Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2023 – 08:38 AM EDT

PDB ID : 4W6Z
Title : YEAST ALCOHOL DEHYDROGENASE I, SACCHAROMYCES CEREVISIAE FERMENTATIVE ENZYME
Authors : plapp, B.v.; savarimuthu, b.r.; ramaswamy, s.
Deposited on : 2014-08-21
Resolution : 2.40 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

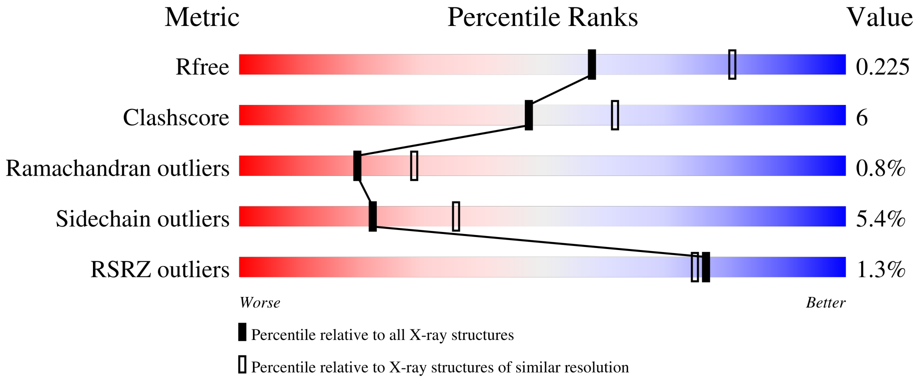
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

1 Overall quality at a glance ⓘ

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

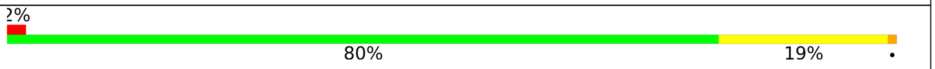
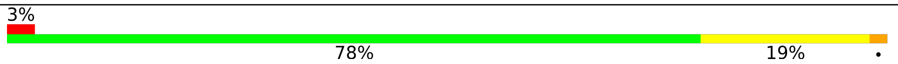
The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	
1	B	347	
1	C	347	
1	D	347	

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 10601 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.

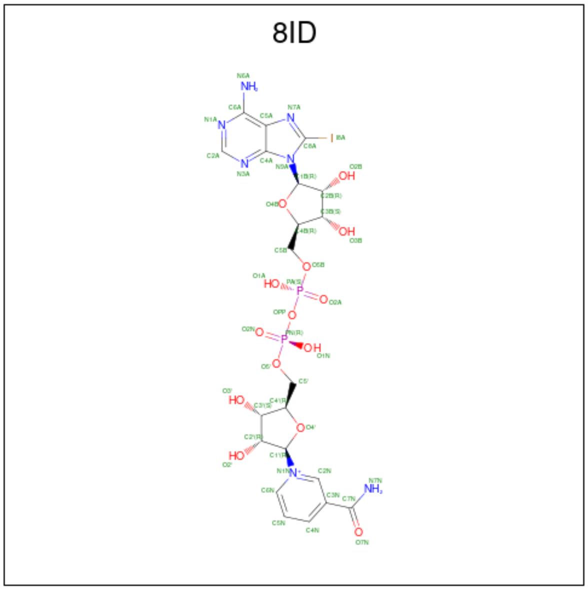
- Molecule 1 is a protein called Alcohol dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total 2582	C 1639	N 440	O 489	S 14	0	0	0
1	B	347	Total 2582	C 1639	N 440	O 489	S 14	0	0	0
1	C	347	Total 2582	C 1639	N 440	O 489	S 14	0	0	0
1	D	347	Total 2582	C 1639	N 440	O 489	S 14	0	0	0

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

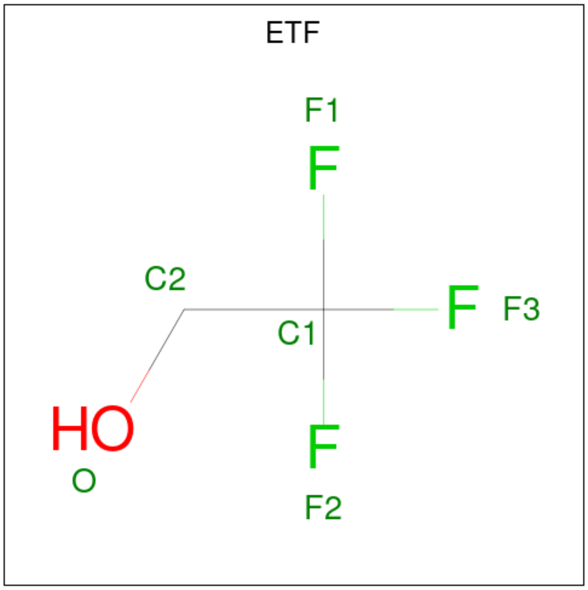
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0

- Molecule 3 is NICOTINAMIDE-8-IODO-ADENINE-DINUCLEOTIDE (three-letter code: 8ID) (formula: $C_{21}H_{27}IN_7O_{14}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C I N O P 45 21 1 7 14 2	0	0
3	C	1	Total C I N O P 45 21 1 7 14 2	0	0

- Molecule 4 is TRIFLUOROETHANOL (three-letter code: ETF) (formula: $C_2H_3F_3O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C F O 6 2 3 1	0	0
4	B	1	Total C F O 6 2 3 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C F O 6 2 3 1	0	0
4	D	1	Total C F O 6 2 3 1	0	0

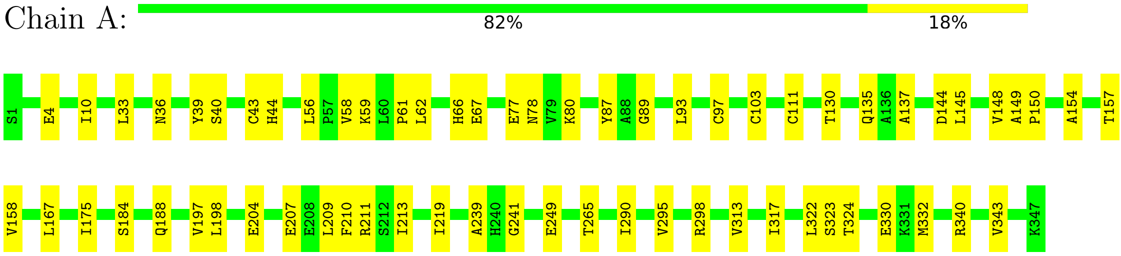
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	41	Total O 41 41	0	0
5	B	33	Total O 33 33	0	0
5	C	51	Total O 51 51	0	0
5	D	26	Total O 26 26	0	0

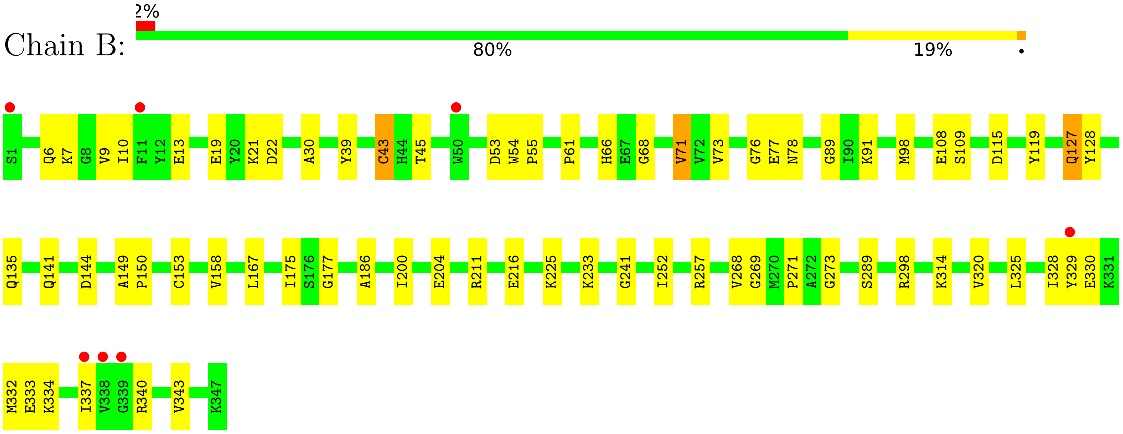
3 Residue-property plots

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.

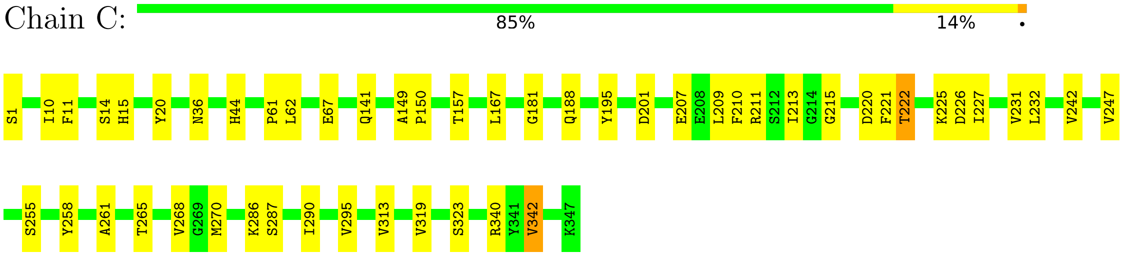
- Molecule 1: Alcohol dehydrogenase 1



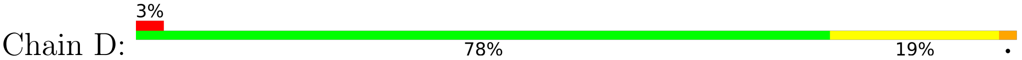
- Molecule 1: Alcohol dehydrogenase 1

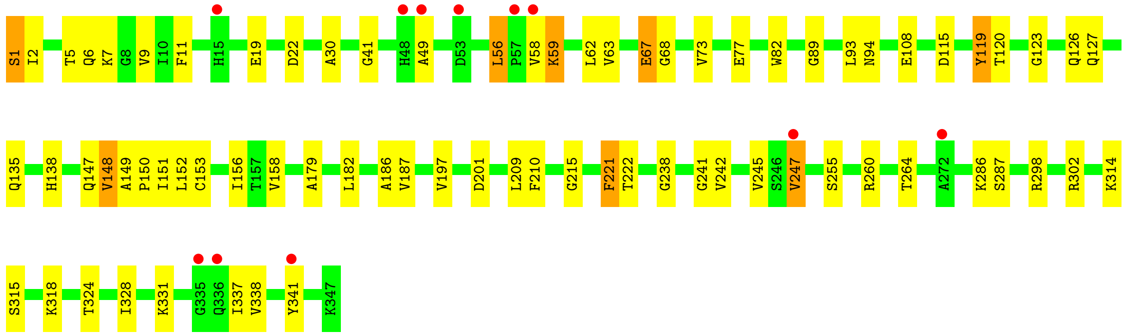


- Molecule 1: Alcohol dehydrogenase 1



- Molecule 1: Alcohol dehydrogenase 1




S1
I2
T5
Q6
K7
G8
V9
I10
F11
H15
E19
D22
A30
G41
H48
A49
D53
L56
P57
V58
K59
L62
V63
E67
G68
V73
E77
W82
G89
L93
N94
E108
D115
Y119
T120
G123
Q126
Q127
Q135
H138
Q147
V148
A149
P150
I151
L152
C153
I156
T157
V158
A179
L182
A186
V187
V197
D201
L209
F210
G215
F221
T222
G238
G241
V242
V245
S246
V247
S255
R260
T264
A272
K286
S287
R298
R302
K314
S315
K318
T324
I328
K331
G335
Q336
I337
V338
Y341
K347

4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α, β, γ	144.34Å 144.34Å 128.20Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.09 – 2.40 28.09 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (28.09-2.40) 98.5 (28.09-2.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.177 , 0.222 0.181 , 0.225	Depositor DCC
R_{free} test set	1499 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 14.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	0.257 for -h,-k,l	Xtriage
Reported twinning fraction	0.713 for H, K, L 0.287 for -h,-k,l	Depositor
Outliers	1 of 59635 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10601	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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 63.41 % 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 9.7127e-06.*

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[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: 8ID, ZN, ETF

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	0.80	0/2636	0.88	1/3571 (0.0%)
1	B	0.75	0/2636	0.89	4/3571 (0.1%)
1	C	0.84	0/2636	0.91	2/3571 (0.1%)
1	D	0.76	0/2636	0.89	2/3571 (0.1%)
All	All	0.79	0/10544	0.89	9/14284 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	115	ASP	CB-CG-OD1	7.28	124.85	118.30
1	A	298	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	C	226	ASP	CB-CG-OD2	-6.67	112.29	118.30
1	D	115	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	71	VAL	CB-CA-C	-6.37	99.29	111.40
1	B	298	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	D	298	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	B	115	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	C	270	MET	CG-SD-CE	-5.04	92.13	100.20

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	2582	0	2565	32	0
1	B	2582	0	2565	30	0
1	C	2582	0	2565	27	0
1	D	2582	0	2565	35	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	45	0	25	2	0
3	C	45	0	25	4	0
4	A	6	0	2	0	0
4	B	6	0	3	1	0
4	C	6	0	2	0	0
4	D	6	0	3	0	0
5	A	41	0	0	0	0
5	B	33	0	0	0	0
5	C	51	0	0	0	0
5	D	26	0	0	0	0
All	All	10601	0	10320	126	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 6.

All (126) 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:9:VAL:HG11	1:B:325:LEU:HD23	1.53	0.89
1:A:87:TYR:CD2	1:A:145:LEU:HD21	2.15	0.81
1:A:59:LYS:O	1:A:62:LEU:HB2	1.82	0.80
1:B:320:VAL:HG21	1:B:328:ILE:HD11	1.71	0.72
1:C:149:ALA:HB3	1:C:150:PRO:HD3	1.76	0.68
1:D:158:VAL:HG21	1:D:186:ALA:HB2	1.75	0.67
1:D:93:LEU:HD23	1:D:135:GLN:CD	2.15	0.66
1:A:324:THR:O	1:A:324:THR:HG22	1.97	0.65
1:A:188:GLN:HB3	1:A:313:VAL:HG12	1.83	0.61
3:A:403:8ID:H2B	3:A:403:8ID:I8A	2.72	0.60
1:D:179:ALA:HB3	1:D:201:ASP:OD2	2.02	0.59
1:C:207:GLU:O	1:C:210:PHE:HB3	2.02	0.59
1:C:220:ASP:OD1	1:C:222:THR:HB	2.02	0.59
1:C:231:VAL:HG11	1:C:258:TYR:CD1	2.38	0.59
1:C:242:VAL:HG11	1:C:255:SER:HB2	1.84	0.58
1:D:56:LEU:O	1:D:119:TYR:CE2	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:VAL:HB	1:D:62:LEU:HD22	1.86	0.57
1:A:184:SER:O	1:A:188:GLN:NE2	2.37	0.57
1:B:167:LEU:HD21	1:B:241:GLY:HA3	1.85	0.57
1:D:123:GLY:O	1:D:126:GLN:NE2	2.37	0.56
1:D:56:LEU:O	1:D:119:TYR:HE2	1.89	0.55
1:D:238:GLY:O	1:D:260:ARG:NH1	2.38	0.55
1:C:261:ALA:HB2	1:C:286:LYS:HD2	1.88	0.55
1:D:6:GLN:O	1:D:22:ASP:HA	2.07	0.55
1:A:144:ASP:C	1:A:144:ASP:OD1	2.44	0.54
1:C:265:THR:HG23	1:C:290:ILE:HG23	1.89	0.54
1:C:10:ILE:HD11	1:C:61:PRO:HB2	1.89	0.54
1:A:58:VAL:HB	1:A:62:LEU:HD22	1.91	0.53
1:A:149:ALA:HB3	1:A:150:PRO:HD3	1.90	0.53
1:B:268:VAL:HG12	1:B:269:GLY:N	2.23	0.53
3:C:403:8ID:I8A	3:C:403:8ID:H2B	2.79	0.52
1:B:30:ALA:O	1:B:78:ASN:HB2	2.09	0.52
1:C:221:PHE:HA	1:C:227:ILE:HD11	1.92	0.52
1:A:209:LEU:O	1:A:213:ILE:HG12	2.09	0.52
1:C:201:ASP:O	1:C:220:ASP:HA	2.08	0.52
1:D:9:VAL:HA	1:D:19:GLU:O	2.10	0.52
1:D:108:GLU:HG3	1:D:135:GLN:NE2	2.25	0.51
1:D:210:PHE:CZ	1:D:215:GLY:HA3	2.45	0.51
1:A:40:SER:HA	1:A:67:GLU:O	2.10	0.51
1:A:324:THR:O	1:A:324:THR:CG2	2.59	0.51
1:A:93:LEU:HD23	1:A:135:GLN:NE2	2.26	0.51
1:B:211:ARG:NH1	1:B:216:GLU:O	2.44	0.50
1:D:59:LYS:HG2	1:D:120:THR:O	2.12	0.50
1:C:268:VAL:O	3:C:403:8ID:H2N	2.11	0.50
1:D:148:VAL:O	1:D:151:ILE:HB	2.12	0.50
1:B:9:VAL:HG11	1:B:325:LEU:CD2	2.35	0.49
1:A:148:VAL:HG22	1:A:148:VAL:O	2.12	0.49
1:D:41:GLY:HA3	1:D:67:GLU:OE1	2.13	0.49
1:D:247:VAL:HG12	1:D:247:VAL:O	2.13	0.49
1:A:89:GLY:HA3	1:A:137:ALA:HB3	1.94	0.49
1:C:210:PHE:CZ	1:C:215:GLY:HA3	2.48	0.48
1:A:154:ALA:O	1:A:158:VAL:HG22	2.14	0.48
1:B:91:LYS:NZ	1:B:135:GLN:O	2.46	0.47
1:B:39:TYR:HA	1:B:343:VAL:O	2.13	0.47
1:D:68:GLY:O	1:D:89:GLY:HA2	2.13	0.47
1:C:44:HIS:CE1	1:C:247:VAL:HG21	2.50	0.47
1:D:242:VAL:HG11	1:D:255:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:THR:HG21	3:A:403:8ID:C4N	2.44	0.47
1:B:54:TRP:HB3	1:B:55:PRO:CD	2.45	0.47
1:C:188:GLN:HB3	1:C:313:VAL:HG12	1.96	0.47
1:B:66:HIS:NE2	4:B:404:ETF:O	2.48	0.47
1:B:332:MET:O	1:B:334:LYS:O	2.32	0.47
1:A:207:GLU:O	1:A:210:PHE:HB3	2.14	0.46
1:A:175:ILE:CD1	1:A:197:VAL:HG13	2.45	0.46
1:A:33:LEU:O	1:A:130:THR:HA	2.17	0.45
1:B:68:GLY:O	1:B:89:GLY:HA2	2.16	0.45
1:A:10:ILE:HD11	1:A:61:PRO:HB2	1.99	0.45
1:A:78:ASN:HD22	1:A:78:ASN:N	2.15	0.45
1:A:103:CYS:SG	1:A:111:CYS:HB2	2.56	0.45
1:A:322:LEU:O	1:A:324:THR:N	2.50	0.45
1:B:325:LEU:HD21	1:B:329:TYR:CE1	2.52	0.45
1:C:286:LYS:O	1:C:287:SER:C	2.55	0.45
1:A:317:ILE:HG22	1:A:340:ARG:HB3	1.98	0.45
1:C:157:THR:HG21	3:C:403:8ID:C4N	2.47	0.45
1:D:221:PHE:C	1:D:221:PHE:CD1	2.89	0.45
1:B:167:LEU:HD21	1:B:241:GLY:CA	2.47	0.44
1:C:210:PHE:CE2	1:C:215:GLY:HA3	2.52	0.44
1:B:144:ASP:OD1	1:B:144:ASP:C	2.56	0.44
1:B:269:GLY:C	1:B:271:PRO:HD3	2.38	0.44
1:B:177:GLY:N	1:B:200:ILE:O	2.50	0.44
1:B:330:GLU:HA	1:B:333:GLU:OE2	2.17	0.44
1:C:11:PHE:CZ	1:C:62:LEU:HD23	2.53	0.44
1:C:44:HIS:HB3	3:C:403:8ID:H3'	1.99	0.44
1:D:94:ASN:O	1:D:135:GLN:HB2	2.17	0.43
1:D:7:LYS:O	1:D:127:GLN:HG2	2.18	0.43
1:A:167:LEU:HD21	1:A:241:GLY:N	2.34	0.43
1:D:187:VAL:HG13	1:D:197:VAL:HG11	2.00	0.43
1:D:331:LYS:HB3	1:D:337:ILE:HG12	2.01	0.43
1:B:43:CYS:SG	1:B:45:THR:HB	2.58	0.43
1:D:149:ALA:N	1:D:150:PRO:CD	2.82	0.43
1:B:19:GLU:HB3	1:B:21:LYS:HD2	1.99	0.43
1:A:43:CYS:HB3	1:A:66:HIS:CE1	2.54	0.42
1:B:149:ALA:N	1:B:150:PRO:CD	2.81	0.42
1:D:82:TRP:CZ2	1:D:138:HIS:CE1	3.07	0.42
1:D:152:LEU:HA	1:D:156:ILE:HD12	2.01	0.42
1:C:181:GLY:HA3	1:C:340:ARG:NH1	2.35	0.42
1:A:59:LYS:NZ	1:A:61:PRO:O	2.53	0.42
1:B:127:GLN:HB3	1:B:128:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:VAL:HG11	1:D:126:GLN:HB2	2.02	0.41
1:B:10:ILE:HD11	1:B:61:PRO:HB2	2.01	0.41
1:C:319:VAL:HG22	1:C:342:VAL:HG22	2.03	0.41
1:C:265:THR:HG23	1:C:265:THR:O	2.21	0.41
1:D:337:ILE:HG23	1:D:341:TYR:CE2	2.54	0.41
1:A:198:LEU:HD11	1:A:219:ILE:HD11	2.02	0.41
1:D:11:PHE:CZ	1:D:62:LEU:HD23	2.55	0.41
1:A:44:HIS:HA	1:A:332:MET:SD	2.61	0.41
1:C:20:TYR:CD1	1:C:323:SER:HA	2.55	0.41
1:B:30:ALA:HA	1:B:76:GLY:HA3	2.03	0.41
1:C:167:LEU:HB2	1:C:195:TYR:CZ	2.56	0.41
1:D:149:ALA:O	1:D:152:LEU:HB2	2.20	0.41
1:D:324:THR:HG22	1:D:328:ILE:HG12	2.03	0.41
1:B:268:VAL:O	1:B:269:GLY:O	2.39	0.41
1:C:67:GLU:OE1	1:C:150:PRO:HA	2.20	0.41
1:D:241:GLY:HA2	1:D:264:THR:O	2.21	0.41
1:A:265:THR:O	1:A:290:ILE:HA	2.21	0.40
1:B:175:ILE:HD13	1:B:186:ALA:HB1	2.04	0.40
1:B:325:LEU:HD21	1:B:329:TYR:HE1	1.86	0.40
1:B:332:MET:HG2	1:B:337:ILE:HG13	2.03	0.40
1:B:6:GLN:O	1:B:22:ASP:HA	2.20	0.40
1:A:239:ALA:HB1	1:A:241:GLY:O	2.20	0.40
1:C:232:LEU:HD23	1:C:232:LEU:HA	1.94	0.40
1:D:49:ALA:O	1:D:58:VAL:HG11	2.21	0.40
1:D:286:LYS:O	1:D:287:SER:C	2.58	0.40
1:A:39:TYR:HA	1:A:343:VAL:O	2.22	0.40
1:C:209:LEU:O	1:C:213:ILE:HG12	2.21	0.40
1:D:1:SER:O	1:D:2:ILE:HD13	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	345/347 (99%)	321 (93%)	22 (6%)	2 (1%)	25	36
1	B	345/347 (99%)	319 (92%)	22 (6%)	4 (1%)	13	19
1	C	345/347 (99%)	321 (93%)	22 (6%)	2 (1%)	25	36
1	D	345/347 (99%)	322 (93%)	20 (6%)	3 (1%)	17	25
All	All	1380/1388 (99%)	1283 (93%)	86 (6%)	11 (1%)	19	29

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	SER
1	D	30	ALA
1	A	295	VAL
1	B	204	GLU
1	C	295	VAL
1	D	119	TYR
1	B	273	GLY
1	C	141	GLN
1	D	247	VAL
1	B	53	ASP
1	B	119	TYR

5.3.2 Protein sidechains ⓘ

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	268/268 (100%)	258 (96%)	10 (4%)	34	53
1	B	268/268 (100%)	248 (92%)	20 (8%)	13	21
1	C	268/268 (100%)	260 (97%)	8 (3%)	41	61
1	D	268/268 (100%)	248 (92%)	20 (8%)	13	21
All	All	1072/1072 (100%)	1014 (95%)	58 (5%)	22	36

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	36	ASN
1	A	56	LEU
1	A	77	GLU
1	A	80	LYS
1	A	97	CYS
1	A	204	GLU
1	A	211	ARG
1	A	249	GLU
1	A	330	GLU
1	B	7	LYS
1	B	13	GLU
1	B	43	CYS
1	B	71	VAL
1	B	73	VAL
1	B	77	GLU
1	B	98	MET
1	B	108	GLU
1	B	109	SER
1	B	127	GLN
1	B	141	GLN
1	B	153	CYS
1	B	158	VAL
1	B	225	LYS
1	B	233	LYS
1	B	252	ILE
1	B	257	ARG
1	B	289	SER
1	B	314	LYS
1	B	340	ARG
1	C	1	SER
1	C	14	SER
1	C	15	HIS
1	C	36	ASN
1	C	211	ARG
1	C	222	THR
1	C	225	LYS
1	C	342	VAL
1	D	1	SER
1	D	5	THR
1	D	56	LEU
1	D	59	LYS
1	D	67	GLU

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Mol	Chain	Res	Type
1	D	73	VAL
1	D	77	GLU
1	D	147	GLN
1	D	148	VAL
1	D	153	CYS
1	D	182	LEU
1	D	209	LEU
1	D	221	PHE
1	D	222	THR
1	D	245	VAL
1	D	302	ARG
1	D	314	LYS
1	D	315	SER
1	D	318	LYS
1	D	338	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	336	GLN
1	B	78	ASN
1	B	107	ASN
1	B	141	GLN
1	B	147	GLN
1	C	107	ASN
1	C	147	GLN
1	D	107	ASN
1	D	135	GLN
1	D	138	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 8 are monoatomic - leaving 6 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	ETF	D	404	-	5,5,5	0.70	0	7,7,7	1.51	1 (14%)
3	8ID	C	403	-	43,49,49	1.27	5 (11%)	50,75,75	1.75	12 (24%)
3	8ID	A	403	-	43,49,49	0.98	2 (4%)	50,75,75	1.42	6 (12%)
4	ETF	C	404	2	5,5,5	0.82	0	7,7,7	1.24	1 (14%)
4	ETF	A	404	2	5,5,5	0.70	0	7,7,7	0.61	0
4	ETF	B	404	-	5,5,5	0.52	0	7,7,7	0.91	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
4	ETF	D	404	-	-	3/3/3/3	-
3	8ID	C	403	-	-	5/26/62/62	0/5/5/5
3	8ID	A	403	-	-	9/26/62/62	0/5/5/5
4	ETF	C	404	2	-	0/3/3/3	-
4	ETF	A	404	2	-	3/3/3/3	-
4	ETF	B	404	-	-	0/3/3/3	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	8ID	C3N-C7N	-3.66	1.45	1.50
3	C	403	8ID	C5A-C4A	3.57	1.50	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	8ID	C5A-C4A	3.06	1.49	1.40
3	C	403	8ID	C2'-C1'	-3.02	1.49	1.53
3	A	403	8ID	C2A-N3A	2.74	1.36	1.32
3	C	403	8ID	O3'-C3'	2.04	1.47	1.43
3	C	403	8ID	O4'-C1'	2.03	1.43	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	403	8ID	O4B-C1B-C2B	-6.66	97.19	106.93
3	A	403	8ID	O4B-C1B-C2B	-4.35	100.56	106.93
3	C	403	8ID	N3A-C2A-N1A	-3.78	122.77	128.68
4	D	404	ETF	F3-C1-F2	3.43	119.04	106.43
3	C	403	8ID	C5N-C4N-C3N	-3.28	116.46	120.34
3	A	403	8ID	N3A-C2A-N1A	-2.98	124.03	128.68
3	C	403	8ID	O7N-C7N-C3N	-2.95	116.11	119.63
3	A	403	8ID	PA-OPP-PN	-2.93	122.78	132.83
3	C	403	8ID	C2A-N1A-C6A	2.92	123.75	118.75
3	C	403	8ID	C2N-C3N-C4N	2.73	121.35	118.26
3	C	403	8ID	N6A-C6A-N1A	2.61	124.00	118.57
3	C	403	8ID	O1N-PN-O2N	2.57	124.96	112.24
4	C	404	ETF	F3-C1-F1	2.47	115.51	106.43
3	C	403	8ID	O7N-C7N-N7N	2.47	126.08	122.58
3	C	403	8ID	O5B-PA-O2A	-2.24	100.32	109.07
3	A	403	8ID	C3N-C7N-N7N	2.15	120.33	117.75
3	A	403	8ID	N6A-C6A-N1A	2.15	123.03	118.57
3	C	403	8ID	C6N-N1N-C2N	-2.14	120.02	121.97
3	C	403	8ID	O1A-PA-O2A	2.09	122.56	112.24
3	A	403	8ID	O3B-C3B-C4B	-2.04	105.15	111.05

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	8ID	O4'-C1'-N1N-C6N
3	A	403	8ID	C2'-C1'-N1N-C2N
3	A	403	8ID	O4'-C1'-N1N-C2N
3	C	403	8ID	O4'-C1'-N1N-C6N
3	C	403	8ID	C2'-C1'-N1N-C2N
3	C	403	8ID	O4'-C1'-N1N-C2N
4	D	404	ETF	F2-C1-C2-O
4	D	404	ETF	F1-C1-C2-O

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Mol	Chain	Res	Type	Atoms
3	A	403	8ID	PN-OPP-PA-O2A
3	C	403	8ID	O4B-C4B-C5B-O5B
3	A	403	8ID	C5B-O5B-PA-OPP
4	D	404	ETF	F3-C1-C2-O
4	A	404	ETF	F3-C1-C2-O
3	A	403	8ID	O4B-C4B-C5B-O5B
4	A	404	ETF	F2-C1-C2-O
3	A	403	8ID	C2'-C1'-N1N-C6N
3	C	403	8ID	C2'-C1'-N1N-C6N
3	A	403	8ID	PN-OPP-PA-O1A
4	A	404	ETF	F1-C1-C2-O
3	A	403	8ID	C5B-O5B-PA-O2A

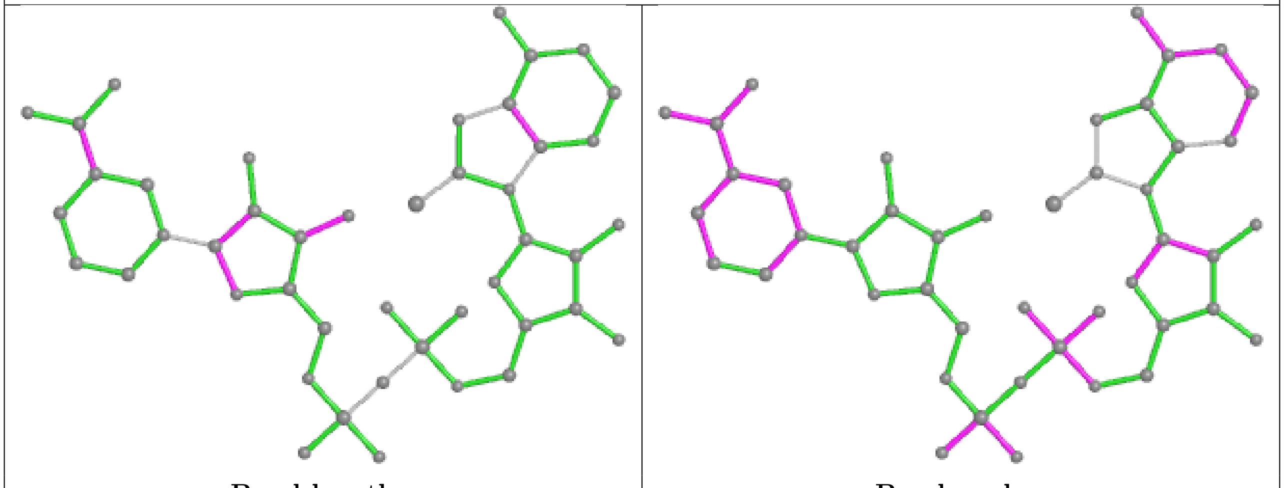
There are no ring outliers.

3 monomers are involved in 7 short contacts:

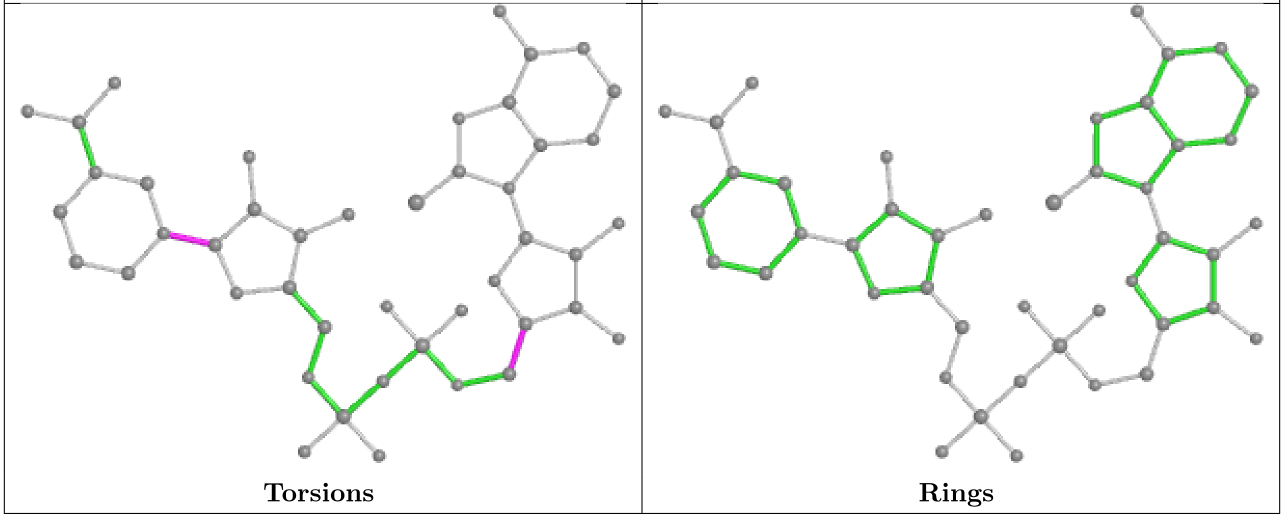
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	403	8ID	4	0
3	A	403	8ID	2	0
4	B	404	ETF	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 8ID C 403

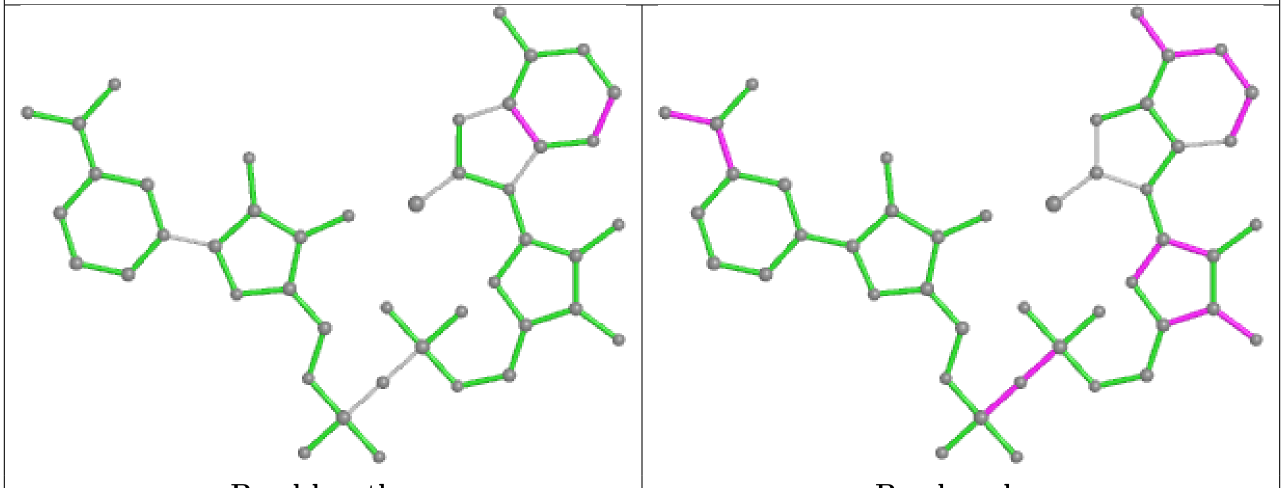


Bond lengths **Bond angles**

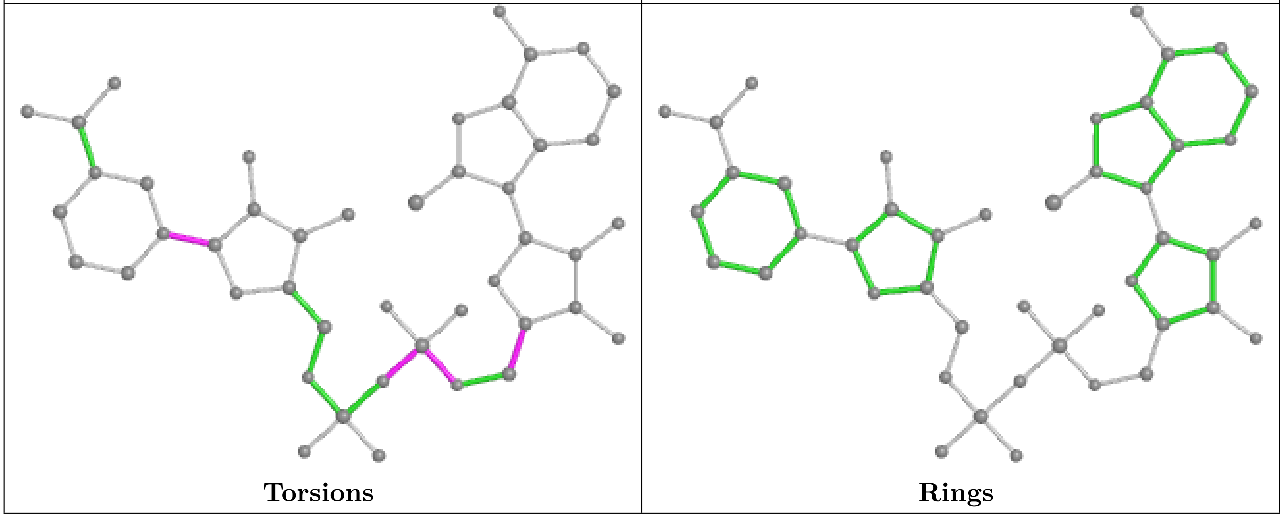


Torsions **Rings**

Ligand 8ID A 403



Bond lengths Bond angles



Torsions Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	347/347 (100%)	-0.47	0	100	100	23, 36, 56, 73	0
1	B	347/347 (100%)	-0.26	7 (2%)	65	63	23, 40, 74, 93	0
1	C	347/347 (100%)	-0.55	0	100	100	21, 31, 47, 64	0
1	D	347/347 (100%)	-0.20	11 (3%)	47	46	22, 39, 83, 120	0
All	All	1388/1388 (100%)	-0.37	18 (1%)	77	75	21, 36, 69, 120	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	336	GLN	6.3
1	B	338	VAL	4.9
1	B	1	SER	4.9
1	D	57	PRO	4.8
1	D	247	VAL	4.6
1	D	335	GLY	4.2
1	D	49	ALA	3.5
1	D	15	HIS	3.5
1	D	53	ASP	3.1
1	D	341	TYR	3.0
1	B	339	GLY	3.0
1	B	337	ILE	3.0
1	D	272	ALA	2.7
1	B	11	PHE	2.7
1	B	50	TRP	2.4
1	D	58	VAL	2.3
1	B	329	TYR	2.2
1	D	48	HIS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

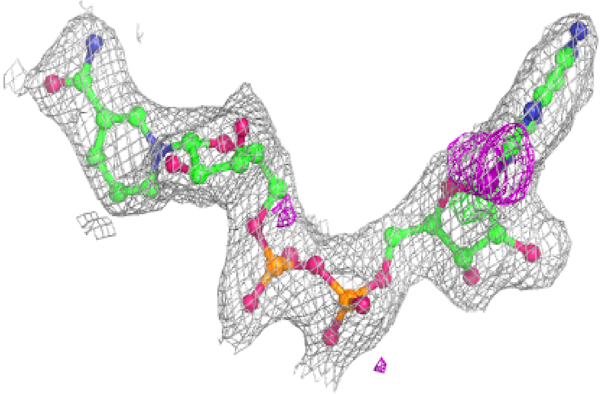
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

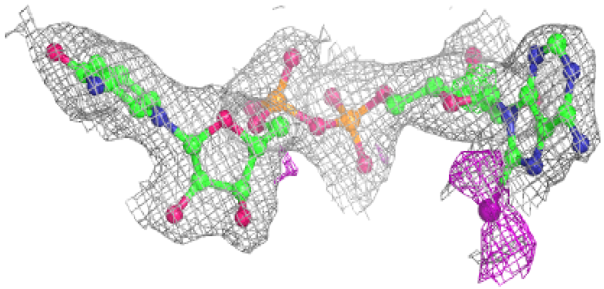
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
4	ETF	B	404	6/6	0.84	0.22	61,71,74,78	0
4	ETF	D	404	6/6	0.86	0.17	47,52,56,61	0
2	ZN	D	401	1/1	0.97	0.06	48,48,48,48	0
3	8ID	A	403	45/45	0.97	0.10	25,32,45,59	0
3	8ID	C	403	45/45	0.99	0.10	20,24,34,44	0
4	ETF	A	404	6/6	0.99	0.09	26,31,31,34	0
2	ZN	B	401	1/1	0.99	0.10	49,49,49,49	0
4	ETF	C	404	6/6	0.99	0.10	18,22,24,25	0
2	ZN	B	402	1/1	0.99	0.11	37,37,37,37	0
2	ZN	C	401	1/1	1.00	0.12	25,25,25,25	0
2	ZN	C	402	1/1	1.00	0.10	30,30,30,30	0
2	ZN	A	401	1/1	1.00	0.11	33,33,33,33	0
2	ZN	D	402	1/1	1.00	0.09	33,33,33,33	0
2	ZN	A	402	1/1	1.00	0.10	35,35,35,35	0

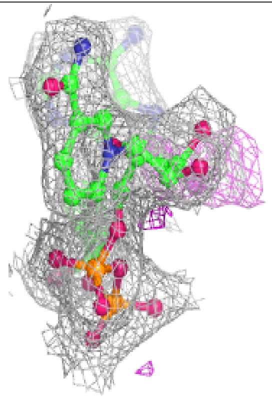
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 8ID A 403:

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

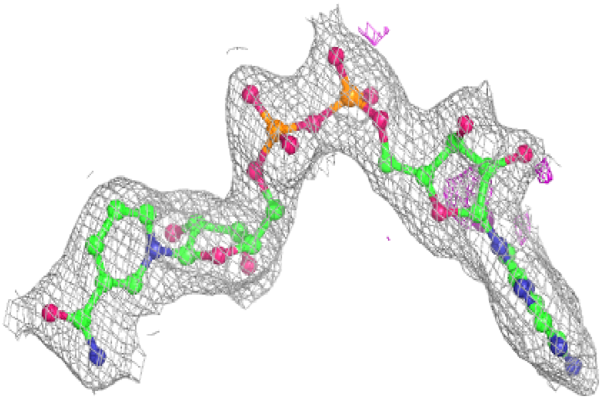


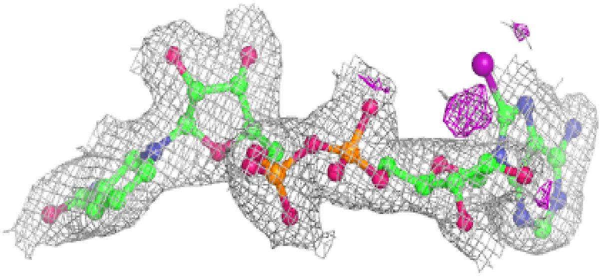


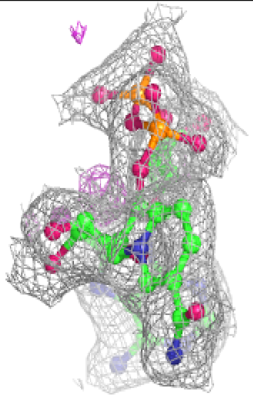


Electron density around 8ID C 403:

$2mF_o$-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 ⓘ

There are no such residues in this entry.