



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:48 PM UTC

PDB ID : 6SY1 / pdb_00006sy1
Title : Crystal structure of the human 2-oxoadipate dehydrogenase DHTKD1 (E1)
Authors : Bezerra, G.A.; Foster, W.; Shrestha, L.; Pena, I.A.; Coker, J.; Kolker, S.; Nicola, B.B.; von Delft, F.; Edwards, A.; Arrowsmith, C.; Bountra, C.; Yue, W.W.; Structural Genomics Consortium (SGC)
Deposited on : 2019-09-26
Resolution : 1.87 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

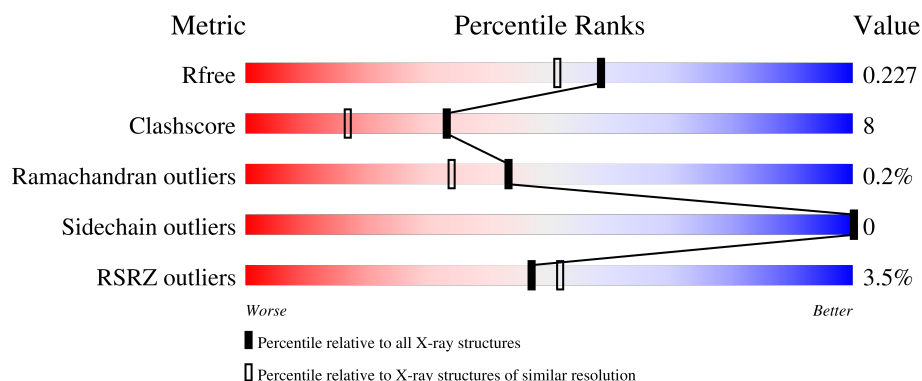
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	898	4% 85% 11% .
1	B	898	3% 83% 12% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14484 atoms, of which 32 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 Probable 2-oxoglutarate dehydrogenase E1 component DHKTD1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	859	Total	C	N	O	S	0	0	0
			6663	4249	1150	1226	38			
1	B	861	Total	C	N	O	S	0	0	0
			6668	4245	1154	1231	38			

There are 46 discrepancies between the modelled and reference sequences:

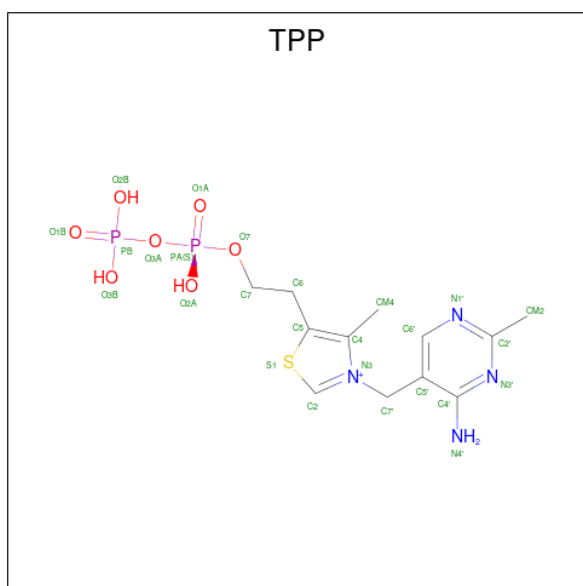
Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP Q96HY7
A	23	HIS	-	expression tag	UNP Q96HY7
A	24	HIS	-	expression tag	UNP Q96HY7
A	25	HIS	-	expression tag	UNP Q96HY7
A	26	HIS	-	expression tag	UNP Q96HY7
A	27	HIS	-	expression tag	UNP Q96HY7
A	28	HIS	-	expression tag	UNP Q96HY7
A	29	SER	-	expression tag	UNP Q96HY7
A	30	SER	-	expression tag	UNP Q96HY7
A	31	GLY	-	expression tag	UNP Q96HY7
A	32	VAL	-	expression tag	UNP Q96HY7
A	33	ASP	-	expression tag	UNP Q96HY7
A	34	LEU	-	expression tag	UNP Q96HY7
A	35	GLY	-	expression tag	UNP Q96HY7
A	36	THR	-	expression tag	UNP Q96HY7
A	37	GLU	-	expression tag	UNP Q96HY7
A	38	ASN	-	expression tag	UNP Q96HY7
A	39	LEU	-	expression tag	UNP Q96HY7
A	40	TYR	-	expression tag	UNP Q96HY7
A	41	PHE	-	expression tag	UNP Q96HY7
A	42	GLN	-	expression tag	UNP Q96HY7
A	43	SER	-	expression tag	UNP Q96HY7
A	44	MET	-	expression tag	UNP Q96HY7
B	22	MET	-	initiating methionine	UNP Q96HY7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	23	HIS	-	expression tag	UNP Q96HY7
B	24	HIS	-	expression tag	UNP Q96HY7
B	25	HIS	-	expression tag	UNP Q96HY7
B	26	HIS	-	expression tag	UNP Q96HY7
B	27	HIS	-	expression tag	UNP Q96HY7
B	28	HIS	-	expression tag	UNP Q96HY7
B	29	SER	-	expression tag	UNP Q96HY7
B	30	SER	-	expression tag	UNP Q96HY7
B	31	GLY	-	expression tag	UNP Q96HY7
B	32	VAL	-	expression tag	UNP Q96HY7
B	33	ASP	-	expression tag	UNP Q96HY7
B	34	LEU	-	expression tag	UNP Q96HY7
B	35	GLY	-	expression tag	UNP Q96HY7
B	36	THR	-	expression tag	UNP Q96HY7
B	37	GLU	-	expression tag	UNP Q96HY7
B	38	ASN	-	expression tag	UNP Q96HY7
B	39	LEU	-	expression tag	UNP Q96HY7
B	40	TYR	-	expression tag	UNP Q96HY7
B	41	PHE	-	expression tag	UNP Q96HY7
B	42	GLN	-	expression tag	UNP Q96HY7
B	43	SER	-	expression tag	UNP Q96HY7
B	44	MET	-	expression tag	UNP Q96HY7

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
2	B	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Mg	0	0
			2	2		
3	B	1	Total	Mg	0	0
			1	1		

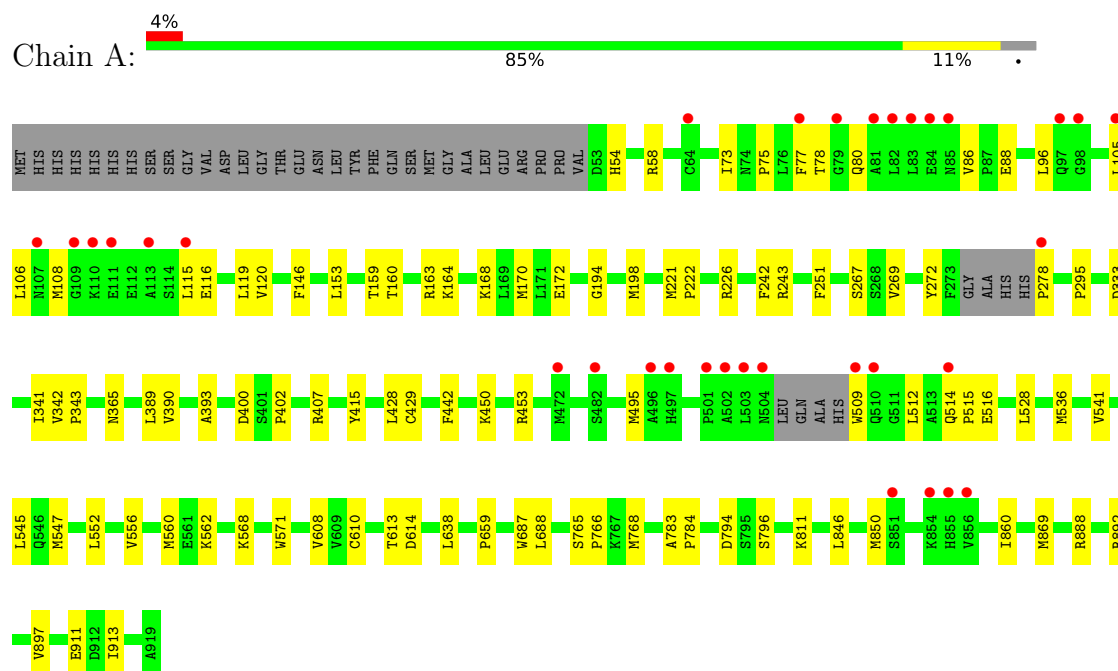
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	524	Total	O	0	0
			524	524		
4	B	542	Total	O	0	0
			542	542		

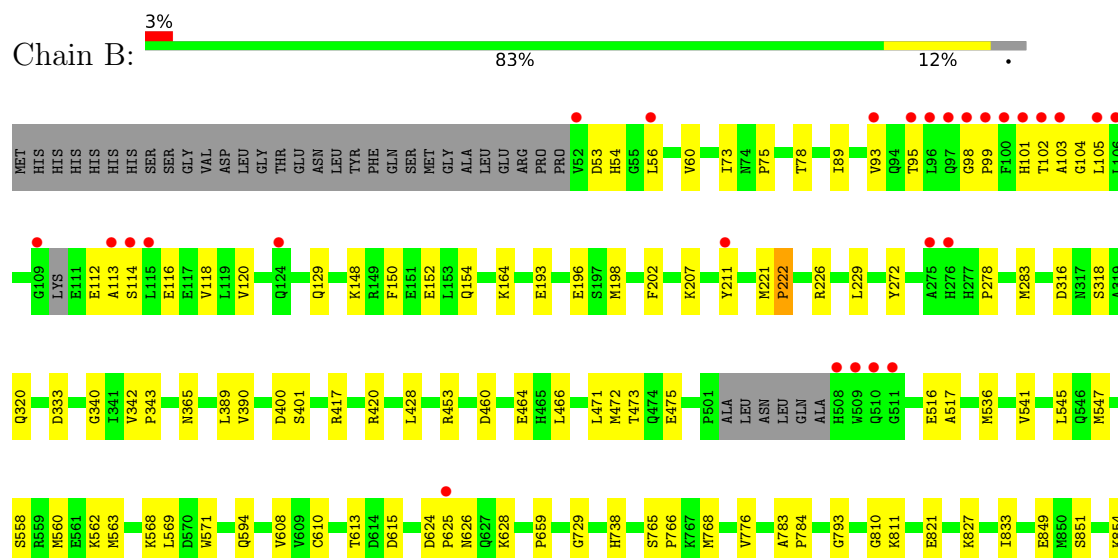
3 Residue-property plots

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: Probable 2-oxoglutarate dehydrogenase E1 component DHKTD1, mitochondrial



- Molecule 1: Probable 2-oxoglutarate dehydrogenase E1 component DHKTD1, mitochondrial



P866
M869
S876
P877
K886
P893
V897
A919

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.55Å 81.22Å 86.90Å 63.43° 76.96° 72.06°	Depositor
Resolution (Å)	46.01 – 1.87 46.01 – 1.87	Depositor EDS
% Data completeness (in resolution range)	96.5 (46.01-1.87) 96.5 (46.01-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.190 , 0.230 0.190 , 0.227	Depositor DCC
R_{free} test set	7091 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14484	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.40% 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: MG, 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	0.31	0/6827	0.50	0/9261
1	B	0.32	0/6829	0.50	0/9264
All	All	0.32	0/13656	0.50	0/18525

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	6663	0	6492	96	0
1	B	6668	0	6496	112	0
2	A	26	16	16	1	0
2	B	26	16	16	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
4	A	524	0	0	6	0
4	B	542	0	0	5	0
All	All	14452	32	13020	207	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 8.

All (207) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ASP:HB3	1:B:102:THR:OG1	1.58	1.03
1:A:811:LYS:HE2	4:A:1148:HOH:O	1.61	0.96
1:B:516:GLU:OE1	4:B:1101:HOH:O	1.87	0.92
1:B:221:MET:HE3	1:B:226:ARG:HG3	1.51	0.91
1:A:389:LEU:HD12	1:A:390:VAL:HG13	1.50	0.90
1:B:613:THR:HG23	1:B:615:ASP:H	1.37	0.88
1:B:628:LYS:HE3	1:B:628:LYS:HA	1.56	0.88
1:B:536:MET:HE3	1:B:563:MET:HB2	1.51	0.88
1:B:886:LYS:NZ	4:B:1102:HOH:O	1.99	0.88
1:B:610:CYS:SG	1:B:613:THR:HG22	2.14	0.87
1:B:562:LYS:HB3	1:B:569:LEU:HD22	1.59	0.84
1:A:536:MET:HE1	1:A:560:MET:HG2	1.60	0.83
1:B:536:MET:HE1	1:B:560:MET:HA	1.58	0.83
1:A:541:VAL:HG11	1:A:545:LEU:HD22	1.62	0.81
1:B:101:HIS:CB	1:B:112:GLU:HA	2.11	0.81
1:A:547:MET:HE2	1:A:552:LEU:HG	1.61	0.80
1:A:547:MET:HG3	1:A:608:VAL:HG11	1.62	0.80
1:A:768:MET:HE2	1:A:811:LYS:HG3	1.62	0.80
1:A:768:MET:HE2	1:A:811:LYS:CG	2.13	0.79
1:B:272:TYR:CE2	1:B:278:PRO:HG3	2.21	0.76
1:B:417:ARG:O	1:B:420:ARG:NH1	2.19	0.76
1:A:545:LEU:HG	1:A:610:CYS:HB2	1.68	0.75
1:A:528:LEU:HD21	1:A:783:ALA:HB2	1.68	0.74
1:B:562:LYS:HB3	1:B:569:LEU:CD2	2.18	0.73
1:B:473:THR:HG21	4:B:1526:HOH:O	1.88	0.72
1:B:628:LYS:HA	1:B:628:LYS:CE	2.19	0.72
1:B:102:THR:HG22	1:B:104:GLY:H	1.56	0.71
1:B:536:MET:HE3	1:B:563:MET:CB	2.21	0.70
1:B:626:ASN:O	1:B:628:LYS:HD2	1.90	0.70
1:B:536:MET:CE	1:B:563:MET:HB2	2.22	0.69
1:A:272:TYR:CE2	1:A:278:PRO:HB3	2.28	0.68
1:B:116:GLU:O	1:B:120:VAL:HG23	1.93	0.68
1:B:541:VAL:CG1	1:B:547:MET:HE2	2.24	0.67
1:A:547:MET:HE2	1:A:552:LEU:CG	2.24	0.67
1:A:116:GLU:O	1:A:120:VAL:HG23	1.93	0.67
1:A:547:MET:HE2	1:A:552:LEU:CD2	2.25	0.67
1:B:101:HIS:CB	1:B:113:ALA:H	2.08	0.66
1:B:272:TYR:HE2	1:B:278:PRO:HG3	1.61	0.66
1:B:473:THR:HG22	1:B:475:GLU:N	2.10	0.66
1:A:198:MET:SD	4:A:1370:HOH:O	2.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:SER:O	1:B:118:VAL:HG23	1.96	0.65
1:A:547:MET:HE1	1:A:556:VAL:HG21	1.79	0.64
1:B:150:PHE:O	1:B:154:GLN:HG3	1.97	0.64
1:B:148:LYS:HE2	1:B:152:GLU:OE2	1.98	0.64
1:B:221:MET:HG3	1:B:222:PRO:HD2	1.79	0.63
1:B:53:ASP:O	1:B:105:LEU:HD11	1.99	0.63
1:B:536:MET:CE	1:B:560:MET:HG2	2.28	0.63
1:B:536:MET:HE1	1:B:560:MET:HG2	1.80	0.63
1:B:821:GLU:OE1	1:B:827:LYS:HE2	1.99	0.62
1:A:243:ARG:HG3	1:A:495:MET:HE3	1.82	0.62
1:B:221:MET:CE	1:B:283:MET:CE	2.78	0.62
1:A:768:MET:SD	1:A:811:LYS:HE3	2.40	0.62
1:B:833:ILE:HD12	1:B:849:GLU:CG	2.29	0.62
1:A:77:PHE:HB3	1:A:80:GLN:HG3	1.82	0.61
1:A:516:GLU:HB2	4:A:1509:HOH:O	1.99	0.61
1:B:536:MET:SD	1:B:560:MET:HG2	2.40	0.61
1:B:207:LYS:HE2	1:B:211:TYR:OH	2.00	0.61
1:B:571:TRP:CE2	1:B:766:PRO:HG3	2.35	0.61
1:A:514:GLN:OE1	1:A:515:PRO:HD2	2.00	0.61
1:A:389:LEU:CD1	1:A:390:VAL:HG13	2.28	0.60
1:A:242:PHE:HB2	1:A:495:MET:SD	2.42	0.60
1:A:547:MET:HG3	1:A:608:VAL:CG1	2.31	0.59
1:B:460:ASP:O	1:B:464:GLU:HG3	2.01	0.59
1:B:78:THR:HG22	4:B:1459:HOH:O	2.02	0.59
1:B:466:LEU:CD1	1:B:472:MET:HE2	2.33	0.59
1:B:541:VAL:HG11	1:B:547:MET:HE2	1.84	0.58
1:B:198:MET:HE2	1:B:202:PHE:HE2	1.68	0.58
1:A:536:MET:HE3	1:A:536:MET:HA	1.84	0.58
1:A:571:TRP:CE2	1:A:766:PRO:HG3	2.39	0.58
1:B:536:MET:CE	1:B:560:MET:HA	2.30	0.58
1:B:102:THR:HG21	1:B:105:LEU:HG	1.86	0.57
1:B:53:ASP:CB	1:B:102:THR:OG1	2.45	0.57
1:B:833:ILE:HD12	1:B:849:GLU:HG2	1.87	0.57
1:A:115:LEU:HD21	1:A:119:LEU:HD11	1.87	0.57
1:A:243:ARG:HG3	1:A:495:MET:CE	2.35	0.57
1:A:160:THR:O	1:A:164:LYS:HG3	2.05	0.56
1:A:768:MET:HE2	1:A:811:LYS:HG2	1.85	0.56
1:A:536:MET:HE1	1:A:560:MET:HE3	1.86	0.56
1:B:793:GLY:HA2	1:B:833:ILE:HD13	1.86	0.56
1:A:846:LEU:O	1:A:850:MET:HG3	2.05	0.56
1:B:221:MET:HE1	1:B:283:MET:HE1	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:MET:HE2	1:B:283:MET:HE2	1.89	0.55
1:B:389:LEU:HD12	1:B:390:VAL:HG13	1.88	0.55
1:B:547:MET:HG3	1:B:608:VAL:HG11	1.89	0.55
1:B:466:LEU:HD12	1:B:472:MET:HE2	1.90	0.54
1:A:75:PRO:HB3	1:A:400:ASP:HB2	1.89	0.54
1:B:768:MET:HE2	1:B:811:LYS:HD3	1.89	0.54
1:B:56:LEU:O	1:B:60:VAL:HG23	2.06	0.54
1:B:866:PRO:HB3	1:B:893:PRO:O	2.07	0.53
1:A:267:SER:OG	1:A:269:VAL:HG13	2.08	0.53
1:A:77:PHE:O	1:A:80:GLN:HG3	2.08	0.53
1:A:272:TYR:CZ	1:A:278:PRO:HB3	2.43	0.53
1:A:509:TRP:CE3	1:A:512:LEU:HD12	2.44	0.53
1:B:417:ARG:HA	1:B:420:ARG:NH1	2.24	0.53
1:A:295:PRO:HG3	1:A:341:ILE:HD11	1.89	0.53
1:B:473:THR:HG22	1:B:475:GLU:H	1.74	0.53
1:B:129:GLN:HG2	1:B:401:SER:OG	2.08	0.53
1:B:417:ARG:HA	1:B:420:ARG:HH11	1.74	0.53
1:B:320:GLN:HG3	4:B:1305:HOH:O	2.08	0.53
1:B:342:VAL:HB	1:B:343:PRO:HD3	1.90	0.53
1:A:911:GLU:OE2	4:A:1101:HOH:O	2.19	0.52
1:B:221:MET:HE1	1:B:229:LEU:HD23	1.91	0.52
1:B:768:MET:CE	1:B:811:LYS:HD3	2.39	0.52
1:A:243:ARG:NE	4:A:1110:HOH:O	2.42	0.52
1:A:251:PHE:CZ	1:A:688:LEU:HD13	2.45	0.51
1:B:164:LYS:HE3	1:B:471:LEU:O	2.09	0.51
1:B:541:VAL:HG13	1:B:547:MET:HE2	1.93	0.51
1:B:783:ALA:HB1	1:B:784:PRO:HD2	1.92	0.51
1:B:628:LYS:HE3	1:B:628:LYS:CA	2.28	0.51
1:B:75:PRO:HB3	1:B:400:ASP:HB2	1.91	0.50
1:B:610:CYS:CB	1:B:613:THR:HG22	2.42	0.50
1:A:442:PHE:HE1	1:A:450:LYS:HG2	1.77	0.49
1:A:77:PHE:O	1:A:80:GLN:CG	2.60	0.49
1:B:536:MET:HE1	1:B:560:MET:CA	2.36	0.49
1:B:221:MET:HE1	1:B:283:MET:CE	2.42	0.48
1:A:73:ILE:HG13	1:A:428:LEU:HD22	1.96	0.48
1:B:102:THR:HG22	1:B:103:ALA:N	2.27	0.48
1:A:159:THR:O	1:A:163:ARG:HG3	2.14	0.48
1:B:869:MET:HE1	1:B:897:VAL:O	2.15	0.47
1:A:242:PHE:CB	1:A:495:MET:SD	3.02	0.47
1:A:765:SER:HB2	1:A:766:PRO:HD2	1.96	0.47
1:B:102:THR:CG2	1:B:105:LEU:HG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:THR:HG23	4:A:1407:HOH:O	2.14	0.47
1:B:198:MET:HE2	1:B:202:PHE:CE2	2.50	0.47
1:B:221:MET:HE2	1:B:283:MET:CE	2.44	0.47
1:A:562:LYS:HD2	1:A:568:LYS:O	2.14	0.46
1:B:89:ILE:O	1:B:93:VAL:HG23	2.15	0.46
1:B:610:CYS:HB3	1:B:613:THR:CG2	2.45	0.46
1:A:146:PHE:CE2	1:A:415:TYR:CD1	3.04	0.46
1:B:545:LEU:C	1:B:545:LEU:HD23	2.40	0.46
1:B:95:THR:HG22	1:B:95:THR:O	2.15	0.46
1:A:105:LEU:O	1:A:106:LEU:HG	2.16	0.46
1:B:340:GLY:C	1:B:343:PRO:HD2	2.40	0.46
1:A:536:MET:CE	1:A:560:MET:HE3	2.46	0.46
1:B:466:LEU:HD12	1:B:472:MET:CE	2.46	0.46
1:B:610:CYS:HB3	1:B:613:THR:HG22	1.98	0.46
1:A:96:LEU:HD23	1:B:54:HIS:NE2	2.31	0.46
1:A:77:PHE:HB3	1:A:80:GLN:CG	2.47	0.45
1:B:102:THR:HG22	1:B:104:GLY:N	2.28	0.45
1:B:389:LEU:CD1	1:B:390:VAL:HG13	2.45	0.45
1:A:547:MET:CE	1:A:552:LEU:HD23	2.45	0.45
1:A:343:PRO:HB3	1:A:389:LEU:HD21	1.99	0.45
1:B:765:SER:HB2	1:B:766:PRO:HD2	1.98	0.45
2:A:1001:TPP:H6'	1:B:594:GLN:OE1	2.16	0.45
1:B:73:ILE:HG13	1:B:428:LEU:HD22	1.98	0.45
1:B:833:ILE:HD12	1:B:849:GLU:HG3	1.96	0.45
1:B:876:SER:HB3	1:B:877:PRO:HD3	1.99	0.45
1:A:541:VAL:CG1	1:A:545:LEU:HD22	2.40	0.45
1:A:783:ALA:HB1	1:A:784:PRO:HD2	1.98	0.45
1:B:568:LYS:HA	1:B:776:VAL:HB	1.99	0.45
1:A:850:MET:HE2	1:A:850:MET:HB3	1.86	0.45
1:B:624:ASP:OD2	1:B:625:PRO:O	2.35	0.45
1:A:168:LYS:O	1:A:172:GLU:HG3	2.16	0.44
1:A:194:GLY:O	1:A:429:CYS:HB2	2.17	0.44
1:A:547:MET:HE2	1:A:552:LEU:HD23	1.98	0.44
1:A:768:MET:CE	1:A:811:LYS:CG	2.91	0.44
1:A:562:LYS:HA	1:A:562:LYS:HD3	1.74	0.44
1:A:638:LEU:HD11	2:B:1001:TPP:HM42	1.99	0.44
1:B:221:MET:CE	1:B:283:MET:HE2	2.46	0.44
1:B:558:SER:OG	1:B:562:LYS:HE2	2.18	0.44
1:B:466:LEU:HD13	1:B:472:MET:HE2	1.99	0.43
1:A:536:MET:HE3	1:A:536:MET:CA	2.46	0.43
1:B:876:SER:HB3	1:B:877:PRO:CD	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:GLY:HA2	1:B:99:PRO:HD3	1.87	0.43
1:A:115:LEU:HD21	1:A:119:LEU:CD1	2.49	0.43
1:A:768:MET:CE	1:A:811:LYS:HG2	2.47	0.43
1:B:164:LYS:HE2	1:B:472:MET:HG2	2.01	0.43
1:A:146:PHE:HE2	1:A:415:TYR:CD1	2.37	0.43
1:A:251:PHE:CZ	1:A:688:LEU:CD1	3.02	0.43
1:A:794:ASP:OD1	1:A:796:SER:OG	2.32	0.43
1:A:453:ARG:HA	1:A:453:ARG:HD3	1.92	0.43
1:A:77:PHE:CB	1:A:80:GLN:HG3	2.48	0.42
1:A:170:MET:HE1	1:A:402:PRO:HG2	1.99	0.42
1:A:86:VAL:CG1	1:A:88:GLU:OE1	2.67	0.42
1:A:869:MET:HE1	1:A:897:VAL:O	2.19	0.42
1:B:453:ARG:HA	1:B:453:ARG:HD3	1.85	0.42
1:A:545:LEU:HD23	1:A:545:LEU:C	2.44	0.42
1:A:243:ARG:CG	1:A:495:MET:CE	2.97	0.42
1:B:517:ALA:O	1:B:729:GLY:HA3	2.20	0.42
1:A:860:ILE:HD11	1:A:888:ARG:NH2	2.35	0.42
1:B:738:HIS:CE1	1:B:810:GLY:HA3	2.55	0.42
1:B:316:ASP:CG	1:B:318:SER:HG	2.28	0.42
1:A:783:ALA:HB1	1:A:784:PRO:CD	2.50	0.41
1:A:892:ARG:HG3	1:A:913:ILE:HD11	2.00	0.41
1:B:563:MET:HA	1:B:563:MET:HE2	2.02	0.41
1:A:153:LEU:O	1:A:407:ARG:HD3	2.20	0.41
1:B:851:SER:HA	1:B:854:LYS:HE2	2.02	0.41
1:A:547:MET:HE1	1:A:556:VAL:CG2	2.49	0.41
1:A:243:ARG:CG	1:A:495:MET:HE1	2.50	0.41
1:A:687:TRP:O	1:A:688:LEU:HB2	2.20	0.41
1:B:389:LEU:HD12	1:B:389:LEU:C	2.46	0.41
1:A:333:ASP:HB3	1:A:365:ASN:HA	2.02	0.41
1:B:221:MET:CG	1:B:222:PRO:HD2	2.50	0.41
1:A:54:HIS:O	1:A:58:ARG:HG3	2.21	0.41
1:A:77:PHE:HB3	1:A:80:GLN:OE1	2.21	0.41
1:A:108:MET:HE2	1:A:108:MET:HB3	1.96	0.41
1:A:536:MET:HE1	1:A:560:MET:CE	2.49	0.41
1:A:613:THR:O	1:A:614:ASP:HB2	2.21	0.41
1:B:193:GLU:HA	1:B:196:GLU:OE2	2.20	0.41
1:A:115:LEU:C	1:A:115:LEU:HD23	2.46	0.40
1:A:342:VAL:HB	1:A:343:PRO:CD	2.50	0.40
1:A:221:MET:HE2	1:A:226:ARG:HA	2.03	0.40
1:B:765:SER:HB2	1:B:766:PRO:CD	2.51	0.40
1:B:102:THR:CG2	1:B:103:ALA:N	2.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:PHE:HB3	1:A:80:GLN:CD	2.47	0.40
1:A:146:PHE:CZ	1:A:393:ALA:HB1	2.56	0.40
1:B:333:ASP:HB3	1:B:365:ASN: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	853/898 (95%)	827 (97%)	24 (3%)	2 (0%)	43	34
1	B	855/898 (95%)	828 (97%)	25 (3%)	2 (0%)	43	34
All	All	1708/1796 (95%)	1655 (97%)	49 (3%)	4 (0%)	43	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	222	PRO
1	B	222	PRO
1	A	659	PRO
1	B	659	PRO

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	711/776 (92%)	711 (100%)	0	100	100
1	B	712/776 (92%)	712 (100%)	0	100	100
All	All	1423/1552 (92%)	1423 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	154	GLN
1	A	174	GLN
1	A	432	GLN
1	A	550	HIS
1	A	882	GLN
1	B	124	GLN
1	B	203	HIS
1	B	320	GLN
1	B	474	GLN
1	B	550	HIS
1	B	738	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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
2	TPP	A	1001	3	26,27,27	1.26	1 (3%)	38,40,40	0.69	1 (2%)
2	TPP	B	1001	3	26,27,27	0.50	0	38,40,40	0.67	1 (2%)

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
2	TPP	A	1001	3	-	2/17/17/17	0/2/2/2
2	TPP	B	1001	3	-	1/17/17/17	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	TPP	PA-O3A	-5.91	1.53	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	TPP	O3B-PB-O3A	2.26	112.20	104.64
2	A	1001	TPP	O2A-PA-O3A	2.17	113.14	107.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

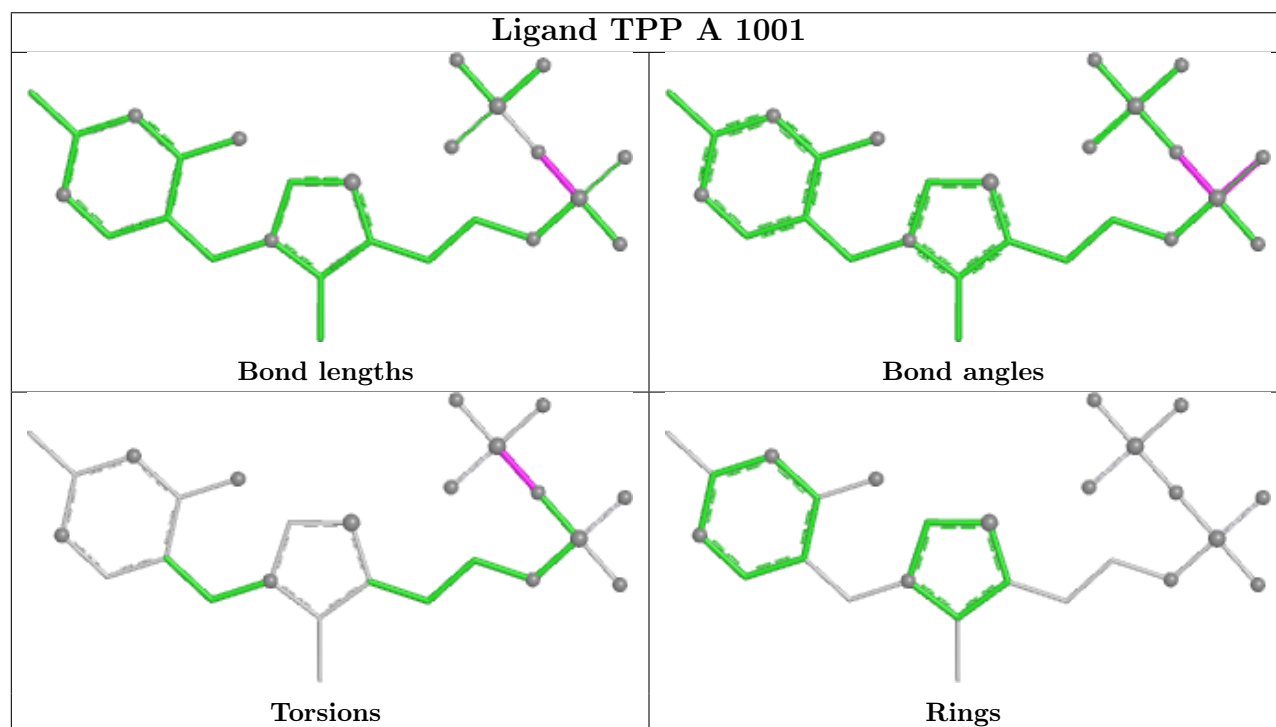
Mol	Chain	Res	Type	Atoms
2	B	1001	TPP	PA-O3A-PB-O1B
2	A	1001	TPP	PA-O3A-PB-O1B
2	A	1001	TPP	PA-O3A-PB-O3B

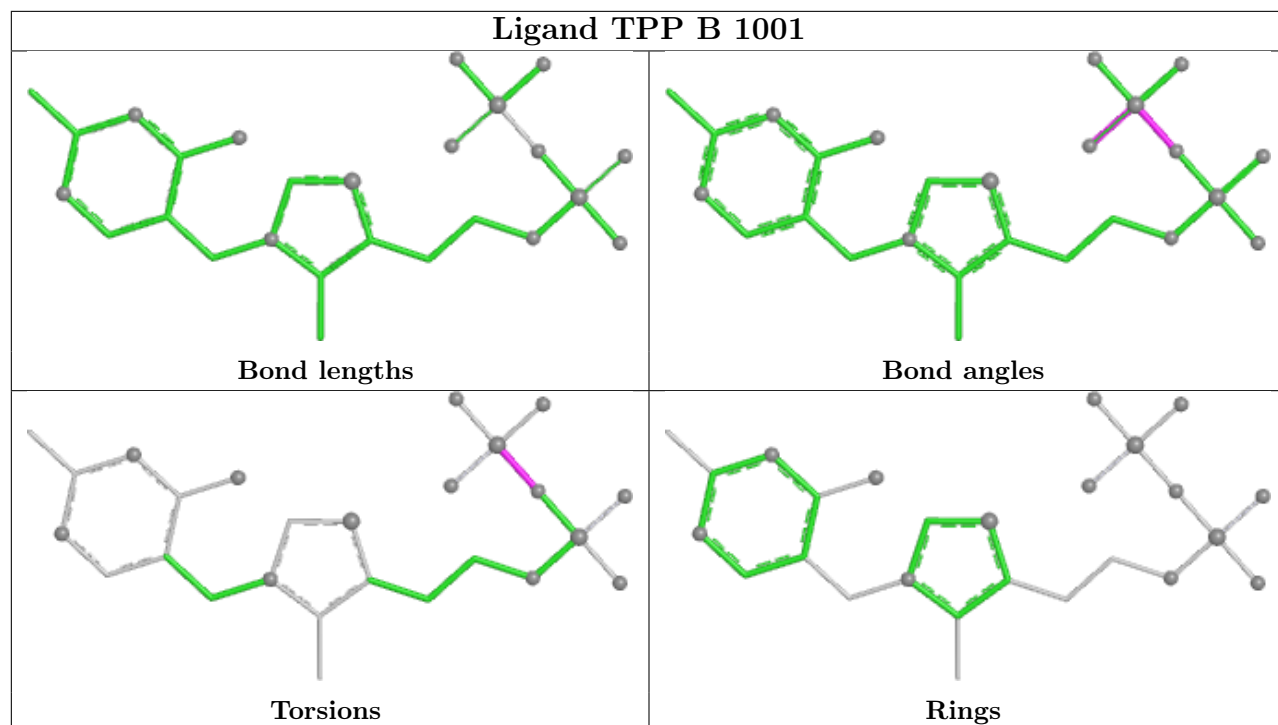
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	TPP	1	0
2	B	1001	TPP	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 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	859/898 (95%)	-0.07	33 (3%) 44 48	14, 23, 46, 72	0
1	B	861/898 (95%)	-0.10	27 (3%) 51 56	14, 24, 46, 87	0
All	All	1720/1796 (95%)	-0.09	60 (3%) 47 52	14, 24, 46, 87	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	503	LEU	5.3
1	B	508	HIS	5.0
1	B	103	ALA	4.9
1	A	502	ALA	4.6
1	B	100	PHE	4.5
1	B	109	GLY	4.4
1	A	109	GLY	4.1
1	B	99	PRO	4.1
1	B	98	GLY	3.9
1	A	115	LEU	3.8
1	A	504	ASN	3.8
1	B	97	GLN	3.7
1	B	511	GLY	3.7
1	B	211	TYR	3.7
1	B	509	TRP	3.7
1	A	510	GLN	3.6
1	A	83	LEU	3.5
1	A	98	GLY	3.5
1	A	110	LYS	3.4
1	B	102	THR	3.4
1	B	105	LEU	3.2
1	A	854	LYS	3.1
1	B	113	ALA	3.1
1	A	82	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	85	ASN	3.0
1	B	95	THR	3.0
1	B	52	VAL	2.9
1	B	625	PRO	2.8
1	B	275	ALA	2.8
1	A	84	GLU	2.7
1	A	496	ALA	2.6
1	B	93	VAL	2.6
1	B	114	SER	2.6
1	A	501	PRO	2.5
1	A	64	CYS	2.4
1	A	509	TRP	2.4
1	B	106	LEU	2.4
1	B	510	GLN	2.4
1	B	101	HIS	2.4
1	B	56	LEU	2.3
1	B	124	GLN	2.3
1	A	107	ASN	2.3
1	A	497	HIS	2.3
1	A	855	HIS	2.3
1	A	856	VAL	2.3
1	B	276	HIS	2.3
1	B	96	LEU	2.3
1	A	851	SER	2.2
1	A	97	GLN	2.2
1	A	81	ALA	2.2
1	A	472	MET	2.1
1	A	105	LEU	2.1
1	B	115	LEU	2.1
1	A	77	PHE	2.1
1	A	113	ALA	2.1
1	A	482	SER	2.1
1	A	278	PRO	2.1
1	A	79	GLY	2.0
1	A	514	GLN	2.0
1	A	111	GLU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

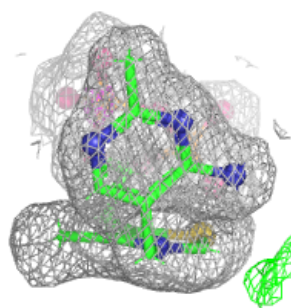
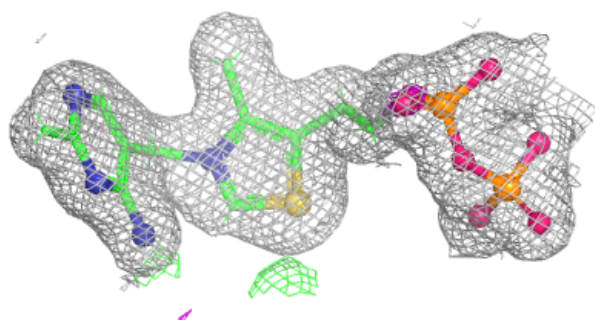
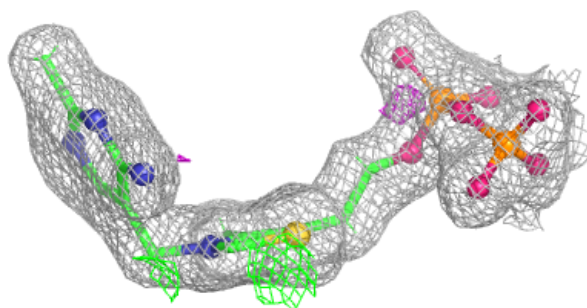
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	TPP	A	1001	26/26	0.98	0.05	15,19,23,24	0
2	TPP	B	1001	26/26	0.98	0.05	17,20,23,25	0
3	MG	A	1003	1/1	0.98	0.03	22,22,22,22	0
3	MG	A	1002	1/1	0.99	0.02	18,18,18,18	0
3	MG	B	1002	1/1	0.99	0.02	18,18,18,18	0

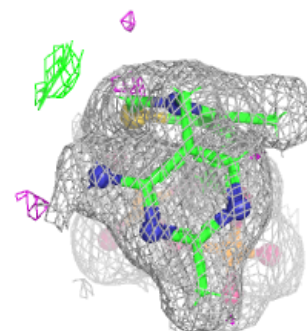
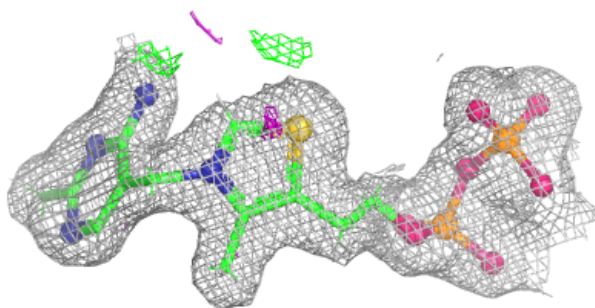
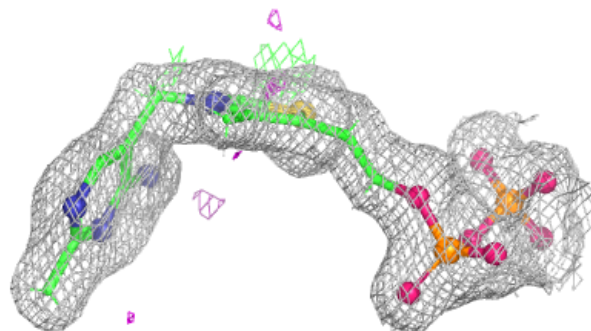
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 1001:

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

**Electron density around TPP B 1001:**

$2mF_o-DF_c$ (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.