



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:11 AM EDT

PDB ID : 2QTA / pdb_00002qta
Title : E. coli Pyruvate dehydrogenase E1 component E401K mutant with thiamin diphosphate
Authors : Furey, W.; Arjunan, P.; Chandrasekhar, K.
Deposited on : 2007-08-01
Resolution : 1.85 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

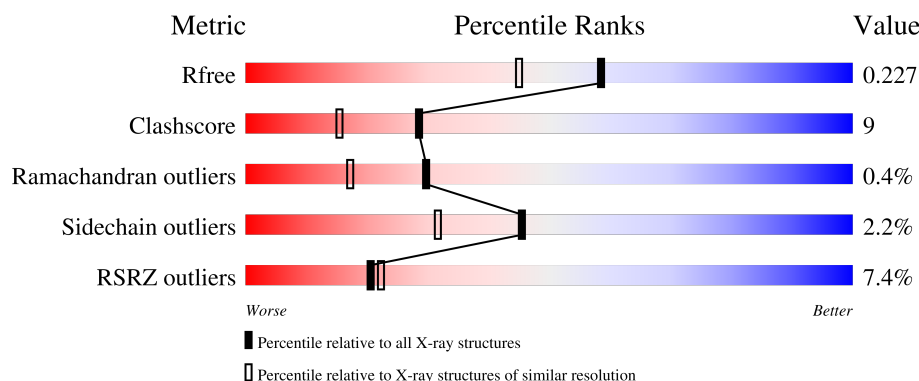
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	886	
1	B	886	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13149 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 Pyruvate dehydrogenase E1 component.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	801	Total	C	N	O	S	0	0	0
			6341	4018	1093	1204	26			
1	B	801	Total	C	N	O	S	0	0	0
			6341	4018	1093	1204	26			

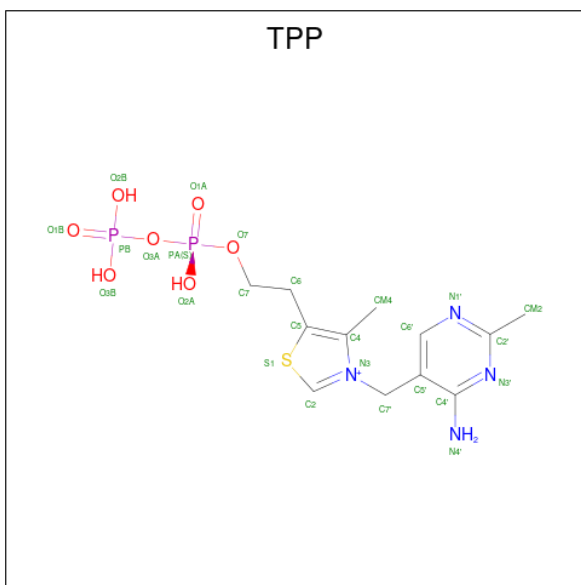
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	401	LYS	GLU	engineered mutation	UNP P0AFG8
B	401	LYS	GLU	engineered mutation	UNP P0AFG8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

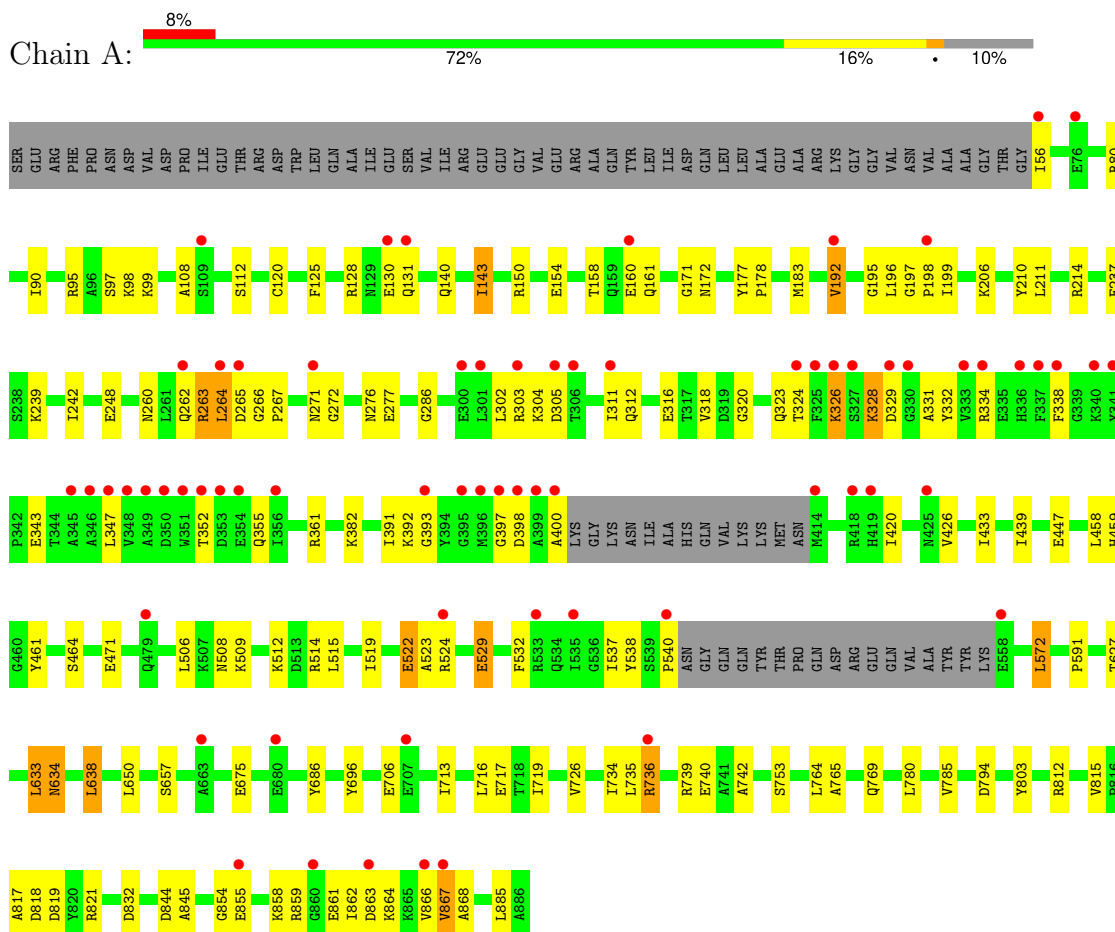
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	200	Total O 200 200	0	0
4	B	213	Total O 213 213	0	0

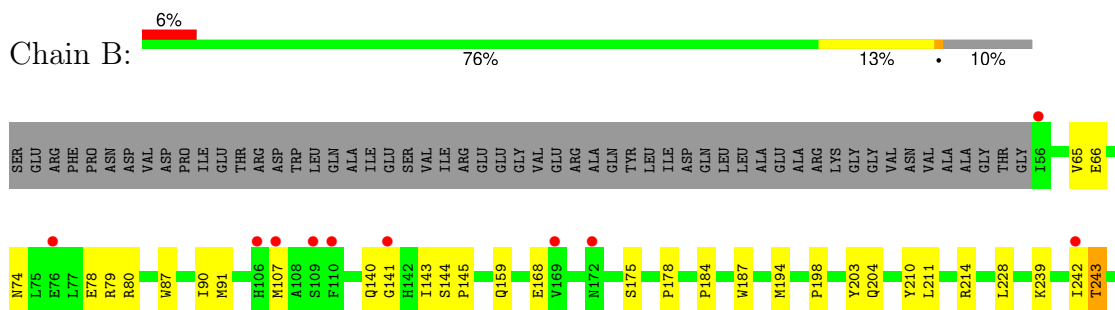
3 Residue-property plots [i](#)

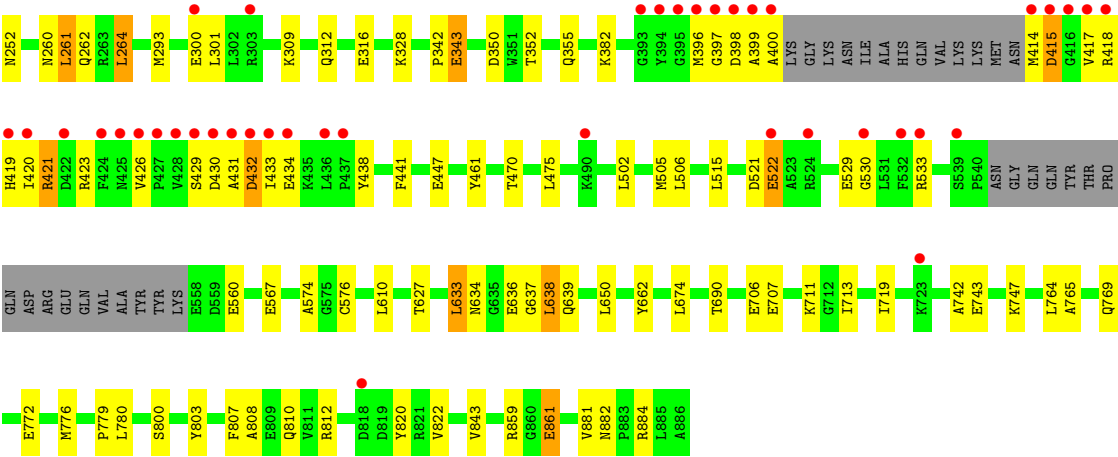
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Pyruvate dehydrogenase E1 component



- Molecule 1: Pyruvate dehydrogenase E1 component





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.81Å 141.83Å 82.56Å 90.00° 102.01° 90.00°	Depositor
Resolution (Å)	38.06 – 1.85 38.06 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.1 (38.06-1.85) 97.1 (38.06-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.27 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.237 0.203 , 0.227	Depositor DCC
R_{free} test set	7685 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13149	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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	0.61	0/6484	0.99	18/8766 (0.2%)
1	B	0.63	0/6484	0.99	14/8766 (0.2%)
All	All	0.62	0/12968	0.99	32/17532 (0.2%)

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	3
1	B	0	1
All	All	0	4

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	634	ASN	N-CA-C	10.75	123.00	111.28
1	A	634	ASN	N-CA-C	10.21	122.41	111.28
1	A	638	LEU	N-CA-C	8.63	121.47	111.11
1	B	638	LEU	N-CA-C	7.90	120.88	111.33
1	A	171	GLY	N-CA-C	7.36	123.44	114.69
1	A	633	LEU	N-CA-C	-7.34	98.61	109.62
1	B	633	LEU	N-CA-C	-7.33	99.37	109.71
1	B	432	ASP	N-CA-C	-7.30	104.52	113.50
1	B	706	GLU	N-CA-C	6.27	118.63	111.11
1	B	662	TYR	N-CA-C	5.96	119.27	109.85
1	A	171	GLY	CA-C-N	-5.75	113.54	123.25
1	A	171	GLY	C-N-CA	-5.75	113.54	123.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ILE	N-CA-C	5.73	117.16	110.62
1	A	785	VAL	N-CA-C	5.68	114.21	107.73
1	A	183	MET	CA-C-N	5.60	125.27	119.56
1	A	183	MET	C-N-CA	5.60	125.27	119.56
1	A	794	ASP	N-CA-C	5.58	120.08	113.16
1	B	204	GLN	N-CA-C	-5.49	105.21	111.14
1	B	636	GLU	N-CA-C	5.47	118.01	111.71
1	A	529	GLU	N-CA-C	5.40	117.92	111.71
1	A	706	GLU	N-CA-C	5.38	117.57	111.11
1	A	143	ILE	N-CA-C	-5.35	107.26	112.29
1	B	293	MET	N-CA-C	5.35	119.74	112.04
1	A	260	ASN	N-CA-C	-5.28	106.69	113.02
1	A	657	SER	N-CA-C	5.24	118.03	109.59
1	A	108	ALA	N-CA-C	5.21	116.96	111.28
1	B	328	LYS	N-CA-C	5.20	113.74	108.75
1	B	637	GLY	N-CA-C	5.18	121.64	112.53
1	B	252	ASN	N-CA-C	-5.16	106.29	112.59
1	B	470	THR	N-CA-C	5.10	119.58	112.90
1	B	184	PRO	N-CA-C	5.07	120.43	113.84
1	A	522	GLU	N-CA-C	5.07	117.51	109.96

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	461	TYR	Sidechain
1	A	686	TYR	Sidechain
1	A	803	TYR	Sidechain
1	B	461	TYR	Sidechain

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	6341	0	6179	136	0
1	B	6341	0	6179	105	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	26	0	16	0	0
3	B	26	0	16	2	0
4	A	200	0	0	2	0
4	B	213	0	0	2	0
All	All	13149	0	12390	221	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 9.

All (221) 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:264:LEU:CD2	1:B:522:GLU:HG3	1.62	1.29
1:A:264:LEU:HD22	1:B:522:GLU:CG	1.64	1.27
1:A:264:LEU:HD22	1:B:522:GLU:CD	1.58	1.26
1:A:177:TYR:CG	1:A:192:VAL:HG11	1.90	1.06
1:A:192:VAL:HG22	4:B:897:HOH:O	1.59	1.02
1:A:264:LEU:HD22	1:B:522:GLU:HG3	1.24	1.02
1:B:800:SER:OG	1:B:843:VAL:HG23	1.64	0.97
1:A:264:LEU:CD2	1:B:522:GLU:CG	2.32	0.97
1:A:264:LEU:HD22	1:B:522:GLU:OE1	1.63	0.97
1:A:277:GLU:OE2	1:B:243:THR:HG21	1.64	0.95
1:A:326:LYS:HD2	1:A:391:ILE:HG23	1.50	0.93
1:A:352:THR:OG1	1:A:355:GLN:HG3	1.72	0.90
1:A:264:LEU:CD2	1:B:522:GLU:CD	2.44	0.89
1:A:177:TYR:CD2	1:A:192:VAL:HG11	2.09	0.87
1:A:264:LEU:HD23	1:A:265:ASP:OD1	1.77	0.85
1:B:417:VAL:O	1:B:420:ILE:HG22	1.74	0.85
1:B:776:MET:HA	1:B:776:MET:HE2	1.60	0.84
1:A:696:TYR:CD2	1:A:736:ARG:HD2	2.15	0.82
1:B:414:MET:O	1:B:434:GLU:HG3	1.80	0.82
1:A:192:VAL:CG2	4:B:897:HOH:O	2.22	0.80
1:A:192:VAL:HG23	1:B:639:GLN:OE1	1.82	0.80
1:A:177:TYR:CG	1:A:192:VAL:CG1	2.67	0.78
1:A:195:GLY:C	1:A:198:PRO:HD2	2.09	0.77
1:A:522:GLU:OE1	1:B:264:LEU:HD23	1.86	0.75
1:A:863:ASP:O	1:A:866:VAL:HG22	1.87	0.75
1:B:90:ILE:HG12	1:B:107:MET:HE3	1.69	0.75
1:B:418:ARG:O	1:B:421:ARG:HG3	1.87	0.75
1:A:719:ILE:HD12	1:A:742:ALA:HB1	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:VAL:HG23	1:B:779:PRO:HG3	1.68	0.74
1:A:264:LEU:HD23	1:B:522:GLU:HG3	1.68	0.73
1:B:90:ILE:HG23	1:B:107:MET:HE3	1.69	0.73
1:B:414:MET:HE3	1:B:434:GLU:HG2	1.70	0.73
1:B:309:LYS:HG3	1:B:343:GLU:HG3	1.70	0.73
1:B:415:ASP:C	1:B:417:VAL:H	1.97	0.73
1:A:130:GLU:HG2	1:A:131:GLN:OE1	1.89	0.73
1:A:286:GLY:O	1:A:382:LYS:HE3	1.89	0.72
1:A:524:ARG:HA	1:A:529:GLU:OE1	1.90	0.72
1:B:884:ARG:HG2	1:B:884:ARG:O	1.88	0.72
1:A:426:VAL:CG1	1:A:439:ILE:HD11	2.21	0.71
1:A:158:THR:OG1	1:A:160:GLU:HG2	1.92	0.69
1:A:195:GLY:O	1:A:198:PRO:HD2	1.92	0.69
1:B:309:LYS:HG3	1:B:343:GLU:CG	2.22	0.68
1:A:864:LYS:O	1:A:867:VAL:HG22	1.94	0.67
1:A:821:ARG:HG2	1:A:821:ARG:HH11	1.59	0.67
1:B:530:GLY:HA2	1:B:533:ARG:NH1	2.10	0.67
1:A:160:GLU:HG3	1:A:172:ASN:OD1	1.94	0.67
1:B:421:ARG:HG2	1:B:433:ILE:HD11	1.77	0.66
1:A:272:GLY:O	1:A:318:VAL:HG22	1.95	0.65
1:A:862:ILE:HD12	1:A:866:VAL:HG21	1.78	0.65
1:B:423:ARG:O	1:B:423:ARG:HD3	1.96	0.65
1:B:418:ARG:HB2	1:B:421:ARG:NH1	2.11	0.64
1:A:312:GLN:O	1:A:316:GLU:HG2	1.98	0.64
1:A:812:ARG:NH2	1:A:818:ASP:O	2.31	0.64
1:A:458:LEU:O	1:A:459:HIS:HB2	1.99	0.63
1:A:867:VAL:CG2	1:B:779:PRO:HG3	2.29	0.62
1:A:264:LEU:CD2	1:B:522:GLU:OE1	2.44	0.62
1:B:194:MET:HE1	3:B:887:TPP:S1	2.40	0.62
1:A:328:LYS:HG3	1:A:332:TYR:CD1	2.35	0.62
1:A:160:GLU:CD	1:A:172:ASN:OD1	2.43	0.62
1:A:862:ILE:HD12	1:A:866:VAL:CG2	2.30	0.61
1:A:160:GLU:HG2	1:A:161:GLN:N	2.16	0.60
1:B:352:THR:OG1	1:B:355:GLN:HG3	2.02	0.60
1:A:140:GLN:O	1:A:143:ILE:HG13	2.01	0.60
1:B:418:ARG:HB2	1:B:421:ARG:HH11	1.67	0.60
1:B:239:LYS:HA	1:B:242:ILE:HG23	1.82	0.60
1:B:239:LYS:O	1:B:242:ILE:HG12	2.02	0.59
1:A:854:GLY:O	1:A:858:LYS:HG3	2.03	0.59
1:A:519:ILE:HD12	1:A:523:ALA:HB2	1.83	0.59
1:A:765:ALA:O	1:A:769:GLN:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:GLU:OE1	1:B:747:LYS:HE3	2.03	0.58
1:B:414:MET:CE	1:B:434:GLU:HG2	2.33	0.58
1:B:396:MET:O	1:B:398:ASP:N	2.36	0.58
1:B:843:VAL:HG22	1:B:843:VAL:O	2.02	0.58
1:A:95:ARG:O	1:A:98:LYS:HD3	2.03	0.57
1:A:237:GLU:HG2	1:A:572:LEU:HD11	1.86	0.57
1:A:197:GLY:N	1:A:198:PRO:HD2	2.18	0.57
1:A:719:ILE:CD1	1:A:742:ALA:HB1	2.34	0.57
1:A:196:LEU:C	1:A:198:PRO:HD2	2.30	0.57
1:A:393:GLY:HA3	1:A:400:ALA:HB1	1.87	0.57
1:A:328:LYS:HE2	1:A:328:LYS:HA	1.87	0.56
1:A:304:LYS:HE3	1:A:347:LEU:CD2	2.35	0.56
1:A:56:ILE:HD13	1:A:276:ASN:HB3	1.87	0.56
1:B:65:VAL:HG23	1:B:66:GLU:CD	2.30	0.56
1:B:423:ARG:HD3	1:B:423:ARG:C	2.31	0.56
1:A:197:GLY:N	1:A:198:PRO:CD	2.69	0.56
1:A:305:ASP:OD1	1:A:347:LEU:HD11	2.05	0.56
1:A:343:GLU:O	1:A:347:LEU:HG	2.07	0.55
1:A:716:LEU:HD21	1:A:739:ARG:NH1	2.22	0.55
1:A:98:LYS:HG2	1:A:99:LYS:N	2.21	0.55
1:B:505:MET:HE2	1:B:674:LEU:HD22	1.89	0.55
4:A:1026:HOH:O	3:B:887:TPP:H2	2.06	0.55
1:A:736:ARG:HG3	4:A:961:HOH:O	2.06	0.54
1:A:195:GLY:O	1:A:198:PRO:HG2	2.08	0.54
1:A:734:ILE:O	1:A:734:ILE:HG22	2.06	0.54
1:A:160:GLU:CG	1:A:172:ASN:OD1	2.56	0.54
1:B:859:ARG:HH12	1:B:861:GLU:CD	2.16	0.53
1:B:627:THR:HB	1:B:633:LEU:HD22	1.90	0.53
1:A:264:LEU:HD13	1:B:522:GLU:OE1	2.08	0.53
1:B:90:ILE:HG12	1:B:107:MET:CE	2.38	0.53
1:A:195:GLY:O	1:A:198:PRO:CG	2.57	0.53
1:A:696:TYR:CG	1:A:736:ARG:HD2	2.43	0.52
1:A:195:GLY:O	1:A:198:PRO:CD	2.58	0.52
1:A:304:LYS:HE3	1:A:347:LEU:HD23	1.91	0.52
1:A:713:ILE:HB	1:A:764:LEU:HD11	1.90	0.52
1:B:210:TYR:CZ	1:B:214:ARG:HD3	2.45	0.52
1:A:95:ARG:O	1:A:98:LYS:CD	2.59	0.51
1:A:522:GLU:CD	1:B:264:LEU:HD23	2.36	0.51
1:B:90:ILE:HG22	1:B:91:MET:HE2	1.92	0.51
1:B:418:ARG:HD3	1:B:430:ASP:OD1	2.10	0.51
1:A:262:GLN:HA	1:A:267:PRO:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ILE:HG23	1:B:107:MET:CE	2.39	0.51
1:B:707:GLU:OE2	1:B:711:LYS:NZ	2.38	0.51
1:A:239:LYS:O	1:A:242:ILE:HG12	2.10	0.51
1:A:471:GLU:OE2	1:A:591:PRO:HD2	2.11	0.50
1:B:812:ARG:HD2	1:B:820:TYR:HD2	1.76	0.50
1:A:819:ASP:OD2	1:A:855:GLU:HG2	2.12	0.50
1:A:859:ARG:NH1	1:A:861:GLU:OE1	2.45	0.50
1:B:419:HIS:O	1:B:423:ARG:HB2	2.12	0.50
1:B:776:MET:HA	1:B:776:MET:CE	2.35	0.50
1:B:396:MET:HB2	1:B:400:ALA:HA	1.94	0.49
1:A:160:GLU:CG	1:A:161:GLN:N	2.75	0.49
1:B:140:GLN:O	1:B:141:GLY:C	2.54	0.49
1:B:239:LYS:HA	1:B:242:ILE:CG2	2.43	0.49
1:A:328:LYS:HG3	1:A:332:TYR:CE1	2.48	0.49
1:A:271:ASN:C	1:A:318:VAL:HG21	2.37	0.49
1:A:717:GLU:CD	1:A:739:ARG:HH21	2.21	0.49
1:A:195:GLY:C	1:A:198:PRO:CD	2.83	0.49
1:B:415:ASP:C	1:B:417:VAL:N	2.61	0.49
1:A:734:ILE:O	1:A:734:ILE:CG2	2.61	0.48
1:A:160:GLU:HG2	1:A:161:GLN:H	1.77	0.48
1:B:421:ARG:HD3	1:B:421:ARG:C	2.38	0.48
1:A:509:LYS:HA	1:A:512:LYS:HE3	1.96	0.48
1:B:260:ASN:O	1:B:261:LEU:HB2	2.11	0.48
1:A:320:GLY:O	1:A:324:THR:HG23	2.14	0.48
1:A:304:LYS:NZ	1:A:347:LEU:O	2.47	0.48
1:A:506:LEU:HD23	1:A:515:LEU:HD12	1.95	0.48
1:A:128:ARG:NH1	1:A:464:SER:OG	2.38	0.47
1:B:506:LEU:HD23	1:B:515:LEU:HD12	1.97	0.47
1:A:522:GLU:OE1	1:B:264:LEU:CD2	2.59	0.47
1:A:326:LYS:HB3	1:A:326:LYS:NZ	2.30	0.47
1:B:765:ALA:O	1:B:769:GLN:HG3	2.14	0.47
1:B:843:VAL:O	1:B:843:VAL:CG2	2.62	0.47
1:A:735:LEU:O	1:A:736:ARG:C	2.56	0.47
1:A:867:VAL:HG21	1:B:779:PRO:CB	2.45	0.46
1:A:532:PHE:CD1	1:A:537:ILE:HD11	2.50	0.46
1:A:634:ASN:HB2	1:A:832:ASP:O	2.16	0.46
1:A:627:THR:HB	1:A:633:LEU:HD22	1.97	0.46
1:B:312:GLN:O	1:B:316:GLU:HG2	2.16	0.46
1:A:426:VAL:HG13	1:A:439:ILE:HD11	1.98	0.46
1:A:508:ASN:O	1:A:512:LYS:HB3	2.15	0.46
1:B:506:LEU:CD2	1:B:515:LEU:HD12	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLN:HE21	1:A:361:ARG:HH22	1.62	0.45
1:A:538:TYR:CZ	1:A:540:PRO:HG3	2.52	0.45
1:A:210:TYR:CZ	1:A:214:ARG:HD3	2.51	0.45
1:B:144:SER:OG	1:B:145:PRO:HD3	2.15	0.45
1:B:168:GLU:CD	1:B:175:SER:HA	2.41	0.45
1:A:206:LYS:HD2	1:A:248:GLU:HG3	1.99	0.45
1:A:150:ARG:O	1:A:154:GLU:HG3	2.16	0.45
1:A:334:ARG:HA	1:A:338:PHE:HB2	1.99	0.45
1:A:638:LEU:C	1:A:638:LEU:HD23	2.42	0.44
1:B:429:SER:O	1:B:433:ILE:HG13	2.17	0.44
1:A:726:VAL:O	1:A:753:SER:HA	2.17	0.44
1:B:808:ALA:HB3	1:B:822:VAL:CG1	2.47	0.44
1:B:159:GLN:HG3	1:B:438:TYR:CD2	2.52	0.44
1:A:821:ARG:HG2	1:A:821:ARG:NH1	2.29	0.44
1:A:821:ARG:CD	1:B:772:GLU:OE2	2.66	0.44
1:B:441:PHE:CE1	1:B:447:GLU:HG2	2.52	0.44
1:B:79:ARG:HG2	1:B:79:ARG:HH11	1.82	0.44
1:B:198:PRO:HD3	1:B:228:LEU:HD22	2.00	0.44
1:B:859:ARG:NH1	1:B:861:GLU:CD	2.75	0.43
1:A:263:ARG:HG3	1:A:266:GLY:O	2.19	0.43
1:A:821:ARG:HD3	1:B:772:GLU:OE2	2.17	0.43
1:B:178:PRO:HA	1:B:187:TRP:CG	2.54	0.43
1:B:418:ARG:C	1:B:421:ARG:HG3	2.42	0.43
1:A:199:ILE:HD13	1:A:572:LEU:HD13	2.01	0.43
1:B:529:GLU:HG2	1:B:530:GLY:N	2.33	0.43
1:B:650:LEU:HD12	1:B:650:LEU:C	2.43	0.43
1:A:324:THR:O	1:A:328:LYS:HG2	2.18	0.43
1:A:177:TYR:HB3	1:A:178:PRO:CD	2.49	0.43
1:A:815:VAL:HG12	1:A:817:ALA:H	1.83	0.43
1:B:342:PRO:HD2	1:B:343:GLU:OE2	2.19	0.43
1:A:740:GLU:HG2	1:A:845:ALA:CB	2.49	0.43
1:A:80:ARG:HD2	1:A:447:GLU:OE2	2.18	0.42
1:A:650:LEU:C	1:A:650:LEU:HD12	2.44	0.42
1:B:530:GLY:HA2	1:B:533:ARG:HH12	1.81	0.42
1:B:418:ARG:HA	1:B:421:ARG:CG	2.49	0.42
1:A:302:LEU:HD22	1:A:311:ILE:HD11	2.02	0.42
1:A:143:ILE:C	1:A:143:ILE:HD12	2.45	0.42
1:A:264:LEU:HD21	1:B:522:GLU:CG	2.42	0.42
1:B:881:VAL:HG22	1:B:882:ASN:N	2.34	0.42
1:B:429:SER:C	1:B:431:ALA:H	2.26	0.42
1:A:329:ASP:OD1	1:A:331:ALA:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ASP:OD1	1:B:350:ASP:N	2.51	0.42
1:A:112:SER:HB3	1:A:392:LYS:HA	2.01	0.42
1:A:323:GLN:NE2	1:A:361:ARG:HH22	2.17	0.41
1:A:120:CYS:HB3	1:A:125:PHE:CZ	2.54	0.41
1:B:65:VAL:HG23	1:B:66:GLU:OE2	2.19	0.41
1:B:780:LEU:HD13	1:B:780:LEU:HA	1.84	0.41
1:A:844:ASP:OD1	1:A:844:ASP:C	2.64	0.41
1:A:90:ILE:HD13	1:A:420:ILE:HD13	2.01	0.41
1:B:74:ASN:O	1:B:78:GLU:HG3	2.21	0.41
1:B:399:ALA:O	1:B:400:ALA:C	2.64	0.41
1:B:567:GLU:HG3	1:B:574:ALA:HA	2.03	0.41
1:B:713:ILE:HB	1:B:764:LEU:HD11	2.02	0.41
1:B:80:ARG:NH1	1:B:447:GLU:OE2	2.54	0.41
1:B:87:TRP:CD2	1:B:426:VAL:HG11	2.56	0.41
1:B:143:ILE:HD12	1:B:143:ILE:C	2.46	0.41
1:B:203:TYR:HB2	1:B:576:CYS:HB3	2.03	0.41
1:B:690:THR:HG21	1:B:803:TYR:OH	2.20	0.41
1:B:807:PHE:O	1:B:810:GLN:HG2	2.20	0.41
1:A:304:LYS:HE3	1:A:347:LEU:HD22	2.02	0.40
1:A:177:TYR:CB	1:A:192:VAL:HG11	2.48	0.40
1:A:506:LEU:CD2	1:A:515:LEU:HD12	2.51	0.40
1:B:638:LEU:C	1:B:638:LEU:HD23	2.46	0.40
1:B:719:ILE:HD12	1:B:742:ALA:HB1	2.02	0.40
1:A:98:LYS:HG2	1:A:99:LYS:HG3	2.03	0.40
1:A:177:TYR:CD1	1:A:192:VAL:CG1	3.04	0.40
1:A:716:LEU:HD21	1:A:739:ARG:CZ	2.52	0.40
1:A:867:VAL:CG2	1:A:868:ALA:N	2.84	0.40
1:B:198:PRO:HD3	1:B:228:LEU:CD2	2.51	0.40
1:A:514:ARG:NH1	1:A:591:PRO:HG2	2.37	0.40

There are no symmetry-related clashes.

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	795/886 (90%)	765 (96%)	26 (3%)	4 (0%)	24	13
1	B	795/886 (90%)	765 (96%)	27 (3%)	3 (0%)	30	17
All	All	1590/1772 (90%)	1530 (96%)	53 (3%)	7 (0%)	30	17

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	LYS
1	A	397	GLY
1	A	398	ASP
1	B	397	GLY
1	B	415	ASP
1	A	736	ARG
1	B	521	ASP

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	665/735 (90%)	653 (98%)	12 (2%)	51	40
1	B	665/735 (90%)	648 (97%)	17 (3%)	40	25
All	All	1330/1470 (90%)	1301 (98%)	29 (2%)	45	32

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	SER
1	A	192	VAL
1	A	211	LEU
1	A	263	ARG
1	A	264	LEU
1	A	303	ARG
1	A	326	LYS
1	A	572	LEU
1	A	675	GLU

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Mol	Chain	Res	Type
1	A	780	LEU
1	A	867	VAL
1	A	885	LEU
1	B	211	LEU
1	B	243	THR
1	B	261	LEU
1	B	262	GLN
1	B	264	LEU
1	B	300	GLU
1	B	301	LEU
1	B	343	GLU
1	B	382	LYS
1	B	421	ARG
1	B	432	ASP
1	B	475	LEU
1	B	502	LEU
1	B	522	GLU
1	B	560	GLU
1	B	610	LEU
1	B	861	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	GLN
1	A	323	GLN
1	A	377	GLN
1	A	454	GLN
1	A	503	ASN
1	A	534	GLN
1	A	695	ASN
1	A	810	GLN
1	B	122	ASN
1	B	172	ASN
1	B	222	GLN
1	B	262	GLN
1	B	336	HIS
1	B	695	ASN

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 4 ligands modelled in this entry, 2 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
3	TPP	A	887	2	26,27,27	1.64	6 (23%)	38,40,40	0.91	1 (2%)
3	TPP	B	887	2	26,27,27	1.68	6 (23%)	38,40,40	0.87	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
3	TPP	A	887	2	-	1/17/17/17	0/2/2/2
3	TPP	B	887	2	-	2/17/17/17	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	887	TPP	C4'-N3'	4.45	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	887	TPP	C4'-N3'	4.23	1.40	1.35
3	B	887	TPP	C5'-C4'	3.51	1.48	1.42
3	A	887	TPP	C5'-C4'	3.49	1.48	1.42
3	B	887	TPP	C2'-N1'	3.32	1.39	1.34
3	B	887	TPP	C6'-N1'	2.94	1.40	1.34
3	A	887	TPP	C2'-N1'	2.57	1.38	1.34
3	A	887	TPP	C6'-N1'	2.52	1.39	1.34
3	B	887	TPP	C7'-N3	2.27	1.53	1.48
3	A	887	TPP	C7'-N3	2.16	1.53	1.48
3	A	887	TPP	PA-O3A	2.11	1.61	1.59
3	B	887	TPP	PA-O2A	-2.08	1.45	1.55

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	887	TPP	C6'-N1'-C2'	2.45	120.10	116.07
3	B	887	TPP	C6'-N1'-C2'	2.23	119.73	116.07

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	887	TPP	PA-O3A-PB-O2B
3	B	887	TPP	PA-O3A-PB-O2B
3	B	887	TPP	PA-O3A-PB-O3B

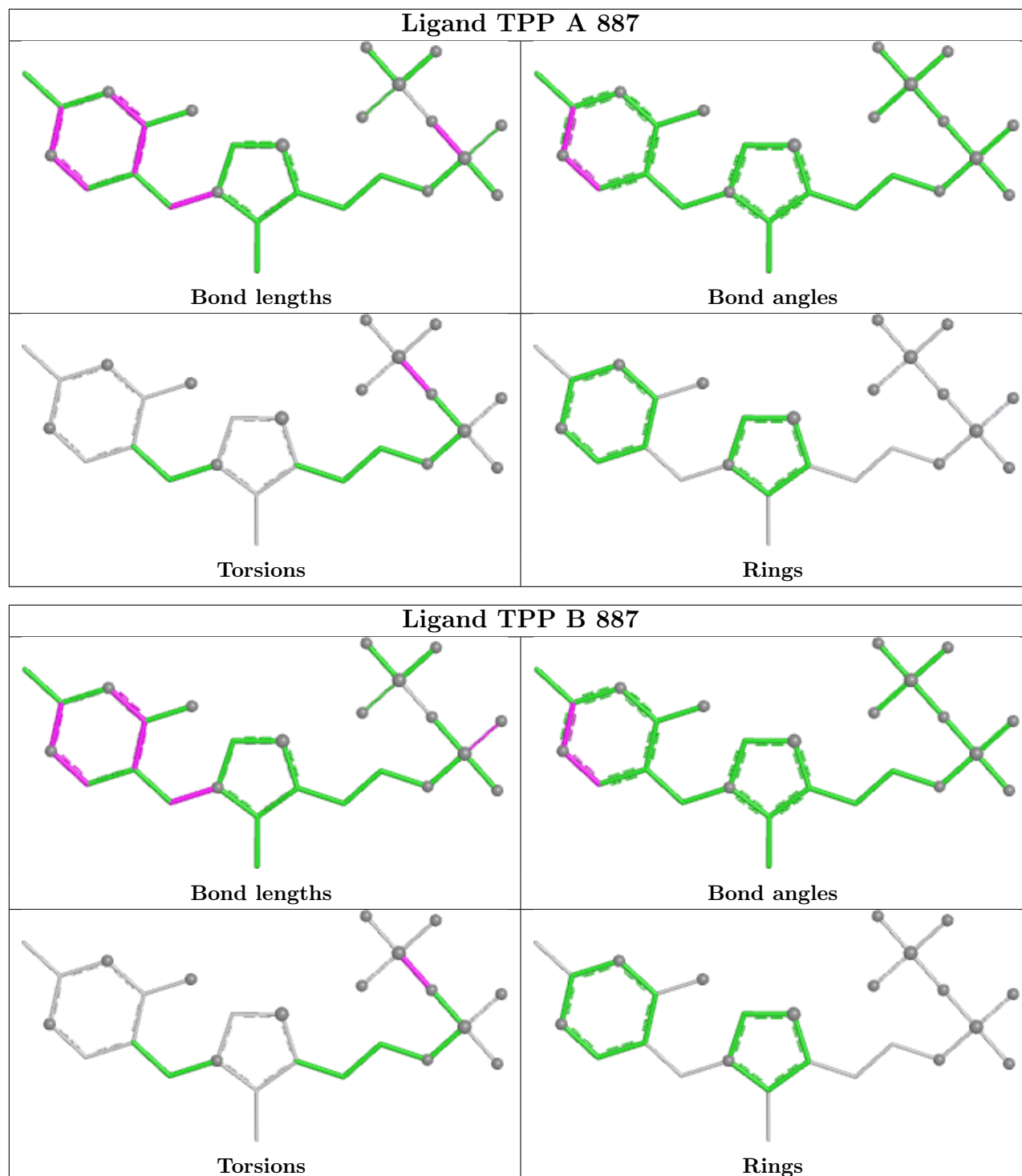
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	887	TPP	2	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 ⓘ

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	801/886 (90%)	0.38	68 (8%) 16 17	11, 20, 37, 41	0
1	B	801/886 (90%)	0.29	50 (6%) 26 29	10, 19, 31, 47	0
All	All	1602/1772 (90%)	0.34	118 (7%) 20 22	10, 19, 36, 47	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	399	ALA	15.5
1	A	400	ALA	9.1
1	B	400	ALA	9.1
1	A	399	ALA	7.3
1	B	414	MET	7.3
1	B	398	ASP	7.2
1	B	415	ASP	6.6
1	B	416	GLY	6.2
1	A	398	ASP	5.8
1	B	397	GLY	5.6
1	B	395	GLY	5.4
1	B	420	ILE	5.4
1	A	397	GLY	5.3
1	A	264	LEU	5.2
1	B	396	MET	5.2
1	B	394	TYR	4.7
1	B	417	VAL	4.7
1	B	56	ILE	4.5
1	B	393	GLY	4.5
1	B	428	VAL	4.4
1	A	351	TRP	4.4
1	A	333	VAL	4.3
1	A	860	GLY	4.0
1	B	431	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	436	LEU	4.0
1	A	349	ALA	3.9
1	B	172	ASN	3.9
1	A	533	ARG	3.8
1	B	426	VAL	3.8
1	A	341	TYR	3.7
1	A	414	MET	3.6
1	B	818	ASP	3.6
1	B	432	ASP	3.5
1	A	396	MET	3.5
1	A	418	ARG	3.4
1	A	305	ASP	3.3
1	B	433	ILE	3.2
1	B	427	PRO	3.2
1	B	533	ARG	3.2
1	B	532	PHE	3.2
1	A	192	VAL	3.2
1	B	425	ASN	3.2
1	B	424	PHE	3.2
1	A	867	VAL	3.1
1	A	350	ASP	3.1
1	A	301	LEU	3.1
1	A	866	VAL	3.1
1	B	430	ASP	3.0
1	A	130	GLU	3.0
1	B	530	GLY	2.9
1	B	110	PHE	2.9
1	A	330	GLY	2.9
1	B	107	MET	2.9
1	A	354	GLU	2.9
1	A	306	THR	2.9
1	A	160	GLU	2.9
1	A	393	GLY	2.8
1	A	56	ILE	2.7
1	B	76	GLU	2.7
1	B	434	GLU	2.7
1	A	348	VAL	2.7
1	A	395	GLY	2.6
1	A	329	ASP	2.6
1	A	262	GLN	2.6
1	B	303	ARG	2.5
1	A	311	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	524	ARG	2.5
1	A	326	LYS	2.5
1	A	338	PHE	2.5
1	A	736	ARG	2.5
1	A	479	GLN	2.5
1	B	522	GLU	2.5
1	B	418	ARG	2.5
1	A	345	ALA	2.5
1	A	327	SER	2.4
1	B	539	SER	2.4
1	A	663	ALA	2.4
1	A	524	ARG	2.4
1	B	169	VAL	2.4
1	A	352	THR	2.4
1	B	419	HIS	2.4
1	A	419	HIS	2.3
1	A	540	PRO	2.3
1	A	109	SER	2.3
1	B	109	SER	2.3
1	A	353	ASP	2.3
1	A	131	GLN	2.3
1	B	429	SER	2.3
1	A	680	GLU	2.3
1	A	336	HIS	2.3
1	B	106	HIS	2.3
1	A	356	ILE	2.3
1	A	346	ALA	2.2
1	A	707	GLU	2.2
1	A	855	GLU	2.2
1	B	300	GLU	2.2
1	B	242	ILE	2.2
1	A	340	LYS	2.2
1	A	198	PRO	2.2
1	A	265	ASP	2.2
1	A	300	GLU	2.2
1	A	558	GLU	2.2
1	B	422	ASP	2.2
1	A	303	ARG	2.2
1	A	325	PHE	2.1
1	A	425	ASN	2.1
1	A	863	ASP	2.1
1	A	347	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	141	GLY	2.1
1	A	337	PHE	2.1
1	A	76	GLU	2.1
1	A	324	THR	2.1
1	A	334	ARG	2.1
1	A	535	ILE	2.0
1	A	271	ASN	2.0
1	B	437	PRO	2.0
1	B	490	LYS	2.0
1	B	723	LYS	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](#)

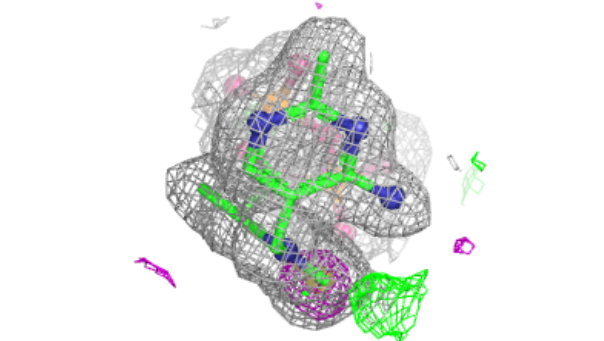
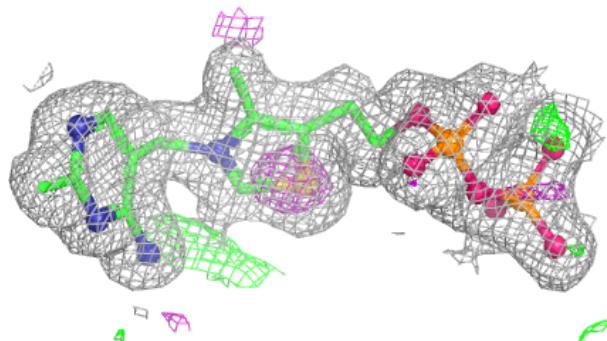
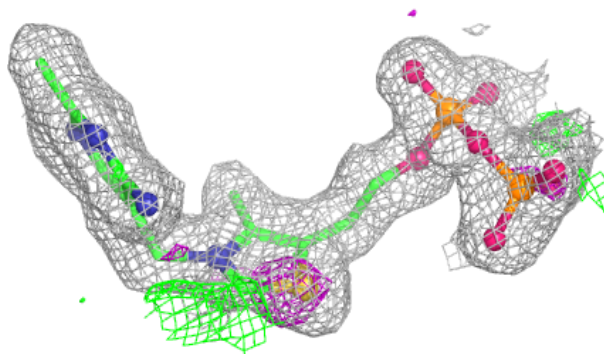
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	MG	A	888	1/1	0.92	0.06	19,19,19,19	0
2	MG	B	888	1/1	0.96	0.06	18,18,18,18	0
3	TPP	A	887	26/26	0.96	0.07	19,21,21,21	0
3	TPP	B	887	26/26	0.97	0.06	17,17,18,19	0

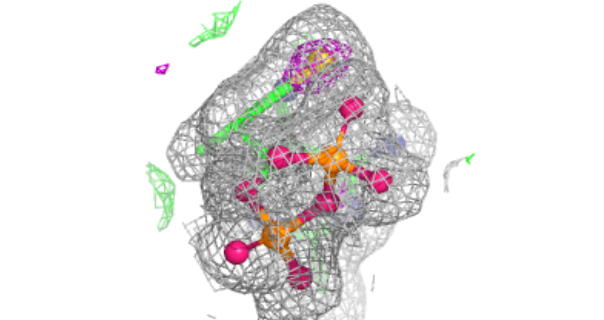
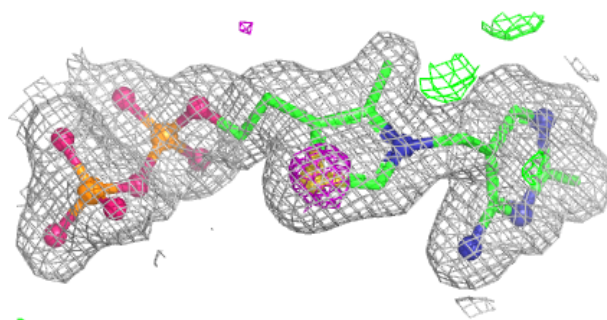
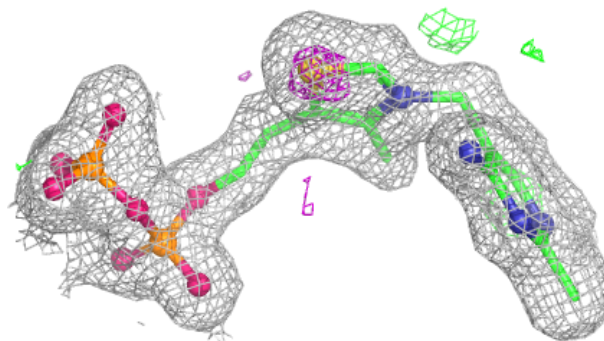
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 887:

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

**Electron density around TPP B 887:**

$2mF_o-DF_c$ (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.