



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 28, 2021 – 07:05 pm BST

PDB ID : 2BFD
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 : 2004-12-06
Resolution : 1.39 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 : 2.22
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) : 2.22

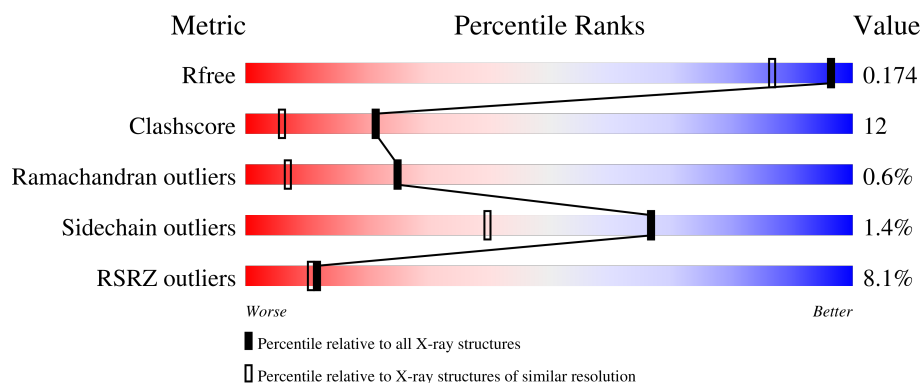
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	400	<div> <div>10%</div> <div> <div></div> <div>74%</div> <div>17%</div> <div>• 6%</div> </div> </div>
2	B	342	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6678 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	374	Total	C	N	O	S	0	32	0
			3312	2085	596	609	22			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ALA	TYR	engineered mutation	UNP P12694
A	292	SER	HIS	conflict	UNP P12694
A	300	PHE	TYR	conflict	UNP P12694

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	332	Total	C	N	O	S	0	14	0
			2721	1746	458	501	16			

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

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

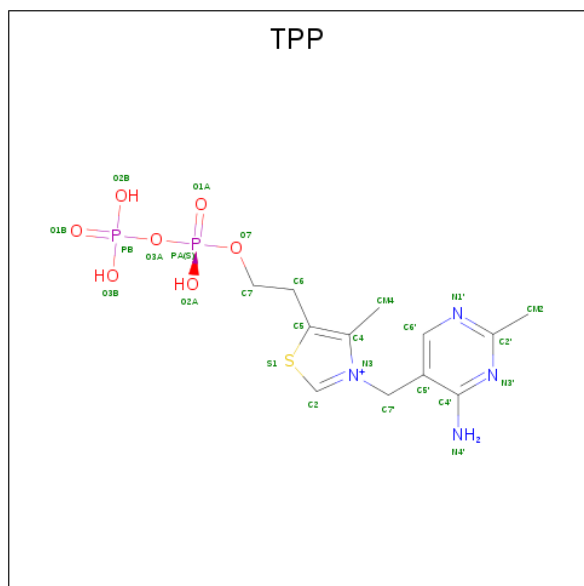
- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

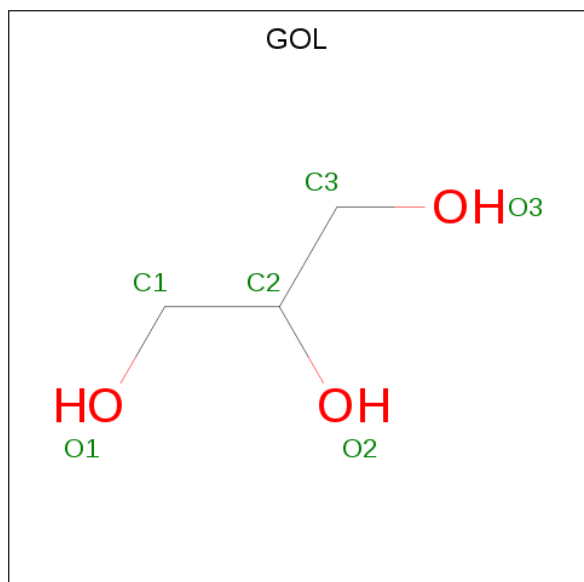
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P S 26 12 4 7 2 1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 8 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			8	6	2		

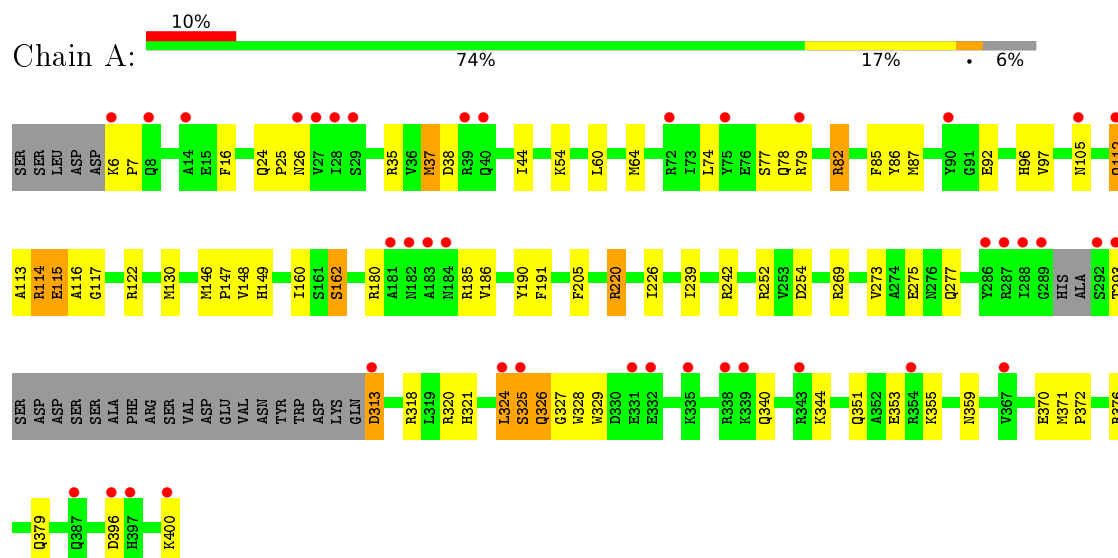
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	340	Total	O	0	0
			340	340		
9	B	261	Total	O	0	0
			261	261		

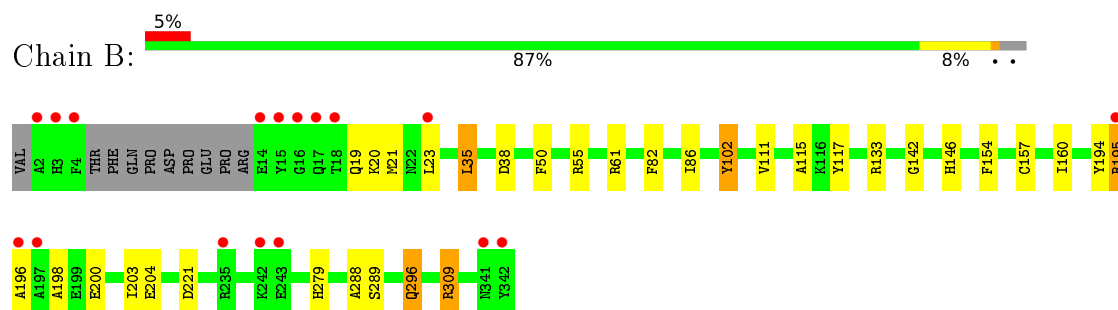
3 Residue-property plots [i](#)

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: 2-OXISOVALERATE DEHYDROGENASE ALPHA SUBUNIT



• Molecule 2: 2-OXISOVALERATE DEHYDROGENASE BETA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.84Å 144.84Å 69.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 1.39 20.31 – 1.39	Depositor EDS
% Data completeness (in resolution range)	97.8 (30.00-1.39) 97.8 (20.31-1.39)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 1.39Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.149 , 0.170 0.151 , 0.174	Depositor DCC
R_{free} test set	1633 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 57.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6678	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, K, CL, MPD, MN, TPP

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	1.03	3/3390 (0.1%)	1.16	13/4576 (0.3%)
2	B	0.91	3/2790 (0.1%)	1.04	8/3788 (0.2%)
All	All	0.98	6/6180 (0.1%)	1.11	21/8364 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	220	ARG	NE-CZ	8.18	1.43	1.33
1	A	162	SER	CA-CB	7.94	1.64	1.52
1	A	162	SER	CB-OG	7.54	1.52	1.42
2	B	61	ARG	CZ-NH1	5.68	1.40	1.33
2	B	102	TYR	CE1-CZ	-5.39	1.31	1.38
2	B	133	ARG	CG-CD	5.09	1.64	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	61	ARG	NE-CZ-NH1	13.03	126.81	120.30
2	B	61	ARG	NE-CZ-NH2	-10.39	115.10	120.30
1	A	220	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	A	252	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	A	180	ARG	NE-CZ-NH1	7.64	124.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	MET	CG-SD-CE	-7.12	88.80	100.20
2	B	309	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	B	195	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	313	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	242	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	A	180	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	82	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	A	254	ASP	CB-CG-OD1	5.31	123.08	118.30
2	B	35[A]	LEU	CB-CG-CD2	-5.20	102.17	111.00
2	B	35[B]	LEU	CB-CG-CD2	-5.20	102.17	111.00
1	A	122	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	38	ASP	CB-CG-OD2	5.14	122.93	118.30
2	B	38	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	326	GLN	O-C-N	5.06	131.79	123.20
1	A	252	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	B	221	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112[B]	GLN	Peptide

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	3312	0	3187	116	1
2	B	2721	0	2667	29	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	26	0	16	0	0
7	B	6	0	8	0	0
8	B	8	0	14	0	0
9	A	340	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	261	0	0	2	0
All	All	6678	0	5892	145	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (145) 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:92[A]:GLU:OE2	1:A:114[A]:ARG:HD2	1.28	1.32
1:A:186[B]:VAL:CG2	1:A:273[B]:VAL:CG2	2.08	1.29
1:A:92[A]:GLU:OE2	1:A:114[A]:ARG:CD	1.85	1.21
1:A:92[A]:GLU:OE1	1:A:220:ARG:HD2	1.34	1.20
1:A:186[B]:VAL:CG2	1:A:273[B]:VAL:HG23	1.67	1.20
1:A:186[B]:VAL:HG23	1:A:273[B]:VAL:CG2	1.75	1.12
1:A:114[B]:ARG:HA	9:A:2124:HOH:O	1.51	1.11
1:A:92[A]:GLU:OE1	1:A:220:ARG:CD	2.07	1.02
1:A:26:ASN:HB3	9:A:2035:HOH:O	1.62	1.00
1:A:149[A]:HIS:CE1	9:A:2162:HOH:O	2.16	0.97
1:A:112[A]:GLN:HE21	1:A:220:ARG:NH2	1.62	0.96
1:A:186[B]:VAL:HG22	1:A:273[B]:VAL:CG2	1.93	0.96
1:A:186[B]:VAL:HG23	1:A:273[B]:VAL:HG21	1.51	0.90
1:A:74:LEU:HD21	1:A:130[A]:MET:SD	2.12	0.88
1:A:112[A]:GLN:NE2	1:A:220:ARG:NH2	2.22	0.87
1:A:92[A]:GLU:OE2	1:A:114[A]:ARG:HD3	1.72	0.86
2:B:111:VAL:HG22	2:B:157[B]:CYS:SG	2.14	0.86
1:A:205[A]:PHE:CD2	9:A:2232:HOH:O	2.28	0.85
1:A:186[B]:VAL:HG21	1:A:273[B]:VAL:HG23	1.55	0.85
1:A:185:ARG:HG2	9:A:2194:HOH:O	1.75	0.84
1:A:149[A]:HIS:ND1	9:A:2162:HOH:O	2.08	0.83
1:A:186[B]:VAL:CG2	1:A:273[B]:VAL:HG22	2.08	0.83
1:A:186[B]:VAL:HG22	1:A:273[B]:VAL:HG23	1.57	0.82
1:A:326:GLN:HB3	1:A:328[A]:TRP:CE2	2.17	0.80
1:A:96[C]:HIS:CE1	1:A:220:ARG:HD3	2.19	0.78
1:A:324[C]:LEU:CD1	1:A:329:TRP:HB3	2.15	0.76
1:A:112[A]:GLN:HB3	1:A:190:TYR:O	1.86	0.76
1:A:112[B]:GLN:HG3	1:A:113[B]:ALA:N	2.01	0.76
1:A:351:GLN:HG2	1:A:355:LYS:HE3	1.67	0.75
1:A:186[B]:VAL:HG22	1:A:273[B]:VAL:HG22	1.65	0.74
1:A:105:ASN:ND2	9:A:2114:HOH:O	2.21	0.74
1:A:64[B]:MET:SD	1:A:97[B]:VAL:HG21	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:GLN:HE21	2:B:203:ILE:CD1	2.02	0.72
2:B:289[B]:SER:OG	2:B:309:ARG:NH1	2.22	0.72
1:A:112[A]:GLN:HE21	1:A:220:ARG:HH21	1.37	0.72
1:A:325[A]:SER:C	1:A:327[A]:GLY:H	1.93	0.72
1:A:82:ARG:NH2	9:A:2090:HOH:O	2.25	0.69
1:A:396:ASP:HB2	9:A:2331:HOH:O	1.94	0.68
1:A:6:LYS:HB3	1:A:7:PRO:HD3	1.75	0.68
1:A:324[C]:LEU:HD11	1:A:329:TRP:HB3	1.75	0.68
1:A:96[A]:HIS:HD1	1:A:117:GLY:H	1.41	0.68
2:B:55[A]:ARG:HD2	2:B:195:ARG:HH22	1.58	0.68
1:A:112[A]:GLN:NE2	1:A:220:ARG:HH22	1.90	0.67
1:A:92[C]:GLU:OE2	1:A:220:ARG:HD2	1.96	0.66
1:A:96[C]:HIS:HE1	1:A:220:ARG:HD3	1.60	0.66
2:B:20:LYS:HE2	2:B:198:ALA:HB3	1.76	0.66
1:A:92[C]:GLU:OE1	9:A:2105:HOH:O	2.15	0.65
1:A:205[A]:PHE:HD2	9:A:2232:HOH:O	1.74	0.65
1:A:112[A]:GLN:HG3	1:A:115[A]:GLU:OE1	1.96	0.65
2:B:55[A]:ARG:HD2	2:B:195:ARG:NH2	2.12	0.64
1:A:112[C]:GLN:HB2	1:A:191:PHE:HA	1.78	0.64
1:A:149[A]:HIS:HE1	1:A:162:SER:OG	1.82	0.62
1:A:92[B]:GLU:OE2	1:A:220:ARG:NH1	2.32	0.62
1:A:92[B]:GLU:HB3	1:A:96[B]:HIS:CE1	2.35	0.62
1:A:112[B]:GLN:HA	1:A:160:ILE:HG23	1.81	0.62
2:B:23[B]:LEU:HB3	2:B:194:TYR:HA	1.80	0.62
1:A:112[A]:GLN:HB2	1:A:191:PHE:HA	1.82	0.61
1:A:359:ASN:ND2	1:A:400:LYS:HB3	2.15	0.61
2:B:279:HIS:CE1	2:B:288:ALA:H	2.19	0.60
1:A:112[B]:GLN:CG	1:A:113[B]:ALA:N	2.64	0.60
1:A:324[C]:LEU:HD12	1:A:329:TRP:HB3	1.81	0.60
1:A:87[B]:MET:CE	1:A:148[B]:VAL:HG21	2.32	0.60
1:A:114[B]:ARG:CA	9:A:2124:HOH:O	2.26	0.60
1:A:351:GLN:CG	1:A:355:LYS:HE3	2.32	0.59
1:A:85:PHE:CZ	1:A:87[B]:MET:HG3	2.38	0.59
1:A:87[B]:MET:HE2	1:A:148[B]:VAL:CG2	2.33	0.59
2:B:19:GLN:HE21	2:B:203:ILE:HD11	1.68	0.58
2:B:19:GLN:NE2	2:B:203:ILE:CD1	2.66	0.58
1:A:376:ARG:NH1	9:A:2315:HOH:O	2.37	0.57
1:A:321:HIS:HA	1:A:324[B]:LEU:HD12	1.86	0.57
2:B:19:GLN:NE2	2:B:203:ILE:HD11	2.20	0.57
2:B:20:LYS:HG3	2:B:200:GLU:OE2	2.03	0.57
1:A:37:MET:O	1:A:318[A]:ARG:NH2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112[B]:GLN:HG3	9:A:2120:HOH:O	2.06	0.56
1:A:92[C]:GLU:CD	9:A:2105:HOH:O	2.45	0.55
1:A:85:PHE:CE2	1:A:87[B]:MET:HG3	2.41	0.55
1:A:112[A]:GLN:NE2	1:A:220:ARG:HH21	1.97	0.55
1:A:205[A]:PHE:CE2	9:A:2232:HOH:O	2.55	0.55
1:A:35[A]:ARG:HG2	1:A:44:ILE:HD12	1.88	0.54
1:A:114[B]:ARG:O	9:A:2124:HOH:O	2.17	0.54
2:B:279:HIS:HE1	2:B:288:ALA:H	1.53	0.54
1:A:64[B]:MET:CG	1:A:97[B]:VAL:HG21	2.38	0.54
1:A:326:GLN:CB	1:A:328[A]:TRP:CE2	2.90	0.53
2:B:19:GLN:HE21	2:B:203:ILE:HD12	1.72	0.53
1:A:78:GLN:NE2	9:A:2084:HOH:O	2.42	0.53
2:B:55[A]:ARG:HH11	2:B:195:ARG:HH22	1.57	0.53
1:A:112[A]:GLN:CB	1:A:190:TYR:O	2.56	0.53
1:A:324[C]:LEU:HD12	1:A:324[C]:LEU:N	2.24	0.52
1:A:87[B]:MET:HE2	1:A:148[B]:VAL:HG21	1.92	0.52
1:A:340:GLN:HE21	1:A:344:LYS:HE3	1.76	0.51
1:A:324[A]:LEU:HD12	1:A:329:TRP:HB3	1.93	0.51
1:A:275:GLU:OE1	1:A:277:GLN:NE2	2.43	0.51
1:A:326:GLN:HB2	1:A:328[A]:TRP:CD2	2.46	0.51
1:A:326:GLN:HB3	1:A:328[A]:TRP:NE1	2.26	0.51
2:B:204:GLU:OE1	9:B:2169:HOH:O	2.20	0.50
2:B:146[C]:HIS:CE1	9:B:2127:HOH:O	2.64	0.50
1:A:326:GLN:HB2	1:A:328[A]:TRP:CG	2.46	0.50
1:A:87[B]:MET:HE3	1:A:148[B]:VAL:HG21	1.94	0.50
1:A:186[B]:VAL:HG23	1:A:273[B]:VAL:HG22	1.80	0.50
1:A:325[A]:SER:C	1:A:327[A]:GLY:N	2.65	0.49
1:A:326:GLN:CB	1:A:328[A]:TRP:CD2	2.96	0.49
1:A:113[B]:ALA:O	1:A:114[B]:ARG:HB2	2.13	0.49
2:B:35[B]:LEU:CD2	2:B:35[B]:LEU:N	2.76	0.49
1:A:370[A]:GLU:O	1:A:372:PRO:HD3	2.12	0.48
2:B:35[B]:LEU:N	2:B:35[B]:LEU:HD23	2.29	0.48
1:A:87[B]:MET:CE	1:A:148[B]:VAL:CG2	2.91	0.48
1:A:396:ASP:CB	9:A:2331:HOH:O	2.55	0.47
1:A:86:TYR:O	1:A:293:THR:HG23	2.14	0.47
1:A:92[A]:GLU:OE1	1:A:220:ARG:NE	2.47	0.47
1:A:146[B]:MET:O	1:A:149[B]:HIS:HD2	1.98	0.47
1:A:147:PRO:O	1:A:149[C]:HIS:HD2	1.97	0.47
2:B:21:MET:CE	2:B:203:ILE:HD13	2.45	0.47
1:A:92[C]:GLU:CD	1:A:220:ARG:HD2	2.34	0.46
1:A:149[A]:HIS:CE1	1:A:162:SER:OG	2.66	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146[B]:MET:HG3	1:A:149[B]:HIS:CD2	2.50	0.46
1:A:359:ASN:HD21	1:A:400:LYS:HD2	1.79	0.46
1:A:359:ASN:ND2	1:A:400:LYS:HD2	2.30	0.46
2:B:19:GLN:NE2	2:B:203:ILE:HD12	2.30	0.45
1:A:92[B]:GLU:OE1	1:A:96[B]:HIS:HE1	2.00	0.45
1:A:113[B]:ALA:HB1	1:A:114[B]:ARG:CZ	2.47	0.45
1:A:82:ARG:HD3	1:A:353:GLU:OE2	2.17	0.44
1:A:96[B]:HIS:CD2	1:A:115[B]:GLU:HA	2.52	0.44
1:A:371[A]:MET:SD	1:A:379[A]:GLN:NE2	2.90	0.44
1:A:77:SER:OG	1:A:82:ARG:HB2	2.17	0.44
1:A:92[B]:GLU:HB3	1:A:96[B]:HIS:ND1	2.32	0.44
1:A:147:PRO:O	1:A:148[B]:VAL:HG22	2.19	0.43
1:A:313:ASP:OD1	1:A:318[B]:ARG:NH2	2.50	0.43
1:A:54:LYS:HA	1:A:328[B]:TRP:CZ3	2.55	0.42
1:A:78:GLN:OE1	1:A:293:THR:HB	2.18	0.42
2:B:55[B]:ARG:HG3	2:B:195:ARG:NH2	2.35	0.42
2:B:142:GLY:O	2:B:146[B]:HIS:HB2	2.19	0.42
1:A:114[B]:ARG:C	1:A:116:ALA:N	2.72	0.42
2:B:102:TYR:OH	2:B:146[C]:HIS:HE1	2.03	0.42
1:A:82:ARG:HD3	1:A:82:ARG:HH11	1.73	0.41
2:B:296[A]:GLN:HE21	2:B:296[A]:GLN:HB3	1.60	0.41
2:B:82:PHE:CE2	2:B:86:ILE:HD11	2.55	0.41
1:A:6:LYS:HD3	1:A:16:PHE:HD2	1.85	0.41
1:A:60:LEU:O	1:A:64[B]:MET:HG3	2.21	0.41
1:A:115[A]:GLU:CD	1:A:115[A]:GLU:N	2.72	0.41
2:B:115:ALA:HB2	2:B:160:ILE:HG23	2.03	0.41
1:A:320:ARG:O	1:A:324[C]:LEU:HD13	2.21	0.41
1:A:24:GLN:HA	1:A:25:PRO:HD3	1.78	0.40
1:A:115[A]:GLU:OE2	1:A:115[A]:GLU:CA	2.66	0.40
2:B:55[A]:ARG:HH11	2:B:195:ARG:NH2	2.20	0.40
2:B:154:PHE:O	2:B:157[B]:CYS:HB2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLN:OE1	1:A:370[A]:GLU:CG[3_664]	1.88	0.32

5.3 Torsion angles

5.3.1 Protein backbone

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	407/400 (102%)	387 (95%)	14 (3%)	6 (2%)	10	1
2	B	344/342 (101%)	333 (97%)	10 (3%)	1 (0%)	41	18
All	All	751/742 (101%)	720 (96%)	24 (3%)	7 (1%)	25	3

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325[A]	SER
1	A	325[B]	SER
1	A	325[C]	SER
1	A	226	ILE
2	B	196	ALA
1	A	114[A]	ARG
1	A	114[B]	ARG

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	346/334 (104%)	338 (98%)	8 (2%)	50	18
2	B	295/289 (102%)	291 (99%)	4 (1%)	67	40
All	All	641/623 (103%)	629 (98%)	12 (2%)	67	25

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	115[A]	GLU
1	A	115[B]	GLU
1	A	239	ILE
1	A	269	ARG
1	A	324[A]	LEU
1	A	324[B]	LEU
1	A	324[C]	LEU
2	B	50	PHE
2	B	117	TYR
2	B	296[A]	GLN
2	B	296[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	A	333	GLN
2	B	19	GLN
2	B	279	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 7 ligands modelled in this entry, 4 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	MPD	B	901	-	7,7,7	0.35	0	9,10,10	1.26	1 (11%)
7	GOL	B	701	-	5,5,5	0.43	0	5,5,5	0.32	0
6	TPP	A	601	4	22,27,27	2.69	5 (22%)	29,40,40	2.01	7 (24%)

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	MPD	B	901	-	-	0/5/5/5	-
7	GOL	B	701	-	-	0/4/4/4	-
6	TPP	A	601	4	-	1/16/17/17	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	601	TPP	C6-C5	-10.52	1.46	1.50
6	A	601	TPP	C4-N3	-3.12	1.37	1.39
6	A	601	TPP	C2-N3	2.99	1.42	1.36
6	A	601	TPP	C7'-C5'	2.49	1.56	1.51
6	A	601	TPP	PA-O2A	-2.30	1.44	1.55

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	601	TPP	C7'-N3-C2	-5.53	115.37	125.35
6	A	601	TPP	C5-C4-N3	4.22	116.02	107.57
6	A	601	TPP	C6-C5-C4	4.15	130.76	127.43
6	A	601	TPP	CM2-C2'-N1'	3.76	121.28	117.14
6	A	601	TPP	C6'-N1'-C2'	3.01	121.08	115.96
8	B	901	MPD	CM-C2-C1	-3.00	104.32	110.57
6	A	601	TPP	N1'-C2'-N3'	-2.36	121.48	125.54
6	A	601	TPP	CM4-C4-N3	-2.09	119.87	122.53

There are no chirality outliers.

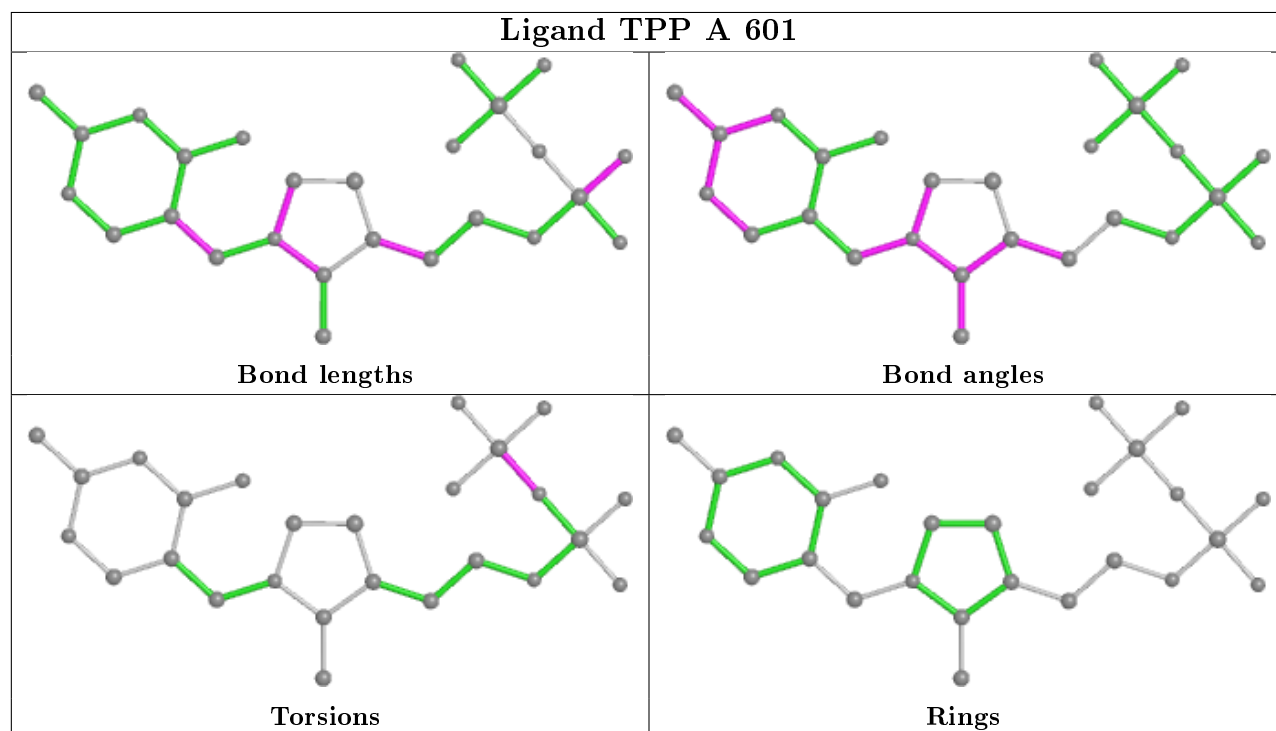
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	601	TPP	PA-O3A-PB-O2B

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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, 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	374/400 (93%)	0.59	40 (10%) 6 5	9, 15, 31, 51	0
2	B	332/342 (97%)	0.22	17 (5%) 28 27	8, 13, 24, 37	0
All	All	706/742 (95%)	0.42	57 (8%) 12 11	8, 14, 28, 51	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	288	ILE	12.4
2	B	2	ALA	9.5
1	A	28	ILE	9.4
1	A	289	GLY	8.1
1	A	293	THR	7.3
2	B	4	PHE	6.8
1	A	286	TYR	6.7
1	A	26	ASN	5.8
2	B	3	HIS	5.5
1	A	287	ARG	5.4
1	A	183	ALA	5.2
2	B	342	TYR	4.9
2	B	15	TYR	4.9
1	A	292	SER	4.8
1	A	324[A]	LEU	4.8
1	A	182	ASN	4.6
1	A	396	ASP	4.2
1	A	8	GLN	4.1
1	A	6	LYS	4.1
1	A	400	LYS	4.0
2	B	14	GLU	3.6
1	A	90	TYR	3.5
1	A	75	TYR	3.4
1	A	343	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	331	GLU	3.4
1	A	39	ARG	3.4
1	A	387	GLN	3.3
2	B	16	GLY	3.2
1	A	338	ARG	3.1
2	B	23[A]	LEU	3.1
2	B	341	ASN	3.0
1	A	79	ARG	3.0
1	A	184	ASN	3.0
2	B	243	GLU	2.9
1	A	335	LYS	2.9
2	B	17	GLN	2.7
1	A	397	HIS	2.7
1	A	325[A]	SER	2.6
1	A	105	ASN	2.6
1	A	332	GLU	2.5
2	B	195	ARG	2.5
1	A	29	SER	2.5
1	A	313	ASP	2.4
1	A	354[A]	ARG	2.4
1	A	40	GLN	2.4
2	B	197	ALA	2.4
1	A	339	LYS	2.4
2	B	196	ALA	2.3
1	A	27	VAL	2.3
1	A	112[A]	GLN	2.3
2	B	235	ARG	2.3
1	A	367	VAL	2.3
2	B	18	THR	2.2
1	A	14	ALA	2.2
1	A	181	ALA	2.1
1	A	72	ARG	2.0
2	B	242	LYS	2.0

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 [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	MPD	B	901	8/8	0.85	0.17	28,35,37,38	0
7	GOL	B	701	6/6	0.96	0.06	14,16,16,16	0
5	CL	A	504	1/1	0.96	0.15	24,24,24,24	0
6	TPP	A	601	26/26	0.98	0.08	8,10,13,16	0
3	K	A	501	1/1	0.99	0.04	10,10,10,10	0
3	K	B	502	1/1	0.99	0.05	11,11,11,11	0
4	MN	A	503	1/1	1.00	0.04	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.