



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:58 PM UTC

PDB ID : 4W6Z / pdb_00004w6z
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)

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

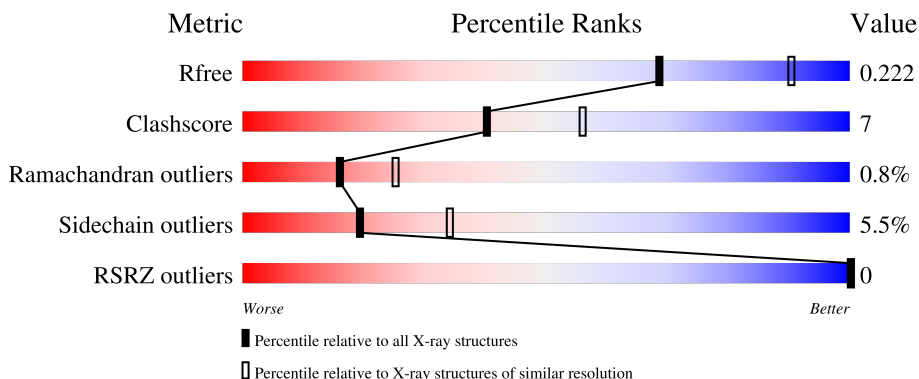
1 Overall quality at a glance

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}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 82% 18% .
1	B	347	 78% 20% .
1	C	347	 83% 16% .
1	D	347	 76% 22% .

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.

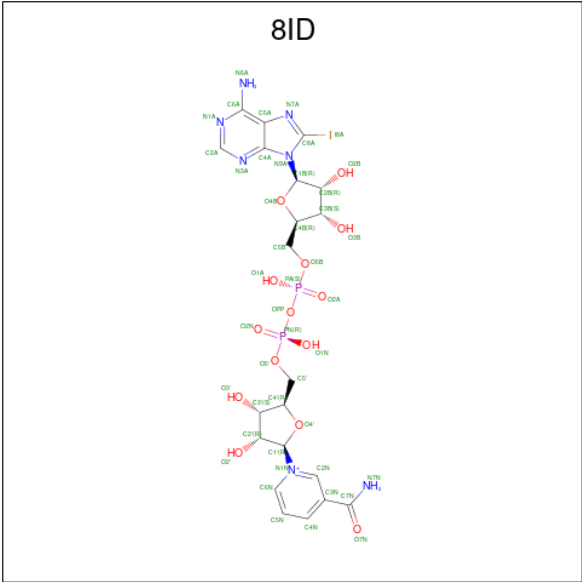
- Molecule 1 is a protein called Alcohol dehydrogenase 1.

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

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

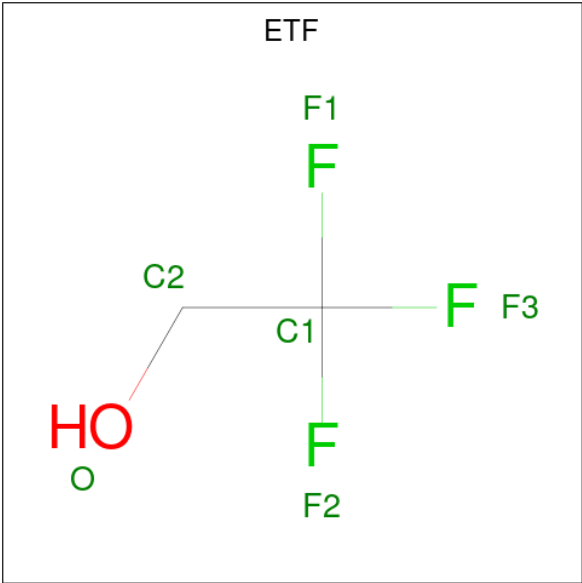
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is NICOTINAMIDE-8-iodo-ADENINE-DINUCLEOTIDE (CCD ID: 8ID) (formula: C₂₁H₂₇IN₇O₁₄P₂).



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

- Molecule 4 is TRIFLUOROETHANOL (CCD ID: ETF) (formula: C₂H₃F₃O).



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

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

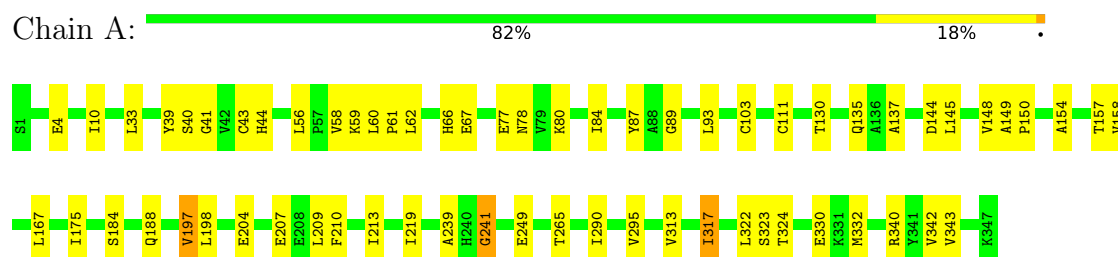
- Molecule 5 is water.

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

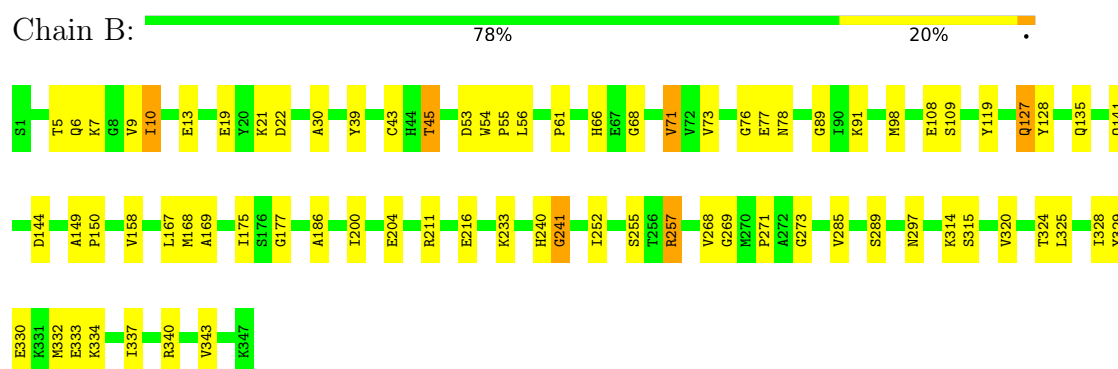
3 Residue-property plots

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.

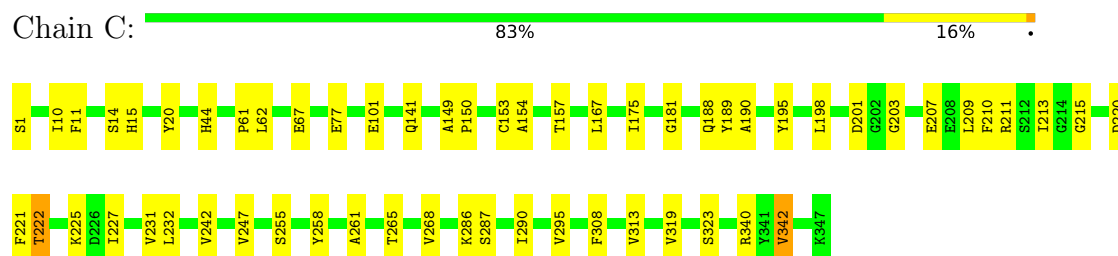
• Molecule 1: Alcohol dehydrogenase 1



• Molecule 1: Alcohol dehydrogenase 1



• Molecule 1: Alcohol dehydrogenase 1



• Molecule 1: Alcohol dehydrogenase 1





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
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.177 , 0.222 (Not available) , 0.222	Depositor DCC
R_{free} test set	1499 reflections (2.47%)	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)	0.35 , 15.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	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	0.95	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1.08	1/2636 (0.0%)	1.14	3/3571 (0.1%)
1	B	1.03	2/2636 (0.1%)	1.16	6/3571 (0.2%)
1	C	1.16	0/2636	1.16	4/3571 (0.1%)
1	D	1.07	1/2636 (0.0%)	1.15	6/3571 (0.2%)
All	All	1.08	4/10544 (0.0%)	1.15	19/14284 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	GLY	N-CA	5.99	1.51	1.45
1	B	240	HIS	C-O	-5.24	1.18	1.24
1	D	294	TYR	CA-C	5.10	1.56	1.53
1	B	241	GLY	N-CA	5.03	1.51	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	203	GLY	N-CA-C	-8.73	103.14	112.04
1	B	71	VAL	CB-CA-C	-7.58	99.29	110.81
1	B	315	SER	CA-C-N	-7.25	112.28	119.90
1	B	315	SER	C-N-CA	-7.25	112.28	119.90
1	A	41	GLY	N-CA-C	-6.89	104.75	112.33
1	B	56	LEU	CA-C-N	6.53	128.00	119.84
1	B	56	LEU	C-N-CA	6.53	128.00	119.84
1	B	240	HIS	N-CA-C	-6.17	104.55	111.28
1	D	293	SER	CA-C-N	6.10	129.66	123.13
1	D	293	SER	C-N-CA	6.10	129.66	123.13
1	A	197	VAL	N-CA-C	5.74	116.13	107.80
1	C	198	LEU	N-CA-C	-5.55	101.12	109.95
1	D	294	TYR	CB-CA-C	-5.31	108.72	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	294	TYR	N-CA-C	5.26	113.80	108.75
1	D	308	PHE	N-CA-C	-5.18	105.08	111.40
1	D	134	VAL	N-CA-C	5.17	115.78	110.36
1	A	317	ILE	N-CA-C	5.14	115.98	108.53
1	C	101	GLU	CB-CA-C	-5.11	102.37	110.84
1	C	77	GLU	N-CA-C	5.01	118.16	111.75

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	34	0
1	B	2582	0	2565	33	0
1	C	2582	0	2565	30	0
1	D	2582	0	2565	38	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	137	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 7.

All (137) 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:D:93:LEU:HD23	1:D:135:GLN:CD	2.15	0.71
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: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:A:144:ASP:C	1:A:144:ASP:OD1	2.44	0.58
1:D:56:LEU:O	1:D:119:TYR:CE2	2.56	0.58
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: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
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:B:268:VAL:HG12	1:B:269:GLY:N	2.23	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:PHE:C	1:D:221:PHE:CD1	2.89	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:C:286:LYS:O	1:C:287:SER:C	2.55	0.49
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:B:269:GLY:C	1:B:271:PRO:HD3	2.38	0.48
1:B:144:ASP:OD1	1:B:144:ASP:C	2.56	0.48
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
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:A:317:ILE:HG22	1:A:340:ARG:HB3	1.98	0.45
1:D:286:LYS:O	1:D:287:SER:C	2.58	0.45
1:C:157:THR:HG21	3:C:403:8ID:C4N	2.47	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:C:189:TYR:O	1:C:190:ALA:C	2.60	0.44
1:D:198:LEU:C	1:D:198:LEU:HD23	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:SER:C	1:D:248:SER:H	2.25	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:C:153:CYS:O	1:C:154:ALA:C	2.59	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:C:308:PHE:CD2	1:C:308:PHE:C	2.97	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:A:60:LEU:HA	1:A:61:PRO:C	2.44	0.42
1:B:127:GLN:HB3	1:B:128:TYR:CD1	2.55	0.42
1:B:297:ASN:OD1	1:B:297:ASN:C	2.63	0.42
1:D:144:ASP:OD1	1:D:144:ASP:C	2.62	0.42
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:B:168:MET:O	1:B:169:ALA:C	2.63	0.41
1:C:319:VAL:HG22	1:C:342:VAL:HG22	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:255:SER:C	1:B:257:ARG:H	2.29	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:A:322:LEU:C	1:A:324:THR:H	2.30	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:C:265:THR:HG23	1:C:265:THR:O	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%)	21	32
1	B	345/347 (99%)	319 (92%)	22 (6%)	4 (1%)	10	16
1	C	345/347 (99%)	321 (93%)	22 (6%)	2 (1%)	21	32
1	D	345/347 (99%)	322 (93%)	20 (6%)	3 (1%)	14	22
All	All	1380/1388 (99%)	1283 (93%)	86 (6%)	11 (1%)	16	25

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	SER

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Mol	Chain	Res	Type
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 [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	268/268 (100%)	259 (97%)	9 (3%)	32	54
1	B	268/268 (100%)	246 (92%)	22 (8%)	10	18
1	C	268/268 (100%)	260 (97%)	8 (3%)	36	58
1	D	268/268 (100%)	248 (92%)	20 (8%)	12	21
All	All	1072/1072 (100%)	1013 (94%)	59 (6%)	19	34

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	56	LEU
1	A	77	GLU
1	A	80	LYS
1	A	84	ILE
1	A	204	GLU
1	A	249	GLU
1	A	330	GLU
1	A	342	VAL
1	B	5	THR
1	B	7	LYS

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Mol	Chain	Res	Type
1	B	10	ILE
1	B	13	GLU
1	B	45	THR
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	158	VAL
1	B	233	LYS
1	B	252	ILE
1	B	257	ARG
1	B	285	VAL
1	B	289	SER
1	B	314	LYS
1	B	324	THR
1	B	340	ARG
1	C	1	SER
1	C	14	SER
1	C	15	HIS
1	C	175	ILE
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	59	LYS
1	D	67	GLU
1	D	73	VAL
1	D	77	GLU
1	D	108	GLU
1	D	147	GLN
1	D	148	VAL
1	D	153	CYS
1	D	182	LEU
1	D	209	LEU
1	D	222	THR
1	D	245	VAL

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Mol	Chain	Res	Type
1	D	285	VAL
1	D	310	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 (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	107	ASN
1	A	126	GLN
1	A	138	HIS
1	A	171	HIS
1	A	336	GLN
1	B	78	ASN
1	B	107	ASN
1	B	141	GLN
1	B	147	GLN
1	C	15	HIS
1	C	107	ASN
1	C	147	GLN
1	C	262	ASN
1	D	107	ASN
1	D	110	ASN
1	D	138	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	B	404	-	5,5,5	0.52	0	7,7,7	0.94	0
4	ETF	D	404	-	5,5,5	0.70	0	7,7,7	1.57	1 (14%)
3	8ID	A	403	-	46,49,49	1.54	5 (10%)	61,75,75	2.03	17 (27%)
4	ETF	A	404	2	5,5,5	0.73	0	7,7,7	0.62	0
4	ETF	C	404	2	5,5,5	0.85	0	7,7,7	1.27	1 (14%)
3	8ID	C	403	-	46,49,49	1.51	6 (13%)	61,75,75	2.05	20 (32%)

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	B	404	-	-	0/3/3/3	-
4	ETF	D	404	-	-	3/3/3/3	-
3	8ID	A	403	-	-	9/30/62/62	0/5/5/5
4	ETF	A	404	2	-	3/3/3/3	-
4	ETF	C	404	2	-	0/3/3/3	-
3	8ID	C	403	-	-	5/30/62/62	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	8ID	C5A-C4A	6.33	1.50	1.39
3	A	403	8ID	C5A-C4A	5.57	1.49	1.39
3	A	403	8ID	PN-OPP	4.53	1.64	1.59
3	C	403	8ID	C3N-C7N	-3.71	1.45	1.50
3	A	403	8ID	C4A-N9A	-3.58	1.33	1.38
3	A	403	8ID	C5A-N7A	-2.90	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	8ID	PN-OPP	2.68	1.62	1.59
3	C	403	8ID	C4A-N9A	-2.66	1.34	1.38
3	A	403	8ID	C5A-C6A	2.59	1.48	1.41
3	C	403	8ID	O4'-C1'	2.30	1.43	1.40
3	C	403	8ID	C5A-N7A	-2.07	1.35	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	8ID	C5A-C4A-N3A	-6.55	117.70	126.72
3	C	403	8ID	I8A-C8A-N7A	-5.28	116.11	122.46
3	C	403	8ID	C5A-C4A-N3A	-5.22	119.53	126.72
3	A	403	8ID	N3A-C4A-N9A	5.22	134.86	127.33
3	C	403	8ID	N3A-C4A-N9A	4.89	134.39	127.33
3	A	403	8ID	I8A-C8A-N7A	-4.42	117.14	122.46
3	C	403	8ID	O4B-C1B-C2B	-4.40	97.19	106.62
3	C	403	8ID	C5N-C4N-C3N	-3.97	116.46	120.36
3	A	403	8ID	C2A-N3A-C4A	3.90	121.36	111.83
3	A	403	8ID	C4'-O4'-C1'	-3.87	106.38	109.92
3	C	403	8ID	N1A-C2A-N3A	-3.84	122.77	128.58
3	C	403	8ID	C2A-N3A-C4A	3.63	120.69	111.83
4	D	404	ETF	F3-C1-F2	3.58	119.04	106.44
3	A	403	8ID	O1N-PN-OPP	-3.43	98.00	107.27
3	A	403	8ID	OPP-PA-O2A	-3.30	100.77	110.70
3	C	403	8ID	C4B-O4B-C1B	-3.12	102.58	109.47
3	C	403	8ID	C2A-N1A-C6A	3.06	123.75	118.73
3	A	403	8ID	C4A-C5A-N7A	-3.04	107.80	110.91
3	A	403	8ID	N1A-C2A-N3A	-3.01	124.03	128.58
3	A	403	8ID	C5A-C4A-N9A	2.88	107.44	105.63
3	C	403	8ID	O7N-C7N-C3N	-2.86	116.11	119.60
3	A	403	8ID	O4B-C1B-C2B	-2.83	100.56	106.62
3	C	403	8ID	OPP-PA-O2A	-2.71	102.56	110.70
3	C	403	8ID	O1N-PN-O2N	2.69	124.96	112.44
3	C	403	8ID	C2N-C3N-C4N	2.66	121.35	118.26
4	C	404	ETF	F3-C1-F1	2.57	115.51	106.44
3	C	403	8ID	N6A-C6A-N1A	2.52	124.00	118.38
3	C	403	8ID	O7N-C7N-N7N	2.40	126.08	122.62
3	A	403	8ID	OPP-PN-O2N	2.20	117.31	110.70
3	C	403	8ID	C6N-N1N-C2N	-2.18	120.02	121.88
3	C	403	8ID	O1A-PA-O2A	2.18	122.56	112.44
3	C	403	8ID	O5B-PA-O2A	-2.17	100.32	108.94
3	C	403	8ID	O4B-C1B-N9A	2.16	111.30	108.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	8ID	C6A-C5A-N7A	2.16	133.86	131.72
3	C	403	8ID	C6A-C5A-N7A	2.15	133.85	131.72
3	A	403	8ID	C3N-C7N-N7N	2.10	120.33	117.74
3	A	403	8ID	N6A-C6A-N1A	2.09	123.03	118.38
3	A	403	8ID	O3B-C3B-C4B	-2.07	105.15	111.08
3	A	403	8ID	O1A-PA-O2A	2.01	121.80	112.44

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
3	A	403	8ID	PN-OPP-PA-O2A
3	A	403	8ID	C5B-O5B-PA-O2A
4	D	404	ETF	F3-C1-C2-O
3	A	403	8ID	C2'-C1'-N1N-C6N
3	C	403	8ID	C2'-C1'-N1N-C6N
3	C	403	8ID	O4B-C4B-C5B-O5B
4	A	404	ETF	F3-C1-C2-O
4	A	404	ETF	F2-C1-C2-O
3	A	403	8ID	PN-OPP-PA-O1A
3	A	403	8ID	C2B-C1B-N9A-C8A
3	A	403	8ID	O4B-C4B-C5B-O5B
4	A	404	ETF	F1-C1-C2-O

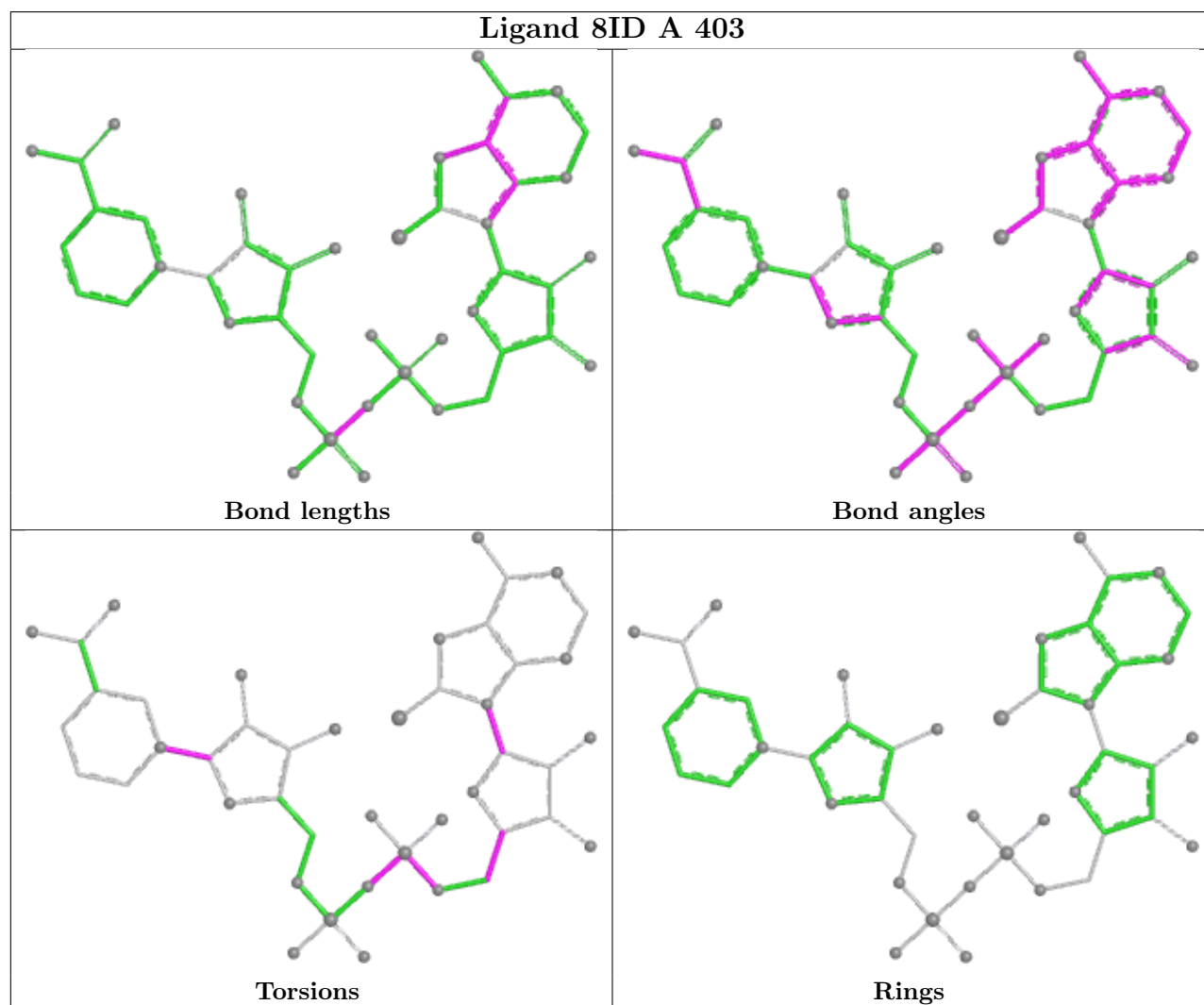
There are no ring outliers.

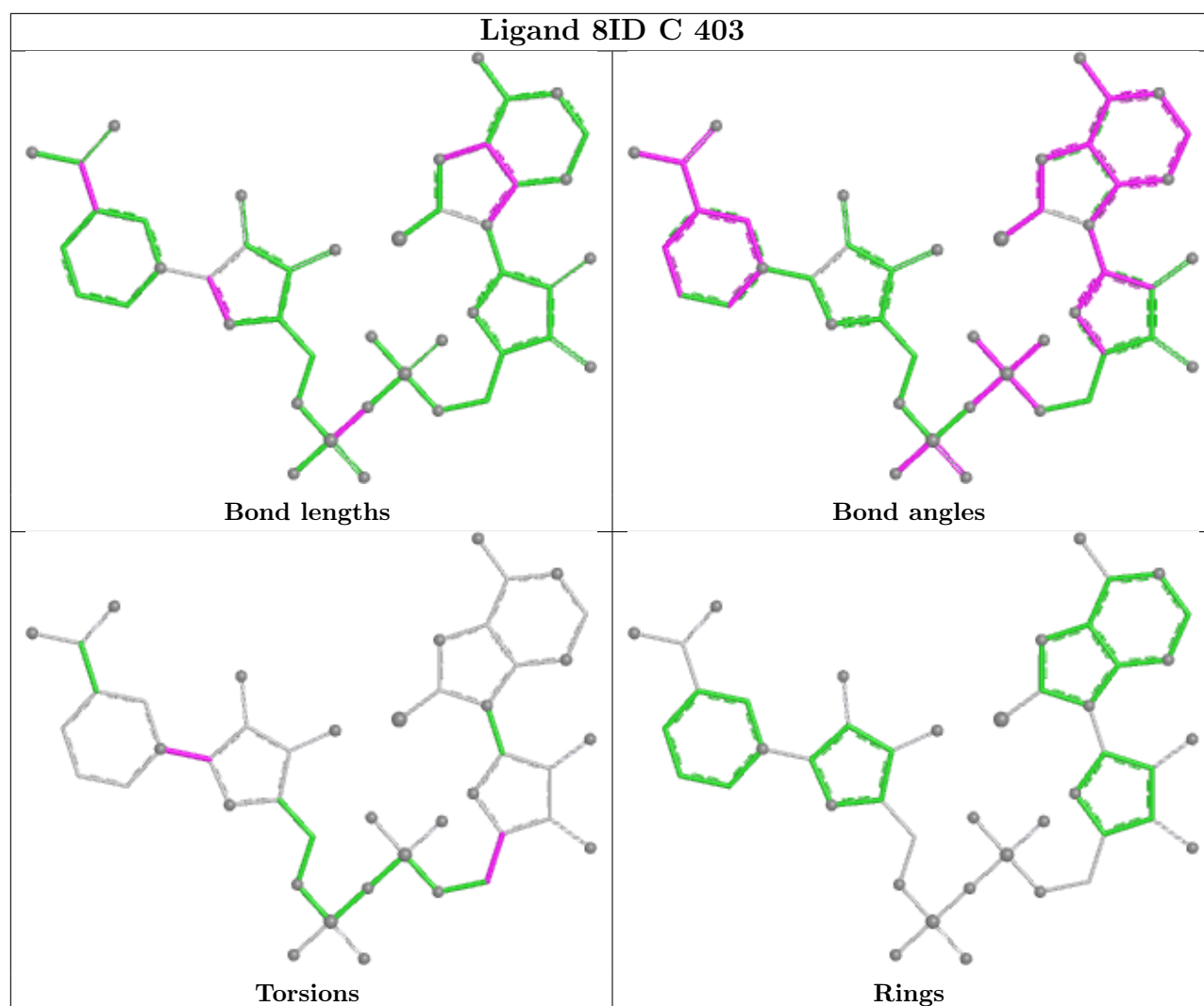
3 monomers are involved in 7 short contacts:

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





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	347/347 (100%)	-1.10	0 100 100	23, 36, 56, 73	0
1	B	347/347 (100%)	-1.02	0 100 100	23, 40, 74, 93	0
1	C	347/347 (100%)	-1.24	0 100 100	21, 31, 47, 64	0
1	D	347/347 (100%)	-1.00	0 100 100	22, 39, 83, 120	0
All	All	1388/1388 (100%)	-1.09	0 100 100	21, 36, 69, 120	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	ETF	D	404	6/6	0.95	0.09	47,52,56,61	0
4	ETF	B	404	6/6	0.96	0.09	61,71,74,78	0
4	ETF	A	404	6/6	0.99	0.04	26,31,31,34	0
2	ZN	D	401	1/1	0.99	0.02	48,48,48,48	0

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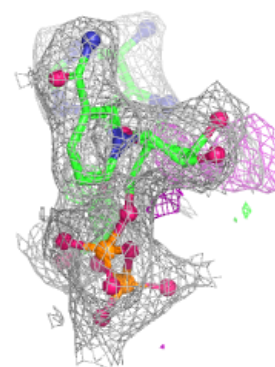
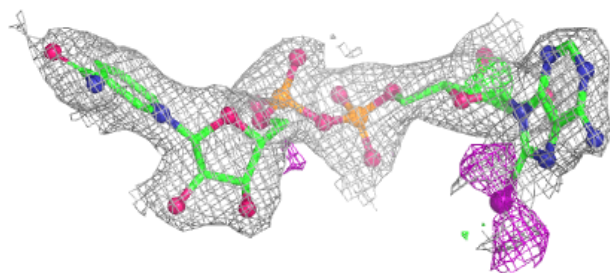
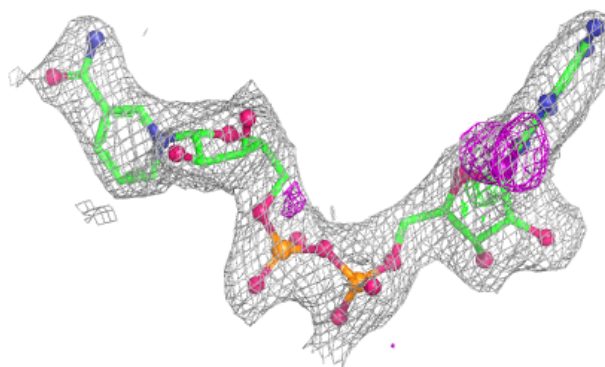
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ETF	C	404	6/6	0.99	0.03	18,22,24,25	0
3	8ID	A	403	45/45	0.99	0.04	25,32,45,59	0
2	ZN	A	401	1/1	1.00	0.01	33,33,33,33	0
2	ZN	D	402	1/1	1.00	0.01	33,33,33,33	0
2	ZN	A	402	1/1	1.00	0.01	35,35,35,35	0
3	8ID	C	403	45/45	1.00	0.03	20,24,34,44	0
2	ZN	B	401	1/1	1.00	0.01	49,49,49,49	0
2	ZN	B	402	1/1	1.00	0.01	37,37,37,37	0
2	ZN	C	401	1/1	1.00	0.01	25,25,25,25	0
2	ZN	C	402	1/1	1.00	0.01	30,30,30,30	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.

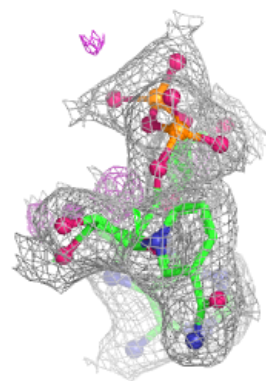
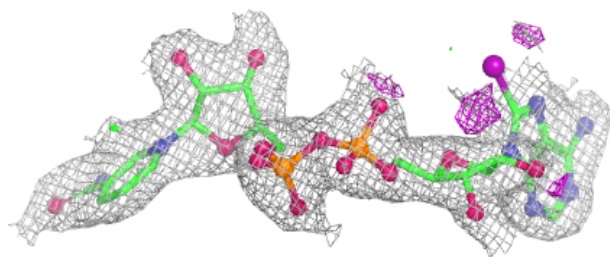
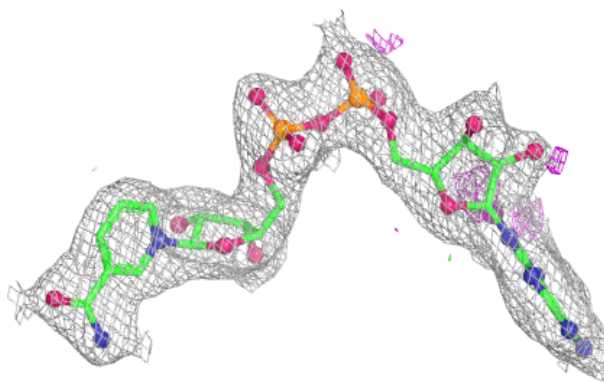
Electron density around 8ID A 403:

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 [i](#)

There are no such residues in this entry.