



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:12 PM UTC

PDB ID : 6EFG / pdb_00006efg
Title : Pyruvate decarboxylase from Kluyveromyces lactis
Authors : Kutter, S.; Konig, S.
Deposited on : 2018-08-16
Resolution : 2.04 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

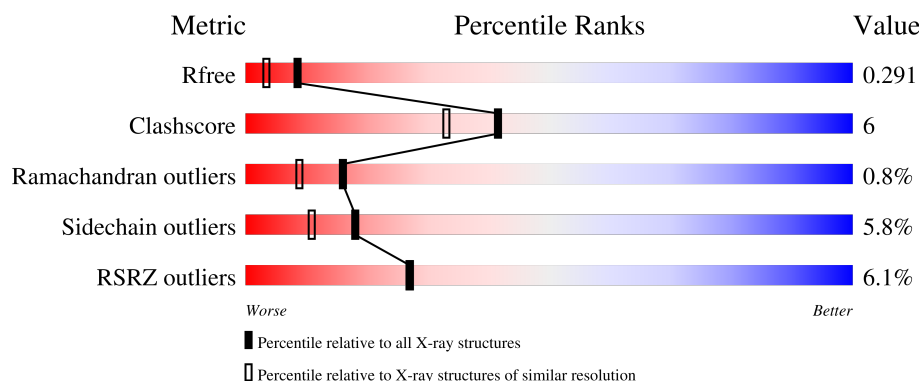
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	563	5% 77% 16% • 5%
1	B	563	7% 74% 19% • 6%
1	D	563	6% 76% 17% • 5%
1	E	563	5% 78% 16% • •

2 Entry composition [i](#)

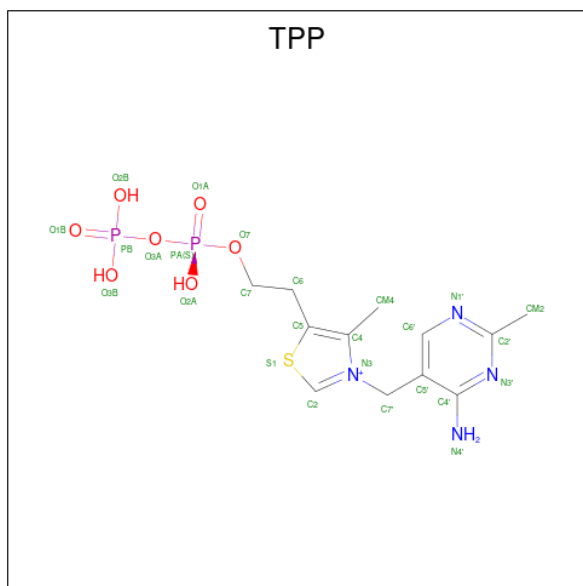
There are 4 unique types of molecules in this entry. The entry contains 16950 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	536	Total	C	N	O	S	0	0	0
			4137	2637	692	794	14			
1	B	532	Total	C	N	O	S	0	0	0
			4099	2609	685	791	14			
1	D	537	Total	C	N	O	S	0	1	0
			4144	2640	691	799	14			
1	E	538	Total	C	N	O	S	0	0	0
			4154	2649	694	797	14			

- Molecule 2 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	
2	E	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	

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

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

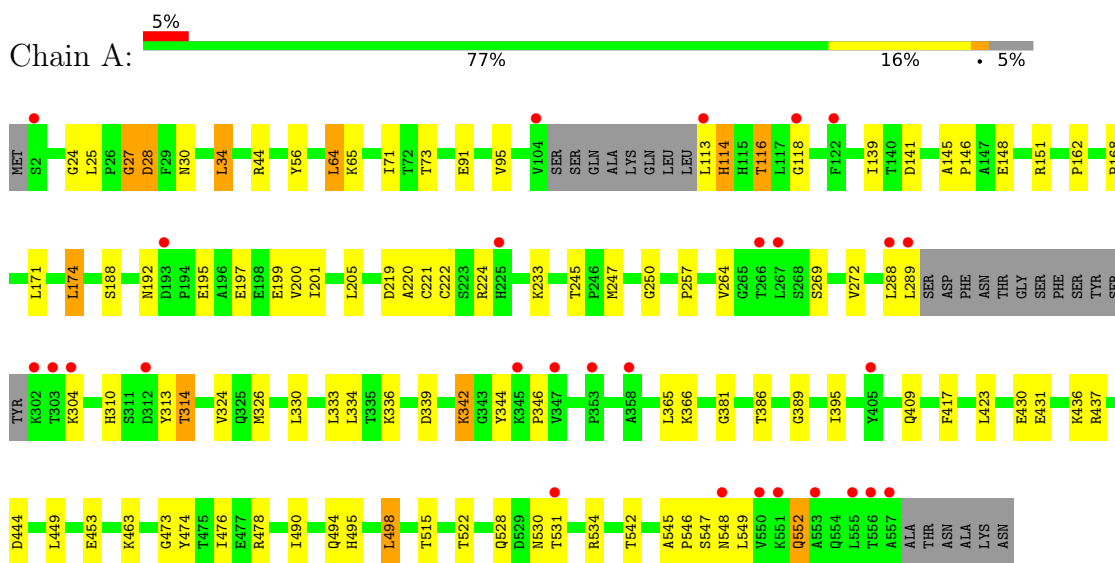
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O		
			75	75	0	0
4	B	78	Total	O		
			78	78	0	0
4	D	64	Total	O		
			64	64	0	0
4	E	91	Total	O		
			91	91	0	0

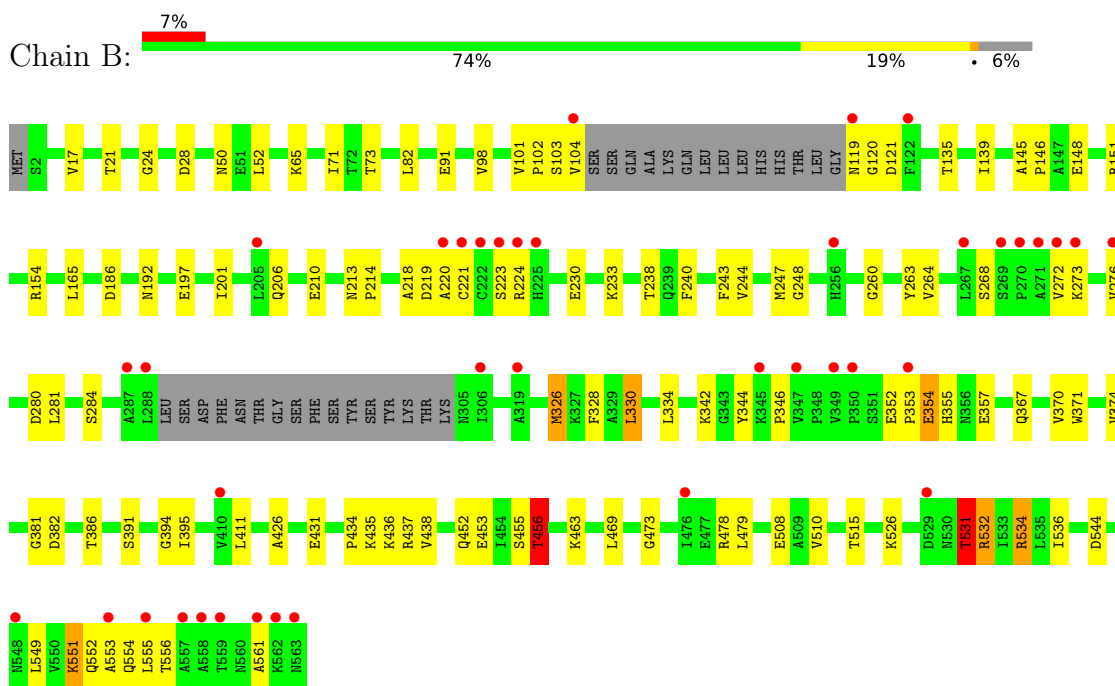
3 Residue-property plots [i](#)

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.

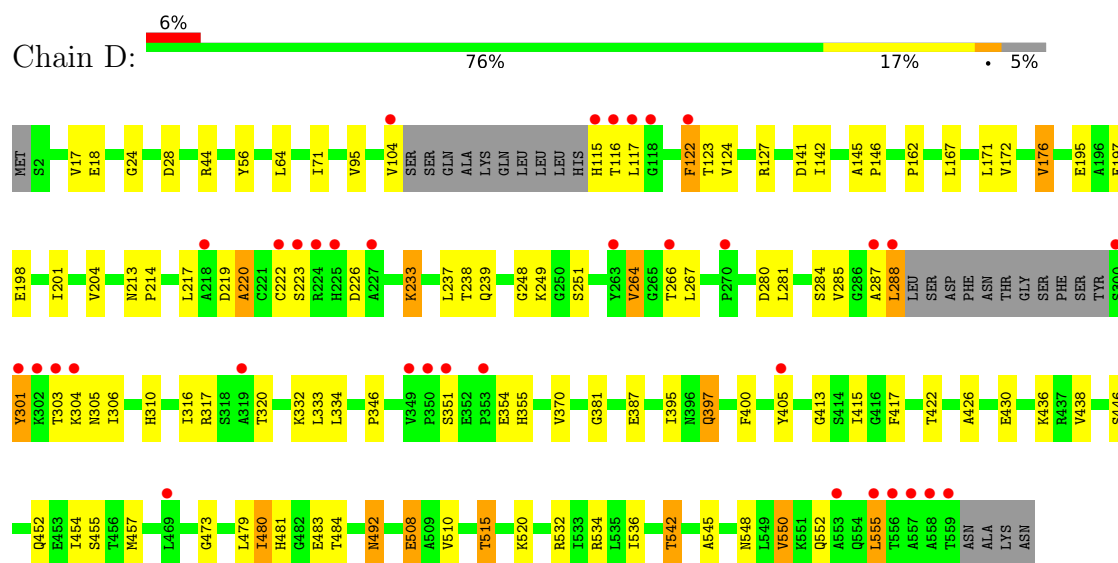
- Molecule 1: Pyruvate decarboxylase



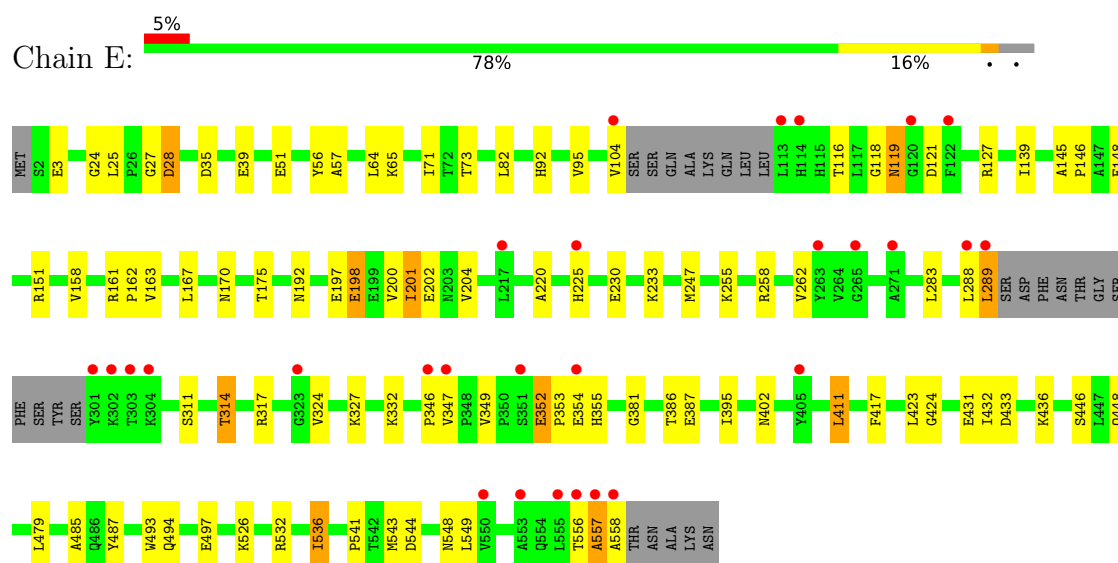
- Molecule 1: Pyruvate decarboxylase



● Molecule 1: Pyruvate decarboxylase



● Molecule 1: Pyruvate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.36Å 78.48Å 100.57Å 80.10° 67.72° 77.40°	Depositor
Resolution (Å)	38.25 – 2.04 38.25 – 2.04	Depositor EDS
% Data completeness (in resolution range)	93.2 (38.25-2.04) 93.2 (38.25-2.04)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.221 , 0.290 0.226 , 0.291	Depositor DCC
R_{free} test set	970 reflections (0.71%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16950	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.38% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.86	0/4223	1.11	6/5748 (0.1%)
1	B	0.85	2/4183 (0.0%)	1.09	4/5695 (0.1%)
1	D	0.86	2/4233 (0.0%)	1.09	2/5762 (0.0%)
1	E	0.90	1/4241 (0.0%)	1.10	1/5773 (0.0%)
All	All	0.87	5/16880 (0.0%)	1.09	13/22978 (0.1%)

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	2
1	B	0	2
1	D	0	1
1	E	0	4
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	163	VAL	N-CA	-6.23	1.38	1.46
1	D	473	GLY	C-O	-5.91	1.21	1.24
1	B	17	VAL	C-O	-5.51	1.17	1.24
1	D	542	THR	N-CA	-5.20	1.39	1.46
1	B	52	LEU	C-O	-5.13	1.18	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	456	THR	CB-CA-C	6.40	122.55	109.55
1	A	141	ASP	CA-CB-CG	6.16	118.76	112.60
1	A	444	ASP	CA-CB-CG	5.71	118.31	112.60
1	A	515	THR	CA-CB-OG1	-5.70	101.05	109.60
1	A	257	PRO	CB-CA-C	-5.53	104.00	111.85
1	E	28	ASP	CB-CA-C	5.41	121.18	110.42
1	B	21	THR	CA-CB-OG1	-5.38	101.53	109.60
1	D	422	THR	CA-CB-OG1	-5.20	101.80	109.60
1	D	515	THR	CA-CB-OG1	-5.20	101.80	109.60
1	B	531	THR	CB-CA-C	5.19	117.80	109.07
1	B	435	LYS	CB-CA-C	-5.14	102.59	110.81
1	A	250	GLY	CA-C-N	5.00	126.99	120.28
1	A	250	GLY	C-N-CA	5.00	126.99	120.28

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	GLY	Peptide
1	A	437	ARG	Sidechain
1	B	532	ARG	Sidechain
1	B	534	ARG	Sidechain
1	D	532	ARG	Sidechain
1	E	118	GLY	Peptide
1	E	27	GLY	Peptide
1	E	317	ARG	Sidechain
1	E	532	ARG	Sidechain

5.2 Too-close contacts [i](#)

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	4137	0	4125	51	0
1	B	4099	0	4077	58	0
1	D	4144	0	4127	61	0
1	E	4154	0	4139	48	0
2	A	26	0	16	1	0
2	B	26	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	26	0	16	2	0
2	E	26	0	16	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	75	0	0	5	0
4	B	78	0	0	2	0
4	D	64	0	0	1	0
4	E	91	0	0	1	0
All	All	16950	0	16532	213	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 6.

All (213) 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:D:287:ALA:O	1:D:288:LEU:HD22	1.70	0.91
1:E:104:VAL:HG22	1:E:170:ASN:HD21	1.41	0.86
4:D:747:HOH:O	1:E:494:GLN:HG3	1.77	0.83
1:D:545:ALA:HB3	1:D:550:VAL:HG23	1.60	0.82
1:B:342:LYS:NZ	4:B:701:HOH:O	2.10	0.82
1:A:548:ASN:HB2	4:A:730:HOH:O	1.82	0.79
1:D:280:ASP:O	1:D:305:ASN:ND2	2.17	0.77
1:A:28:ASP:OD1	4:A:701:HOH:O	2.02	0.77
1:A:339:ASP:O	1:A:342:LYS:HB2	1.88	0.74
1:B:453:GLU:OE2	1:B:456:THR:HG21	1.91	0.71
1:D:198:GLU:OE2	1:D:332:LYS:NZ	2.23	0.70
1:B:381:GLY:O	1:B:436:LYS:HG3	1.90	0.70
1:B:154:ARG:NH2	1:B:186:ASP:O	2.20	0.70
1:B:233:LYS:HG2	1:B:334:LEU:HD22	1.77	0.66
1:B:549:LEU:O	1:B:552:GLN:HB3	1.96	0.65
1:A:522:THR:O	1:A:528:GLN:NE2	2.22	0.64
1:E:494:GLN:HB3	1:E:497:GLU:HG2	1.81	0.63
1:A:549:LEU:O	1:A:552:GLN:HB3	1.99	0.63
1:B:326:MET:O	1:B:330:LEU:HB2	2.00	0.62
1:E:536:ILE:HD12	1:E:536:ILE:N	2.15	0.61
1:D:267:LEU:HD22	1:D:548:ASN:O	2.01	0.61
1:E:200:VAL:O	1:E:204:VAL:HG23	2.00	0.60
1:E:220:ALA:HB2	1:E:247:MET:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:255:LYS:HG2	1:E:402:ASN:OD1	2.02	0.59
1:D:492:ASN:OD1	1:D:492:ASN:N	2.36	0.59
1:A:494:GLN:HG3	4:A:729:HOH:O	2.03	0.58
1:B:370:VAL:O	1:B:374:VAL:HG23	2.03	0.58
1:D:481:HIS:NE2	1:E:35:ASP:OD2	2.24	0.58
1:B:220:ALA:HB2	1:B:247:MET:HB3	1.85	0.57
1:B:214:PRO:HA	1:B:281:LEU:O	2.05	0.57
1:E:381:GLY:O	1:E:436:LYS:NZ	2.33	0.57
1:E:121:ASP:OD2	1:E:127:ARG:NH2	2.37	0.56
1:A:30:ASN:O	1:A:34:LEU:HG	2.04	0.56
1:A:116:THR:HG22	1:A:118:GLY:H	1.70	0.56
1:D:213:ASN:N	1:D:280:ASP:OD1	2.39	0.56
1:B:453:GLU:OE2	1:B:456:THR:CG2	2.54	0.56
1:A:24:GLY:HA3	1:A:71:ILE:O	2.05	0.56
1:A:205:LEU:HD11	1:A:336:LYS:HB2	1.87	0.56
1:D:287:ALA:HB3	1:D:310:HIS:NE2	2.22	0.55
1:A:95:VAL:O	1:A:162:PRO:HA	2.06	0.55
1:B:426:ALA:HA	1:B:438:VAL:HG21	1.87	0.55
1:E:541:PRO:HB2	1:E:544:ASP:HB2	1.89	0.55
1:B:192:ASN:ND2	1:B:328:PHE:HB2	2.22	0.55
1:D:64:LEU:HD21	1:D:405:TYR:CD2	2.42	0.54
1:A:114:HIS:ND1	1:B:411:LEU:O	2.40	0.54
1:D:354:GLU:HG3	1:D:355:HIS:CE1	2.43	0.54
1:B:353:PRO:O	1:B:355:HIS:N	2.41	0.54
1:D:397:GLN:OE1	1:D:548:ASN:ND2	2.41	0.53
1:E:258:ARG:HH12	1:E:349:VAL:HG13	1.73	0.53
1:E:448:GLN:HA	1:E:493:TRP:CH2	2.43	0.53
1:B:243:PHE:CE2	1:B:260:GLY:HA3	2.43	0.53
1:E:148:GLU:OE1	1:E:151:ARG:NH2	2.36	0.53
1:A:145:ALA:HB3	1:A:146:PRO:HD3	1.89	0.53
1:B:148:GLU:OE1	1:B:151:ARG:NH2	2.39	0.53
1:D:267:LEU:HD21	1:D:552:GLN:HB2	1.91	0.53
1:B:148:GLU:CD	1:B:151:ARG:HH21	2.16	0.52
1:D:123:THR:OG1	1:D:127:ARG:NH1	2.42	0.52
1:A:64:LEU:N	1:A:64:LEU:HD23	2.25	0.52
1:D:214:PRO:HB3	1:D:281:LEU:HB3	1.90	0.52
1:E:145:ALA:HB3	1:E:146:PRO:HD3	1.91	0.52
1:A:381:GLY:O	1:A:436:LYS:HG3	2.10	0.52
1:D:95:VAL:O	1:D:162:PRO:HA	2.09	0.52
1:D:536:ILE:N	1:D:536:ILE:HD12	2.25	0.52
1:D:301:TYR:CD1	1:D:301:TYR:N	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:411:LEU:HD23	1:E:411:LEU:O	2.10	0.52
1:A:545:ALA:HB1	1:A:546:PRO:HD2	1.91	0.51
1:D:104:VAL:HG12	1:D:122:PHE:HE2	1.75	0.51
1:B:508:GLU:HB2	1:B:534:ARG:HG2	1.92	0.51
1:E:230:GLU:OE1	1:E:230:GLU:N	2.44	0.51
1:A:56:TYR:CD2	1:A:417:PHE:HA	2.45	0.51
1:D:266:THR:HG23	1:D:301:TYR:HE2	1.76	0.51
1:A:171:LEU:HD23	1:A:174:LEU:HD22	1.93	0.50
1:B:536:ILE:N	1:B:536:ILE:HD12	2.26	0.50
1:D:145:ALA:HB3	1:D:146:PRO:HD3	1.94	0.50
1:A:449:LEU:HA	1:B:50:ASN:HB3	1.94	0.50
1:B:456:THR:HB	4:B:735:HOH:O	2.12	0.50
1:D:249:LYS:HG2	1:D:400:PHE:CE2	2.47	0.49
1:E:200:VAL:HG21	1:E:324:VAL:HG11	1.94	0.49
1:A:344:TYR:CE2	1:A:346:PRO:HA	2.48	0.49
1:B:272:VAL:O	1:B:273:LYS:C	2.54	0.49
1:B:553:ALA:HA	1:B:556:THR:OG1	2.13	0.49
1:B:411:LEU:C	1:B:411:LEU:HD23	2.37	0.49
1:D:266:THR:HG23	1:D:301:TYR:CE2	2.47	0.48
1:B:382:ASP:OD1	1:B:437:ARG:HB2	2.14	0.48
1:A:44:ARG:NH2	1:A:430:GLU:OE1	2.45	0.48
1:A:473:GLY:HA2	1:A:490:ILE:HG12	1.94	0.48
1:B:139:ILE:CD1	1:B:165:LEU:HD11	2.43	0.48
1:D:219:ASP:CG	1:D:220:ALA:H	2.21	0.48
1:D:387:GLU:HG2	1:D:446:SER:CB	2.43	0.48
1:E:354:GLU:HB3	1:E:355:HIS:CD2	2.49	0.48
1:D:264:VAL:HG13	1:D:264:VAL:O	2.14	0.48
1:D:479:LEU:HD11	1:D:545:ALA:HB2	1.96	0.48
1:A:65:LYS:NZ	1:A:431:GLU:OE1	2.46	0.48
1:A:219:ASP:OD1	1:A:245:THR:HG21	2.13	0.48
1:B:551:LYS:HA	1:B:554:GLN:HG3	1.96	0.48
1:D:249:LYS:HE2	1:D:395:ILE:O	2.14	0.48
1:E:386:THR:HG21	1:E:395:ILE:HB	1.95	0.48
1:B:206:GLN:NE2	1:B:210:GLU:OE1	2.44	0.48
1:B:220:ALA:HA	1:B:248:GLY:HA2	1.96	0.47
1:B:473:GLY:HA3	1:B:478:ARG:HH12	1.79	0.47
1:E:411:LEU:HD23	1:E:411:LEU:C	2.39	0.47
1:A:494:GLN:CG	4:A:729:HOH:O	2.62	0.47
1:E:288:LEU:O	1:E:289:LEU:C	2.57	0.47
1:A:495:HIS:HA	1:A:498:LEU:HD22	1.96	0.47
1:E:56:TYR:CD2	1:E:417:PHE:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:GLU:O	1:B:201:ILE:HG12	2.15	0.47
1:E:201:ILE:N	1:E:201:ILE:HD13	2.30	0.47
1:D:117:LEU:HD22	1:D:124:VAL:HG11	1.96	0.46
1:E:352:GLU:O	1:E:353:PRO:C	2.57	0.46
1:B:354:GLU:HG3	1:B:355:HIS:CE1	2.51	0.46
1:D:64:LEU:CD2	1:D:405:TYR:CD2	2.98	0.46
1:A:463:LYS:HD3	1:A:531:THR:C	2.40	0.46
1:D:452:GLN:O	1:D:455:SER:HB3	2.16	0.46
1:E:479:LEU:HD12	1:E:543:MET:HE3	1.98	0.46
1:A:200:VAL:HG21	1:A:324:VAL:HG11	1.96	0.46
1:D:454:ILE:O	1:D:457:MET:HB2	2.15	0.46
1:E:119:ASN:OD1	1:E:119:ASN:N	2.48	0.46
1:D:284:SER:OG	1:D:287:ALA:HB2	2.14	0.46
1:E:3:GLU:HB3	1:E:175:THR:HB	1.96	0.46
1:A:44:ARG:NH1	1:A:430:GLU:OE1	2.47	0.46
1:D:219:ASP:OD2	1:D:288:LEU:N	2.49	0.46
1:B:139:ILE:HD12	1:B:165:LEU:HD11	1.98	0.46
1:B:552:GLN:O	1:B:556:THR:HG23	2.15	0.46
1:D:381:GLY:O	1:D:436:LYS:HE3	2.16	0.46
1:A:192:ASN:ND2	1:A:197:GLU:OE1	2.36	0.46
1:B:24:GLY:HA3	1:B:71:ILE:O	2.16	0.46
1:B:220:ALA:HB2	1:B:247:MET:CB	2.46	0.46
1:E:485:ALA:HB1	1:E:487:TYR:CE2	2.51	0.46
1:E:411:LEU:C	1:E:411:LEU:CD2	2.90	0.45
1:D:508:GLU:O	1:D:534:ARG:HA	2.16	0.45
1:D:64:LEU:HD23	1:D:405:TYR:CE2	2.51	0.45
1:E:258:ARG:NH1	1:E:349:VAL:HG13	2.30	0.45
1:D:44:ARG:NH2	1:D:430:GLU:OE1	2.46	0.45
1:B:531:THR:HG23	1:B:532:ARG:NH1	2.32	0.45
1:A:220:ALA:HB2	1:A:247:MET:HB3	1.99	0.45
1:A:474:TYR:HB3	2:A:600:TPP:H62	1.99	0.45
1:D:204:VAL:CG2	1:D:316:ILE:HD11	2.47	0.45
1:D:248:GLY:O	1:D:251[A]:SER:HB2	2.17	0.45
1:A:91:GLU:OE1	1:A:409:GLN:HA	2.17	0.44
1:A:310:HIS:O	1:A:326:MET:HB3	2.16	0.44
1:B:353:PRO:O	1:B:354:GLU:C	2.60	0.44
1:D:222:CYS:SG	1:D:285:VAL:HG12	2.57	0.44
1:A:195:GLU:O	1:A:199:GLU:HG3	2.17	0.44
1:D:233:LYS:HG2	1:D:334:LEU:HD13	1.99	0.44
1:E:432:ILE:O	1:E:433:ASP:HB2	2.17	0.44
1:B:371:TRP:CZ2	1:B:391:SER:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:GLY:HA3	1:D:71:ILE:O	2.17	0.44
1:D:233:LYS:O	1:D:237:LEU:HG	2.18	0.44
1:D:305:ASN:OD1	1:D:317:ARG:NH2	2.51	0.44
1:B:71:ILE:HA	1:B:98:VAL:O	2.17	0.44
1:D:480:ILE:O	1:D:481:HIS:HB2	2.18	0.44
1:A:148:GLU:CD	1:A:151:ARG:HH21	2.25	0.44
1:B:344:TYR:CE2	1:B:346:PRO:HA	2.52	0.44
1:E:39:GLU:HG3	4:E:748:HOH:O	2.18	0.44
1:A:365:LEU:O	1:A:366:LYS:HD3	2.18	0.43
1:B:91:GLU:CD	1:B:247:MET:HE1	2.43	0.43
1:D:142:ILE:HD11	1:D:176:VAL:HG12	2.00	0.43
1:E:24:GLY:HA3	1:E:71:ILE:O	2.18	0.43
1:B:352:GLU:O	1:B:354:GLU:N	2.50	0.43
1:B:561:ALA:HA	1:D:320:THR:O	2.18	0.43
1:D:17:VAL:O	1:D:18:GLU:HB2	2.18	0.43
1:E:192:ASN:ND2	1:E:197:GLU:OE1	2.36	0.43
1:E:557:ALA:O	1:E:558:ALA:C	2.61	0.43
1:B:65:LYS:NZ	1:B:431:GLU:OE1	2.50	0.43
1:A:221:CYS:HA	1:A:224:ARG:HG3	2.01	0.43
1:A:474:TYR:O	1:A:478:ARG:HG3	2.18	0.43
1:B:213:ASN:N	1:B:280:ASP:OD1	2.48	0.43
1:D:223:SER:N	1:D:251[A]:SER:OG	2.52	0.43
1:E:95:VAL:O	1:E:162:PRO:HA	2.19	0.43
1:D:238:THR:O	1:D:239:GLN:HB2	2.19	0.43
1:D:197:GLU:O	1:D:201:ILE:HG12	2.18	0.43
2:D:600:TPP:N1'	1:E:51:GLU:OE2	2.52	0.42
1:E:387:GLU:HG2	1:E:446:SER:CB	2.49	0.42
1:A:314:THR:HG22	1:A:324:VAL:O	2.19	0.42
1:A:269:SER:OG	1:A:272:VAL:HG23	2.19	0.42
1:A:27:GLY:O	1:A:28:ASP:C	2.62	0.42
1:B:101:VAL:HB	1:B:102:PRO:CD	2.50	0.42
1:D:167:LEU:HG	1:D:172:VAL:HG12	2.02	0.42
1:D:288:LEU:HD13	1:D:288:LEU:HA	1.91	0.42
1:E:148:GLU:OE2	1:E:148:GLU:HA	2.20	0.42
1:D:56:TYR:CD2	1:D:417:PHE:HA	2.55	0.42
1:E:386:THR:HG21	1:E:395:ILE:CB	2.50	0.42
1:A:310:HIS:CE1	1:A:313:TYR:OH	2.73	0.42
1:A:531:THR:HG22	1:A:534:ARG:HH22	1.85	0.42
1:D:415:ILE:HB	1:D:446:SER:OG	2.19	0.42
1:A:330:LEU:O	1:A:334:LEU:HG	2.19	0.42
1:A:139:ILE:O	1:A:168:PRO:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLY:HA3	1:A:478:ARG:HH12	1.85	0.41
1:E:289:LEU:HD22	1:E:289:LEU:H	1.84	0.41
1:E:314:THR:HG22	1:E:324:VAL:O	2.20	0.41
1:E:65:LYS:NZ	1:E:431:GLU:OE1	2.47	0.41
1:B:218:ALA:HB3	1:B:244:VAL:HG12	2.03	0.41
1:B:238:THR:HB	1:B:240:PHE:CG	2.55	0.41
1:B:551:LYS:O	1:B:554:GLN:HB2	2.20	0.41
1:D:415:ILE:HG12	2:D:600:TPP:C4'	2.50	0.41
1:B:452:GLN:O	1:B:455:SER:HB3	2.20	0.41
1:E:57:ALA:O	1:E:424:GLY:HA3	2.20	0.41
1:B:386:THR:HG21	1:B:395:ILE:HB	2.03	0.41
1:D:426:ALA:HA	1:D:438:VAL:HG21	2.03	0.41
1:A:386:THR:HG21	1:A:395:ILE:HB	2.03	0.41
1:B:411:LEU:O	1:B:411:LEU:HD23	2.21	0.41
1:A:423:LEU:HD22	1:A:453:GLU:HG3	2.04	0.40
1:A:548:ASN:CB	4:A:730:HOH:O	2.54	0.40
1:B:367:GLN:N	1:B:544:ASP:OD2	2.44	0.40
1:A:389:GLY:HA2	1:A:476:ILE:HG21	2.02	0.40
1:B:263:TYR:CD1	1:B:276:VAL:HG21	2.57	0.40
1:E:198:GLU:OE1	1:E:202:GLU:OE1	2.40	0.40
1:B:145:ALA:HB3	1:B:146:PRO:HD3	2.03	0.40
1:D:116:THR:HA	1:E:411:LEU:CD2	2.51	0.40
1:D:483:GLU:HG2	1:D:484:THR:HG23	2.04	0.40
1:B:371:TRP:CE2	1:B:394:GLY:HA3	2.57	0.40
1:D:204:VAL:HG22	1:D:316:ILE:HD11	2.03	0.40
1:E:92:HIS:NE2	1:E:161:ARG:NH1	2.70	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	530/563 (94%)	508 (96%)	19 (4%)	3 (1%)	21	13
1	B	526/563 (93%)	494 (94%)	28 (5%)	4 (1%)	16	9
1	D	532/563 (94%)	499 (94%)	27 (5%)	6 (1%)	11	5
1	E	532/563 (94%)	505 (95%)	23 (4%)	4 (1%)	16	9
All	All	2120/2252 (94%)	2006 (95%)	97 (5%)	17 (1%)	16	9

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	E	28	ASP
1	A	114	HIS
1	A	552	GLN
1	B	121	ASP
1	B	354	GLU
1	D	346	PRO
1	E	346	PRO
1	E	556	THR
1	D	226	ASP
1	E	557	ALA
1	B	120	GLY
1	D	220	ALA
1	D	555	LEU
1	B	103	SER
1	D	264	VAL
1	D	413	GLY

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	451/474 (95%)	429 (95%)	22 (5%)	22	15
1	B	446/474 (94%)	418 (94%)	28 (6%)	16	9
1	D	452/474 (95%)	425 (94%)	27 (6%)	17	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	452/474 (95%)	424 (94%)	28 (6%)	16 9
All	All	1801/1896 (95%)	1696 (94%)	105 (6%)	18 11

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	34	LEU
1	A	64	LEU
1	A	73	THR
1	A	113	LEU
1	A	116	THR
1	A	174	LEU
1	A	188	SER
1	A	201	ILE
1	A	222	CYS
1	A	233	LYS
1	A	264	VAL
1	A	288	LEU
1	A	289	LEU
1	A	304	LYS
1	A	314	THR
1	A	333	LEU
1	A	342	LYS
1	A	498	LEU
1	A	530	ASN
1	A	542	THR
1	A	547	SER
1	B	28	ASP
1	B	73	THR
1	B	82	LEU
1	B	104	VAL
1	B	119	ASN
1	B	135	THR
1	B	219	ASP
1	B	221	CYS
1	B	223	SER
1	B	224	ARG
1	B	230	GLU
1	B	264	VAL
1	B	268	SER
1	B	284	SER

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Mol	Chain	Res	Type
1	B	326	MET
1	B	330	LEU
1	B	357	GLU
1	B	434	PRO
1	B	456	THR
1	B	463	LYS
1	B	469	LEU
1	B	479	LEU
1	B	510	VAL
1	B	515	THR
1	B	526	LYS
1	B	531	THR
1	B	551	LYS
1	B	555	LEU
1	D	28	ASP
1	D	115	HIS
1	D	122	PHE
1	D	141	ASP
1	D	171	LEU
1	D	176	VAL
1	D	195	GLU
1	D	217	LEU
1	D	233	LYS
1	D	288	LEU
1	D	301	TYR
1	D	303	THR
1	D	304	LYS
1	D	306	ILE
1	D	333	LEU
1	D	351	SER
1	D	370	VAL
1	D	397	GLN
1	D	480	ILE
1	D	492	ASN
1	D	508	GLU
1	D	510	VAL
1	D	515	THR
1	D	520	LYS
1	D	542	THR
1	D	550	VAL
1	D	555	LEU
1	E	25	LEU

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Mol	Chain	Res	Type
1	E	64	LEU
1	E	73	THR
1	E	82	LEU
1	E	116	THR
1	E	119	ASN
1	E	139	ILE
1	E	158	VAL
1	E	167	LEU
1	E	198	GLU
1	E	201	ILE
1	E	225	HIS
1	E	233	LYS
1	E	262	VAL
1	E	283	LEU
1	E	289	LEU
1	E	311	SER
1	E	314	THR
1	E	327	LYS
1	E	332	LYS
1	E	347	VAL
1	E	352	GLU
1	E	411	LEU
1	E	423	LEU
1	E	526	LYS
1	E	536	ILE
1	E	548	ASN
1	E	549	LEU

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	83	ASN
1	A	203	ASN
1	A	325	GLN
1	A	530	ASN
1	A	552	GLN
1	B	20	GLN
1	B	119	ASN
1	D	239	GLN
1	E	213	ASN
1	E	325	GLN
1	E	492	ASN

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Mol	Chain	Res	Type
1	E	548	ASN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	B	600	3	26,27,27	1.70	5 (19%)	38,40,40	1.87	12 (31%)
2	TPP	E	600	3	26,27,27	1.76	6 (23%)	38,40,40	2.44	13 (34%)
2	TPP	A	600	3	26,27,27	1.60	4 (15%)	38,40,40	1.57	9 (23%)
2	TPP	D	600	3	26,27,27	1.81	4 (15%)	38,40,40	2.18	15 (39%)

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	B	600	3	-	3/17/17/17	0/2/2/2
2	TPP	E	600	3	-	2/17/17/17	0/2/2/2
2	TPP	A	600	3	-	1/17/17/17	0/2/2/2
2	TPP	D	600	3	-	2/17/17/17	0/2/2/2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	TPP	C5-C4	6.09	1.48	1.35
2	E	600	TPP	C5-C4	5.43	1.46	1.35
2	B	600	TPP	C5-C4	4.68	1.45	1.35
2	A	600	TPP	C5-C4	4.66	1.45	1.35
2	B	600	TPP	C5'-C4'	3.80	1.49	1.42
2	B	600	TPP	PA-O3A	3.64	1.63	1.59
2	E	600	TPP	C2'-N1'	3.64	1.39	1.34
2	D	600	TPP	C5'-C4'	3.37	1.48	1.42
2	A	600	TPP	C5'-C4'	3.27	1.48	1.42
2	A	600	TPP	PA-O3A	3.04	1.62	1.59
2	D	600	TPP	PA-O3A	2.84	1.62	1.59
2	E	600	TPP	C2-N3	2.59	1.38	1.32
2	E	600	TPP	C5'-C4'	2.57	1.47	1.42
2	E	600	TPP	C2-S1	2.52	1.76	1.69
2	A	600	TPP	C2-S1	2.52	1.76	1.69
2	D	600	TPP	C2-S1	2.24	1.76	1.69
2	E	600	TPP	C4-N3	-2.17	1.35	1.39
2	B	600	TPP	C2'-N1'	2.11	1.37	1.34
2	B	600	TPP	C6'-C5'	2.02	1.41	1.37

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	600	TPP	CM2-C2'-N1'	7.87	125.58	117.20
2	E	600	TPP	C2-S1-C5	-5.80	87.37	91.22
2	D	600	TPP	CM2-C2'-N1'	5.66	123.23	117.20
2	D	600	TPP	C2-S1-C5	-4.26	88.40	91.22
2	B	600	TPP	C2-S1-C5	-4.16	88.46	91.22
2	B	600	TPP	CM4-C4-N3	3.98	129.75	120.57
2	E	600	TPP	S1-C2-N3	3.95	117.29	112.30
2	E	600	TPP	C2-N3-C4	-3.93	108.75	114.06
2	B	600	TPP	CM4-C4-C5	-3.93	117.68	127.75
2	E	600	TPP	C6'-N1'-C2'	3.63	122.03	116.07
2	D	600	TPP	S1-C2-N3	3.62	116.88	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	TPP	C2-S1-C5	-3.52	88.88	91.22
2	D	600	TPP	N1'-C2'-N3'	-3.50	119.70	125.53
2	B	600	TPP	C6'-N1'-C2'	3.48	121.78	116.07
2	D	600	TPP	O2A-PA-O3A	3.42	116.51	107.27
2	D	600	TPP	C6-C5-S1	-3.35	113.07	120.90
2	D	600	TPP	O3B-PB-O2B	3.18	119.74	107.80
2	D	600	TPP	C2-N3-C4	-3.02	109.97	114.06
2	A	600	TPP	S1-C2-N3	3.01	116.11	112.30
2	D	600	TPP	C2'-N3'-C4'	3.00	122.72	118.10
2	D	600	TPP	O3A-PA-O1A	-2.97	101.76	110.70
2	A	600	TPP	C6'-N1'-C2'	2.97	120.95	116.07
2	B	600	TPP	S1-C2-N3	2.91	115.98	112.30
2	E	600	TPP	N1'-C2'-N3'	-2.90	120.70	125.53
2	E	600	TPP	O3A-PB-O1B	-2.89	95.85	111.04
2	A	600	TPP	C2-N3-C4	-2.87	110.18	114.06
2	A	600	TPP	CM4-C4-C5	-2.86	120.42	127.75
2	E	600	TPP	C7'-C5'-C4'	-2.83	117.20	122.36
2	D	600	TPP	C6'-N1'-C2'	2.82	120.70	116.07
2	E	600	TPP	C5'-C6'-N1'	-2.77	119.33	123.83
2	E	600	TPP	C7'-C5'-C6'	2.73	125.83	120.69
2	D	600	TPP	C6-C5-C4	2.70	134.95	128.17
2	B	600	TPP	O3B-PB-O2B	2.66	117.78	107.80
2	A	600	TPP	CM2-C2'-N1'	2.63	120.00	117.20
2	B	600	TPP	O3A-PA-O1A	2.59	118.50	110.70
2	D	600	TPP	C7'-C5'-C6'	2.57	125.53	120.69
2	B	600	TPP	N1'-C2'-N3'	-2.46	121.44	125.53
2	E	600	TPP	CM4-C4-C5	-2.39	121.63	127.75
2	A	600	TPP	N1'-C2'-N3'	-2.33	121.66	125.53
2	B	600	TPP	N4'-C4'-N3'	2.32	120.16	117.03
2	B	600	TPP	CM2-C2'-N3'	2.31	120.58	117.13
2	B	600	TPP	C2-N3-C4	-2.30	110.96	114.06
2	E	600	TPP	CM2-C2'-N3'	-2.27	113.72	117.13
2	D	600	TPP	CM4-C4-C5	-2.23	122.03	127.75
2	B	600	TPP	C5'-C6'-N1'	-2.23	120.21	123.83
2	A	600	TPP	C5'-C6'-N1'	-2.12	120.38	123.83
2	E	600	TPP	O3B-PB-O1B	2.05	118.84	110.83
2	D	600	TPP	CM4-C4-N3	2.04	125.27	120.57
2	A	600	TPP	C2'-N3'-C4'	2.02	121.20	118.10

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	600	TPP	PA-O3A-PB-O3B
2	E	600	TPP	PA-O3A-PB-O3B
2	B	600	TPP	PA-O3A-PB-O1B
2	A	600	TPP	PA-O3A-PB-O3B
2	E	600	TPP	PA-O3A-PB-O1B
2	B	600	TPP	PA-O3A-PB-O2B
2	B	600	TPP	PA-O3A-PB-O3B
2	D	600	TPP	PA-O3A-PB-O2B

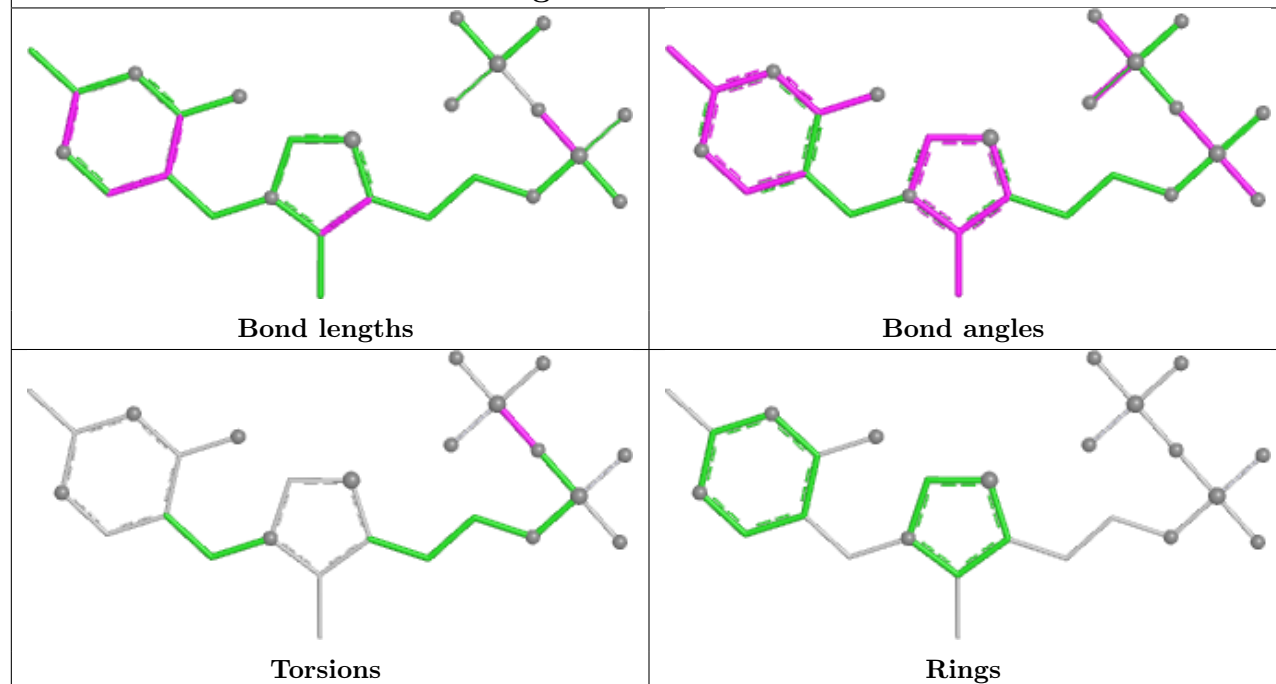
There are no ring outliers.

2 monomers are involved in 3 short contacts:

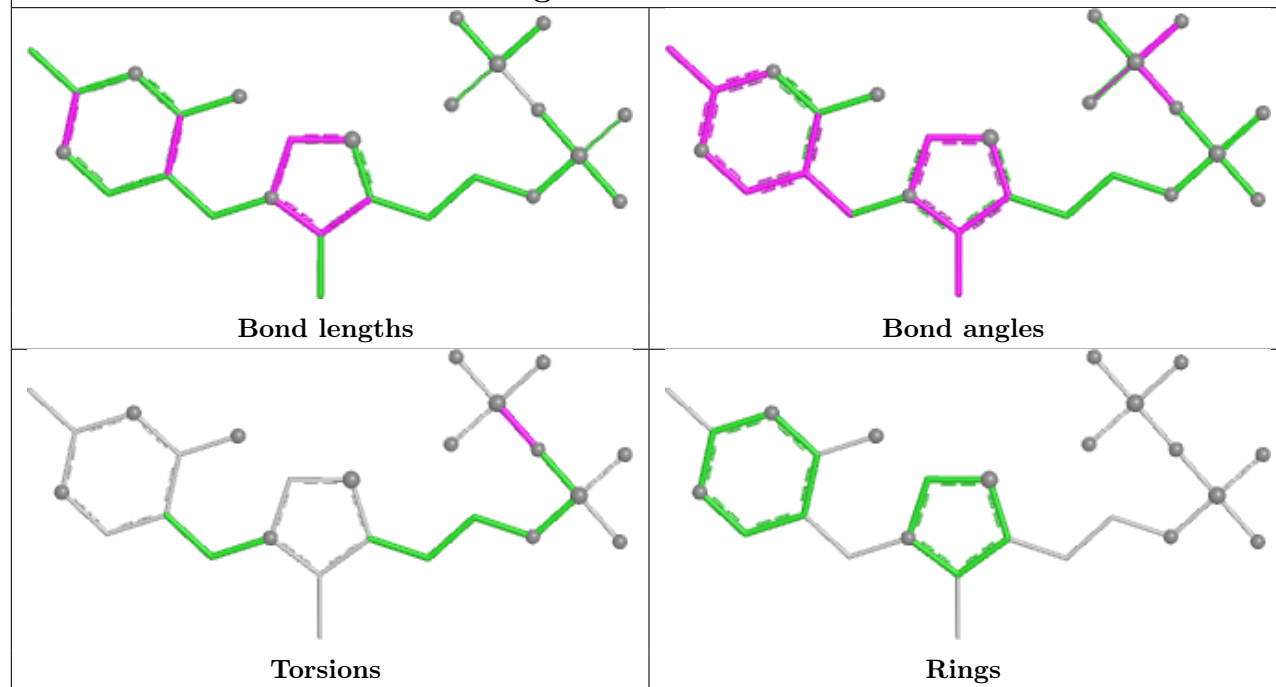
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	TPP	1	0
2	D	600	TPP	2	0

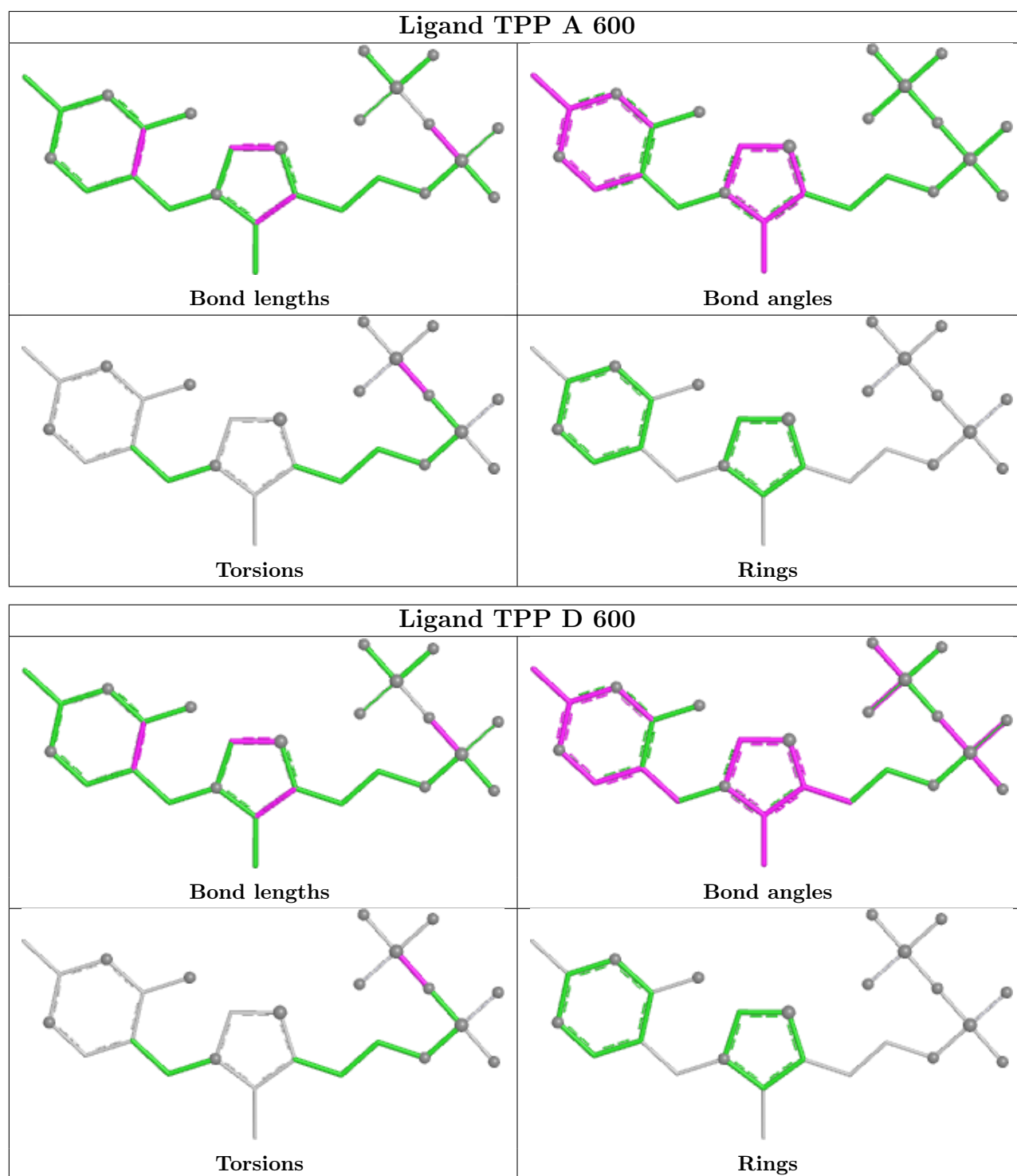
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand TPP B 600



Ligand TPP E 600





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	536/563 (95%)	0.40	28 (5%)	33 33	20, 35, 65, 102	0
1	B	532/563 (94%)	0.52	39 (7%)	21 21	21, 37, 77, 110	0
1	D	537/563 (95%)	0.50	35 (6%)	25 24	21, 37, 74, 122	1 (0%)
1	E	538/563 (95%)	0.33	28 (5%)	33 33	20, 33, 63, 95	0
All	All	2143/2252 (95%)	0.44	130 (6%)	27 27	20, 35, 68, 122	1 (0%)

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	113	LEU	5.6
1	B	557	ALA	5.6
1	D	288	LEU	5.0
1	B	288	LEU	4.9
1	B	225	HIS	4.9
1	D	557	ALA	4.8
1	D	104	VAL	4.8
1	B	353	PRO	4.7
1	E	555	LEU	4.6
1	E	347	VAL	4.5
1	E	558	ALA	4.4
1	A	113	LEU	4.4
1	D	303	THR	4.3
1	B	104	VAL	4.2
1	D	116	THR	4.2
1	D	224	ARG	4.1
1	D	118	GLY	4.0
1	A	555	LEU	3.9
1	B	561	ALA	3.9
1	D	223	SER	3.9
1	B	555	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	555	LEU	3.8
1	D	301	TYR	3.8
1	A	289	LEU	3.7
1	D	558	ALA	3.6
1	B	287	ALA	3.6
1	E	289	LEU	3.6
1	A	104	VAL	3.5
1	A	225	HIS	3.5
1	D	115	HIS	3.5
1	E	304	LYS	3.4
1	A	557	ALA	3.4
1	B	548	ASN	3.4
1	D	353	PRO	3.4
1	A	303	THR	3.3
1	D	287	ALA	3.3
1	E	557	ALA	3.3
1	A	122	PHE	3.3
1	B	563	ASN	3.3
1	D	122	PHE	3.3
1	B	559	THR	3.2
1	D	222	CYS	3.2
1	B	319	ALA	3.2
1	E	553	ALA	3.2
1	B	122	PHE	3.2
1	E	346	PRO	3.2
1	B	558	ALA	3.1
1	E	271	ALA	3.1
1	B	270	PRO	3.0
1	E	302	LYS	3.0
1	B	349	VAL	3.0
1	A	347	VAL	3.0
1	D	270	PRO	3.0
1	D	227	ALA	2.9
1	D	225	HIS	2.9
1	E	303	THR	2.9
1	A	550	VAL	2.8
1	A	345	LYS	2.7
1	D	319	ALA	2.7
1	D	349	VAL	2.7
1	B	222	CYS	2.7
1	D	351	SER	2.7
1	A	553	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	405	TYR	2.7
1	A	193	ASP	2.7
1	A	288	LEU	2.7
1	E	556	THR	2.6
1	E	114	HIS	2.6
1	B	224	ARG	2.6
1	E	263	TYR	2.6
1	E	301	TYR	2.6
1	B	221	CYS	2.6
1	E	120	GLY	2.6
1	B	223	SER	2.6
1	E	323	GLY	2.5
1	A	548	ASN	2.5
1	A	551	LYS	2.5
1	B	271	ALA	2.5
1	A	302	LYS	2.5
1	D	556	THR	2.5
1	B	553	ALA	2.5
1	E	104	VAL	2.5
1	A	556	THR	2.5
1	D	266	THR	2.5
1	D	559	THR	2.5
1	B	350	PRO	2.4
1	B	306	ILE	2.4
1	D	263	TYR	2.4
1	E	225	HIS	2.4
1	E	354	GLU	2.4
1	B	529	ASP	2.4
1	B	220	ALA	2.4
1	D	469	LEU	2.4
1	B	119	ASN	2.3
1	D	117	LEU	2.3
1	E	288	LEU	2.3
1	E	351	SER	2.3
1	A	2	SER	2.3
1	B	273	LYS	2.3
1	D	218	ALA	2.3
1	A	353	PRO	2.2
1	B	562	LYS	2.2
1	A	358	ALA	2.2
1	D	553	ALA	2.2
1	A	267	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	405	TYR	2.2
1	A	304	LYS	2.2
1	B	476	ILE	2.2
1	D	350	PRO	2.2
1	B	276	VAL	2.2
1	E	550	VAL	2.2
1	B	410	VAL	2.1
1	B	345	LYS	2.1
1	A	312	ASP	2.1
1	D	304	LYS	2.1
1	A	531	THR	2.1
1	B	272	VAL	2.1
1	E	217	LEU	2.1
1	B	256	HIS	2.1
1	D	405	TYR	2.1
1	A	118	GLY	2.1
1	E	265	GLY	2.1
1	D	300	SER	2.1
1	A	266	THR	2.0
1	B	347	VAL	2.0
1	E	122	PHE	2.0
1	B	269	SER	2.0
1	B	205	LEU	2.0
1	B	267	LEU	2.0
1	D	302	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 oligosaccharides in this entry.

6.4 Ligands ⓘ

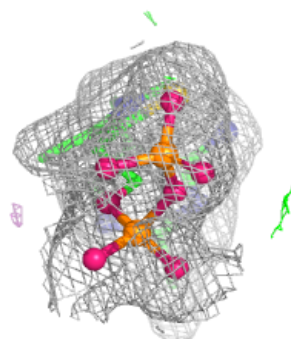
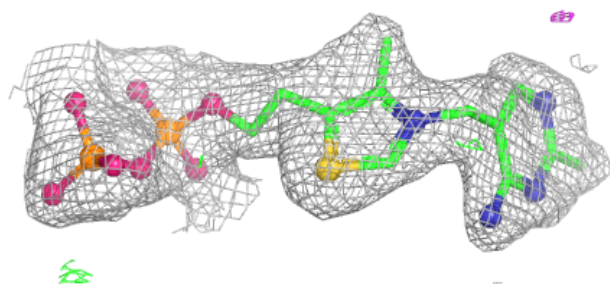
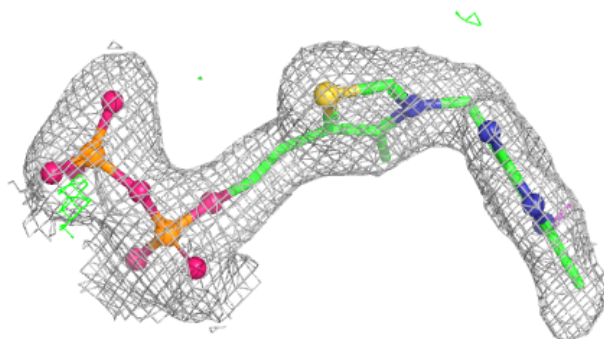
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	600	26/26	0.96	0.07	25,28,31,34	0
3	MG	E	601	1/1	0.96	0.03	21,21,21,21	0
2	TPP	E	600	26/26	0.97	0.06	21,26,30,31	0
3	MG	B	601	1/1	0.97	0.03	38,38,38,38	0
2	TPP	D	600	26/26	0.97	0.06	22,26,31,32	0
2	TPP	A	600	26/26	0.98	0.05	20,24,28,30	0
3	MG	D	601	1/1	0.98	0.06	23,23,23,23	0
3	MG	A	601	1/1	0.98	0.04	30,30,30,30	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.

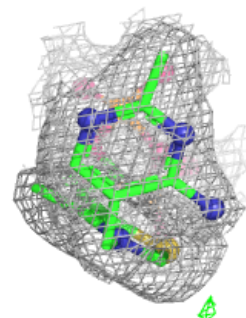
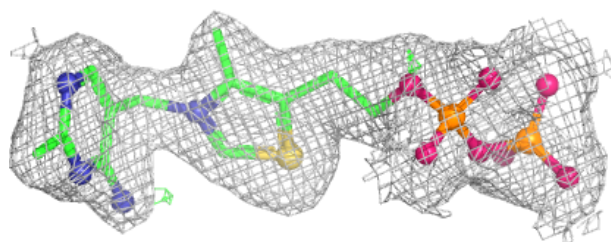
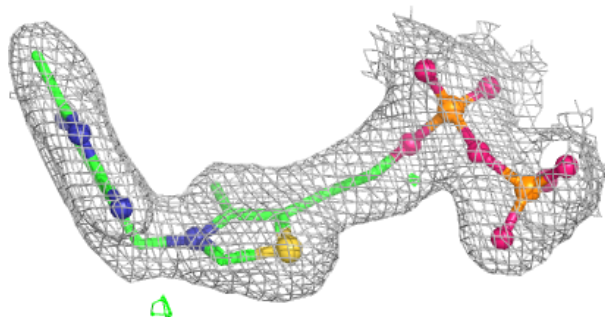
Electron density around TPP B 600:

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

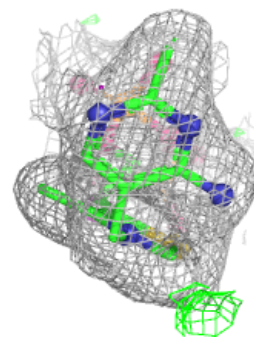
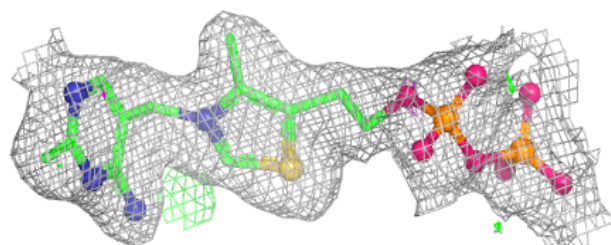
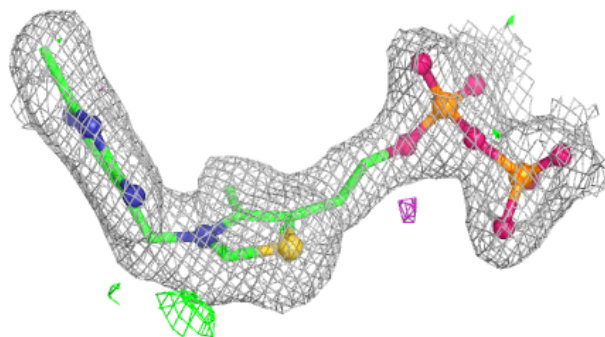


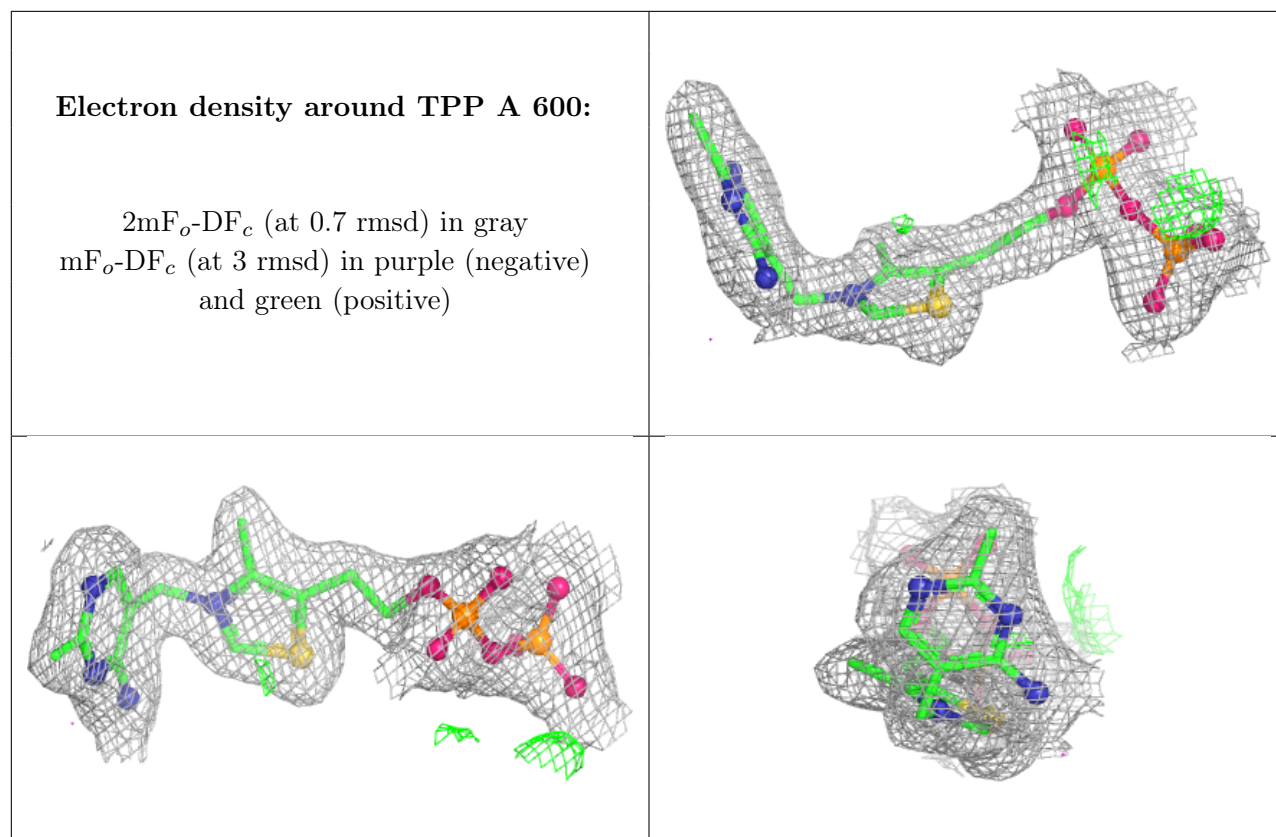
Electron density around TPP E 600:

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

**Electron density around TPP D 600:**

$2mF_o-DF_c$ (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.