Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 08:13 AM EST

PDB ID	:	8W0H
Title	:	Crystal structure of Acetyl-CoA synthetase 2 from Candida albicans in complex with an isopropyl AMP ester inhibitor (trigonal form)
Authors	:	Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2024-02-13
Resolution	:	2.95 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:

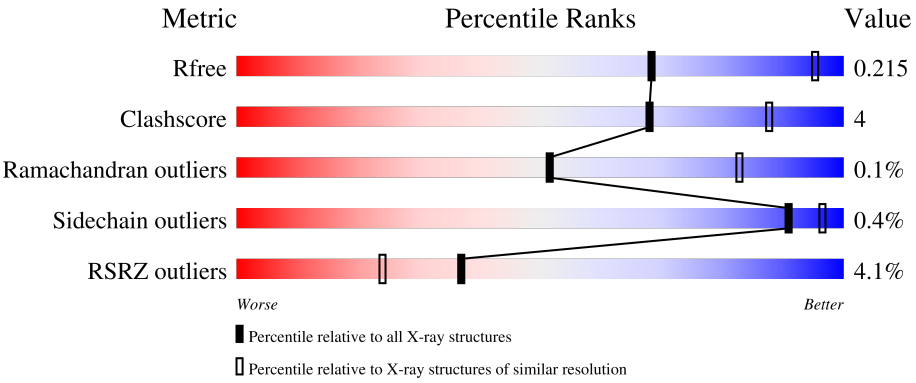
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	686	3% 86% 10% .
1	B	686	4% 87% 9% .
1	C	686	4% 87% 9% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 15515 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 Acetyl-coenzyme A synthetase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	660	Total	C	N	O	S	0	0	0
			5115	3266	868	967	14			
1	B	660	Total	C	N	O	S	0	0	0
			5125	3271	871	969	14			
1	C	654	Total	C	N	O	S	0	0	0
			5081	3244	861	962	14			

There are 51 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q8NJN3
A	2	HIS	-	expression tag	UNP Q8NJN3
A	3	HIS	-	expression tag	UNP Q8NJN3
A	4	HIS	-	expression tag	UNP Q8NJN3
A	5	HIS	-	expression tag	UNP Q8NJN3
A	6	HIS	-	expression tag	UNP Q8NJN3
A	7	HIS	-	expression tag	UNP Q8NJN3
A	8	HIS	-	expression tag	UNP Q8NJN3
A	9	HIS	-	expression tag	UNP Q8NJN3
A	10	GLU	-	expression tag	UNP Q8NJN3
A	11	ASN	-	expression tag	UNP Q8NJN3
A	12	LEU	-	expression tag	UNP Q8NJN3
A	13	TYR	-	expression tag	UNP Q8NJN3
A	14	PHE	-	expression tag	UNP Q8NJN3
A	15	GLN	-	expression tag	UNP Q8NJN3
A	16	GLY	-	expression tag	UNP Q8NJN3
A	403	ALA	VAL	engineered mutation	UNP Q8NJN3
B	1	MET	-	initiating methionine	UNP Q8NJN3
B	2	HIS	-	expression tag	UNP Q8NJN3
B	3	HIS	-	expression tag	UNP Q8NJN3
B	4	HIS	-	expression tag	UNP Q8NJN3
B	5	HIS	-	expression tag	UNP Q8NJN3
B	6	HIS	-	expression tag	UNP Q8NJN3

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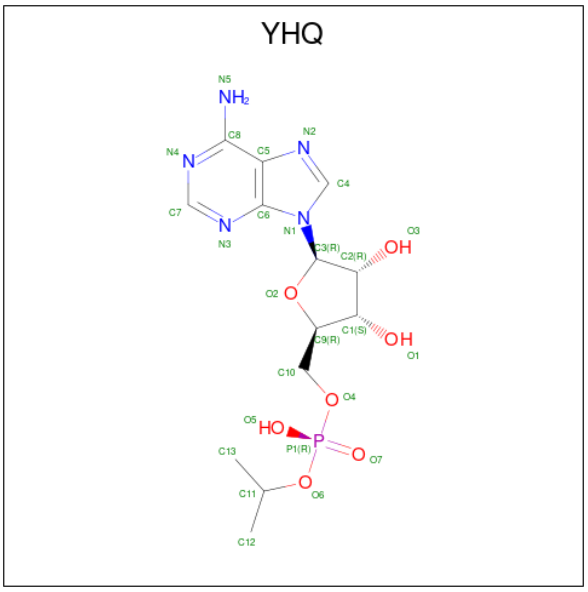
Chain	Residue	Modelled	Actual	Comment	Reference
B	7	HIS	-	expression tag	UNP Q8NJN3
B	8	HIS	-	expression tag	UNP Q8NJN3
B	9	HIS	-	expression tag	UNP Q8NJN3
B	10	GLU	-	expression tag	UNP Q8NJN3
B	11	ASN	-	expression tag	UNP Q8NJN3
B	12	LEU	-	expression tag	UNP Q8NJN3
B	13	TYR	-	expression tag	UNP Q8NJN3
B	14	PHE	-	expression tag	UNP Q8NJN3
B	15	GLN	-	expression tag	UNP Q8NJN3
B	16	GLY	-	expression tag	UNP Q8NJN3
B	403	ALA	VAL	engineered mutation	UNP Q8NJN3
C	1	MET	-	initiating methionine	UNP Q8NJN3
C	2	HIS	-	expression tag	UNP Q8NJN3
C	3	HIS	-	expression tag	UNP Q8NJN3
C	4	HIS	-	expression tag	UNP Q8NJN3
C	5	HIS	-	expression tag	UNP Q8NJN3
C	6	HIS	-	expression tag	UNP Q8NJN3
C	7	HIS	-	expression tag	UNP Q8NJN3
C	8	HIS	-	expression tag	UNP Q8NJN3
C	9	HIS	-	expression tag	UNP Q8NJN3
C	10	GLU	-	expression tag	UNP Q8NJN3
C	11	ASN	-	expression tag	UNP Q8NJN3
C	12	LEU	-	expression tag	UNP Q8NJN3
C	13	TYR	-	expression tag	UNP Q8NJN3
C	14	PHE	-	expression tag	UNP Q8NJN3
C	15	GLN	-	expression tag	UNP Q8NJN3
C	16	GLY	-	expression tag	UNP Q8NJN3
C	403	ALA	VAL	engineered mutation	UNP Q8NJN3

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

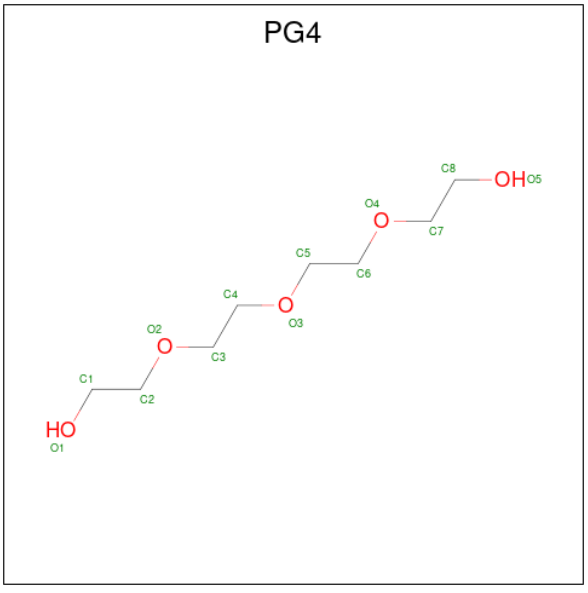
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is 5'-O-{(R)-hydroxy[(propan-2-yl)oxy]phosphoryl}adenosine (three-letter code: YHQ) (formula: $C_{13}H_{20}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			26	13	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			26	13	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			26	13	5	7	1		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	8	5		

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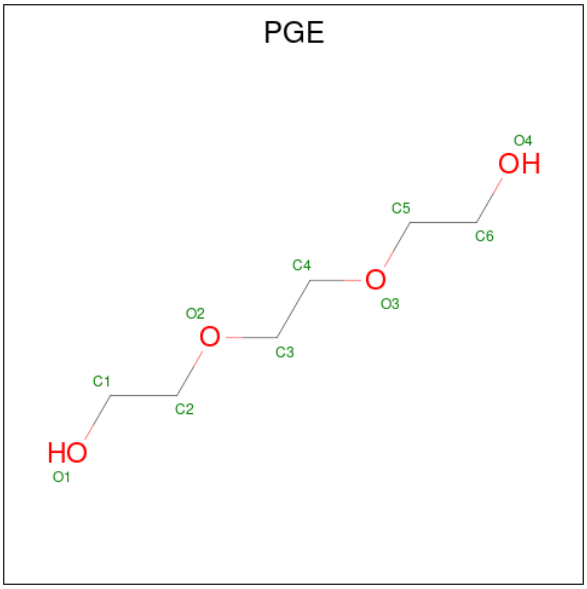
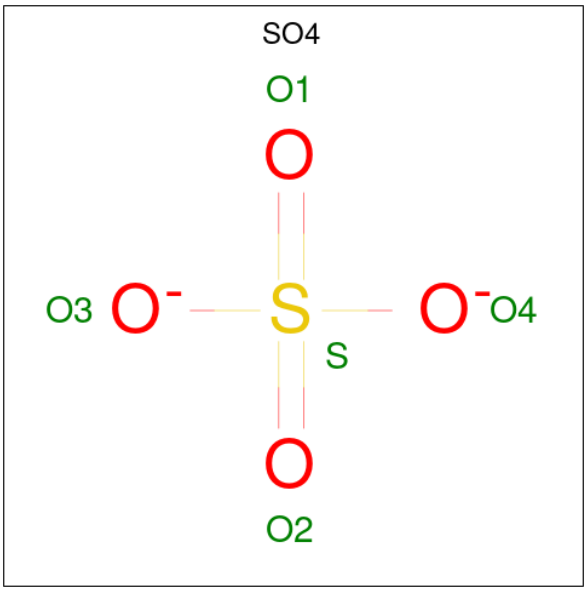
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0
4	B	1	Total C O 13 8 5	0	0
4	C	1	Total C O 13 8 5	0	0
4	C	1	Total C O 13 8 5	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 10 6 4	0	0
5	B	1	Total C O 10 6 4	0	0
5	C	1	Total C O 10 6 4	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

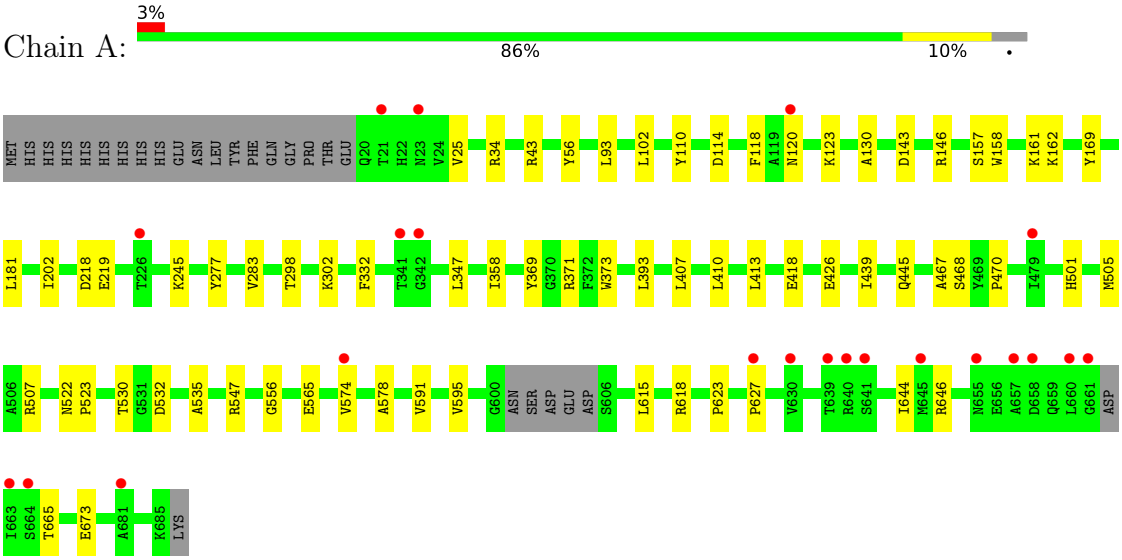


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0

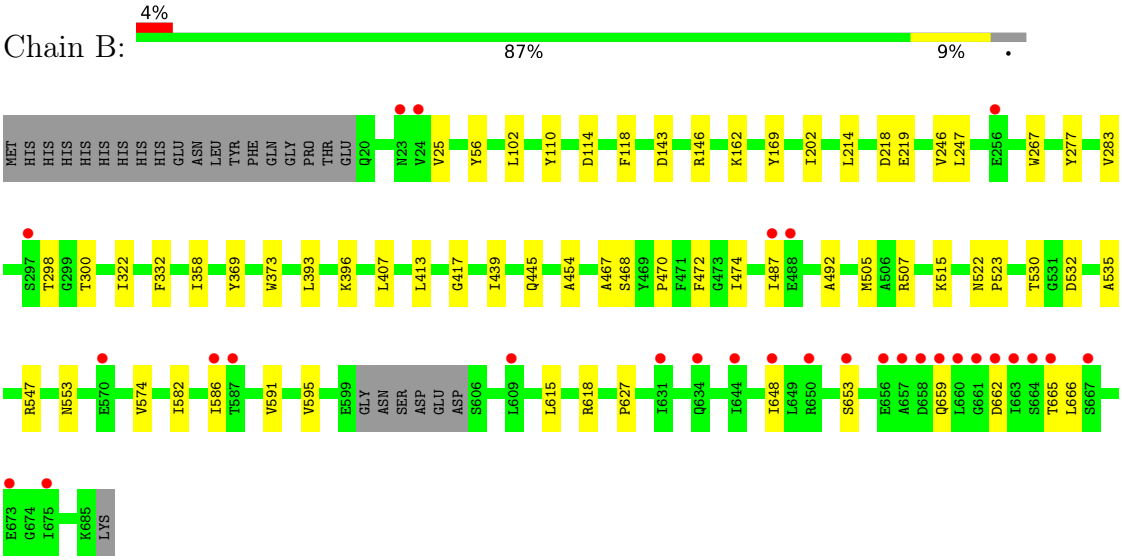
3 Residue-property plots (i)

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: Acetyl-coenzyme A synthetase 2

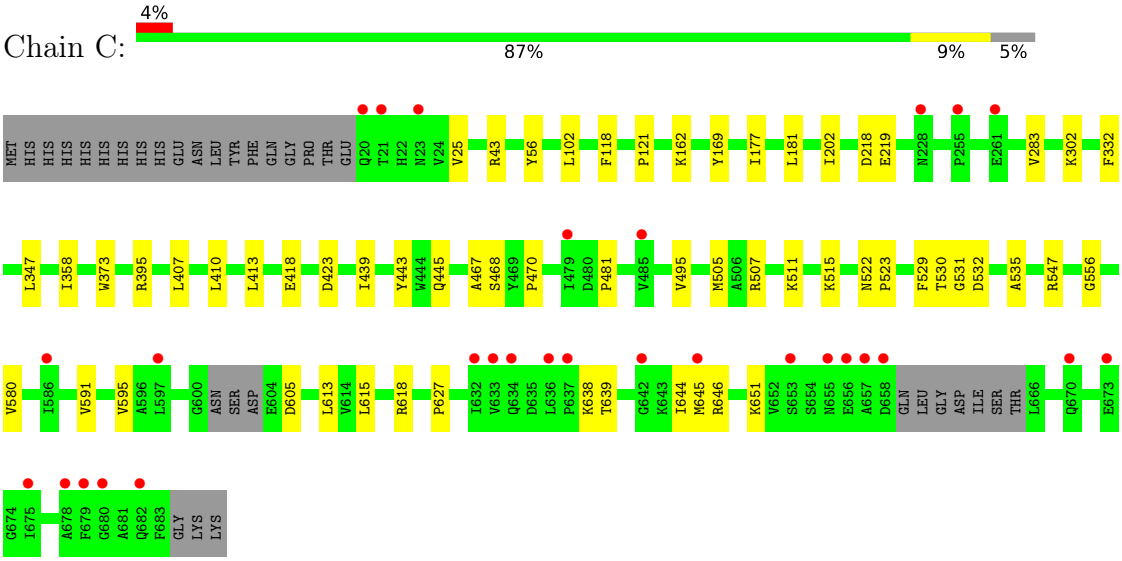


• Molecule 1: Acetyl-coenzyme A synthetase 2



• Molecule 1: Acetyl-coenzyme A synthetase 2

Chain C:


4%
87%
9%
5%
MET HIS HIS HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY PRO THR GLU Q20 T21 H22 N23 V24 V25 R43 Y56 L102 F118 P121 K162 Y169 I177 L181 I202 D218 E219 N228 P255 E261 V283 K302 F332
L347 I358 W373 R395 L407 L410 L413 E418 D423 I439 Y443 W444 Q445 A467 S468 Y469 P470 I479 D480 P481 V485 V495 M505 A506 R507 K511 K515 N522 P523 F529 T530 G531 D532 A535 R547 G556
V580 I586 V591 V595 A596 L597 G600 ASN SER ASP E604 D605 L613 V614 L615 R618 P627 I632 V633 Q634 D635 L636 P637 K638 T639 G642 K643 I644 M645 R646 K651 V652 S653 S654 N655 E656 A657 D658 GLN LEU GLY ASP ILE SER THR L666 Q670 E673
G674 I675 A678 F679 G680 A681 Q682 F683 GLY LYS LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	113.92Å 113.92Å 354.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.33 – 2.95 49.33 – 2.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.33-2.95) 100.0 (49.33-2.95)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.96Å)	Xtriage
Refinement program	PHENIX (dev_5233: ???)	Depositor
R, R_{free}	0.188 , 0.224 0.188 , 0.215	Depositor DCC
R_{free} test set	2981 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å^2)	71.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15515	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.94% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: YHQ, SO4, PG4, CL, PGE

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	0.26	0/5243	0.47	0/7127
1	B	0.25	0/5254	0.47	0/7143
1	C	0.26	0/5209	0.47	0/7081
All	All	0.25	0/15706	0.47	0/21351

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5115	0	5009	45	0
1	B	5125	0	5022	37	0
1	C	5081	0	4969	39	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	26	0	0	1	0
3	B	26	0	0	1	0
3	C	26	0	0	1	0
4	A	26	0	36	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	26	0	36	0	0
4	C	26	0	36	0	0
5	A	10	0	14	0	0
5	B	10	0	14	1	0
5	C	10	0	14	0	0
6	B	5	0	0	0	0
All	All	15515	0	15150	115	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 4.

All (115) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:532:ASP:OD1	1:C:547:ARG:HD2	1.75	0.86
1:A:120:ASN:ND2	1:A:123:LYS:HD2	2.10	0.67
1:A:591:VAL:HG23	1:A:627:PRO:HA	1.75	0.67
1:A:120:ASN:O	1:A:120:ASN:OD1	2.13	0.67
1:A:565:GLU:OE2	1:A:646:ARG:NH1	2.30	0.65
1:A:25:VAL:HG22	1:A:535:ALA:HB1	1.79	0.64
1:B:332:PHE:HB2	1:B:358:ILE:HD12	1.80	0.64
1:C:25:VAL:HG22	1:C:535:ALA:HB1	1.79	0.64
1:C:332:PHE:HB2	1:C:358:ILE:HD12	1.79	0.63
1:A:615:LEU:HD23	1:A:618:ARG:HD3	1.81	0.62
1:B:591:VAL:HG23	1:B:627:PRO:HA	1.81	0.60
1:A:332:PHE:HB2	1:A:358:ILE:HD12	1.84	0.60
1:B:467:ALA:O	1:B:468:SER:OG	2.19	0.60
1:C:591:VAL:HG23	1:C:627:PRO:HA	1.83	0.60
1:B:25:VAL:HG22	1:B:535:ALA:HB1	1.83	0.60
1:A:102:LEU:HD22	1:B:118:PHE:CZ	2.38	0.59
1:A:120:ASN:HD21	1:A:123:LYS:CD	2.17	0.58
1:A:162:LYS:HD2	1:A:283:VAL:HG12	1.86	0.58
1:B:413:LEU:HB2	1:B:439:ILE:HD13	1.85	0.58
1:C:445:GLN:NE2	1:C:530:THR:O	2.35	0.58
1:B:615:LEU:HD23	1:B:618:ARG:HD3	1.86	0.57
1:B:56:TYR:OH	1:B:470:PRO:O	2.22	0.57
1:A:445:GLN:NE2	1:A:530:THR:O	2.36	0.56
1:C:56:TYR:OH	1:C:470:PRO:O	2.23	0.56
1:B:532:ASP:OD2	3:B:703:YHQ:O1	2.23	0.56
1:A:413:LEU:HB2	1:A:439:ILE:HD13	1.88	0.56
1:B:373:TRP:HB3	1:B:407:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532:ASP:OD2	3:A:702:YHQ:O1	2.23	0.55
1:B:532:ASP:OD1	1:B:547:ARG:HD2	2.05	0.55
1:A:120:ASN:ND2	1:A:123:LYS:CD	2.70	0.55
1:A:143:ASP:OD1	1:A:146:ARG:NH2	2.41	0.54
1:A:373:TRP:HB3	1:A:407:LEU:HD11	1.88	0.54
1:B:417:GLY:O	1:B:553:ASN:ND2	2.38	0.53
1:B:445:GLN:NE2	1:B:530:THR:O	2.36	0.53
1:A:578:ALA:HB2	1:A:644:ILE:HD13	1.89	0.53
1:A:467:ALA:O	1:A:468:SER:OG	2.22	0.52
1:C:418:GLU:OE2	1:C:556:GLY:N	2.43	0.52
1:C:302:LYS:HB3	1:C:515:LYS:HZ3	1.73	0.52
1:A:162:LYS:NZ	4:A:703:PG4:O1	2.43	0.51
1:C:443:TYR:HE1	1:C:532:ASP:OD2	1.94	0.51
1:B:169:TYR:CZ	1:B:202:ILE:HD11	2.45	0.51
1:A:56:TYR:OH	1:A:470:PRO:O	2.29	0.51
1:A:574:VAL:HG13	1:A:595:VAL:HG13	1.95	0.49
1:B:298:THR:HG21	1:B:515:LYS:CE	2.42	0.49
1:B:102:LEU:H	1:B:102:LEU:HD12	1.77	0.49
1:C:169:TYR:CZ	1:C:202:ILE:HD11	2.47	0.49
1:A:102:LEU:HD12	1:A:102:LEU:H	1.77	0.48
1:A:120:ASN:HD21	1:A:123:LYS:HD2	1.76	0.48
1:A:43:ARG:NH1	1:A:410:LEU:O	2.44	0.48
1:C:639:THR:CG2	1:C:645:MET:HG2	2.43	0.48
1:B:396:LYS:HD3	1:B:586:ILE:HD11	1.94	0.48
1:B:162:LYS:HD2	1:B:283:VAL:HG12	1.96	0.48
1:C:615:LEU:HD23	1:C:618:ARG:HD3	1.96	0.48
1:A:120:ASN:HD21	1:A:123:LYS:HD3	1.79	0.48
1:C:162:LYS:HD2	1:C:283:VAL:HG12	1.94	0.48
1:A:93:LEU:HD13	1:A:501:HIS:HB3	1.95	0.47
1:B:474:ILE:N	1:B:474:ILE:HD12	2.29	0.47
1:A:158:TRP:CG	1:A:245:LYS:HD2	2.50	0.47
1:B:648:ILE:CD1	1:B:666:LEU:HD11	2.44	0.47
1:A:673:GLU:OE1	1:A:673:GLU:N	2.46	0.47
1:C:638:LYS:HG2	1:C:644:ILE:HD13	1.95	0.47
1:C:467:ALA:O	1:C:468:SER:OG	2.24	0.47
1:A:169:TYR:CZ	1:A:202:ILE:HD11	2.50	0.46
1:C:181:LEU:HD21	1:C:347:LEU:HD21	1.96	0.46
1:A:157:SER:HB2	1:C:511:LYS:NZ	2.31	0.46
1:A:522:ASN:N	1:A:523:PRO:CD	2.79	0.46
1:A:418:GLU:OE2	1:A:556:GLY:N	2.48	0.46
1:B:582:ILE:HG21	1:B:653:SER:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ASP:OD1	1:C:219:GLU:N	2.46	0.45
1:A:34:ARG:NH1	1:A:426:GLU:OE2	2.45	0.45
1:C:395:ARG:NH1	1:C:423:ASP:OD2	2.43	0.45
1:C:522:ASN:N	1:C:523:PRO:CD	2.79	0.45
1:C:373:TRP:HB3	1:C:407:LEU:HD11	1.99	0.45
1:B:369:TYR:HE1	1:B:393:LEU:HD21	1.82	0.45
1:B:218:ASP:OD1	1:B:219:GLU:N	2.48	0.45
1:C:102:LEU:H	1:C:102:LEU:HD12	1.82	0.44
1:A:118:PHE:CZ	1:C:102:LEU:HD22	2.52	0.44
1:B:662:ASP:OD2	1:B:665:THR:HG23	2.17	0.44
1:C:532:ASP:OD2	3:C:702:YHQ:O1	2.35	0.44
1:B:322:ILE:HD13	1:B:454:ALA:HB3	1.99	0.44
1:B:505:MET:O	1:B:507:ARG:NH1	2.50	0.44
1:C:43:ARG:NH1	1:C:410:LEU:O	2.49	0.44
1:A:277:TYR:CZ	1:C:102:LEU:HD23	2.54	0.43
1:B:298:THR:HG21	1:B:515:LYS:HE2	1.99	0.43
1:B:487:ILE:HG21	1:B:492:ALA:HB1	2.00	0.43
1:B:522:ASN:N	1:B:523:PRO:CD	2.81	0.43
1:A:102:LEU:HD23	1:B:277:TYR:CZ	2.53	0.43
1:A:110:TYR:CD1	1:A:114:ASP:HB2	2.54	0.43
1:A:532:ASP:OD1	1:A:547:ARG:HD2	2.18	0.43
1:B:574:VAL:HG13	1:B:595:VAL:HG13	2.00	0.43
1:C:347:LEU:C	1:C:347:LEU:HD23	2.39	0.43
1:C:595:VAL:HG21	1:C:613:LEU:HD13	2.01	0.43
1:B:143:ASP:OD1	1:B:146:ARG:NH2	2.49	0.43
1:C:177:ILE:CD1	1:C:347:LEU:HD12	2.48	0.43
1:C:443:TYR:CE1	1:C:532:ASP:OD2	2.72	0.42
1:A:369:TYR:CE2	1:A:393:LEU:HD21	2.54	0.42
1:C:505:MET:O	1:C:507:ARG:NH1	2.52	0.42
1:C:639:THR:HG22	1:C:645:MET:HG2	2.01	0.42
1:B:102:LEU:HD22	1:C:118:PHE:CZ	2.55	0.41
1:B:214:LEU:HB3	1:B:246:VAL:HG22	2.02	0.41
1:A:181:LEU:HD21	1:A:347:LEU:HD21	2.03	0.41
1:B:247:LEU:HD11	1:B:267:TRP:HA	2.03	0.41
1:B:472:PHE:O	1:B:474:ILE:HD12	2.20	0.41
5:B:706:PGE:H32	1:C:121:PRO:HG3	2.03	0.41
1:A:218:ASP:OD1	1:A:219:GLU:N	2.49	0.41
1:C:481:PRO:HG3	1:C:495:VAL:HG23	2.02	0.41
1:A:130:ALA:O	1:A:371:ARG:NH2	2.54	0.41
1:A:162:LYS:HZ1	4:A:703:PG4:C2	2.34	0.41
1:C:177:ILE:HD12	1:C:347:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:LEU:O	1:C:439:ILE:HA	2.21	0.41
1:C:580:VAL:HG12	1:C:646:ARG:HB3	2.03	0.41
1:A:618:ARG:HG2	1:A:623:PRO:HA	2.03	0.41
1:C:529:PHE:CZ	1:C:531:GLY:HA2	2.57	0.40
1:A:505:MET:O	1:A:507:ARG:NH1	2.54	0.40
1:B:110:TYR:CD1	1:B:114:ASP:HB2	2.56	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	654/686 (95%)	628 (96%)	26 (4%)	0	100	100
1	B	656/686 (96%)	634 (97%)	22 (3%)	0	100	100
1	C	648/686 (94%)	625 (96%)	22 (3%)	1 (0%)	47	79
All	All	1958/2058 (95%)	1887 (96%)	70 (4%)	1 (0%)	51	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	605	ASP

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	540/568 (95%)	536 (99%)	4 (1%)	84 93
1	B	542/568 (95%)	540 (100%)	2 (0%)	91 96
1	C	537/568 (94%)	536 (100%)	1 (0%)	93 98
All	All	1619/1704 (95%)	1612 (100%)	7 (0%)	91 96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	LYS
1	A	298	THR
1	A	302	LYS
1	A	665	THR
1	B	300	THR
1	B	659	GLN
1	C	651	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	C	343	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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	PG4	A	704	-	12,12,12	0.29	0	11,11,11	0.17	0
6	SO4	B	701	-	4,4,4	0.63	0	6,6,6	0.05	0
4	PG4	C	704	-	12,12,12	0.28	0	11,11,11	0.23	0
5	PGE	A	705	-	9,9,9	0.30	0	8,8,8	0.50	0
5	PGE	B	706	-	9,9,9	0.29	0	8,8,8	0.60	0
4	PG4	C	703	-	12,12,12	0.29	0	11,11,11	0.17	0
4	PG4	A	703	-	12,12,12	0.29	0	11,11,11	0.17	0
3	YHQ	A	702	-	25,28,28	0.65	0	27,42,42	0.76	1 (3%)
4	PG4	B	704	-	12,12,12	0.29	0	11,11,11	0.17	0
3	YHQ	C	702	-	25,28,28	0.64	0	27,42,42	0.75	1 (3%)
4	PG4	B	705	-	12,12,12	0.29	0	11,11,11	0.14	0
5	PGE	C	705	-	9,9,9	0.28	0	8,8,8	0.52	0
3	YHQ	B	703	-	25,28,28	0.64	0	27,42,42	0.76	1 (3%)

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	PG4	A	704	-	-	0/10/10/10	-
4	PG4	C	704	-	-	2/10/10/10	-
5	PGE	A	705	-	-	3/7/7/7	-
5	PGE	B	706	-	-	1/7/7/7	-
4	PG4	C	703	-	-	3/10/10/10	-
4	PG4	A	703	-	-	2/10/10/10	-
3	YHQ	A	702	-	-	0/11/31/31	0/3/3/3
4	PG4	B	704	-	-	2/10/10/10	-
3	YHQ	C	702	-	-	0/11/31/31	0/3/3/3
4	PG4	B	705	-	-	3/10/10/10	-
5	PGE	C	705	-	-	2/7/7/7	-
3	YHQ	B	703	-	-	0/11/31/31	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	702	YHQ	C5-C8-N5	2.30	123.85	120.35
3	B	703	YHQ	C5-C8-N5	2.27	123.81	120.35
3	C	702	YHQ	C5-C8-N5	2.27	123.80	120.35

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	703	PG4	O2-C3-C4-O3
4	C	703	PG4	O4-C7-C8-O5
4	B	704	PG4	O2-C3-C4-O3
4	B	705	PG4	O1-C1-C2-O2
4	C	703	PG4	O1-C1-C2-O2
5	C	705	PGE	O3-C5-C6-O4
4	B	704	PG4	O4-C7-C8-O5
4	C	704	PG4	O4-C7-C8-O5
5	A	705	PGE	O2-C3-C4-O3
4	B	705	PG4	O4-C7-C8-O5
4	C	704	PG4	C5-C6-O4-C7
5	C	705	PGE	C3-C4-O3-C5
5	A	705	PGE	C1-C2-O2-C3
4	A	703	PG4	C6-C5-O3-C4
4	B	705	PG4	O2-C3-C4-O3
5	A	705	PGE	C6-C5-O3-C4
5	B	706	PGE	C4-C3-O2-C2
4	A	703	PG4	C3-C4-O3-C5

There are no ring outliers.

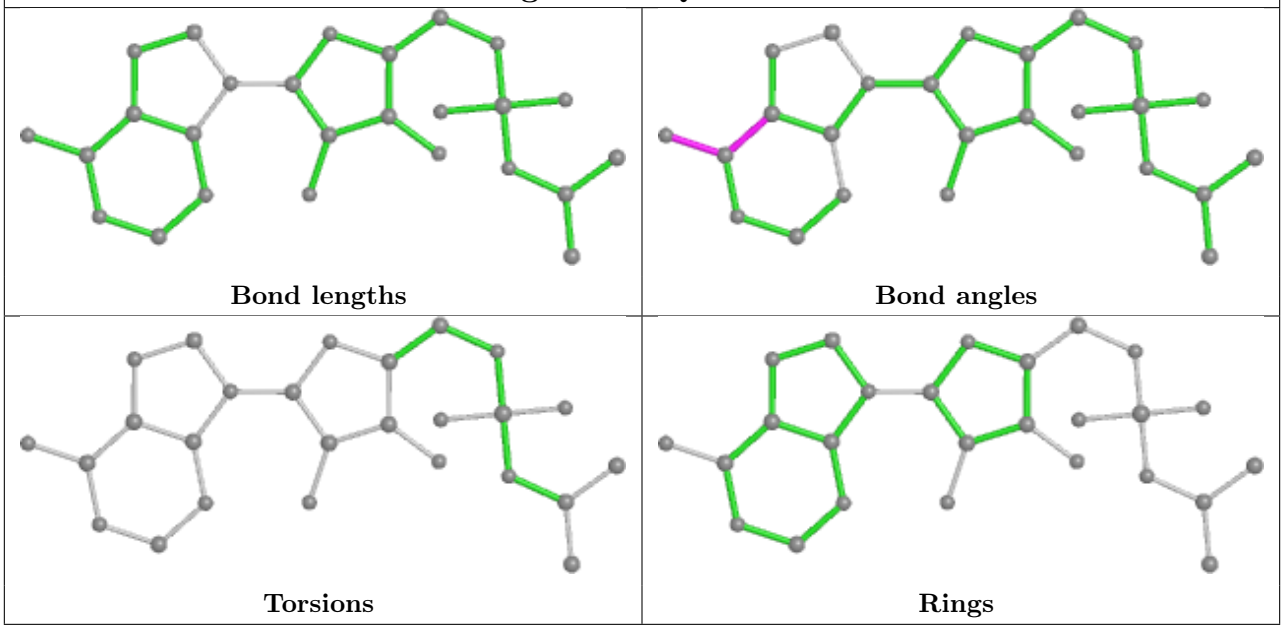
5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	706	PGE	1	0
4	A	703	PG4	2	0
3	A	702	YHQ	1	0
3	C	702	YHQ	1	0
3	B	703	YHQ	1	0

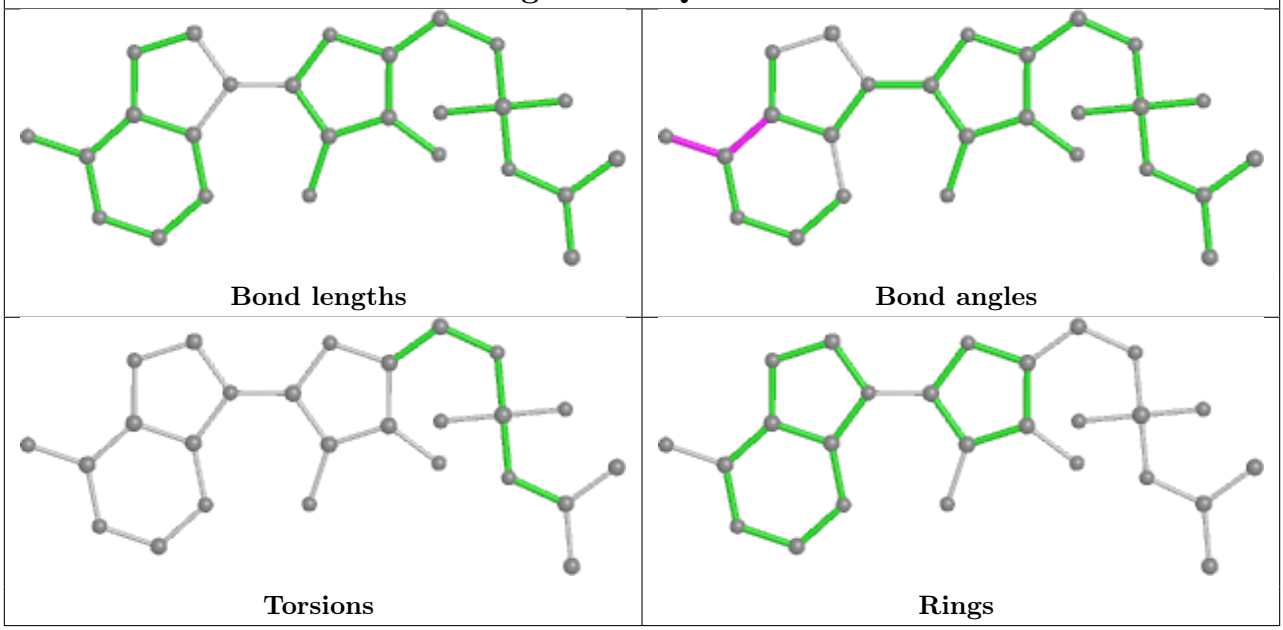
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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.

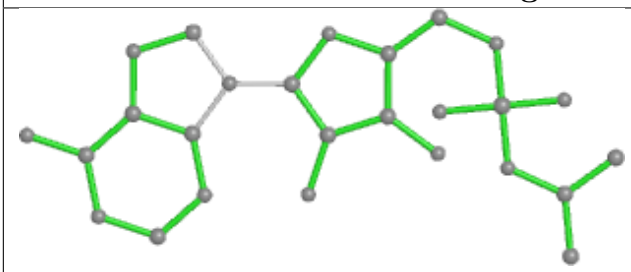
Ligand YHQ A 702



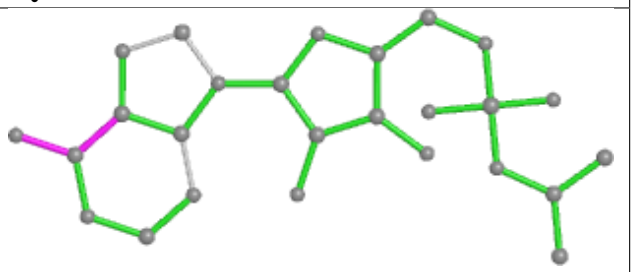
Ligand YHQ C 702



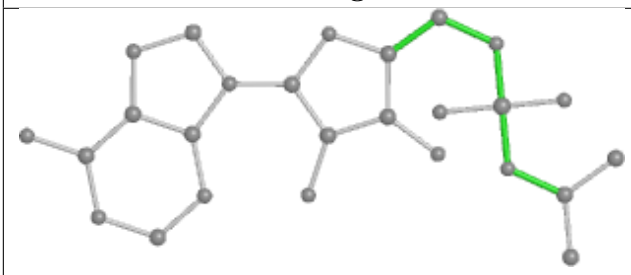
Ligand YHQ B 703



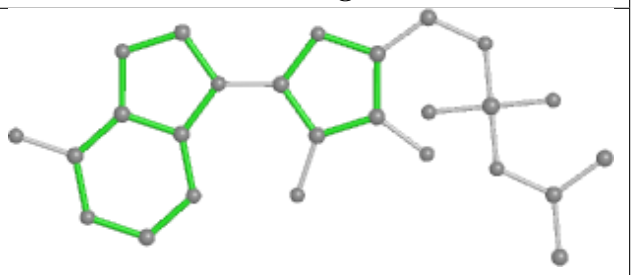
Bond lengths



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

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	660/686 (96%)	0.13	22 (3%)	46	30	42, 72, 122, 153	0
1	B	660/686 (96%)	0.14	29 (4%)	34	21	42, 70, 130, 170	0
1	C	654/686 (95%)	0.08	29 (4%)	34	21	42, 70, 131, 185	0
All	All	1974/2058 (95%)	0.11	80 (4%)	37	24	42, 71, 128, 185	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	657	ALA	6.3
1	B	658	ASP	5.6
1	C	658	ASP	5.0
1	B	659	GLN	4.8
1	A	640	ARG	4.6
1	B	657	ALA	4.3
1	A	641	SER	4.1
1	C	645	MET	4.1
1	B	660	LEU	3.8
1	A	655	ASN	3.7
1	B	653	SER	3.6
1	C	679	PHE	3.5
1	A	663	ILE	3.5
1	B	673	GLU	3.3
1	B	656	GLU	3.3
1	A	658	ASP	3.3
1	A	639	THR	3.1
1	A	660	LEU	3.1
1	B	297	SER	3.1
1	C	636	LEU	3.1
1	C	21	THR	3.1
1	B	663	ILE	3.0
1	C	653	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	630	VAL	3.0
1	B	662	ASP	2.9
1	B	665	THR	2.9
1	C	682	GLN	2.9
1	C	23	ASN	2.8
1	A	226	THR	2.8
1	C	479	ILE	2.8
1	A	341	THR	2.7
1	B	488	GLU	2.7
1	A	23	ASN	2.7
1	B	487	ILE	2.7
1	C	255	PRO	2.6
1	B	661	GLY	2.6
1	C	670	GLN	2.6
1	C	637	PRO	2.6
1	C	642	GLY	2.6
1	B	23	ASN	2.6
1	C	656	GLU	2.6
1	B	675	ILE	2.5
1	B	570	GLU	2.5
1	A	681	ALA	2.5
1	B	587	THR	2.5
1	A	645	MET	2.5
1	C	632	ILE	2.5
1	C	675	ILE	2.5
1	C	634	GLN	2.5
1	C	261	GLU	2.4
1	C	586	ILE	2.4
1	A	120	ASN	2.4
1	B	634	GLN	2.3
1	B	24	VAL	2.3
1	A	479	ILE	2.3
1	C	673	GLU	2.3
1	C	597	LEU	2.3
1	B	664	SER	2.3
1	C	228	ASN	2.3
1	B	644	ILE	2.2
1	B	631	ILE	2.2
1	C	655	ASN	2.2
1	C	678	ALA	2.2
1	C	680	GLY	2.2
1	B	648	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	664	SER	2.2
1	C	633	VAL	2.2
1	A	627	PRO	2.1
1	A	342	GLY	2.1
1	A	21	THR	2.1
1	C	485	VAL	2.1
1	A	574	VAL	2.1
1	B	256	GLU	2.1
1	B	586	ILE	2.1
1	C	20	GLN	2.0
1	B	609	LEU	2.0
1	B	650	ARG	2.0
1	A	661	GLY	2.0
1	A	657	ALA	2.0
1	B	667	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGE	A	705	10/10	0.71	0.36	65,77,83,95	0
4	PG4	C	704	13/13	0.80	0.32	75,81,96,99	0
2	CL	A	701	1/1	0.80	0.34	95,95,95,95	0
4	PG4	B	705	13/13	0.81	0.29	63,77,85,89	0
4	PG4	A	704	13/13	0.84	0.30	65,78,97,97	0
4	PG4	A	703	13/13	0.86	0.28	61,69,78,85	0
4	PG4	B	704	13/13	0.87	0.27	65,75,82,87	0
4	PG4	C	703	13/13	0.87	0.28	66,71,78,80	0

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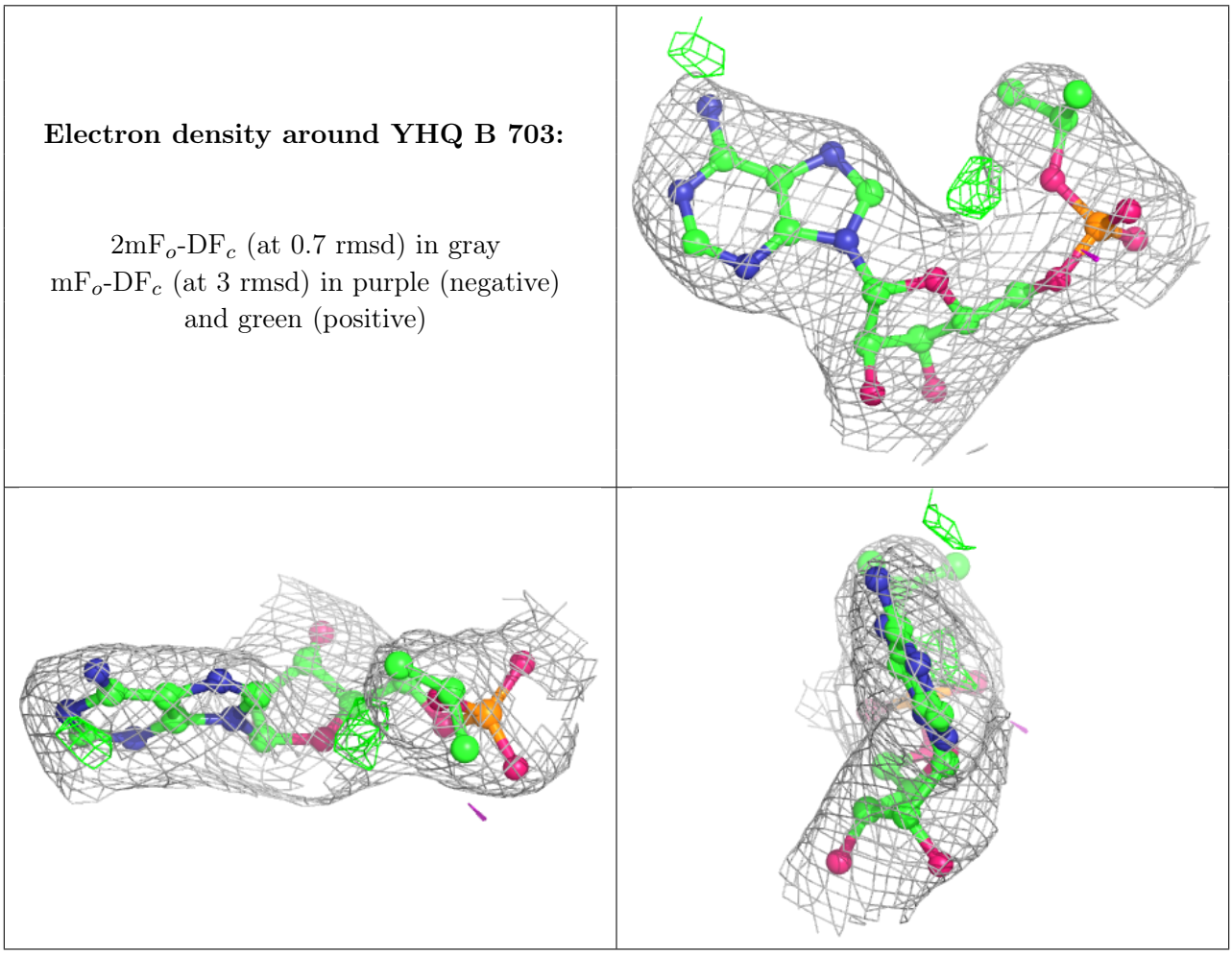
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	PGE	B	706	10/10	0.91	0.38	60,69,80,86	0
6	SO4	B	701	5/5	0.91	0.36	85,86,90,131	0
5	PGE	C	705	10/10	0.92	0.42	69,77,85,88	0
2	CL	C	701	1/1	0.94	0.37	83,83,83,83	0
3	YHQ	B	703	26/26	0.96	0.23	54,62,68,74	0
2	CL	B	702	1/1	0.97	0.17	81,81,81,81	0
3	YHQ	C	702	26/26	0.97	0.20	53,63,72,74	0
3	YHQ	A	702	26/26	0.97	0.25	51,63,68,76	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.

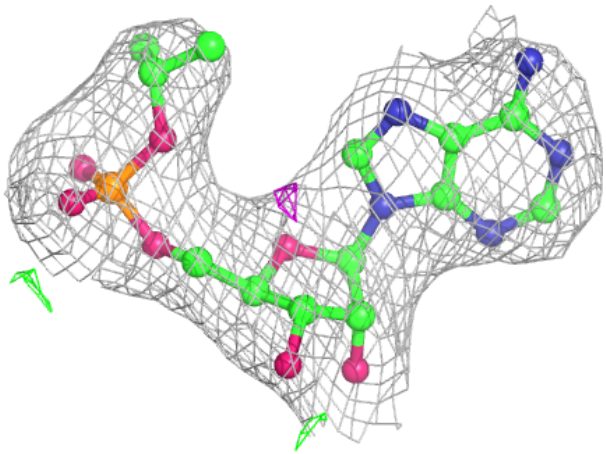
Electron density around YHQ B 703:

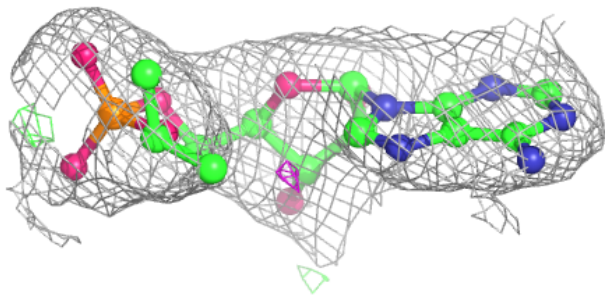
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

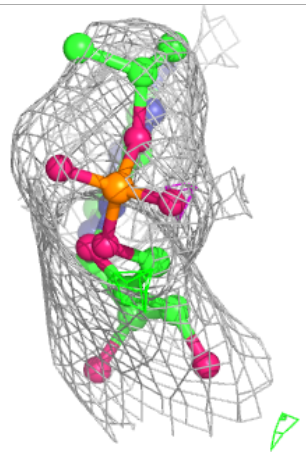


Electron density around YHQ C 702:

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

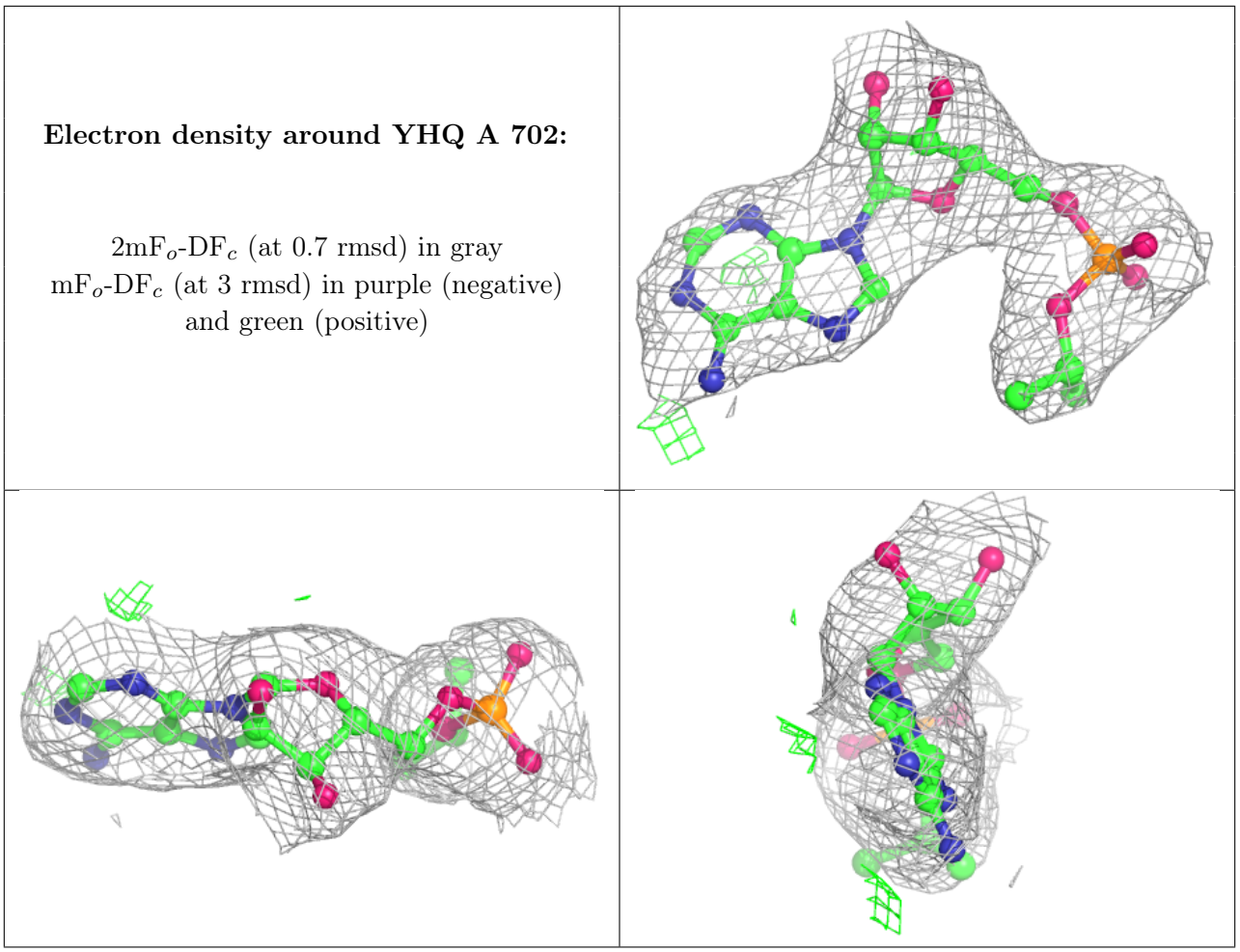






Electron density around YHQ A 702:

$2mF_o$-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.