule 1: ADENOSINE DEAMINASE

Chain C: 68% 28% •



- Molecule 1: ADENOSINE DEAMINASE

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.93Å 93.36Å 101.95Å 90.00° 102.94° 90.00°	Depositor
Resolution (Å)	8.00 – 2.60 19.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.0 (8.00-2.60) 92.0 (19.92-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 2.59Å)	Xtriage
Refinement program	X-PLOR 3.85	Depositor
R, R_{free}	0.185 , 0.272 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	18.9	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11473	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 62.55 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1066e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: ZN, DCF

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	0.42	0/2854	0.69	1/3863 (0.0%)
1	B	0.43	0/2854	0.69	1/3863 (0.0%)
1	C	0.42	0/2854	0.69	1/3863 (0.0%)
1	D	0.42	0/2854	0.71	2/3863 (0.1%)
All	All	0.42	0/11416	0.70	5/15452 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1325	LEU	CA-CB-CG	7.39	132.31	115.30
1	A	325	LEU	CA-CB-CG	7.24	131.95	115.30
1	D	1825	LEU	CA-CB-CG	6.58	130.44	115.30
1	B	825	LEU	CA-CB-CG	6.36	129.93	115.30
1	D	1675	LYS	N-CA-C	-5.09	97.27	111.00

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	2790	0	2757	67	0
1	B	2790	0	2757	72	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2790	0	2757	65	0
1	D	2790	0	2757	70	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	19	0	15	1	0
3	B	19	0	15	1	0
3	C	19	0	15	3	0
3	D	19	0	15	2	0
4	A	54	0	0	3	0
4	B	53	0	0	1	0
4	C	46	0	0	2	0
4	D	80	0	0	0	0
All	All	11473	0	11088	271	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 12.

All (271) 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:528:LEU:HD13	1:B:546:LEU:HD22	1.51	0.93
1:D:1613:ASP:HB3	1:D:1614:PRO:HD3	1.55	0.89
1:C:1039:PRO:HB2	1:C:1049:ILE:HD13	1.63	0.81
1:A:113:ASP:HB3	1:A:114:PRO:HD3	1.63	0.80
1:B:837:GLU:O	1:B:841:LYS:HG2	1.86	0.76
1:C:1028:LEU:HD13	1:C:1046:LEU:HD22	1.69	0.74
1:A:109:ASN:HD21	1:A:124:VAL:H	1.35	0.73
1:B:539:PRO:HB2	1:B:549:ILE:HD13	1.68	0.73
1:C:1113:ASP:HB3	1:C:1114:PRO:HD3	1.68	0.72
1:D:1720:SER:HB2	1:D:1721:PRO:HD2	1.71	0.72
1:C:1157:HIS:CD2	1:C:1158:GLN:HG2	2.25	0.72
1:B:794:THR:HG21	1:B:797:PRO:HG3	1.72	0.71
1:D:1625:THR:HG22	1:D:1626:PRO:HD2	1.72	0.71
1:B:613:ASP:HB3	1:B:614:PRO:HD3	1.70	0.71
1:A:13:GLU:OE2	1:A:294:THR:HG22	1.89	0.70
1:B:794:THR:CG2	1:B:797:PRO:HG3	2.22	0.69
1:C:1095:VAL:HG11	1:C:1098:VAL:HG22	1.75	0.69
1:D:1837:GLU:O	1:D:1841:LYS:HG2	1.93	0.69
1:A:337:GLU:O	1:A:341:LYS:HG2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:792:LEU:HD22	1:B:825:LEU:HD11	1.76	0.68
1:A:39:PRO:HB2	1:A:49:ILE:HD13	1.78	0.66
1:C:1109:ASN:HD21	1:C:1124:VAL:H	1.42	0.65
1:A:213:VAL:HG23	1:A:233:THR:HG23	1.79	0.64
1:C:1227:ALA:HA	1:C:1231:LEU:HB2	1.78	0.64
1:D:1809:GLN:HB3	1:D:1813:LYS:HE3	1.80	0.64
1:D:1750:ASN:O	1:D:1754:LYS:HB2	1.98	0.63
1:C:1095:VAL:CG1	1:C:1098:VAL:HG22	2.29	0.62
1:D:1631:ASP:O	1:D:1635:GLN:HG3	2.00	0.62
1:D:1735:ARG:HH21	1:D:1833:SER:HA	1.65	0.61
1:C:1145:GLY:HA2	4:C:2172:HOH:O	2.01	0.61
1:D:1609:ASN:HD21	1:D:1624:VAL:H	1.47	0.61
1:B:570:PRO:HG3	1:B:617:TRP:HB3	1.81	0.61
1:B:514:LEU:H	1:B:793:ASN:HD21	1.46	0.61
1:D:1634:ASN:ND2	1:D:1676:THR:OG1	2.34	0.61
1:C:1268:LEU:HD23	1:C:1300:PHE:CD1	2.35	0.61
1:C:1134:ASN:ND2	1:C:1176:THR:OG1	2.34	0.60
1:A:13:GLU:HG3	1:A:293:ASN:HD22	1.66	0.60
1:D:1713:VAL:HB	1:D:1733:THR:HG21	1.82	0.59
1:D:1802:SER:HB2	1:D:1806:THR:OG1	2.02	0.58
1:D:1758:HIS:HA	1:D:1789:ASN:O	2.02	0.58
1:B:596:VAL:HG11	1:B:846:ARG:NH1	2.17	0.58
1:A:58:LEU:HB3	1:A:59:PRO:HD3	1.85	0.58
1:A:159:PRO:HG3	1:A:194:PHE:HD2	1.69	0.57
1:A:224:VAL:O	1:A:228:VAL:HG23	2.03	0.57
1:A:70:PRO:HG3	1:A:117:TRP:HB3	1.87	0.57
1:A:292:LEU:HD13	1:A:325:LEU:HD11	1.87	0.57
1:D:1657:HIS:CD2	1:D:1658:GLN:HG2	2.38	0.57
1:A:198:VAL:HG11	1:C:1043:VAL:HG21	1.85	0.57
1:B:561:PHE:CD1	1:B:799:ILE:HG21	2.40	0.57
1:C:1047:ARG:HD3	4:C:2153:HOH:O	2.05	0.57
1:D:1662:SER:OG	1:D:1697:HIS:HD2	1.88	0.57
1:A:125:THR:HG22	1:A:127:ASP:H	1.69	0.56
1:D:1514:LEU:H	1:D:1793:ASN:ND2	2.04	0.56
1:D:1848:TYR:O	1:D:1852:GLN:HG2	2.05	0.56
1:C:1294:THR:CG2	1:C:1297:PRO:HG3	2.35	0.56
1:D:1821:GLU:O	1:D:1825:LEU:HD13	2.06	0.56
1:C:1126:PRO:O	1:C:1129:VAL:HG22	2.06	0.55
1:D:1768:LEU:HD23	1:D:1800:PHE:CD1	2.41	0.55
1:C:1166:LEU:HG	1:C:1170:LYS:HE3	1.88	0.55
1:B:722:GLU:O	1:B:726:GLU:HG3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:PHE:HD1	1:B:799:ILE:HG21	1.71	0.55
1:A:220:SER:HB2	1:A:221:PRO:HD2	1.89	0.55
1:A:31:GLY:HA3	1:A:38:LEU:CD2	2.37	0.55
1:D:1512:VAL:H	1:D:1826:ASN:ND2	2.04	0.55
1:A:125:THR:HG23	1:A:126:PRO:HD2	1.89	0.54
1:B:655:MET:CE	1:B:683:ALA:HB3	2.37	0.54
1:A:14:LEU:H	1:A:293:ASN:HD21	1.55	0.54
1:B:609:ASN:HD21	1:B:624:VAL:H	1.55	0.54
1:B:655:MET:HE2	1:B:683:ALA:HB3	1.90	0.54
1:C:1129:VAL:O	1:C:1133:VAL:HG23	2.06	0.54
1:A:162:SER:OG	1:A:197:HIS:HD2	1.91	0.53
1:B:641:GLU:HG3	1:B:646:ILE:O	2.08	0.53
1:D:1649:ARG:HD3	1:D:1676:THR:HA	1.89	0.53
1:D:1737:GLY:O	1:D:1738:HIS:HB2	2.09	0.53
1:C:1294:THR:HG21	1:C:1297:PRO:HG3	1.89	0.53
1:C:1348:TYR:O	1:C:1352:GLN:HG2	2.08	0.53
1:D:1539:PRO:HB2	1:D:1549:ILE:HD13	1.90	0.53
1:B:593:GLU:OE1	1:B:804:LEU:HB2	2.08	0.53
1:C:1222:GLU:O	1:C:1226:GLU:HG3	2.08	0.53
1:A:97:TYR:HD1	1:A:147:LYS:HB3	1.74	0.52
1:B:679:ALA:HB2	1:B:834:PHE:CD2	2.44	0.52
1:A:65:PHE:CZ	3:A:353:DCF:H2S2	2.45	0.52
1:B:662:SER:OG	1:B:697:HIS:HD2	1.93	0.52
1:C:1110:SER:O	1:C:1126:PRO:HD3	2.10	0.52
1:D:1514:LEU:H	1:D:1793:ASN:HD21	1.57	0.52
1:A:13:GLU:HB3	1:A:98:VAL:HG13	1.92	0.52
1:A:109:ASN:C	1:A:109:ASN:HD22	2.12	0.52
1:B:814:ASP:O	1:B:815:MET:HB2	2.10	0.52
1:A:31:GLY:HA3	1:A:38:LEU:HD21	1.91	0.52
1:B:631:ASP:O	1:B:635:GLN:HG3	2.09	0.52
1:C:1240:TYR:HE1	1:C:1261:VAL:HG13	1.75	0.52
1:C:1309:GLN:HB3	1:C:1313:LYS:HE3	1.91	0.52
1:C:1013:GLU:HG3	1:C:1293:ASN:HD22	1.75	0.52
1:B:657:HIS:CD2	1:B:658:GLN:HG2	2.45	0.52
1:D:1611:LYS:HB2	1:D:1625:THR:HG23	1.91	0.52
1:C:1237:GLY:O	1:C:1238:HIS:HB2	2.10	0.51
1:A:126:PRO:O	1:A:129:VAL:HG22	2.10	0.51
1:A:335:LEU:HG	1:A:339:GLU:HB2	1.91	0.51
1:C:1156:ARG:HD3	1:C:1191:SER:OG	2.10	0.51
1:B:609:ASN:HD22	1:B:609:ASN:C	2.14	0.51
1:B:713:VAL:HB	1:B:733:THR:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1065:PHE:CZ	3:C:1353:DCF:H2S2	2.46	0.51
1:C:1141:GLU:HG3	1:C:1146:ILE:O	2.10	0.51
1:D:1603:SER:HB2	1:D:1655:MET:HE3	1.91	0.50
1:B:656:ARG:HA	1:B:697:HIS:CE1	2.45	0.50
1:A:14:LEU:H	1:A:293:ASN:ND2	2.09	0.50
1:B:737:GLY:O	1:B:738:HIS:HB2	2.11	0.50
1:A:109:ASN:ND2	1:A:124:VAL:H	2.05	0.50
1:D:1666:LEU:HG	1:D:1670:LYS:HE3	1.93	0.50
1:B:728:VAL:HG11	1:B:752:LEU:HD11	1.93	0.50
1:C:1213:VAL:CG2	1:C:1233:THR:HG21	2.42	0.50
1:B:522:ILE:HG23	1:B:582:ILE:HG22	1.94	0.49
1:D:1595:VAL:HG11	1:D:1598:VAL:HG22	1.94	0.49
1:D:1641:GLU:HG3	1:D:1646:ILE:O	2.13	0.49
1:C:1213:VAL:HB	1:C:1233:THR:HG21	1.95	0.49
1:A:198:VAL:CG1	1:C:1043:VAL:HG21	2.43	0.49
1:B:586:PHE:CZ	1:B:600:VAL:HG13	2.48	0.49
1:B:681:ASP:OD2	1:B:714:HIS:HE1	1.96	0.49
1:B:515:HIS:H	1:B:793:ASN:ND2	2.11	0.48
1:D:1635:GLN:O	1:D:1639:GLU:HG3	2.12	0.48
1:D:1838:GLU:O	1:D:1842:GLU:HG3	2.13	0.48
1:B:575:CYS:O	1:B:579:ILE:HG13	2.14	0.48
1:C:1015:HIS:HB2	1:C:1260:GLU:HB3	1.93	0.48
1:D:1626:PRO:O	1:D:1630:VAL:HG23	2.13	0.48
1:B:531:GLY:HA3	1:B:538:LEU:CD2	2.44	0.48
1:A:294:THR:OG1	1:A:297:PRO:HG3	2.13	0.48
1:C:1155:MET:HE2	1:C:1183:ALA:HB3	1.95	0.48
1:D:1666:LEU:HD22	1:D:1700:ALA:O	2.13	0.48
1:D:1825:LEU:HA	1:D:1828:ASN:HB2	1.96	0.48
1:C:1322:PHE:HA	1:C:1325:LEU:HD13	1.95	0.48
1:D:1754:LYS:HB3	1:D:1754:LYS:HE2	1.68	0.48
1:C:1220:SER:HB2	1:C:1221:PRO:HD2	1.96	0.47
1:D:1558:LEU:HD11	3:D:1853:DCF:H72	1.96	0.47
1:A:237:GLY:O	1:A:238:HIS:HB2	2.14	0.47
1:D:1666:LEU:HB2	1:D:1680:MET:HE1	1.95	0.47
1:D:1609:ASN:HB3	1:D:1619:GLN:NE2	2.30	0.47
1:B:794:THR:HG23	1:B:797:PRO:HG3	1.96	0.47
1:D:1556:LEU:HB3	1:D:1557:SER:H	1.49	0.47
1:D:1570:PRO:HG3	1:D:1617:TRP:HB3	1.96	0.47
1:D:1706:LYS:NZ	1:D:1707:ASN:HD21	2.12	0.47
1:A:15:HIS:H	1:A:293:ASN:ND2	2.12	0.47
1:B:717:GLU:O	1:B:771:ALA:HB1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1097:TYR:HD1	1:C:1147:LYS:HB3	1.79	0.47
1:C:1346:ARG:HG2	1:C:1350:GLU:OE2	2.15	0.47
1:D:1601:ARG:HA	1:D:1651:ILE:O	2.15	0.47
1:A:102:TYR:OH	1:A:130:VAL:HA	2.14	0.46
1:A:237:GLY:HA2	1:A:260:GLU:HB2	1.98	0.46
1:C:1078:ALA:O	1:C:1082:ILE:HG23	2.15	0.46
1:C:1109:ASN:HD21	1:C:1124:VAL:N	2.10	0.46
1:D:1522:ILE:HD13	1:D:1572:ILE:HG13	1.96	0.46
1:C:1217:GLU:OE2	3:C:1353:DCF:H71	2.15	0.46
1:D:1625:THR:HG22	1:D:1626:PRO:CD	2.43	0.46
1:C:1101:ARG:HA	1:C:1151:ILE:O	2.16	0.46
1:C:1211:ARG:NH1	1:C:1232:LYS:O	2.48	0.46
1:A:156:ARG:HA	1:A:197:HIS:CE1	2.51	0.46
1:B:732:LYS:NZ	1:D:1532:LYS:HZ3	2.14	0.46
1:D:1749:TYR:CE1	1:D:1753:LEU:HD13	2.51	0.46
1:D:1674:GLN:C	1:D:1676:THR:H	2.19	0.46
1:A:153:CYS:HB3	1:A:155:MET:CE	2.46	0.45
1:C:1109:ASN:ND2	1:C:1124:VAL:HB	2.32	0.45
1:B:515:HIS:N	1:B:793:ASN:ND2	2.65	0.45
1:B:528:LEU:CD1	1:B:546:LEU:HD22	2.33	0.45
1:D:1768:LEU:HD23	1:D:1800:PHE:HD1	1.82	0.45
1:A:137:LEU:HD22	1:A:148:VAL:HG11	1.98	0.45
1:B:515:HIS:H	1:B:793:ASN:HD22	1.64	0.45
1:B:735:ARG:HD3	1:B:758:HIS:CD2	2.52	0.45
1:D:1698:VAL:O	1:D:1702:GLU:HG3	2.17	0.45
1:C:1069:MET:N	1:C:1070:PRO:CD	2.80	0.45
1:C:1182:LEU:HB3	1:C:1213:VAL:HG13	1.99	0.45
1:A:134:ASN:ND2	1:A:176:THR:OG1	2.49	0.45
1:B:649:ARG:HD3	1:B:676:THR:HA	1.98	0.45
1:C:1090:LYS:HA	1:C:1090:LYS:HD3	1.80	0.45
1:A:55:PRO:HA	1:A:268:LEU:O	2.16	0.45
1:B:512:VAL:HG12	1:B:514:LEU:HD13	1.99	0.44
1:C:1156:ARG:HD2	1:C:1185:ASP:O	2.17	0.44
1:C:1058:LEU:HB3	1:C:1059:PRO:HD3	1.99	0.44
1:B:609:ASN:C	1:B:609:ASN:ND2	2.70	0.44
1:D:1659:PRO:HG3	1:D:1694:PHE:HD2	1.82	0.44
1:D:1625:THR:CG2	1:D:1626:PRO:HD2	2.44	0.44
1:C:1159:PRO:HG3	1:C:1197:HIS:CE1	2.52	0.44
1:B:613:ASP:O	1:B:615:MET:N	2.51	0.44
1:A:162:SER:OG	1:A:197:HIS:CD2	2.71	0.44
1:A:291:SER:HB2	4:A:2095:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1086:PHE:CE2	1:C:1100:VAL:HG22	2.53	0.43
1:A:109:ASN:C	1:A:109:ASN:ND2	2.71	0.43
1:A:338:GLU:HG3	4:A:2096:HOH:O	2.17	0.43
1:B:601:ARG:HB2	1:B:653:CYS:SG	2.58	0.43
1:C:1314:ASP:O	1:C:1315:MET:HB2	2.18	0.43
1:B:666:LEU:HG	1:B:670:LYS:HE3	2.00	0.43
1:D:1637:LEU:HD22	1:D:1648:VAL:HG11	1.99	0.43
1:A:330:ALA:HB1	1:A:343:LEU:HD13	2.00	0.43
1:B:512:VAL:H	1:B:826:ASN:ND2	2.15	0.43
1:B:704:ALA:HB1	1:B:709:ILE:HB	2.00	0.43
1:A:210:HIS:HA	1:A:234:GLU:OE2	2.19	0.43
1:A:213:VAL:HB	1:A:233:THR:HG21	2.00	0.43
1:D:1558:LEU:HB3	1:D:1559:PRO:HD3	2.00	0.43
1:D:1649:ARG:HD3	1:D:1649:ARG:HA	1.86	0.43
1:D:1767:TYR:CD2	1:D:1768:LEU:HD13	2.54	0.43
1:B:752:LEU:HD12	1:B:752:LEU:HA	1.86	0.43
1:A:13:GLU:O	1:A:98:VAL:HA	2.19	0.43
1:D:1522:ILE:HG23	1:D:1582:ILE:HG22	2.01	0.43
1:D:1674:GLN:C	1:D:1676:THR:N	2.72	0.43
1:D:1656:ARG:O	1:D:1697:HIS:HE1	2.01	0.43
1:A:166:LEU:HB2	1:A:180:MET:HE1	2.00	0.43
1:A:252:LEU:HG	1:A:257:MET:HG2	2.01	0.43
1:C:1155:MET:CE	1:C:1183:ALA:HB3	2.48	0.43
1:C:1125:THR:HG22	1:C:1128:ASP:H	1.83	0.42
1:A:77:GLU:O	1:A:81:ARG:HB2	2.19	0.42
1:C:1110:SER:HB2	1:C:1122:GLY:O	2.19	0.42
1:A:161:TRP:O	1:A:165:VAL:HG23	2.20	0.42
1:A:330:ALA:CB	1:A:343:LEU:HD13	2.49	0.42
1:B:637:LEU:HD22	1:B:648:VAL:HG11	2.02	0.42
1:B:767:TYR:CD2	1:B:768:LEU:HD13	2.54	0.42
1:D:1517:HIS:CE1	3:D:1853:DCF:C2	3.02	0.42
1:B:651:ILE:HG12	1:B:679:ALA:HB3	2.01	0.42
1:C:1227:ALA:O	1:C:1233:THR:HG23	2.18	0.42
1:D:1540:ALA:HB3	1:D:1546:LEU:HD13	2.01	0.42
1:B:686:GLU:O	1:B:686:GLU:HG2	2.19	0.42
1:C:1023:LYS:HB3	1:C:1023:LYS:HE3	1.81	0.42
1:A:75:CYS:O	1:A:79:ILE:HG13	2.20	0.42
1:B:615:MET:HA	1:B:616:PRO:HD3	1.92	0.42
1:A:88:GLU:HB2	1:A:144:PHE:CE2	2.55	0.42
1:A:109:ASN:HB3	1:A:119:GLN:NE2	2.35	0.42
1:B:787:LYS:HE2	4:B:2145:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:LEU:H	1:B:793:ASN:ND2	2.15	0.42
1:B:701:TYR:CD2	1:B:711:ARG:HG2	2.55	0.42
1:C:1045:GLU:O	1:C:1049:ILE:HG22	2.19	0.42
1:B:720:SER:HB2	1:B:721:PRO:HD2	2.01	0.42
1:B:787:LYS:HA	1:B:787:LYS:HD3	1.89	0.42
1:A:213:VAL:CG2	1:A:233:THR:HG23	2.47	0.41
1:B:613:ASP:HB3	1:B:614:PRO:CD	2.46	0.41
1:D:1506:ALA:HB1	1:D:1812:LYS:HD2	2.02	0.41
1:A:235:ARG:HD3	1:A:258:HIS:CD2	2.54	0.41
1:A:346:ARG:HA	1:A:349:ARG:NH1	2.35	0.41
1:B:838:GLU:O	1:B:842:GLU:HG3	2.20	0.41
1:A:56:LEU:HB3	1:A:57:SER:H	1.54	0.41
1:B:668:LEU:HD12	1:B:668:LEU:HA	1.92	0.41
1:D:1656:ARG:HA	1:D:1697:HIS:CE1	2.55	0.41
1:B:507:PHE:HB2	1:B:822:PHE:CD2	2.55	0.41
1:B:764:TRP:CE3	1:B:764:TRP:HA	2.55	0.41
1:D:1713:VAL:HG21	1:D:1731:LEU:HD23	2.02	0.41
1:A:104:PRO:HA	1:A:129:VAL:HG21	2.02	0.41
1:B:656:ARG:HG3	1:B:683:ALA:O	2.20	0.41
1:B:681:ASP:OD2	1:B:714:HIS:CE1	2.74	0.41
1:A:134:ASN:ND2	4:A:2064:HOH:O	2.53	0.41
1:A:181:ASP:HA	1:A:212:THR:O	2.20	0.41
1:A:227:ALA:HA	1:A:231:LEU:HB2	2.01	0.41
1:B:595:VAL:CG1	1:B:598:VAL:HG22	2.50	0.41
1:C:1081:ARG:HD3	1:C:1085:GLU:OE2	2.20	0.41
1:D:1662:SER:OG	1:D:1697:HIS:CD2	2.72	0.41
1:C:1109:ASN:HD22	1:C:1109:ASN:H	1.68	0.41
1:B:634:ASN:ND2	1:B:676:THR:OG1	2.54	0.41
1:C:1065:PHE:CE1	3:C:1353:DCF:H2S2	2.55	0.41
1:B:595:VAL:HG11	1:B:598:VAL:HG22	2.02	0.41
1:D:1838:GLU:H	1:D:1838:GLU:CD	2.25	0.41
1:D:1575:CYS:HB3	1:D:1578:ALA:HB3	2.03	0.40
1:C:1186:GLU:OE1	1:C:1217:GLU:HB3	2.21	0.40
1:D:1513:GLU:OE2	1:D:1794:THR:HG22	2.21	0.40
1:B:517:HIS:ND1	3:B:853:DCF:O5S	2.49	0.40
1:C:1028:LEU:CD1	1:C:1046:LEU:HD22	2.43	0.40
1:C:1292:LEU:HD22	1:C:1325:LEU:HD11	2.02	0.40
1:D:1583:ALA:HB3	1:D:1636:GLY:HA3	2.04	0.40
1:A:173:ASN:C	1:A:175:LYS:H	2.25	0.40
1:A:254:LYS:HE2	1:A:254:LYS:HB3	1.85	0.40
1:B:531:GLY:HA3	1:B:538:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1030:PHE:O	1:C:1034:ARG:HG3	2.21	0.40
1:D:1569:MET:N	1:D:1570:PRO:CD	2.84	0.40
1:D:1572:ILE:HG21	1:D:1582:ILE:HD13	2.02	0.40
1:A:86:PHE:CE2	1:A:100:VAL:HG22	2.57	0.40
1:A:338:GLU:H	1:A:338:GLU:CD	2.24	0.40
1:C:1164:GLU:O	1:C:1168:LEU:HD22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	347/349 (99%)	326 (94%)	17 (5%)	4 (1%)	13	27
1	B	347/349 (99%)	321 (92%)	23 (7%)	3 (1%)	17	35
1	C	347/349 (99%)	327 (94%)	17 (5%)	3 (1%)	17	35
1	D	347/349 (99%)	327 (94%)	18 (5%)	2 (1%)	25	47
All	All	1388/1396 (99%)	1301 (94%)	75 (5%)	12 (1%)	17	35

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	238	HIS
1	C	1238	HIS
1	B	738	HIS
1	D	1738	HIS
1	A	176	THR
1	B	795	ASP
1	C	1176	THR
1	A	295	ASP
1	B	619	GLN

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Mol	Chain	Res	Type
1	C	1295	ASP
1	D	1763	PRO
1	A	10	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	304/304 (100%)	283 (93%)	21 (7%)	15 31
1	B	304/304 (100%)	280 (92%)	24 (8%)	12 24
1	C	304/304 (100%)	276 (91%)	28 (9%)	9 17
1	D	304/304 (100%)	284 (93%)	20 (7%)	16 33
All	All	1216/1216 (100%)	1123 (92%)	93 (8%)	13 26

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	38	LEU
1	A	43	VAL
1	A	53	ASP
1	A	56	LEU
1	A	61	PHE
1	A	81	ARG
1	A	98	VAL
1	A	100	VAL
1	A	109	ASN
1	A	112	VAL
1	A	129	VAL
1	A	132	LEU
1	A	142	GLN
1	A	168	LEU
1	A	193	LEU
1	A	211	ARG
1	A	233	THR

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Mol	Chain	Res	Type
1	A	252	LEU
1	A	268	LEU
1	A	343	LEU
1	B	538	LEU
1	B	581	ARG
1	B	598	VAL
1	B	600	VAL
1	B	607	LEU
1	B	609	ASN
1	B	632	LEU
1	B	642	GLN
1	B	668	LEU
1	B	689	GLU
1	B	695	PRO
1	B	711	ARG
1	B	718	VAL
1	B	722	GLU
1	B	731	LEU
1	B	733	THR
1	B	752	LEU
1	B	768	LEU
1	B	789	ASN
1	B	792	LEU
1	B	794	THR
1	B	825	LEU
1	B	835	LEU
1	B	843	LEU
1	C	1028	LEU
1	C	1038	LEU
1	C	1044	GLU
1	C	1053	ASP
1	C	1056	LEU
1	C	1061	PHE
1	C	1081	ARG
1	C	1107	LEU
1	C	1109	ASN
1	C	1112	VAL
1	C	1125	THR
1	C	1132	LEU
1	C	1142	GLN
1	C	1160	SER
1	C	1168	LEU

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Mol	Chain	Res	Type
1	C	1189	GLU
1	C	1218	VAL
1	C	1231	LEU
1	C	1233	THR
1	C	1252	LEU
1	C	1256	ASN
1	C	1268	LEU
1	C	1292	LEU
1	C	1294	THR
1	C	1314	ASP
1	C	1325	LEU
1	C	1338	GLU
1	C	1343	LEU
1	D	1538	LEU
1	D	1543	VAL
1	D	1556	LEU
1	D	1581	ARG
1	D	1600	VAL
1	D	1607	LEU
1	D	1609	ASN
1	D	1626	PRO
1	D	1632	LEU
1	D	1668	LEU
1	D	1692	SER
1	D	1718	VAL
1	D	1731	LEU
1	D	1752	LEU
1	D	1768	LEU
1	D	1792	LEU
1	D	1814	ASP
1	D	1825	LEU
1	D	1843	LEU
1	D	1846	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	119	GLN
1	A	134	ASN
1	A	197	HIS
1	A	210	HIS

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Mol	Chain	Res	Type
1	A	214	HIS
1	A	256	ASN
1	A	289	ASN
1	A	293	ASN
1	B	609	ASN
1	B	619	GLN
1	B	634	ASN
1	B	657	HIS
1	B	697	HIS
1	B	707	ASN
1	B	714	HIS
1	B	750	ASN
1	B	789	ASN
1	B	793	ASN
1	B	826	ASN
1	C	1109	ASN
1	C	1134	ASN
1	C	1157	HIS
1	C	1207	ASN
1	C	1210	HIS
1	C	1241	HIS
1	C	1256	ASN
1	C	1289	ASN
1	C	1293	ASN
1	D	1609	ASN
1	D	1619	GLN
1	D	1634	ASN
1	D	1697	HIS
1	D	1707	ASN
1	D	1710	HIS
1	D	1756	ASN
1	D	1789	ASN
1	D	1793	ASN
1	D	1826	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)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
3	DCF	B	853	2	14,21,21	2.41	2 (14%)	12,30,30	0.86	0
3	DCF	A	353	2	14,21,21	2.48	2 (14%)	12,30,30	0.89	0
3	DCF	C	1353	2	14,21,21	2.37	2 (14%)	12,30,30	0.84	0
3	DCF	D	1853	2	14,21,21	2.37	2 (14%)	12,30,30	0.92	0

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
3	DCF	B	853	2	-	0/2/29/29	0/2/3/3
3	DCF	A	353	2	-	0/2/29/29	0/2/3/3
3	DCF	C	1353	2	-	0/2/29/29	0/2/3/3
3	DCF	D	1853	2	-	0/2/29/29	0/2/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	353	DCF	O8-C8	8.13	1.61	1.42
3	D	1853	DCF	O8-C8	7.91	1.60	1.42
3	B	853	DCF	O8-C8	7.90	1.60	1.42
3	C	1353	DCF	O8-C8	7.76	1.60	1.42
3	A	353	DCF	C10-N4	-3.15	1.38	1.41
3	B	853	DCF	C10-N4	-3.05	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1853	DCF	C10-N4	-2.85	1.38	1.41
3	C	1353	DCF	C10-N4	-2.84	1.38	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

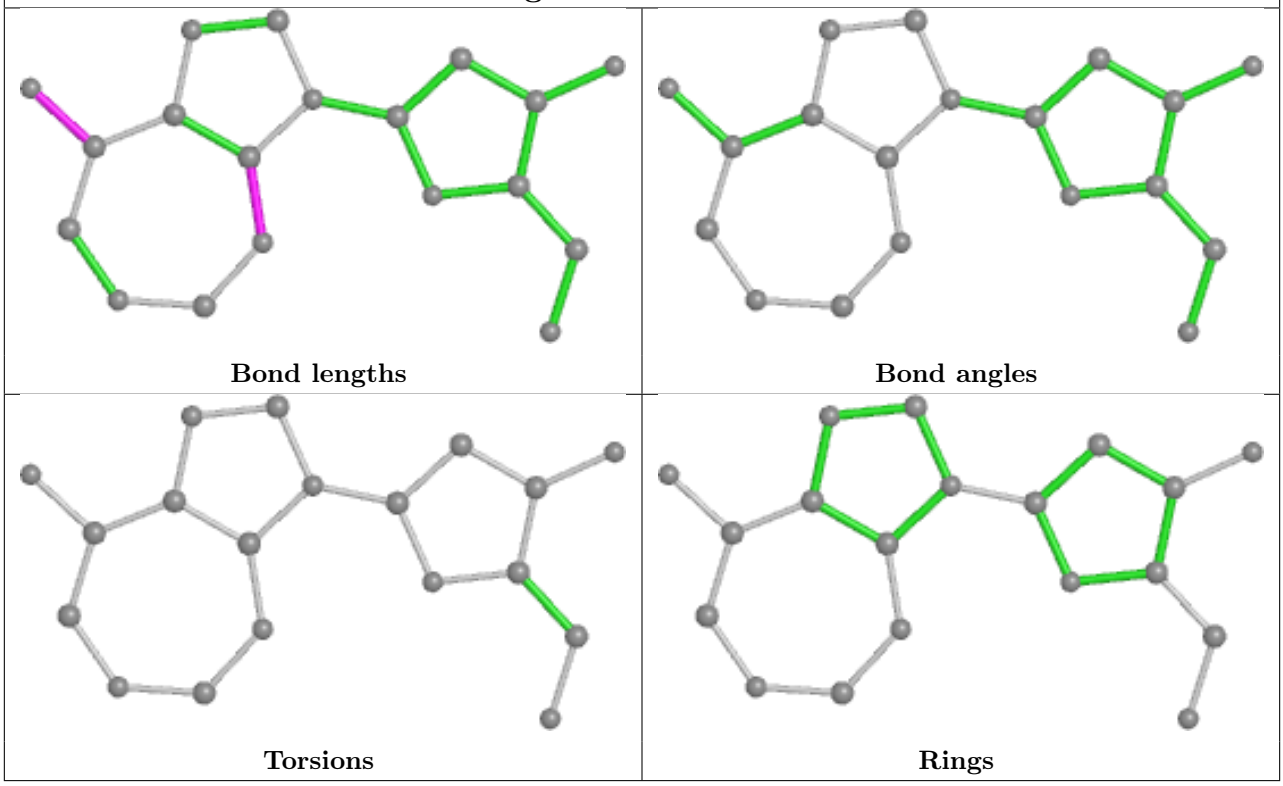
There are no ring outliers.

4 monomers are involved in 7 short contacts:

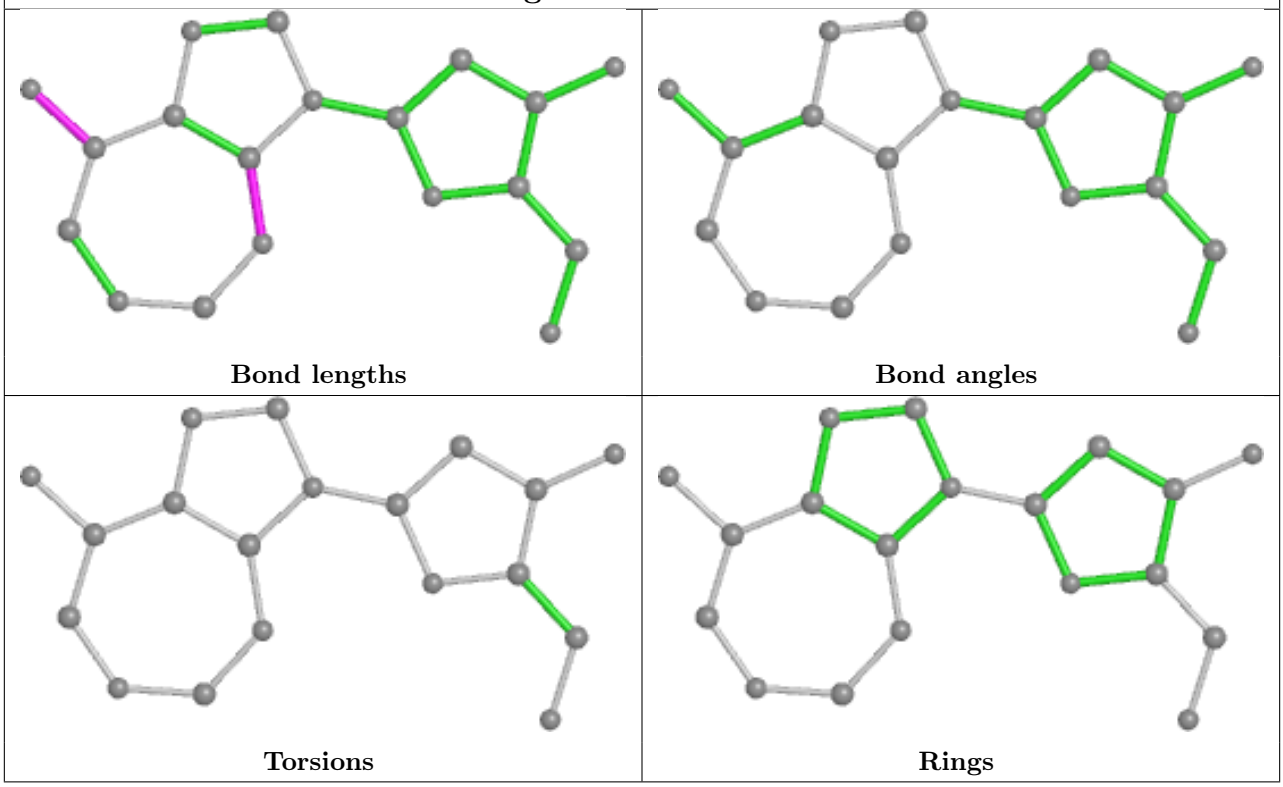
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	853	DCF	1	0
3	A	353	DCF	1	0
3	C	1353	DCF	3	0
3	D	1853	DCF	2	0

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.

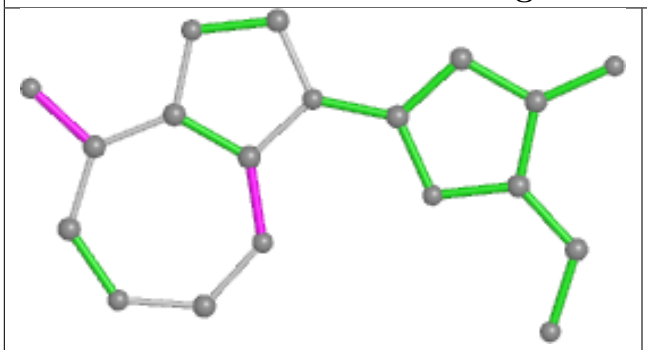
Ligand DCF B 853



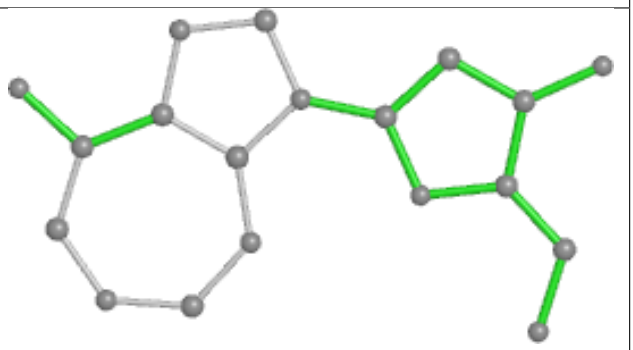
Ligand DCF A 353



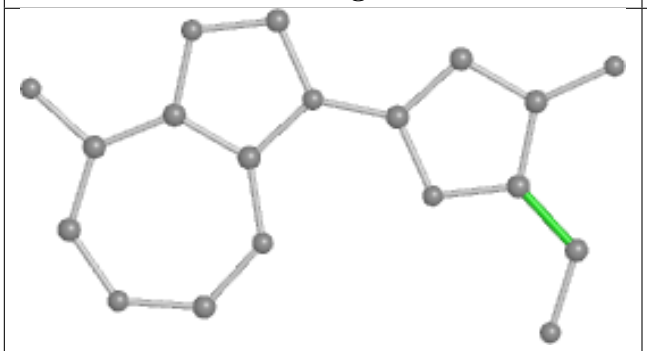
Ligand DCF C 1353



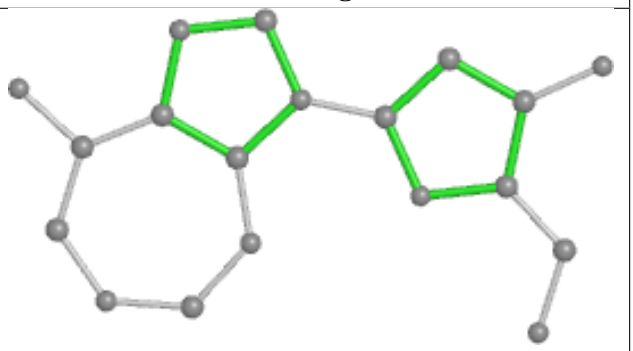
Bond lengths



Bond angles

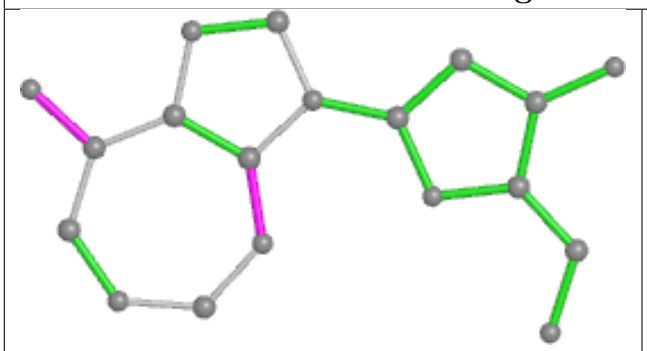


Torsions

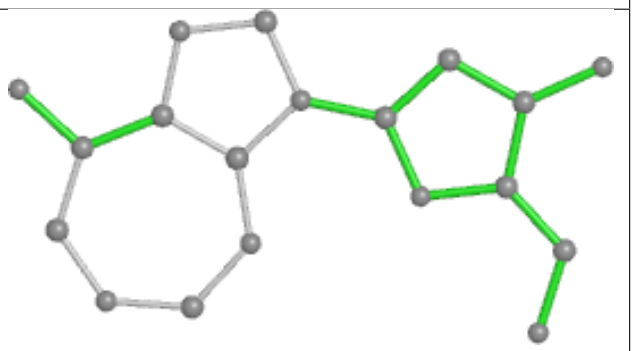


Rings

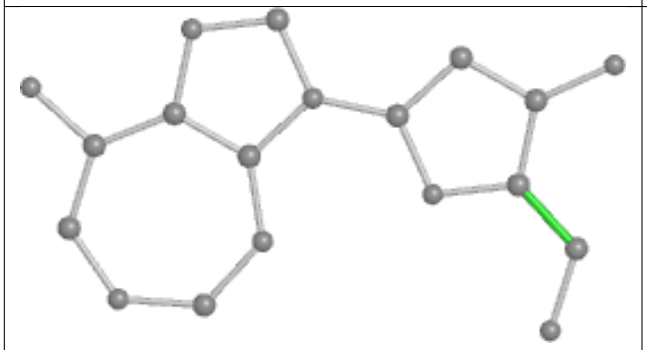
Ligand DCF D 1853



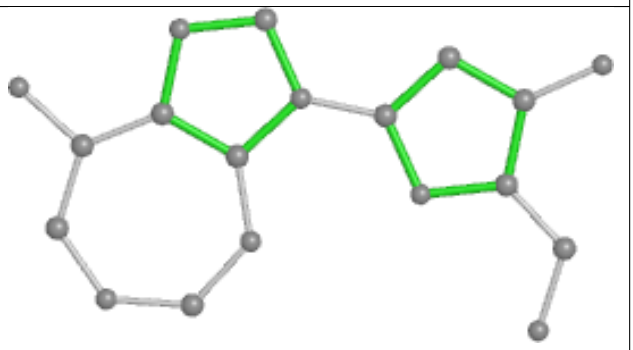
Bond lengths



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	349/349 (100%)	-0.79	0	100	100	2, 11, 25, 38	0
1	B	349/349 (100%)	-0.74	0	100	100	4, 11, 25, 43	0
1	C	349/349 (100%)	-0.72	1 (0%)	94	93	3, 11, 26, 38	0
1	D	349/349 (100%)	-0.74	1 (0%)	94	93	3, 11, 27, 37	0
All	All	1396/1396 (100%)	-0.75	2 (0%)	95	95	2, 11, 26, 43	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1113	ASP	3.6
1	D	1613	ASP	2.6

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)

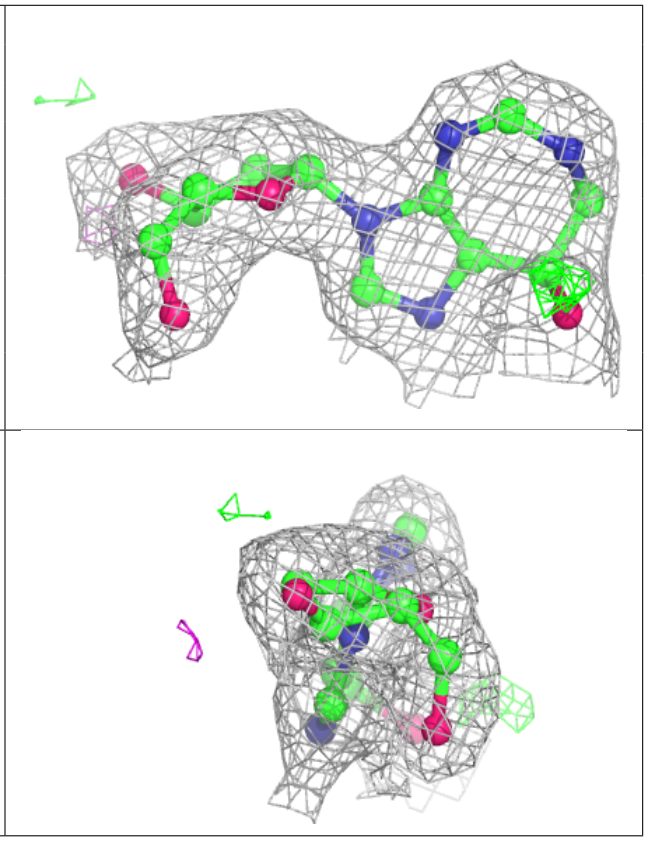
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	DCF	D	1853	19/19	0.96	0.12	2,7,12,13	0
3	DCF	C	1353	19/19	0.97	0.10	2,6,10,12	0
3	DCF	A	353	19/19	0.97	0.11	2,8,14,16	0
3	DCF	B	853	19/19	0.98	0.10	2,5,12,13	0
2	ZN	C	1400	1/1	0.99	0.05	15,15,15,15	0
2	ZN	D	1900	1/1	0.99	0.06	11,11,11,11	0
2	ZN	A	400	1/1	0.99	0.11	25,25,25,25	0
2	ZN	B	900	1/1	1.00	0.10	20,20,20,20	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.

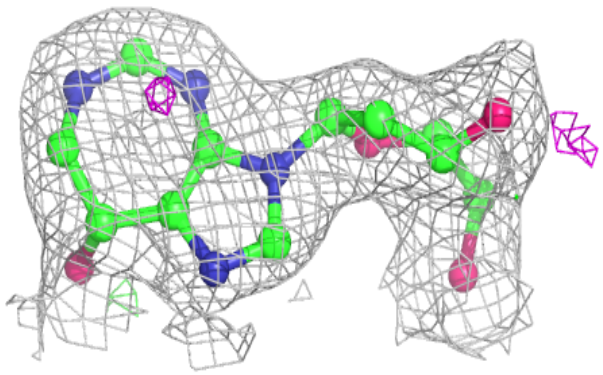
Electron density around DCF D 1853:

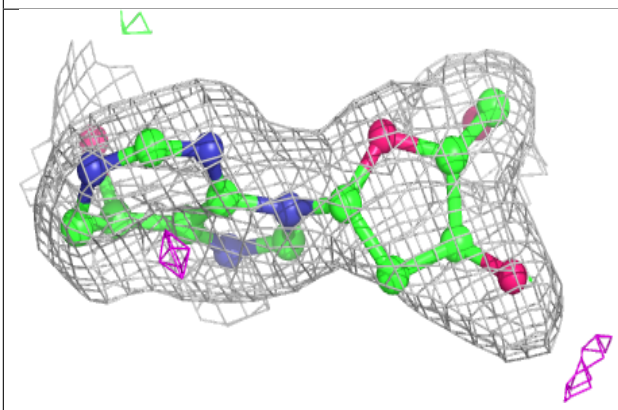
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

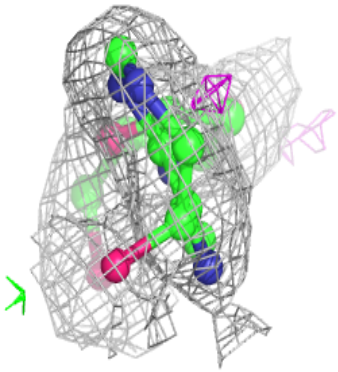


Electron density around DCF C 1353:

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

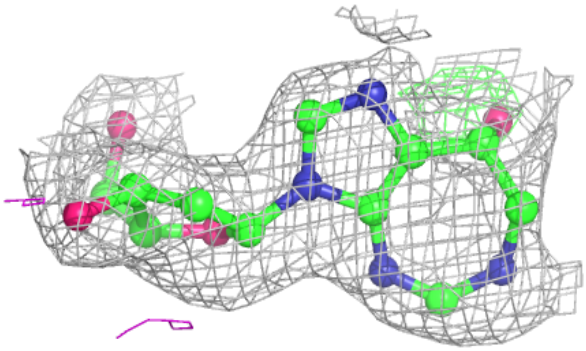


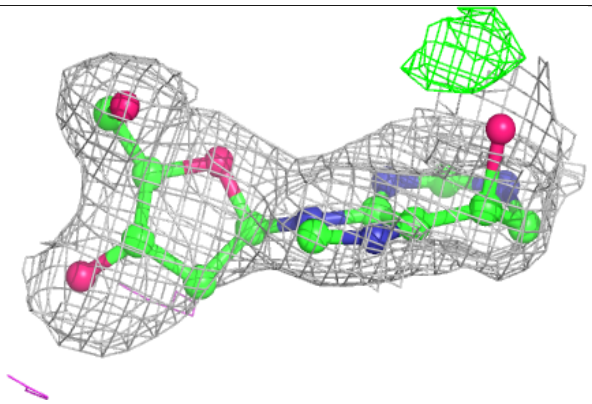


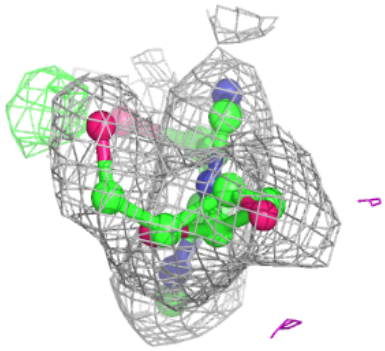


Electron density around DCF A 353:

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

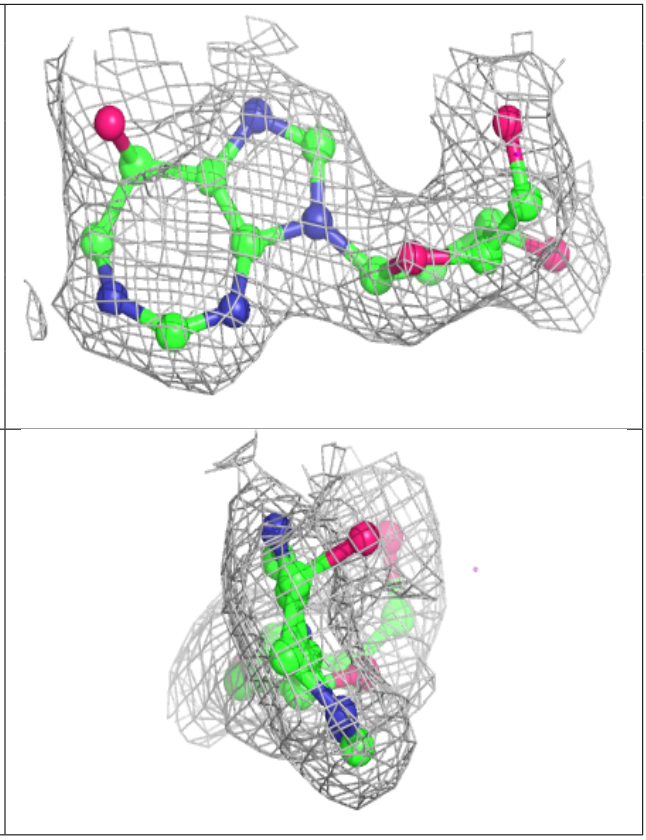






Electron density around DCF B 853:

$2mF_o$-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.