



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:48 am BST

PDB ID : 2BEW
Title : Reactivity modulation of human branched-chain alpha-ketoacid dehydrogenase by an internal molecular switch
Authors : Machius, M.; Wynn, R.M.; Chuang, J.L.; Tomchick, D.R.; Brautigam, C.A.; Chuang, D.T.
Deposited on : 2004-11-30
Resolution : 1.79 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 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 : 2.11
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) : 2.11

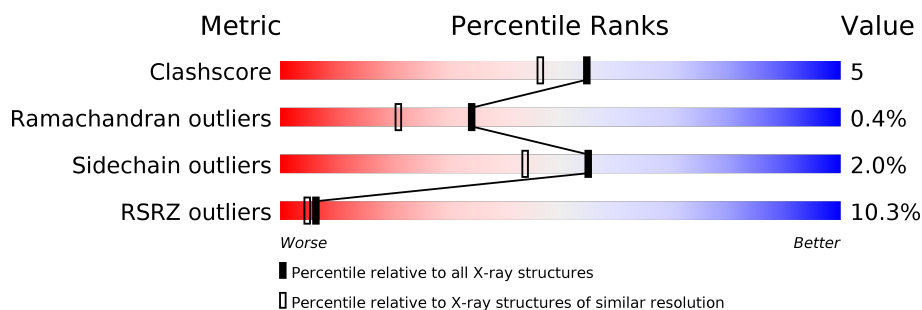
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.79 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	400	<div> <div>12%</div> <div>86%</div> <div>11%</div> <div>••</div> </div>
2	B	342	<div> <div>8%</div> <div>89%</div> <div>9%</div> <div>•</div> </div>
3	C	3	<div> <div>100%</div> <div>67%</div> <div>33%</div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6556 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 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	6	0
			3187	2007	572	590	18			

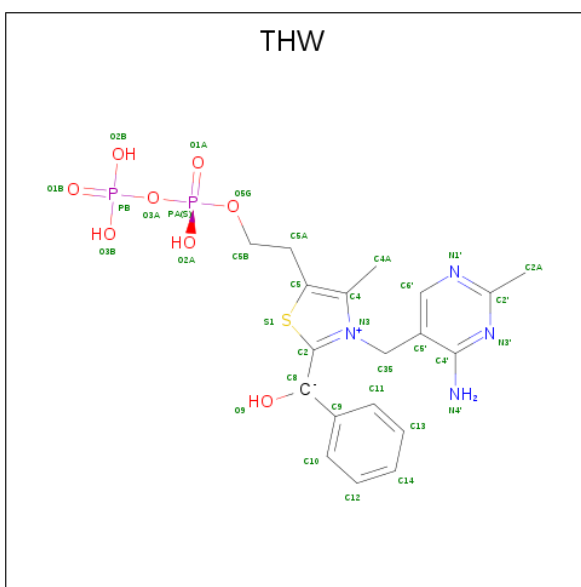
- Molecule 2 is a protein called 2-OXOISOVALERATE DEHYDROGENASE BETA SUB-UNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	336	Total	C	N	O	S	0	6	0
			2666	1719	439	493	15			

- Molecule 3 is a protein called PEPTIDE ALA-TYR-ARG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	3	Total	C	N	O	0	0	0
			28	18	6	4			

- Molecule 4 is C2-1-HYDROXYPHENYL-THIAMIN DIPHOSPHATE (three-letter code: THW) (formula: C₁₉H₂₄N₄O₈P₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	
			34	19	4	8	2	1	0

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 6 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mn		
			1	1	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			6	3	3		
8	B	1	Total	C	O	0	0
			6	3	3		

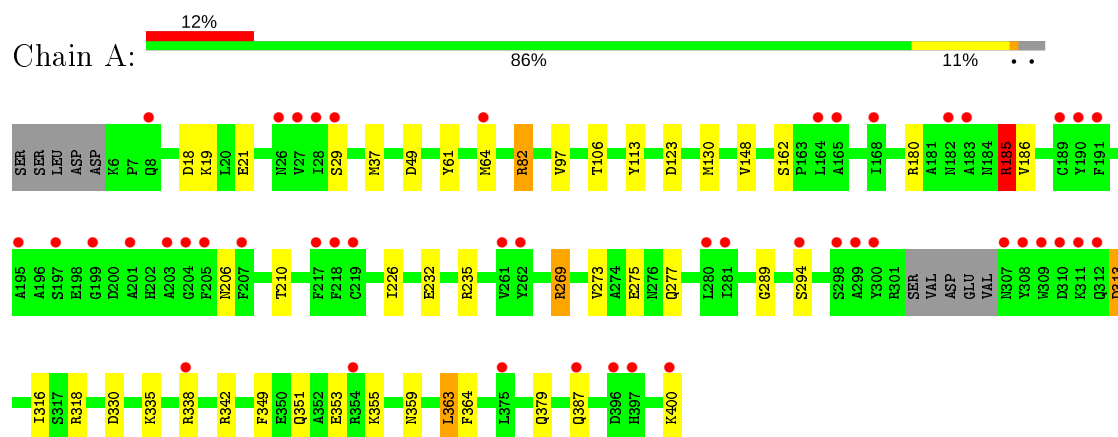
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	350	Total	O	0	0
			350	350		
9	B	270	Total	O	0	0
			270	270		
9	C	4	Total	O	0	0
			4	4		

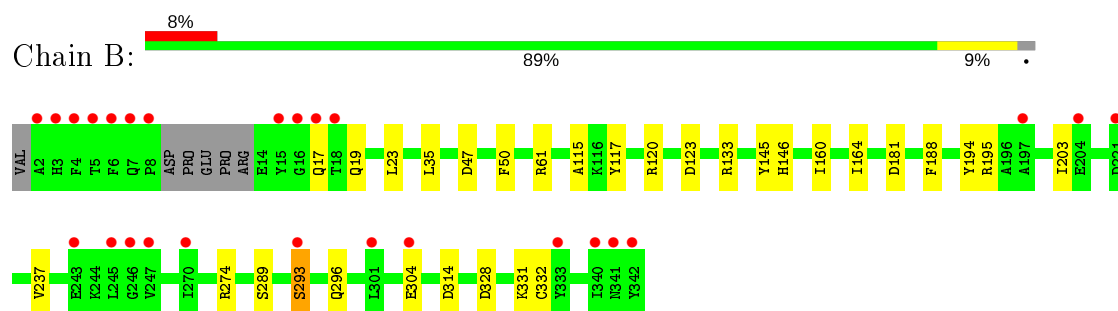
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

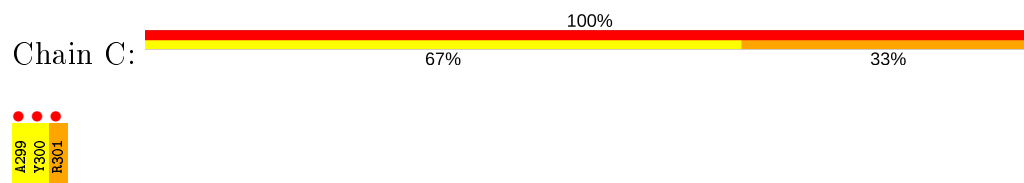
• Molecule 1: 2-OXISOVALERATE DEHYDROGENASE ALPHA SUBUNIT



• Molecule 2: 2-OXISOVALERATE DEHYDROGENASE BETA SUBUNIT



• Molecule 3: PEPTIDE ALA-TYR-ARG



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.56 Å 144.56 Å 69.49 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.79 36.14 – 1.79	Depositor EDS
% Data completeness (in resolution range)	99.4 (30.00-1.79) 99.4 (36.14-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.98 (at 1.79 Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.146 , 0.170 0.163 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.021 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6556	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: THW, GOL, K, MN, CL

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	0.95	2/3266 (0.1%)	1.01	12/4412 (0.3%)
2	B	0.95	0/2735	0.99	9/3718 (0.2%)
3	C	0.99	0/28	1.05	0/36
All	All	0.95	2/6029 (0.0%)	1.00	21/8166 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	232	GLU	CD-OE2	-5.85	1.19	1.25
1	A	162	SER	CB-OG	5.37	1.49	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	LEU	CA-CB-CG	8.95	135.89	115.30
1	A	185	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	A	82	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	A	185	ARG	NE-CZ-NH2	-7.43	116.58	120.30
2	B	47	ASP	CB-CG-OD2	7.23	124.81	118.30
2	B	123	ASP	CB-CG-OD2	6.30	123.97	118.30
1	A	49	ASP	CB-CG-OD1	5.96	123.66	118.30
2	B	274	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	18	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	269	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	313	ASP	CB-CG-OD2	5.61	123.35	118.30
2	B	328	ASP	CB-CG-OD2	5.57	123.31	118.30
2	B	181	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	180	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	37	MET	CG-SD-CE	-5.46	91.46	100.20
2	B	314	ASP	CB-CG-OD2	5.22	123.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	61	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	B	331	LYS	CD-CE-NZ	-5.11	99.94	111.70
1	A	330	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	123	ASP	CB-CG-OD2	5.07	122.86	118.30
2	B	120	ARG	NE-CZ-NH1	-5.00	117.80	120.30

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	3187	0	3071	46	0
2	B	2666	0	2618	10	0
3	C	28	0	26	9	0
4	A	34	0	20	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	B	12	0	16	1	0
9	A	350	0	0	2	0
9	B	270	0	0	3	0
9	C	4	0	0	1	0
All	All	6556	0	5751	61	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 5.

All (61) 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:A:294:SER:CB	3:C:300:TYR:HD1	1.54	1.19
1:A:186[A]:VAL:CG2	1:A:273:VAL:CG2	2.22	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:SER:CB	3:C:300:TYR:CD1	2.29	1.15
1:A:294:SER:HB3	3:C:300:TYR:CD1	1.85	1.10
1:A:294:SER:HB3	3:C:300:TYR:HD1	0.94	1.05
1:A:186[A]:VAL:CG2	1:A:273:VAL:HG22	1.84	1.04
1:A:294:SER:HB2	3:C:300:TYR:CD1	1.94	1.02
1:A:294:SER:HB2	3:C:300:TYR:CE1	1.97	0.99
1:A:186[A]:VAL:HG23	1:A:273:VAL:CG2	1.94	0.97
1:A:186[A]:VAL:HG22	1:A:273:VAL:HG22	1.45	0.97
2:B:146[B]:HIS:HE1	9:B:2130:HOH:O	1.52	0.90
1:A:64[B]:MET:SD	1:A:316:ILE:HG12	2.13	0.89
2:B:146[B]:HIS:CE1	9:B:2130:HOH:O	2.27	0.84
1:A:186[A]:VAL:CG2	1:A:273:VAL:HG23	2.16	0.75
1:A:186[A]:VAL:HG23	1:A:273:VAL:HG21	1.72	0.71
1:A:359:ASN:ND2	1:A:400:LYS:HB2	2.06	0.71
1:A:359:ASN:HD22	1:A:400:LYS:HD3	1.56	0.70
1:A:338:ARG:O	1:A:342:ARG:HG3	1.92	0.70
1:A:61:TYR:O	1:A:64[B]:MET:HG2	1.93	0.69
4:A:601:THW:H4'1	4:A:601:THW:C8	2.07	0.67
1:A:186[A]:VAL:HG23	1:A:273:VAL:HG22	1.65	0.66
3:C:299:ALA:N	9:C:2002:HOH:O	2.30	0.65
2:B:289:SER:O	2:B:293[B]:SER:HB3	1.98	0.63
1:A:186[A]:VAL:HG22	1:A:273:VAL:CG2	2.08	0.63
1:A:351:GLN:HG2	1:A:355:LYS:HE3	1.79	0.63
1:A:185:ARG:NH2	8:B:1346:GOL:O1	2.32	0.62
1:A:359:ASN:HD22	1:A:400:LYS:HB2	1.63	0.62
1:A:313:ASP:OD1	1:A:318[B]:ARG:NH2	2.31	0.61
1:A:294:SER:HB2	3:C:300:TYR:HE1	1.62	0.61
1:A:106:THR:O	1:A:185:ARG:HD2	2.02	0.59
1:A:64[B]:MET:CE	1:A:316:ILE:HG12	2.32	0.59
1:A:130:MET:SD	1:A:349:PHE:HA	2.47	0.55
1:A:82:ARG:HD3	1:A:353:GLU:OE2	2.08	0.54
1:A:186[A]:VAL:HG21	1:A:273:VAL:CG2	2.31	0.53
1:A:186[A]:VAL:HG21	1:A:273:VAL:HG23	1.88	0.52
1:A:351:GLN:CG	1:A:355:LYS:HE3	2.40	0.51
2:B:195:ARG:NH1	9:B:2165:HOH:O	2.42	0.51
1:A:206:ASN:O	1:A:210:THR:HG23	2.10	0.50
1:A:64[A]:MET:SD	1:A:97:VAL:HG21	2.53	0.49
1:A:64[B]:MET:HE2	1:A:316:ILE:HG12	1.96	0.48
1:A:359:ASN:HD22	1:A:400:LYS:CD	2.25	0.48
2:B:19:GLN:HE21	2:B:203:ILE:CD1	2.27	0.48
4:A:601:THW:O9	4:A:601:THW:H351	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:TYR:O	2:B:146[B]:HIS:HD2	1.97	0.47
1:A:269:ARG:O	1:A:273:VAL:HG23	2.16	0.46
1:A:335:LYS:HB2	1:A:335:LYS:NZ	2.32	0.44
1:A:275:GLU:OE1	1:A:277:GLN:NE2	2.45	0.44
1:A:186[A]:VAL:HG21	1:A:269:ARG:HG2	2.00	0.43
1:A:294:SER:O	3:C:301:ARG:C	2.56	0.43
2:B:164:ILE:HG12	2:B:188:PHE:HB2	2.00	0.43
1:A:289:GLY:HA3	9:A:2258:HOH:O	2.19	0.42
4:A:601:THW:H4'1	4:A:601:THW:C2	2.33	0.42
1:A:64[B]:MET:HB2	1:A:64[B]:MET:HE2	1.67	0.42
1:A:235:ARG:HD3	1:A:235:ARG:HA	1.87	0.41
1:A:29:SER:CB	9:A:2035:HOH:O	2.68	0.41
4:A:601:THW:H4A1	4:A:601:THW:H352	1.82	0.41
2:B:115:ALA:HB2	2:B:160:ILE:HG23	2.01	0.41
2:B:237:VAL:HG21	2:B:332:CYS:HB2	2.03	0.41
1:A:364:PHE:CD2	1:A:379:GLN:HG3	2.56	0.41
1:A:19:LYS:HG3	1:A:21:GLU:OE2	2.21	0.40
2:B:23[B]:LEU:HB3	2:B:194:TYR:HA	2.03	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	392/400 (98%)	382 (97%)	7 (2%)	3 (1%)	19	7
2	B	338/342 (99%)	328 (97%)	10 (3%)	0	100	100
3	C	1/3 (33%)	1 (100%)	0	0	100	100
All	All	731/745 (98%)	711 (97%)	17 (2%)	3 (0%)	34	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	TYR
1	A	148	VAL
1	A	226	ILE

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	332/336 (99%)	329 (99%)	3 (1%)	78	75
2	B	289/289 (100%)	280 (97%)	9 (3%)	40	25
3	C	2/2 (100%)	1 (50%)	1 (50%)	0	0
All	All	623/627 (99%)	610 (98%)	13 (2%)	55	42

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	ARG
1	A	363	LEU
1	A	387	GLN
2	B	17	GLN
2	B	35	LEU
2	B	50	PHE
2	B	117	TYR
2	B	133	ARG
2	B	293[A]	SER
2	B	293[B]	SER
2	B	296	GLN
2	B	304	GLU
3	C	301	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	A	276	ASN

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Mol	Chain	Res	Type
1	A	312	GLN
1	A	321	HIS
1	A	387	GLN
2	B	19	GLN
2	B	296	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	$\# Z > 2$
8	GOL	B	1346	-	5,5,5	0.38	0	5,5,5	0.64	0
4	THW	A	601	6	30,36,36	3.10	8 (26%)	37,53,53	2.29	12 (32%)
8	GOL	B	1345	-	5,5,5	0.51	0	5,5,5	0.49	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
8	GOL	B	1346	-	-	0/4/4/4	-
4	THW	A	601	6	-	2/20/25/25	0/3/3/3
8	GOL	B	1345	-	-	0/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	THW	C5A-C5	13.86	1.57	1.50
4	A	601	THW	O9-C8	-4.83	1.27	1.42
4	A	601	THW	C35-C5'	4.23	1.60	1.51
4	A	601	THW	C4'-N3'	3.90	1.40	1.35
4	A	601	THW	PB-O1B	3.37	1.61	1.50
4	A	601	THW	C4A-C4	2.43	1.54	1.49
4	A	601	THW	C6'-C5'	2.10	1.42	1.37
4	A	601	THW	C4-N3	-2.03	1.35	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	THW	C5A-C5-C4	7.03	133.07	127.43
4	A	601	THW	C2A-C2'-N1'	5.17	122.83	117.14
4	A	601	THW	C5-C4-N3	4.30	116.64	107.66
4	A	601	THW	N1'-C2'-N3'	-4.08	118.52	125.54
4	A	601	THW	C6'-N1'-C2'	3.81	122.44	115.96
4	A	601	THW	C13-C11-C9	-3.03	116.90	120.65
4	A	601	THW	C11-C9-C10	2.77	121.74	118.29
4	A	601	THW	C5'-C35-N3	-2.41	109.27	113.26
4	A	601	THW	O3B-PB-O1B	2.37	119.97	110.68
4	A	601	THW	C35-C5'-C4'	2.09	127.99	121.83
4	A	601	THW	C4A-C4-N3	-2.06	120.09	122.69
4	A	601	THW	C4A-C4-C5	-2.01	123.21	127.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

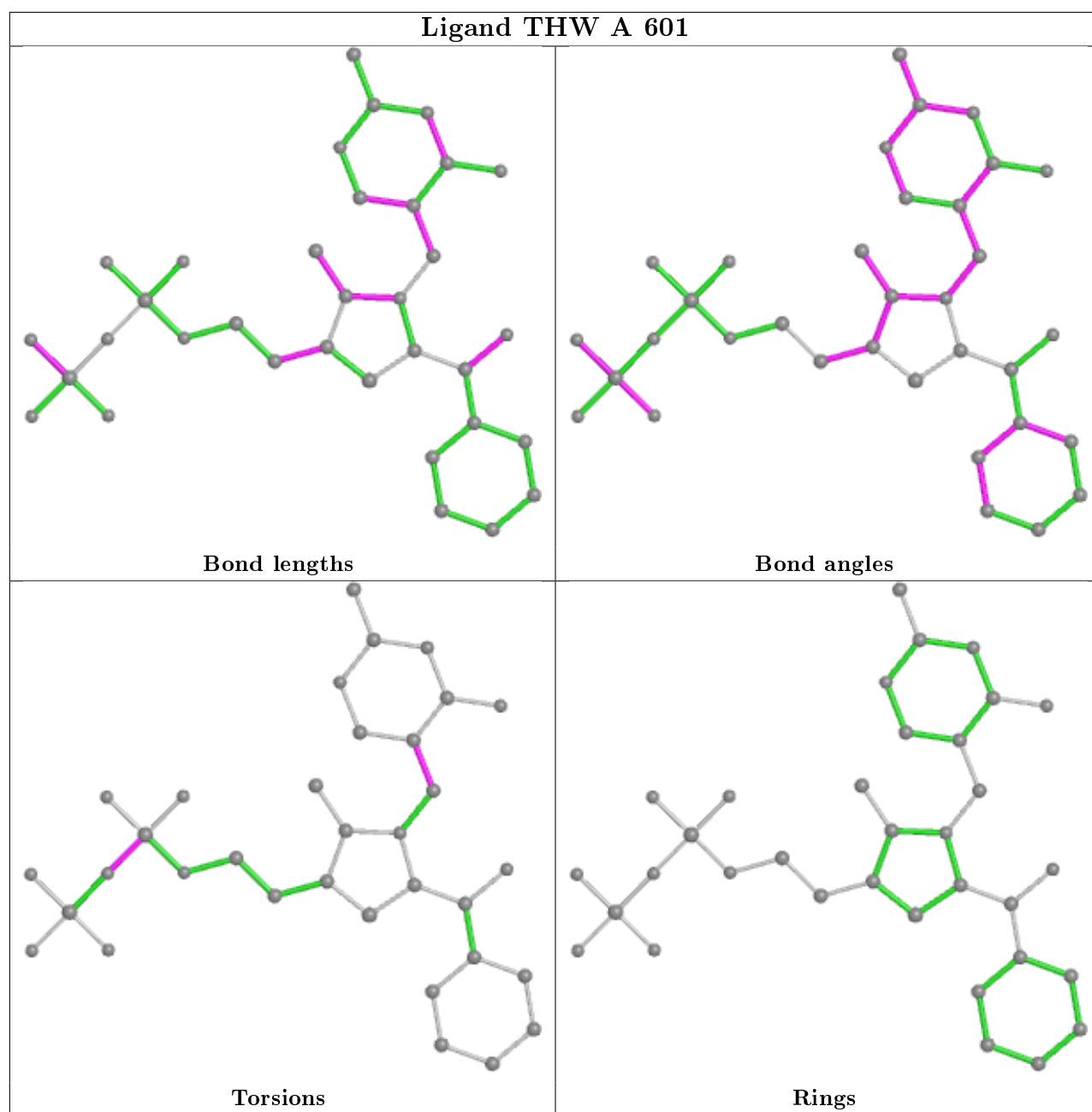
Mol	Chain	Res	Type	Atoms
4	A	601	THW	N3-C35-C5'-C4'
4	A	601	THW	PB-O3A-PA-O5G

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1346	GOL	1	0
4	A	601	THW	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 ⓘ

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, 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	390/400 (97%)	0.66	46 (11%) 4 3	15, 21, 38, 54	0
2	B	336/342 (98%)	0.13	26 (7%) 13 10	13, 19, 33, 48	0
3	C	3/3 (100%)	4.49	3 (100%) 0 0	42, 42, 44, 47	0
All	All	729/745 (97%)	0.43	75 (10%) 6 5	13, 20, 37, 54	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	308	TYR	8.6
2	B	5	THR	6.3
1	A	299	ALA	6.0
2	B	8	PRO	6.0
2	B	2	ALA	5.9
2	B	197	ALA	5.9
2	B	7	GLN	5.6
1	A	312	GLN	5.6
1	A	309	TRP	5.6
3	C	299	ALA	5.5
1	A	64[A]	MET	5.5
2	B	6	PHE	5.1
1	A	311	LYS	4.8
2	B	15	TYR	4.8
2	B	3	HIS	4.6
2	B	301	LEU	4.5
2	B	342	TYR	4.3
3	C	300	TYR	4.2
2	B	247	VAL	4.0
1	A	300	TYR	4.0
2	B	245	LEU	3.9
3	C	301	ARG	3.9
2	B	4	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	17	GLN	3.6
1	A	310	ASP	3.4
1	A	28	ILE	3.3
2	B	246	GLY	3.2
1	A	182	ASN	3.1
1	A	375	LEU	3.1
2	B	340	ILE	3.1
1	A	298	SER	3.1
2	B	341	ASN	3.0
1	A	168	ILE	2.9
2	B	293[A]	SER	2.9
1	A	218	PHE	2.9
1	A	400	LYS	2.8
1	A	29	SER	2.8
2	B	270	ILE	2.8
2	B	333	TYR	2.8
1	A	26	ASN	2.8
1	A	201	ALA	2.8
1	A	387	GLN	2.7
1	A	219	CYS	2.7
2	B	16	GLY	2.6
1	A	164	LEU	2.6
1	A	280	LEU	2.6
1	A	338	ARG	2.4
2	B	221	ASP	2.4
1	A	307	ASN	2.4
1	A	261	VAL	2.4
1	A	195	ALA	2.4
1	A	203	ALA	2.4
1	A	8	GLN	2.4
1	A	204	GLY	2.3
1	A	165	ALA	2.3
1	A	217	PHE	2.3
1	A	397	HIS	2.3
2	B	243	GLU	2.2
1	A	396	ASP	2.2
1	A	281	ILE	2.2
1	A	197	SER	2.2
1	A	205	PHE	2.2
1	A	354	ARG	2.2
1	A	294	SER	2.2
2	B	304	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	199	GLY	2.1
1	A	27	VAL	2.1
2	B	18	THR	2.1
1	A	191	PHE	2.1
1	A	207	PHE	2.1
2	B	204	GLU	2.1
1	A	183	ALA	2.1
1	A	189	CYS	2.1
1	A	190	TYR	2.0
1	A	262	TYR	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 carbohydrates in this entry.

6.4 Ligands [i](#)

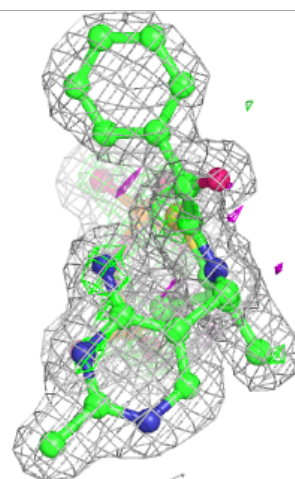
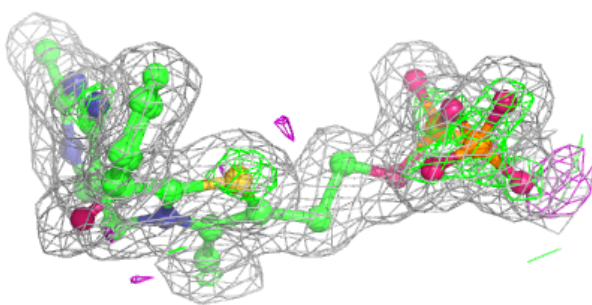
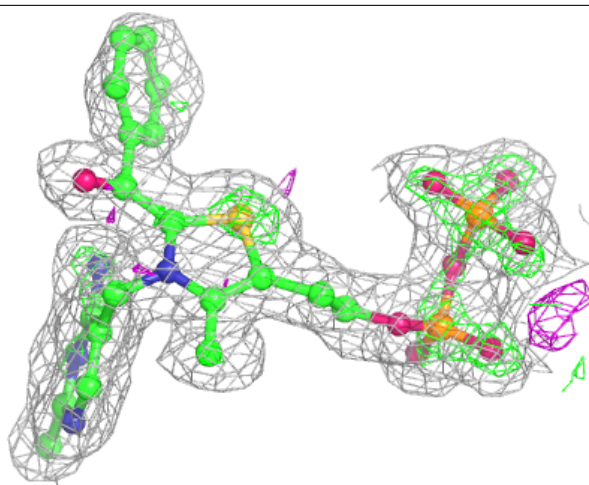
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	GOL	B	1346	6/6	0.89	0.26	32,37,38,40	0
7	CL	A	1404	1/1	0.90	0.06	63,63,63,63	0
8	GOL	B	1345	6/6	0.97	0.07	14,16,17,18	0
7	CL	B	1344	1/1	0.98	0.10	31,31,31,31	0
4	THW	A	601	34/34	0.98	0.18	13,16,29,30	0
5	K	B	1343	1/1	0.99	0.13	24,24,24,24	0
6	MN	A	1402	1/1	0.99	0.03	13,13,13,13	0
5	K	A	1401	1/1	1.00	0.08	20,20,20,20	0

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

Electron density around THW A 601:

$2mF_o-DF_c$ (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.