



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:54 AM UTC

PDB ID : 2J9F / pdb_00002j9f
Title : Human branched-chain alpha-ketoacid dehydrogenase-decarboxylase E1b
Authors : Jun, L.; Machius, M.; Chuang, J.L.; Wynn, R.M.; Chuang, D.T.
Deposited on : 2006-11-07
Resolution : 1.88 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

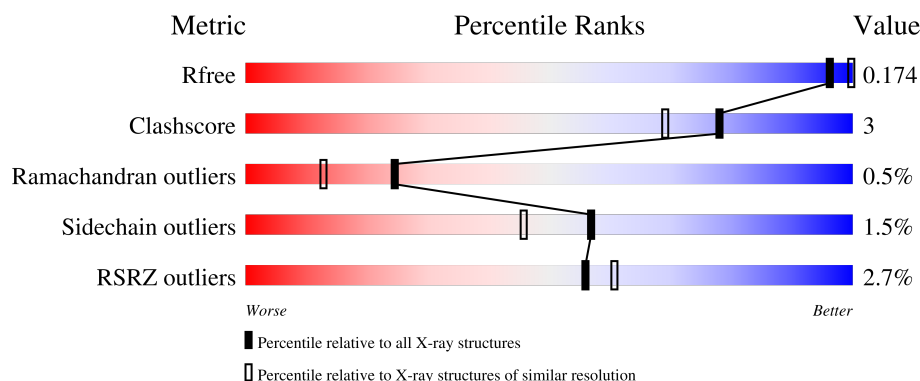
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	4% 84% 11% .
1	C	400	4% 84% 11% .
2	B	350	% 85% 9% 6%
2	D	350	88% 6% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12596 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	383	Total	C	N	O	S	0	9	0
			3135	1972	559	585	19			
1	C	383	Total	C	N	O	S	0	9	0
			3143	1977	565	584	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	PRO	SER	engineered mutation	UNP P12694
C	302	PRO	SER	engineered mutation	UNP P12694

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	0	5	1
			2597	1672	428	482	15			
2	D	330	Total	C	N	O	S	0	1	1
			2566	1652	423	476	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	343	GLY	-	expression tag	UNP P21953
B	344	GLY	-	expression tag	UNP P21953
B	345	HIS	-	expression tag	UNP P21953
B	346	HIS	-	expression tag	UNP P21953
B	347	HIS	-	expression tag	UNP P21953
B	348	HIS	-	expression tag	UNP P21953
B	349	HIS	-	expression tag	UNP P21953
B	350	HIS	-	expression tag	UNP P21953

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Chain	Residue	Modelled	Actual	Comment	Reference
D	343	GLY	-	expression tag	UNP P21953
D	344	GLY	-	expression tag	UNP P21953
D	345	HIS	-	expression tag	UNP P21953
D	346	HIS	-	expression tag	UNP P21953
D	347	HIS	-	expression tag	UNP P21953
D	348	HIS	-	expression tag	UNP P21953
D	349	HIS	-	expression tag	UNP P21953
D	350	HIS	-	expression tag	UNP P21953

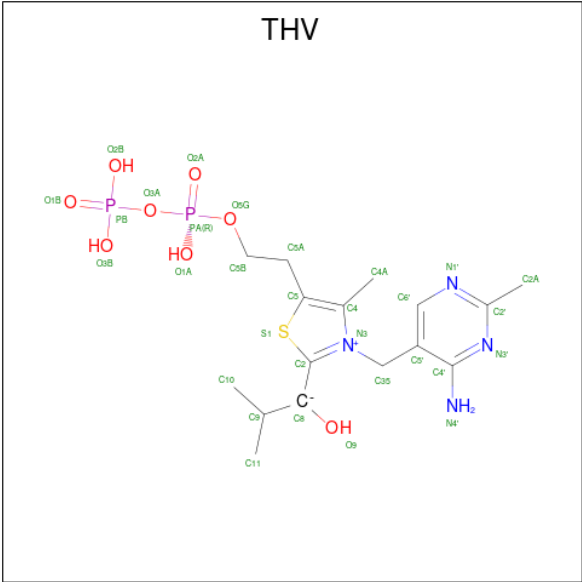
- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0

- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

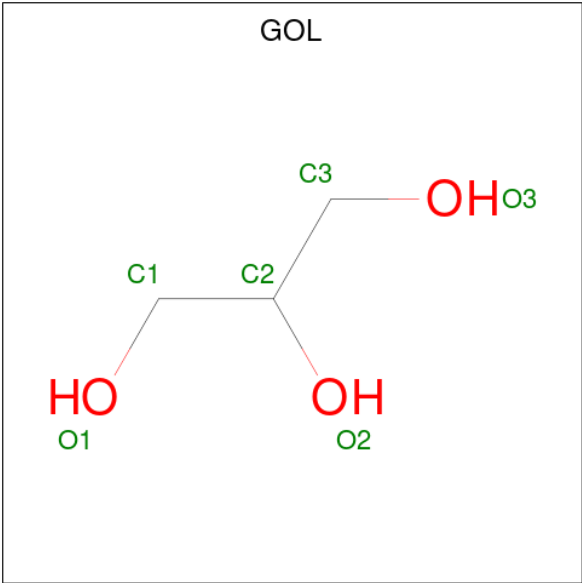
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total K 1 1	0	0
4	B	1	Total K 1 1	0	0
4	C	1	Total K 1 1	0	0
4	D	1	Total K 1 1	0	0

- Molecule 5 is C2-1-HYDROXY-3-METHYL-PROPYL-THIAMIN DIPHOSPHATE (CCD ID: THV) (formula: C₁₆H₂₆N₄O₈P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			31	16	4	8	2	1		
5	C	1	Total	C	N	O	P	S	0	0
			31	16	4	8	2	1		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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

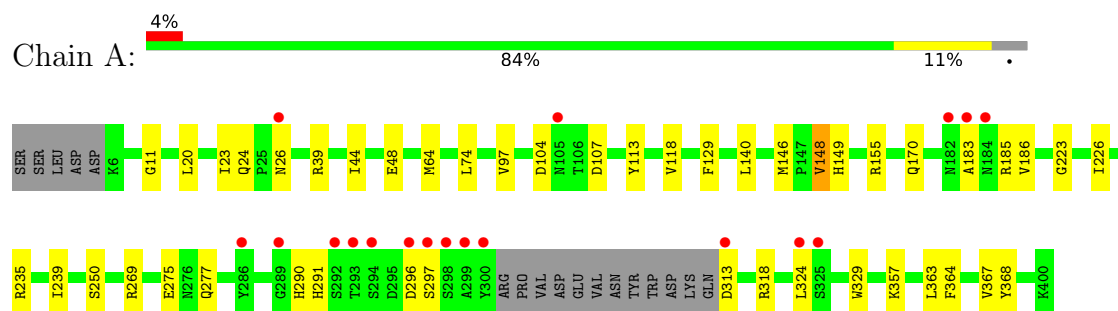
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	291	Total	O	0	0
			291	291		
7	B	243	Total	O	0	0
			243	243		
7	C	297	Total	O	0	0
			297	297		
7	D	238	Total	O	0	0
			238	238		

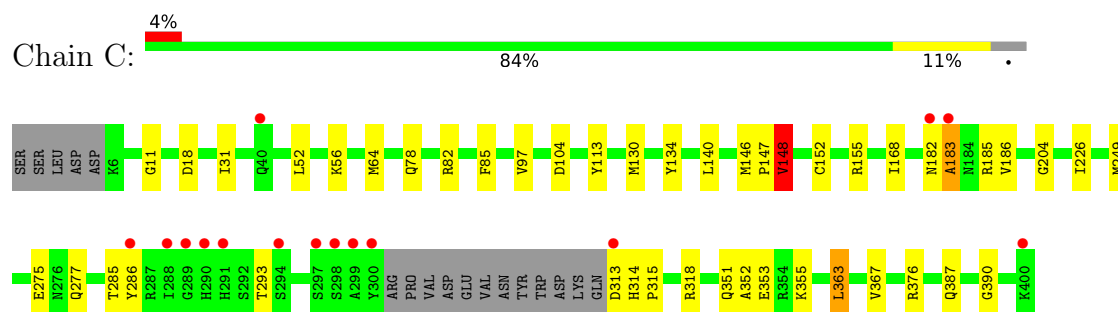
3 Residue-property plots

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.

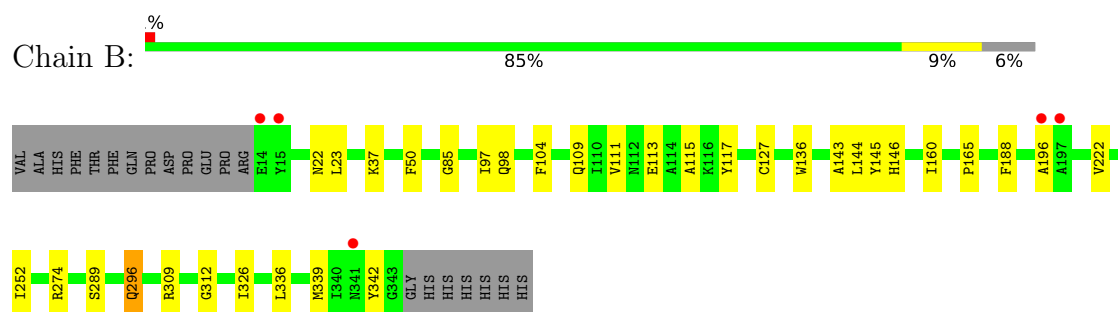
• Molecule 1: 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUBUNIT



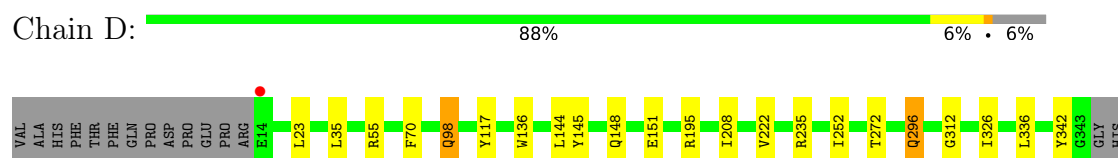
• Molecule 1: 2-OXOISOVALERATE DEHYDROGENASE ALPHA SUBUNIT



• Molecule 2: 2-OXOISOVALERATE DEHYDROGENASE BETA SUBUNIT



• Molecule 2: 2-OXOISOVALERATE DEHYDROGENASE BETA SUBUNIT



HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.34Å 145.34Å 138.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.64 – 1.88 26.64 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.2 (26.64-1.88) 99.1 (26.64-1.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.200 (Not available) , 0.174	Depositor DCC
R_{free} test set	1491 reflections (1.10%)	wwPDB-VP
Wilson B-factor (Å ²)	14.7	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12596	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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 56.53 % 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 2.6991e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: MN, GOL, THV, K

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	0.76	0/3211	1.01	13/4336 (0.3%)
1	C	0.75	0/3219	1.00	6/4345 (0.1%)
2	B	0.82	1/2662 (0.0%)	1.06	12/3619 (0.3%)
2	D	0.83	1/2631 (0.0%)	1.05	15/3577 (0.4%)
All	All	0.79	2/11723 (0.0%)	1.03	46/15877 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	342	TYR	C-N	-6.64	1.24	1.33
2	D	342	TYR	C-N	-6.24	1.24	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183	ALA	N-CA-C	7.91	120.90	111.33
1	C	367	VAL	N-CA-C	-7.82	103.18	110.53
1	A	367	VAL	N-CA-C	-7.53	103.45	110.53
2	B	326	ILE	N-CA-C	7.05	116.71	108.96
1	C	104	ASP	N-CA-C	-7.03	100.08	110.48
2	B	98	GLN	N-CA-C	6.98	119.77	111.33
1	A	104[A]	ASP	N-CA-C	-6.29	101.17	110.48
1	A	104[B]	ASP	N-CA-C	-6.29	101.17	110.48
2	D	145	TYR	N-CA-C	6.29	120.99	112.88
1	C	183	ALA	N-CA-C	6.21	118.86	111.71
2	D	326	ILE	N-CA-C	6.19	115.77	108.96
2	B	312	GLY	N-CA-C	-5.98	104.88	112.54
2	D	151	GLU	N-CA-C	5.96	117.78	111.28
2	B	144	LEU	N-CA-C	5.91	117.73	111.28
2	D	208	ILE	N-CA-C	-5.88	100.61	107.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	97	ILE	N-CA-C	-5.76	99.44	107.80
1	A	357	LYS	N-CA-C	-5.74	103.53	110.13
2	D	98	GLN	N-CA-C	5.70	118.23	111.33
1	C	363	LEU	CA-CB-CG	5.69	136.23	116.30
1	A	368	TYR	N-CA-C	-5.68	101.11	109.81
2	B	111	VAL	N-CA-C	5.68	115.87	110.53
1	C	11	GLY	N-CA-C	5.68	121.26	113.99
2	D	312	GLY	N-CA-C	-5.65	105.31	112.54
2	D	148	GLN	N-CA-C	5.62	117.99	110.35
1	A	129	PHE	N-CA-C	-5.57	105.11	111.07
1	A	11	GLY	N-CA-C	5.56	121.10	113.99
1	A	118	VAL	N-CA-C	-5.55	105.31	110.53
1	A	364	PHE	N-CA-C	5.50	120.27	113.50
1	A	44	ILE	N-CA-C	5.50	116.28	110.72
2	D	144	LEU	N-CA-C	5.39	117.16	111.28
2	D	70	PHE	N-CA-C	5.38	117.26	109.07
2	B	145	TYR	N-CA-C	5.32	120.44	112.94
2	D	272	THR	N-CA-C	5.31	118.22	111.69
2	D	252	ILE	N-CA-C	5.29	115.52	108.11
1	A	223	GLY	N-CA-C	5.27	122.11	115.42
1	A	250	SER	N-CA-C	5.22	117.61	109.52
2	B	22	ASN	N-CA-C	-5.21	102.28	110.36
2	B	127	CYS	N-CA-C	-5.17	104.26	110.88
2	D	136	TRP	N-CA-CB	-5.09	102.84	111.69
2	B	252	ILE	N-CA-C	5.09	115.23	108.11
1	C	390	GLY	N-CA-C	5.08	119.03	112.83
2	D	136	TRP	CA-CB-CG	5.07	123.23	113.60
2	D	235	ARG	N-CA-C	-5.05	105.85	111.36
2	B	104	PHE	N-CA-C	5.04	120.46	113.45
2	B	136	TRP	N-CA-CB	-5.02	102.96	111.69
2	D	23	LEU	N-CA-C	5.00	116.42	111.07

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	3135	0	3024	23	0
1	C	3143	0	3036	31	0
2	B	2597	0	2562	12	0
2	D	2566	0	2531	4	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	22	3	0
5	C	31	0	22	2	0
6	B	6	0	8	0	0
6	D	12	0	16	0	0
7	A	291	0	0	2	0
7	B	243	0	0	0	0
7	C	297	0	0	6	0
7	D	238	0	0	0	0
All	All	12596	0	11221	63	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 3.

All (63) 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:146[A]:MET:HE2	7:C:2146:HOH:O	1.57	1.03
1:A:155[A]:ARG:NH1	7:A:2137:HOH:O	1.99	0.94
1:C:183:ALA:HB1	1:C:185[B]:ARG:HD3	1.53	0.90
1:C:155[A]:ARG:NH1	7:C:2141:HOH:O	1.84	0.89
2:B:146:HIS:CE1	1:C:146[A]:MET:HE1	2.12	0.83
2:B:146:HIS:ND1	1:C:146[A]:MET:HE1	1.94	0.81
1:A:185:ARG:HG2	7:A:2076:HOH:O	1.86	0.75
1:C:52:LEU:HD22	1:C:56[A]:LYS:HD3	1.70	0.73
1:C:387:GLN:NE2	7:C:2286:HOH:O	2.22	0.71
1:C:185[B]:ARG:HG2	7:C:2091:HOH:O	1.90	0.70
2:B:274:ARG:NH1	2:B:339:MET:O	2.28	0.67
1:C:82:ARG:HD3	1:C:353:GLU:OE2	1.95	0.66
1:C:313:ASP:OD1	1:C:318:ARG:NH1	2.25	0.66
5:C:1403:THV:H4'1	5:C:1403:THV:C8	2.12	0.62
1:A:290:HIS:HD2	1:A:297:SER:H	1.46	0.61
1:A:275:GLU:OE1	1:A:277:GLN:NE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:GLN:HG3	2:D:296:GLN:HG3	1.84	0.59
1:C:275:GLU:OE1	1:C:277:GLN:NE2	2.38	0.56
2:D:55:ARG:HH21	2:D:195:ARG:HD2	1.71	0.56
2:B:289[B]:SER:OG	2:B:309:ARG:NH1	2.39	0.56
1:C:134:TYR:CZ	1:C:353:GLU:HG2	2.41	0.55
1:A:64:MET:HG3	1:A:97:VAL:HG21	1.89	0.54
1:C:85:PHE:CD2	1:C:146[B]:MET:HE2	2.42	0.54
1:A:23:ILE:HD11	1:C:31:ILE:HG23	1.89	0.53
1:C:351:GLN:HG2	1:C:355:LYS:HE3	1.91	0.52
5:A:1403:THV:C8	5:A:1403:THV:H4'1	2.23	0.51
1:A:107:ASP:CG	1:A:186:VAL:HG12	2.38	0.49
1:A:313:ASP:OD2	1:A:318:ARG:CD	2.61	0.48
1:A:170:GLN:O	2:B:85:GLY:HA3	2.14	0.48
1:A:313:ASP:OD2	1:A:318:ARG:HD3	2.14	0.48
1:A:186:VAL:HG11	1:A:269:ARG:HG3	1.95	0.47
1:C:147:PRO:O	1:C:148:VAL:HG22	2.14	0.47
1:C:64:MET:HG3	1:C:97:VAL:HG21	1.96	0.47
1:A:39:ARG:HA	1:A:318:ARG:HD2	1.96	0.46
2:B:115:ALA:HB2	2:B:160:ILE:HG23	1.96	0.46
2:B:146:HIS:ND1	1:C:146[A]:MET:CE	2.75	0.45
1:C:152:CYS:SG	1:C:155[B]:ARG:HG3	2.57	0.45
1:A:23:ILE:CD1	1:C:31:ILE:HG23	2.46	0.44
1:A:290:HIS:CD2	1:A:297:SER:H	2.31	0.44
2:B:222:VAL:HG11	2:B:336:LEU:HD11	1.98	0.44
1:A:140:LEU:HD23	1:A:140:LEU:HA	1.77	0.44
1:C:285:THR:HB	1:C:286:TYR:H	1.57	0.44
1:A:20:LEU:C	1:A:20:LEU:HD23	2.43	0.44
1:C:168:ILE:HG22	1:C:204:GLY:HA3	2.00	0.43
2:D:222:VAL:HG11	2:D:336:LEU:HD11	2.00	0.43
1:A:24:GLN:HG2	1:C:249:MET:HE1	1.99	0.43
5:C:1403:THV:O9	5:C:1403:THV:H351	2.19	0.43
1:A:48:GLU:HG3	1:C:18:ASP:O	2.19	0.43
1:C:185[B]:ARG:CG	7:C:2091:HOH:O	2.60	0.43
2:B:143:ALA:HB3	1:C:146[A]:MET:HG3	2.01	0.42
1:A:291:HIS:CE1	5:A:1403:THV:S1	3.12	0.42
5:A:1403:THV:H352	2:D:98:GLN:OE1	2.20	0.42
1:A:146[B]:MET:HG3	1:A:149:HIS:CE1	2.54	0.41
1:C:314:HIS:CG	1:C:315:PRO:HD2	2.55	0.41
1:C:140:LEU:HD23	1:C:140:LEU:HA	1.88	0.41
1:A:235:ARG:HD3	1:A:235:ARG:HA	1.82	0.41
1:C:78:GLN:OE1	1:C:293:THR:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LEU:HD23	1:A:74:LEU:HA	1.96	0.41
1:A:324:LEU:HD23	1:A:329:TRP:O	2.21	0.41
2:B:109:GLN:O	2:B:113:GLU:HB2	2.20	0.41
2:B:165:PRO:HD2	2:B:188:PHE:O	2.20	0.41
1:C:130:MET:HB3	1:C:352:ALA:CB	2.51	0.40
1:C:146[A]:MET:HG2	7:C:2066:HOH:O	2.22	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	388/400 (97%)	379 (98%)	6 (2%)	3 (1%)	16	5
1	C	388/400 (97%)	379 (98%)	6 (2%)	3 (1%)	16	5
2	B	333/350 (95%)	322 (97%)	10 (3%)	1 (0%)	36	26
2	D	329/350 (94%)	317 (96%)	12 (4%)	0	100	100
All	All	1438/1500 (96%)	1397 (97%)	34 (2%)	7 (0%)	24	13

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	TYR
1	C	113	TYR
1	A	148	VAL
1	C	148	VAL
1	C	226	ILE
1	A	226	ILE
2	B	196	ALA

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	328/336 (98%)	323 (98%)	5 (2%)	57	46
1	C	328/336 (98%)	323 (98%)	5 (2%)	57	46
2	B	282/295 (96%)	277 (98%)	5 (2%)	51	38
2	D	278/295 (94%)	275 (99%)	3 (1%)	65	56
All	All	1216/1262 (96%)	1198 (98%)	18 (2%)	57	46

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	148	VAL
1	A	239	ILE
1	A	296	ASP
1	A	363	LEU
2	B	23	LEU
2	B	37	LYS
2	B	50	PHE
2	B	117	TYR
2	B	296	GLN
1	C	148	VAL
1	C	182	ASN
1	C	186	VAL
1	C	363	LEU
1	C	376	ARG
2	D	35	LEU
2	D	117	TYR
2	D	296	GLN

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

Mol	Chain	Res	Type
1	A	105	ASN

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Mol	Chain	Res	Type
1	A	156	HIS
1	A	290	HIS
2	B	141	HIS
1	C	374	GLN
1	C	387	GLN
2	D	212	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 6 are monoatomic - leaving 5 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	$\# Z > 2$
5	THV	C	1403	3	29,32,32	2.29	8 (27%)	36,48,48	1.79	7 (19%)
5	THV	A	1403	3	29,32,32	2.51	8 (27%)	36,48,48	1.91	10 (27%)
6	GOL	B	1344	-	5,5,5	0.34	0	5,5,5	0.45	0
6	GOL	D	1345	-	5,5,5	0.44	0	5,5,5	0.60	0
6	GOL	D	1344	-	5,5,5	0.25	0	5,5,5	0.45	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
5	THV	C	1403	3	-	7/25/25/25	0/2/2/2
5	THV	A	1403	3	-	6/25/25/25	0/2/2/2
6	GOL	B	1344	-	-	0/4/4/4	-
6	GOL	D	1345	-	-	3/4/4/4	-
6	GOL	D	1344	-	-	0/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1403	THV	O9-C8	-8.77	1.25	1.42
5	A	1403	THV	O9-C8	-8.76	1.25	1.42
5	A	1403	THV	C35-C5'	5.15	1.60	1.51
5	A	1403	THV	C8-C2	4.08	1.57	1.51
5	C	1403	THV	C35-C5'	3.56	1.57	1.51
5	A	1403	THV	C4'-N3'	3.35	1.39	1.35
5	A	1403	THV	C4A-C4	3.35	1.56	1.49
5	C	1403	THV	C4'-N3'	2.77	1.38	1.35
5	A	1403	THV	C2'-N3'	2.64	1.38	1.34
5	C	1403	THV	C4A-C4	2.58	1.55	1.49
5	A	1403	THV	C5-C4	2.56	1.40	1.35
5	A	1403	THV	C4-N3	-2.55	1.36	1.40
5	C	1403	THV	C2'-N3'	2.47	1.38	1.34
5	C	1403	THV	C5-C4	2.43	1.40	1.35
5	C	1403	THV	C4-N3	-2.41	1.37	1.40
5	C	1403	THV	C8-C2	2.37	1.55	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1403	THV	C2A-C2'-N1'	5.61	123.17	117.20
5	C	1403	THV	C2A-C2'-N1'	4.90	122.42	117.20
5	A	1403	THV	N1'-C2'-N3'	-4.54	117.98	125.53
5	C	1403	THV	O9-C8-C9	4.15	120.02	110.15
5	C	1403	THV	C4-C5-S1	-3.90	106.52	110.56
5	C	1403	THV	N1'-C2'-N3'	-3.77	119.26	125.53
5	A	1403	THV	O9-C8-C9	3.64	118.79	110.15
5	A	1403	THV	C4-C5-S1	-3.56	106.87	110.56
5	A	1403	THV	C6'-N1'-C2'	3.30	121.48	116.07
5	C	1403	THV	C6'-N1'-C2'	3.14	121.24	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1403	THV	C4A-C4-C5	-2.62	121.03	127.75
5	A	1403	THV	C2'-N3'-C4'	2.38	121.76	118.10
5	A	1403	THV	C35-C5'-C4'	2.33	126.62	122.36
5	A	1403	THV	C4A-C4-C5	-2.16	122.21	127.75
5	C	1403	THV	C5A-C5-S1	2.11	123.81	119.29
5	A	1403	THV	C35-N3-C4	-2.09	120.47	123.95
5	A	1403	THV	C6'-C5'-C4'	-2.01	113.07	115.55

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1403	THV	S1-C2-C8-C9
5	A	1403	THV	N3-C2-C8-C9
5	A	1403	THV	C2-C8-C9-C10
5	A	1403	THV	C2-C8-C9-C11
5	C	1403	THV	S1-C2-C8-C9
5	C	1403	THV	N3-C2-C8-C9
5	C	1403	THV	C2-C8-C9-C10
5	C	1403	THV	C2-C8-C9-C11
6	D	1345	GOL	C1-C2-C3-O3
6	D	1345	GOL	O2-C2-C3-O3
6	D	1345	GOL	O1-C1-C2-O2
5	C	1403	THV	PA-O3A-PB-O1B
5	A	1403	THV	S1-C2-C8-O9
5	C	1403	THV	S1-C2-C8-O9
5	A	1403	THV	N3-C2-C8-O9
5	C	1403	THV	N3-C2-C8-O9

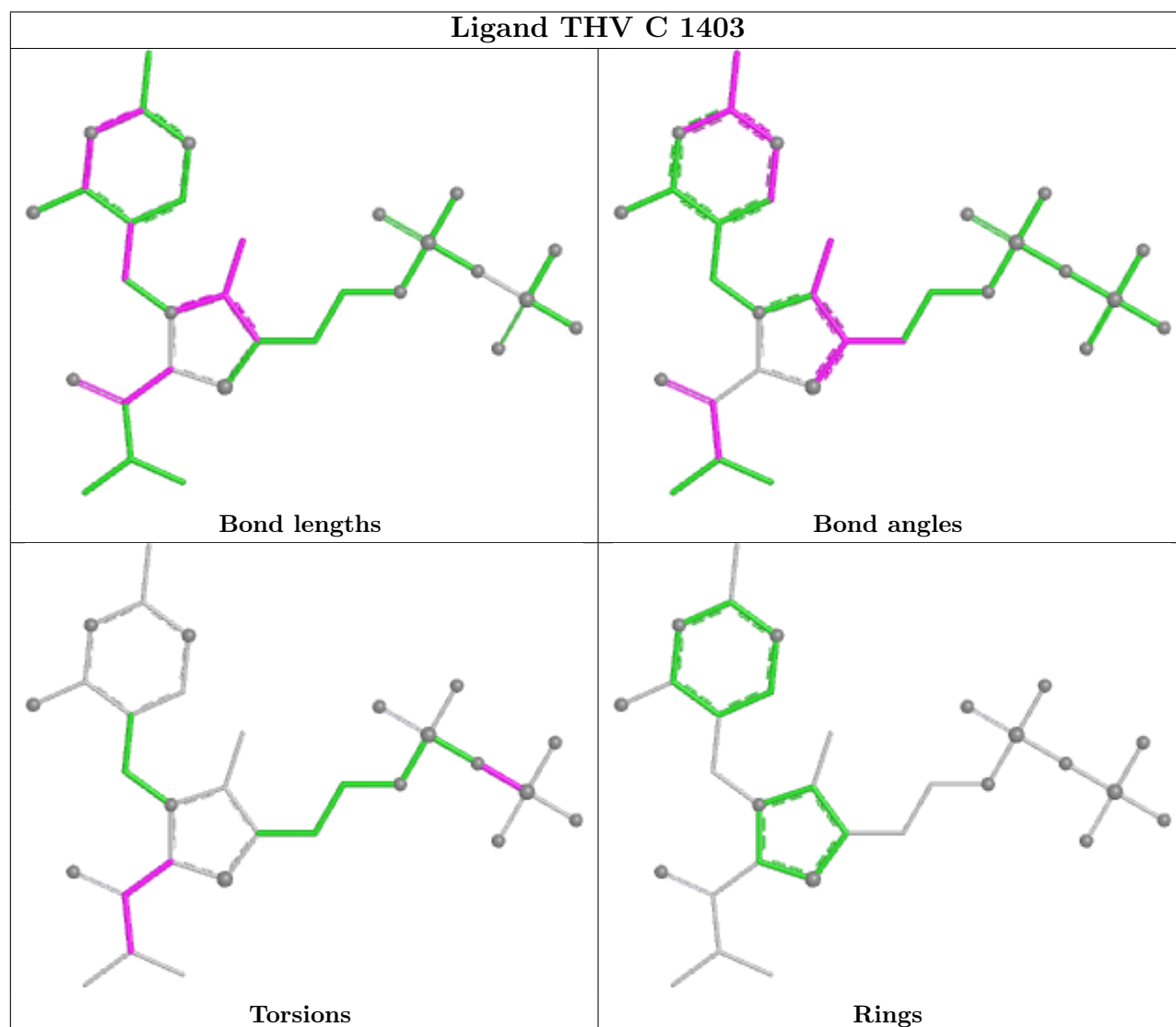
There are no ring outliers.

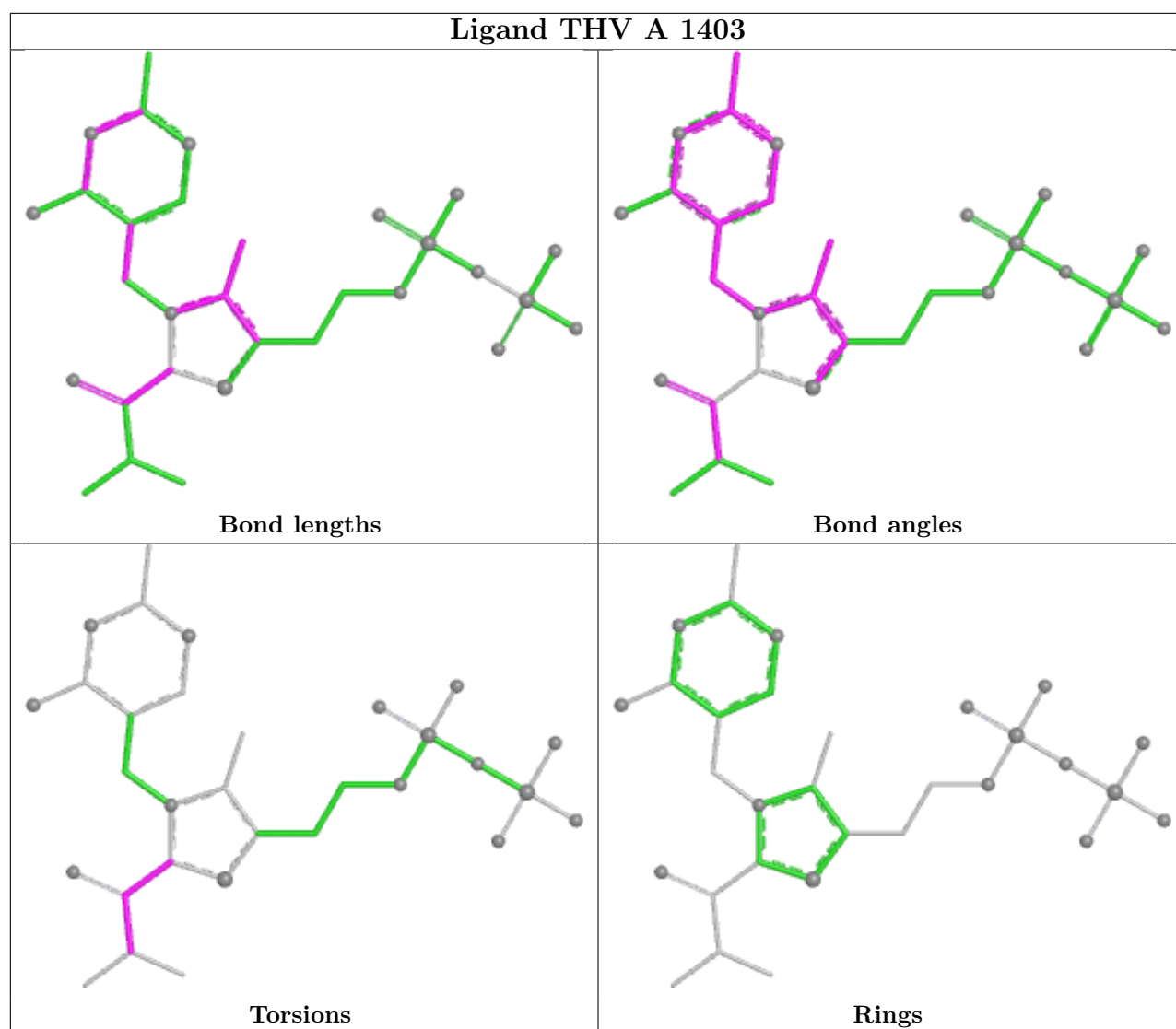
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1403	THV	2	0
5	A	1403	THV	3	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	383/400 (95%)	-0.12	18 (4%)	36 38	5, 15, 32, 52	9 (2%)
1	C	383/400 (95%)	-0.16	15 (3%)	43 47	5, 14, 32, 47	9 (2%)
2	B	330/350 (94%)	-0.43	5 (1%)	72 77	5, 11, 28, 41	5 (1%)
2	D	330/350 (94%)	-0.44	1 (0%)	90 93	6, 12, 28, 38	1 (0%)
All	All	1426/1500 (95%)	-0.28	39 (2%)	56 61	5, 13, 31, 52	24 (1%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	299	ALA	6.2
1	A	299	ALA	6.1
1	A	300	TYR	5.0
1	C	300	TYR	4.7
2	D	14	GLU	4.1
1	A	297	SER	3.8
1	A	296	ASP	3.8
2	B	14	GLU	3.6
1	C	183	ALA	3.6
2	B	197	ALA	3.5
1	C	294	SER	3.5
1	C	298	SER	3.4
1	A	289	GLY	3.3
1	A	183	ALA	3.3
1	A	298	SER	3.2
2	B	15	TYR	3.2
1	C	290	HIS	3.0
1	C	297	SER	3.0
1	A	293	THR	2.9
1	A	313	ASP	2.8
1	C	313	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	325	SER	2.6
1	C	400	LYS	2.6
1	A	292	SER	2.5
1	C	288	ILE	2.4
1	A	184	ASN	2.4
1	C	291	HIS	2.3
1	C	182	ASN	2.3
1	C	286	TYR	2.2
1	A	182	ASN	2.2
1	A	294	SER	2.2
1	C	289	GLY	2.2
1	A	286	TYR	2.1
2	B	196	ALA	2.1
1	A	105	ASN	2.0
1	C	40	GLN	2.0
2	B	341	ASN	2.0
1	A	324	LEU	2.0
1	A	26	ASN	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 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($\text{\AA}^2$)	Q<0.9
6	GOL	D	1345	6/6	0.89	0.12	23,30,32,34	0
6	GOL	D	1344	6/6	0.97	0.06	12,15,18,19	0
5	THV	A	1403	31/31	0.98	0.05	6,10,18,22	0
5	THV	C	1403	31/31	0.98	0.05	6,10,19,23	0
6	GOL	B	1344	6/6	0.99	0.03	15,15,16,17	0

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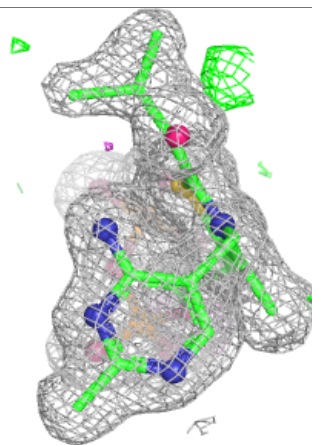
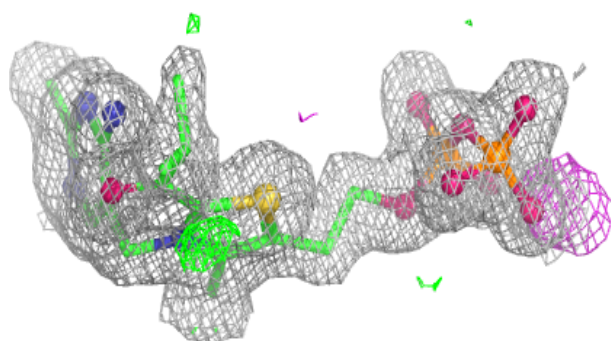
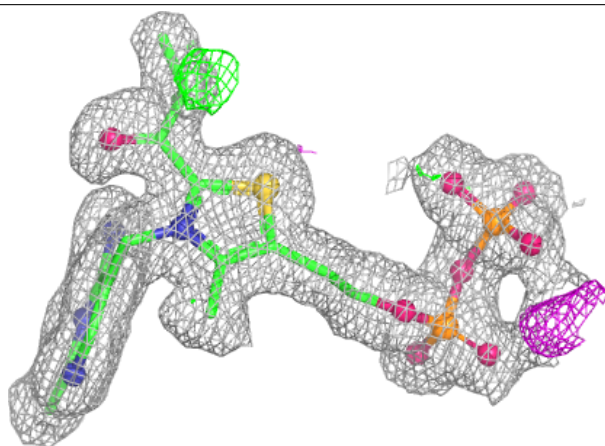
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	K	B	1343	1/1	0.99	0.10	19,19,19,19	0
4	K	C	1402	1/1	0.99	0.11	18,18,18,18	0
3	MN	A	1401	1/1	1.00	0.08	17,17,17,17	0
3	MN	C	1401	1/1	1.00	0.07	17,17,17,17	0
4	K	D	1343	1/1	1.00	0.10	21,21,21,21	0
4	K	A	1402	1/1	1.00	0.09	17,17,17,17	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.

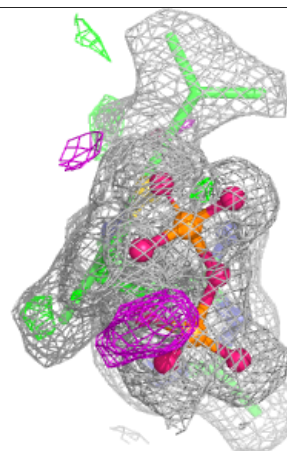
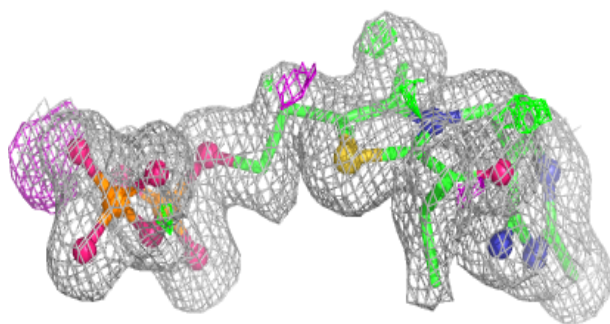
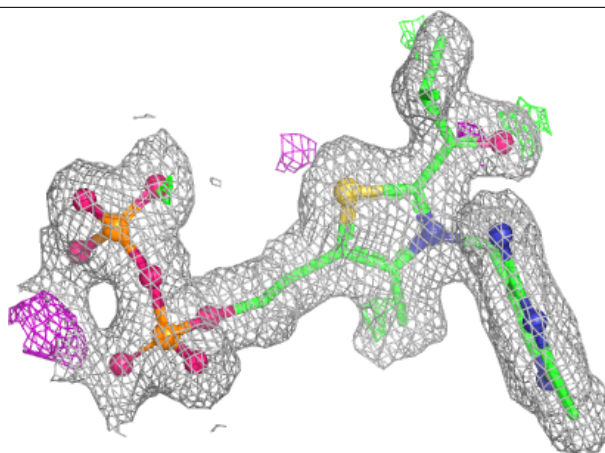
Electron density around THV A 1403:

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 THV C 1403:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.