



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:38 PM UTC

PDB ID : 2VK4 / pdb_00002vk4
Title : Crystal structure of pyruvate decarboxylase from Kluyveromyces lactis
Authors : Kutter, S.; Relle, S.; Wille, G.; Weiss, M.S.; Konig, S.
Deposited on : 2007-12-17
Resolution : 1.95 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

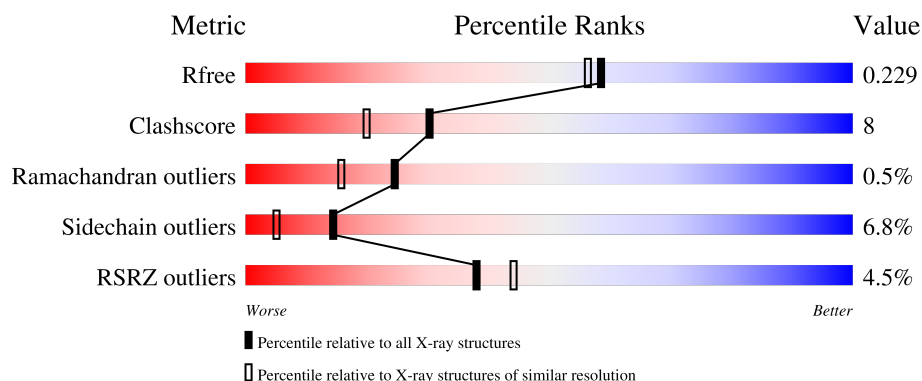
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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% 80% 15% ..
1	B	563	4% 81% 14% ..
1	C	563	5% 80% 16% ...
1	D	563	4% 79% 18% ..

2 Entry composition [i](#)

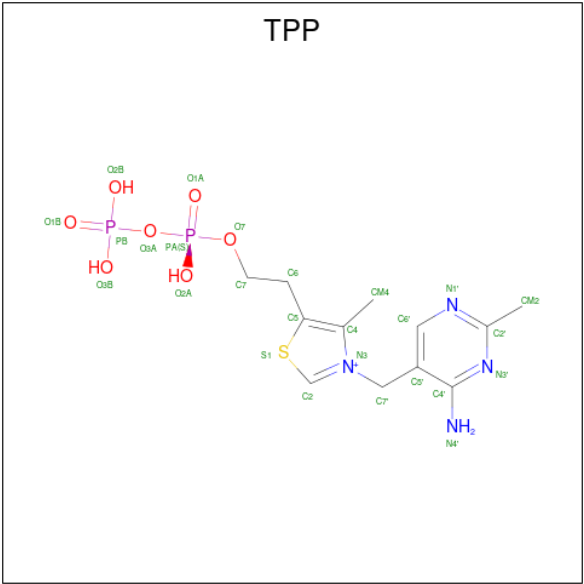
There are 4 unique types of molecules in this entry. The entry contains 18654 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	560	Total	C	N	O	S	0	0	0
			4324	2754	723	833	14			
1	B	557	Total	C	N	O	S	0	0	0
			4293	2733	716	830	14			
1	C	555	Total	C	N	O	S	0	0	0
			4286	2731	715	826	14			
1	D	560	Total	C	N	O	S	0	0	0
			4324	2754	723	833	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	C	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	
2	D	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	C	1	Total	Mg		
			1	1	0	0
3	D	1	Total	Mg		
			1	1	0	0

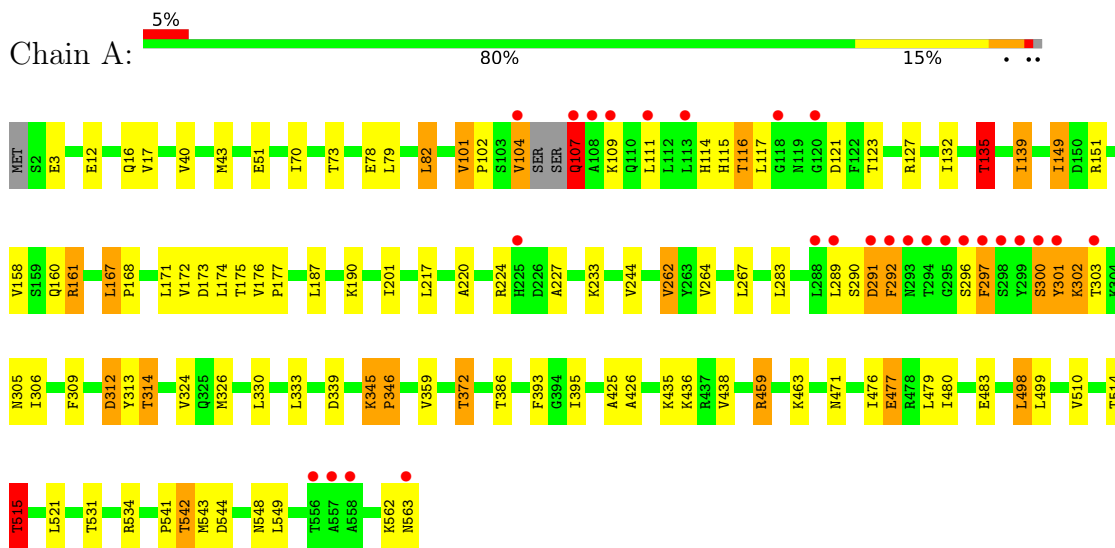
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total	O		
			310	310	0	0
4	B	326	Total	O		
			326	326	0	0
4	C	376	Total	O		
			376	376	0	0
4	D	307	Total	O		
			307	307	0	0

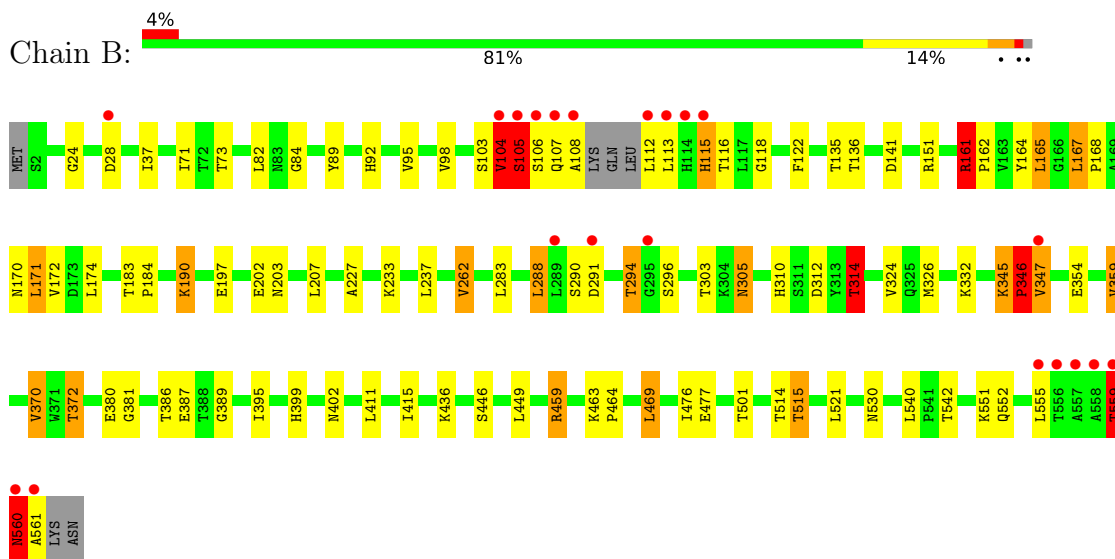
3 Residue-property plots [i](#)

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

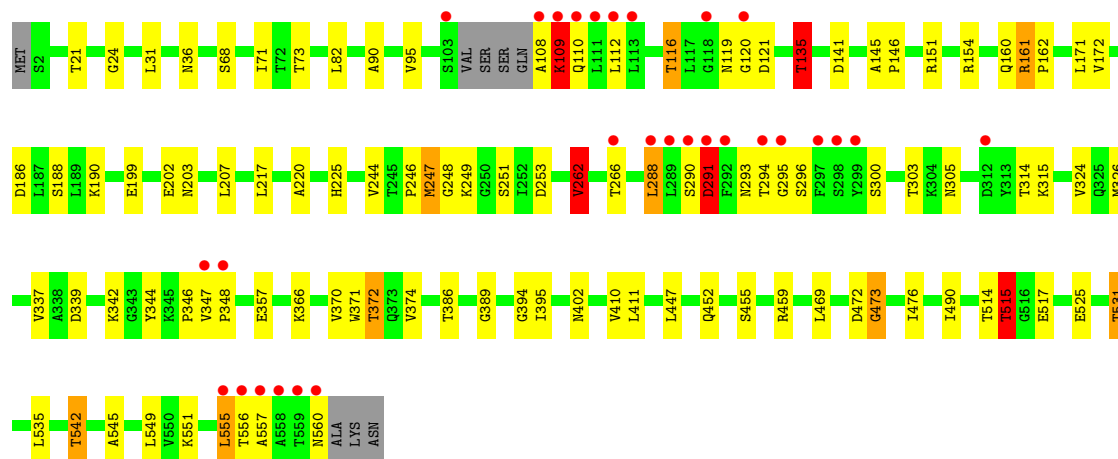


• Molecule 1: PYRUVATE DECARBOXYLASE

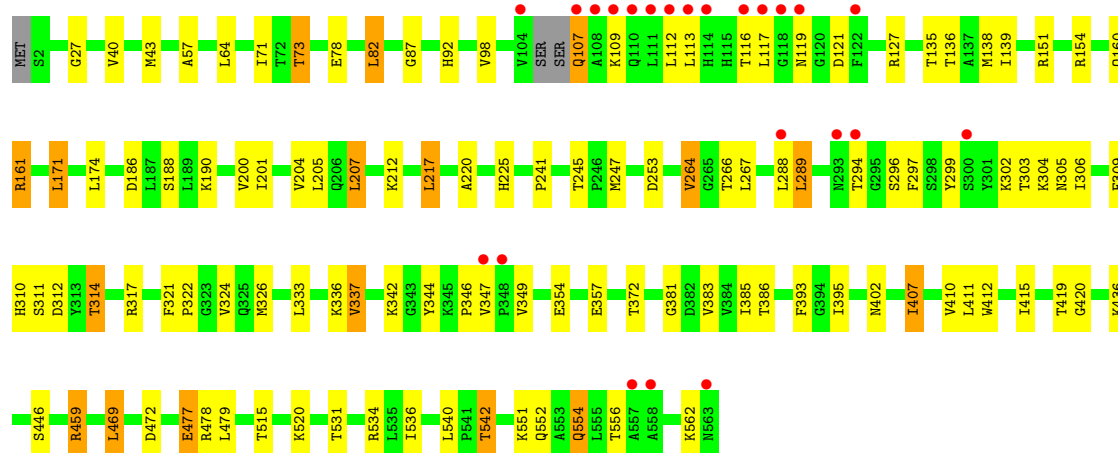
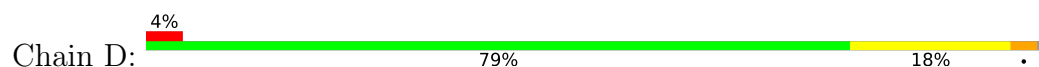


• Molecule 1: PYRUVATE DECARBOXYLASE





• Molecule 1: PYRUVATE DECARBOXYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.71Å 203.18Å 79.81Å 90.00° 91.81° 90.00°	Depositor
Resolution (Å)	48.45 – 1.95 48.45 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.45-1.95) 85.9 (48.45-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.178 , 0.230 0.177 , 0.229	Depositor DCC
R_{free} test set	7829 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for l,k,-h 0.033 for h,-k,-l 0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18654	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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	1.09	8/4415 (0.2%)	1.12	19/6009 (0.3%)
1	B	1.08	5/4384 (0.1%)	1.18	19/5969 (0.3%)
1	C	1.13	5/4377 (0.1%)	1.12	10/5958 (0.2%)
1	D	1.10	7/4415 (0.2%)	1.10	8/6009 (0.1%)
All	All	1.10	25/17591 (0.1%)	1.13	56/23945 (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	4	1
1	B	4	2
1	C	6	1
1	D	7	0
All	All	21	4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	HIS	CA-CB	-17.35	1.24	1.53
1	D	73	THR	C-O	-10.04	1.11	1.23
1	D	107	GLN	CA-CB	-9.37	1.34	1.53
1	A	115	HIS	N-CA	8.41	1.57	1.46
1	B	561	ALA	CA-C	7.67	1.69	1.52
1	A	372	THR	C-O	-7.67	1.15	1.24
1	D	542	THR	C-O	-6.79	1.16	1.24
1	A	101	VAL	C-O	-6.28	1.16	1.24
1	D	407	ILE	CA-CB	6.21	1.61	1.53
1	B	37	ILE	CA-CB	6.13	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	542	THR	C-O	-5.98	1.17	1.24
1	B	370	VAL	CA-CB	5.87	1.61	1.54
1	C	337	VAL	CA-CB	5.57	1.61	1.54
1	A	425	ALA	CA-CB	5.50	1.61	1.53
1	D	536	ILE	CA-CB	5.47	1.61	1.53
1	D	117	LEU	C-O	-5.43	1.17	1.24
1	C	36	ASN	C-O	-5.42	1.17	1.24
1	A	116	THR	C-O	-5.35	1.16	1.24
1	A	201	ILE	CA-CB	5.31	1.60	1.54
1	C	372	THR	C-O	-5.30	1.17	1.24
1	D	347	VAL	CA-CB	5.26	1.60	1.54
1	C	262	VAL	CA-CB	5.25	1.60	1.54
1	B	92	HIS	C-O	-5.23	1.16	1.23
1	A	117	LEU	CG-CD1	-5.12	1.35	1.52
1	B	227	ALA	CA-CB	5.00	1.60	1.53

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	561	ALA	N-CA-C	-25.60	39.32	111.00
1	B	115	HIS	N-CA-C	10.11	125.39	111.74
1	D	107	GLN	N-CA-CB	9.71	127.01	110.50
1	B	560	ASN	N-CA-C	-8.77	100.65	110.91
1	C	515	THR	N-CA-CB	-7.98	98.39	110.12
1	A	115	HIS	N-CA-CB	7.67	123.45	110.49
1	C	545	ALA	CA-C-N	-7.48	111.92	119.92
1	C	545	ALA	C-N-CA	-7.48	111.92	119.92
1	D	337	VAL	N-CA-C	7.11	117.90	110.72
1	A	312	ASP	N-CA-CB	-7.09	100.12	110.47
1	A	345	LYS	CA-C-N	6.82	128.37	119.84
1	A	345	LYS	C-N-CA	6.82	128.37	119.84
1	A	515	THR	N-CA-CB	-6.77	99.85	109.94
1	A	301	TYR	N-CA-C	6.76	125.21	110.80
1	A	292	PHE	N-CA-C	6.62	116.60	107.73
1	C	135	THR	CB-CA-C	-6.41	96.71	111.95
1	B	345	LYS	CA-C-N	6.34	127.77	119.84
1	B	345	LYS	C-N-CA	6.34	127.77	119.84
1	A	149	ILE	N-CA-CB	6.31	119.12	110.54
1	C	473	GLY	N-CA-C	6.11	117.73	111.56
1	A	135	THR	CB-CA-C	-6.09	98.33	111.11
1	B	105	SER	N-CA-CB	-5.98	101.56	111.06
1	B	561	ALA	N-CA-CB	-5.87	101.60	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	559	THR	N-CA-C	-5.83	98.39	110.80
1	B	84	GLY	N-CA-C	-5.68	105.91	112.50
1	A	114	HIS	CA-C-N	5.66	132.35	121.54
1	A	114	HIS	C-N-CA	5.66	132.35	121.54
1	B	82	LEU	N-CA-C	5.61	117.40	111.28
1	B	108	ALA	N-CA-C	5.61	126.72	111.00
1	D	264	VAL	CB-CA-C	5.51	120.33	111.29
1	D	321	PHE	CA-C-N	5.46	126.67	119.84
1	D	321	PHE	C-N-CA	5.46	126.67	119.84
1	A	114	HIS	N-CA-C	5.45	118.14	111.82
1	A	514	THR	CA-C-N	5.42	127.86	120.54
1	A	514	THR	C-N-CA	5.42	127.86	120.54
1	A	115	HIS	CB-CA-C	5.40	121.17	110.42
1	B	514	THR	CA-C-N	5.40	127.46	120.44
1	B	514	THR	C-N-CA	5.40	127.46	120.44
1	B	288	LEU	N-CA-C	-5.39	103.31	111.56
1	A	176	VAL	N-CA-C	-5.32	103.00	109.01
1	B	104	VAL	N-CA-C	5.31	120.39	109.34
1	B	314	THR	CB-CA-C	5.28	119.80	109.35
1	A	499	LEU	CA-C-N	-5.27	113.61	119.19
1	A	499	LEU	C-N-CA	-5.27	113.61	119.19
1	C	531	THR	N-CA-CB	-5.20	102.33	110.44
1	C	247	MET	CG-SD-CE	-5.19	89.49	100.90
1	D	107	GLN	CB-CA-C	5.16	119.90	110.10
1	A	220	ALA	N-CA-C	5.13	117.54	111.33
1	C	337	VAL	N-CA-C	5.11	115.88	110.72
1	C	220	ALA	N-CA-C	5.10	117.50	111.33
1	B	161	ARG	NE-CZ-NH2	-5.09	114.62	119.20
1	D	419	THR	N-CA-C	-5.08	105.66	111.14
1	B	312	ASP	N-CA-CB	-5.06	103.09	110.47
1	D	306	ILE	CB-CA-C	-5.03	102.98	110.33
1	B	262	VAL	N-CA-C	5.03	115.09	107.80
1	C	116	THR	N-CA-C	-5.01	105.56	113.02

All (21) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	73	THR	CB
1	A	116	THR	CB
1	A	303	THR	CB
1	A	372	THR	CB
1	B	73	THR	CB

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Mol	Chain	Res	Type	Atom
1	B	135	THR	CB
1	B	303	THR	CB
1	B	542	THR	CB
1	C	73	THR	CB
1	C	116	THR	CB
1	C	303	THR	CB
1	C	314	THR	CB
1	C	372	THR	CB
1	C	542	THR	CB
1	D	73	THR	CB
1	D	116	THR	CB
1	D	135	THR	CB
1	D	303	THR	CB
1	D	372	THR	CB
1	D	531	THR	CB
1	D	542	THR	CB

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	GLN	Peptide
1	B	104	VAL	Mainchain
1	B	107	GLN	Peptide
1	C	108	ALA	Peptide

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	4324	0	4300	85	0
1	B	4293	0	4259	76	0
1	C	4286	0	4259	68	0
1	D	4324	0	4300	80	0
2	A	26	0	16	0	0
2	B	26	0	16	1	0
2	C	26	0	16	1	0
2	D	26	0	16	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	310	0	0	15	0
4	B	326	0	0	9	0
4	C	376	0	0	18	0
4	D	307	0	0	11	0
All	All	18654	0	17182	290	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 (290) 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:303:THR:HG22	1:D:305:ASN:N	1.67	1.09
1:B:303:THR:HG22	1:B:305:ASN:H	1.15	1.08
1:D:303:THR:HG22	1:D:305:ASN:H	0.91	1.06
1:B:294:THR:HG22	1:B:296:SER:H	1.15	1.06
1:D:303:THR:CG2	1:D:305:ASN:H	1.70	1.05
1:A:372:THR:HG22	4:A:2205:HOH:O	1.56	1.02
1:A:107:GLN:O	1:A:107:GLN:HG3	1.60	0.99
1:A:303:THR:HG22	1:A:305:ASN:H	1.25	0.99
1:D:477:GLU:HG2	4:D:2252:HOH:O	1.60	0.97
1:C:303:THR:HG22	1:C:305:ASN:H	1.33	0.94
1:D:372:THR:HG22	4:D:2203:HOH:O	1.67	0.94
1:A:393:PHE:HE2	1:A:476:ILE:HD11	1.34	0.91
1:C:203:ASN:HB3	4:C:2130:HOH:O	1.72	0.88
1:C:542:THR:HG21	4:C:2300:HOH:O	1.71	0.88
1:B:141:ASP:OD2	1:D:135:THR:HG23	1.74	0.86
1:B:112:LEU:HD11	1:B:122:PHE:HE2	1.41	0.86
1:C:21:THR:O	4:C:2018:HOH:O	1.92	0.86
1:B:113:LEU:O	1:B:116:THR:HG22	1.76	0.85
1:C:288:LEU:HD13	1:C:411:LEU:HD13	1.58	0.84
1:C:135:THR:HG21	1:C:151:ARG:HH12	1.42	0.84
1:A:135:THR:HG21	1:A:151:ARG:HH12	1.42	0.83
1:B:372:THR:HG21	4:B:2188:HOH:O	1.79	0.82
1:A:393:PHE:CE2	1:A:476:ILE:HD11	2.16	0.80
1:B:542:THR:HG21	4:B:2260:HOH:O	1.81	0.79
1:B:104:VAL:HG22	1:B:104:VAL:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:542:THR:HG21	4:D:2241:HOH:O	1.82	0.79
1:B:135:THR:HG21	1:B:151:ARG:HH12	1.48	0.79
1:B:303:THR:HG22	1:B:305:ASN:N	1.96	0.79
1:A:302:LYS:H	1:D:304:LYS:HZ2	1.31	0.78
1:A:515:THR:CG2	4:A:2179:HOH:O	2.31	0.77
1:D:294:THR:HG22	1:D:296:SER:H	1.49	0.77
1:C:515:THR:HG23	4:C:2224:HOH:O	1.85	0.76
1:B:346:PRO:O	1:B:347:VAL:HB	1.86	0.76
1:A:121:ASP:OD1	1:A:127:ARG:NH1	2.19	0.76
1:B:112:LEU:HD12	1:B:112:LEU:C	2.12	0.75
1:A:302:LYS:H	1:D:304:LYS:NZ	1.84	0.75
1:A:515:THR:HG23	4:A:2179:HOH:O	1.84	0.74
1:A:300:SER:O	1:A:302:LYS:HG3	1.87	0.74
1:B:294:THR:HG22	1:B:296:SER:N	1.97	0.74
1:B:112:LEU:HD12	1:B:112:LEU:O	1.88	0.73
1:C:303:THR:HG22	1:C:305:ASN:N	2.04	0.72
1:B:190:LYS:HG3	4:B:2104:HOH:O	1.92	0.70
1:A:267:LEU:HD11	1:A:297:PHE:HB3	1.73	0.70
1:C:372:THR:HG21	4:C:2216:HOH:O	1.92	0.69
1:C:357:GLU:HG2	4:C:2219:HOH:O	1.93	0.69
1:A:173:ASP:OD1	4:A:2091:HOH:O	2.11	0.69
1:C:135:THR:HG21	1:C:151:ARG:NH1	2.07	0.69
1:D:267:LEU:HD12	1:D:297:PHE:HB3	1.76	0.68
1:B:559:THR:HG22	1:B:560:ASN:OD1	1.93	0.67
1:A:116:THR:HB	1:B:411:LEU:HD21	1.75	0.67
1:C:160:GLN:OE1	4:C:2096:HOH:O	2.12	0.67
1:A:303:THR:HG22	1:A:305:ASN:N	2.03	0.67
1:D:303:THR:HG21	1:D:305:ASN:HB3	1.76	0.66
1:A:292:PHE:HB3	1:B:113:LEU:HD13	1.77	0.66
1:A:459:ARG:NH2	4:A:2234:HOH:O	2.28	0.66
1:D:135:THR:HG21	1:D:151:ARG:HH12	1.60	0.66
1:C:225:HIS:HB2	1:C:326:MET:HE1	1.77	0.65
1:A:386:THR:HG21	1:A:395:ILE:HB	1.77	0.65
1:B:303:THR:CG2	1:B:305:ASN:HB2	2.27	0.65
1:C:314:THR:HG22	4:C:2188:HOH:O	1.98	0.64
1:A:477:GLU:HG2	4:A:2243:HOH:O	1.98	0.64
1:C:288:LEU:CD1	1:C:411:LEU:HD13	2.28	0.64
1:C:411:LEU:O	1:D:116:THR:HG21	1.98	0.64
1:A:127:ARG:NH2	4:A:2068:HOH:O	2.25	0.63
1:B:104:VAL:O	1:B:104:VAL:CG2	2.47	0.63
1:A:123:THR:OG1	1:A:127:ARG:NH1	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:THR:HG21	1:D:411:LEU:O	2.00	0.62
1:C:372:THR:HG22	4:C:2263:HOH:O	2.00	0.62
1:B:165:LEU:HD22	1:B:167:LEU:HD13	1.82	0.62
1:C:348:PRO:HB3	4:C:2203:HOH:O	1.99	0.61
1:A:227:ALA:HB3	1:A:326:MET:HE3	1.81	0.61
1:C:339:ASP:O	1:C:342:LYS:HB2	2.00	0.60
1:D:309:PHE:HB3	1:D:326:MET:HG3	1.83	0.60
1:C:290:SER:O	1:C:291:ASP:HB3	2.02	0.60
1:A:116:THR:HB	1:B:411:LEU:CD2	2.32	0.60
1:A:116:THR:HG21	1:B:411:LEU:O	2.02	0.59
1:A:127:ARG:NE	4:A:2068:HOH:O	2.29	0.59
1:C:95:VAL:O	1:C:162:PRO:HA	2.03	0.59
1:B:346:PRO:O	1:B:347:VAL:CB	2.51	0.59
1:B:203:ASN:HB3	4:B:2112:HOH:O	2.02	0.58
1:D:469:LEU:HD13	1:D:540:LEU:HD11	1.85	0.58
1:D:121:ASP:OD1	1:D:127:ARG:NH1	2.36	0.58
1:C:154:ARG:NE	1:C:186:ASP:O	2.32	0.58
1:C:386:THR:HG21	1:C:395:ILE:HB	1.86	0.58
1:D:73:THR:HG22	4:D:2045:HOH:O	2.03	0.58
1:C:199:GLU:OE1	4:C:2129:HOH:O	2.17	0.58
1:C:344:TYR:CE2	1:C:346:PRO:HA	2.39	0.58
1:A:227:ALA:CB	1:A:326:MET:HE3	2.34	0.57
1:A:289:LEU:HD23	1:A:292:PHE:HE2	1.68	0.57
1:B:354:GLU:HG3	1:B:399:HIS:CE1	2.39	0.57
1:A:135:THR:HG22	1:C:141:ASP:OD2	2.03	0.57
1:B:559:THR:C	1:B:560:ASN:OD1	2.48	0.57
1:D:78:GLU:O	1:D:82:LEU:HD13	2.05	0.57
1:A:82:LEU:HG	1:A:132:ILE:HD11	1.86	0.56
1:D:220:ALA:HB2	1:D:247:MET:HB3	1.87	0.56
1:A:548:ASN:HB3	4:A:2148:HOH:O	2.06	0.56
1:D:317:ARG:HD3	4:D:2152:HOH:O	2.06	0.56
1:D:241:PRO:HB3	1:D:349:VAL:HG12	1.87	0.55
1:B:112:LEU:CD1	1:B:122:PHE:HE2	2.17	0.55
1:C:372:THR:HG22	4:C:2212:HOH:O	2.06	0.55
1:D:247:MET:HE2	1:D:410:VAL:HB	1.89	0.55
1:A:302:LYS:N	1:D:304:LYS:HZ2	2.03	0.55
1:D:225:HIS:HB2	1:D:326:MET:HE1	1.88	0.55
1:A:139:ILE:HG22	1:A:171:LEU:HD12	1.89	0.54
1:D:478:ARG:NH2	4:D:2243:HOH:O	2.38	0.54
1:A:135:THR:HG21	1:A:151:ARG:NH1	2.17	0.54
1:A:542:THR:HG21	4:A:2239:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:THR:HG21	4:A:2287:HOH:O	2.08	0.54
1:A:73:THR:HG22	4:A:2044:HOH:O	2.07	0.54
1:A:542:THR:HG22	4:A:2295:HOH:O	2.08	0.54
1:C:294:THR:HG22	1:C:296:SER:H	1.73	0.53
1:C:248:GLY:O	1:C:251:SER:HB2	2.08	0.53
1:D:225:HIS:CD2	1:D:311:SER:HB3	2.44	0.53
1:A:121:ASP:CG	1:A:127:ARG:HH12	2.16	0.53
1:B:459:ARG:NH2	4:B:2250:HOH:O	2.33	0.53
1:D:478:ARG:NE	4:D:2243:HOH:O	1.96	0.53
1:D:207:LEU:HD11	1:D:317:ARG:HH21	1.74	0.53
1:A:562:LYS:HB3	1:D:322:PRO:HG2	1.91	0.53
1:D:217:LEU:HD11	1:D:245:THR:HG23	1.91	0.52
1:A:78:GLU:O	1:A:82:LEU:HD13	2.09	0.52
1:A:477:GLU:CG	4:A:2243:HOH:O	2.57	0.52
1:B:135:THR:CG2	1:B:151:ARG:HH12	2.21	0.52
1:B:112:LEU:HD11	1:B:122:PHE:CE2	2.32	0.52
1:D:303:THR:HG21	1:D:305:ASN:CB	2.40	0.52
1:D:303:THR:CG2	1:D:305:ASN:CB	2.88	0.51
1:A:393:PHE:CE2	1:A:476:ILE:CD1	2.92	0.51
1:B:112:LEU:C	1:B:112:LEU:CD1	2.83	0.51
1:C:459:ARG:NH2	4:C:2290:HOH:O	2.32	0.51
1:A:562:LYS:HE3	4:A:2307:HOH:O	2.10	0.51
1:B:28:ASP:CG	4:B:2012:HOH:O	2.52	0.51
1:A:51:GLU:OE2	2:B:600:TPP:N1'	2.44	0.51
1:C:452:GLN:O	1:C:455:SER:HB3	2.11	0.51
1:B:303:THR:HG22	1:B:305:ASN:HB2	1.93	0.50
1:D:135:THR:CG2	1:D:151:ARG:HH12	2.24	0.50
1:C:160:GLN:O	1:C:161:ARG:HG2	2.11	0.50
1:A:531:THR:HG22	1:A:534:ARG:HH22	1.75	0.50
1:D:245:THR:HG22	1:D:299:TYR:OH	2.12	0.50
1:B:135:THR:HG22	1:B:136:THR:N	2.27	0.50
1:C:288:LEU:HD13	1:C:411:LEU:CD1	2.37	0.50
1:A:104:VAL:HG22	1:A:168:PRO:CB	2.42	0.50
1:A:483:GLU:HG3	1:A:543:MET:CE	2.41	0.50
1:B:411:LEU:C	1:B:411:LEU:HD23	2.36	0.50
1:C:370:VAL:O	1:C:374:VAL:HG23	2.12	0.50
1:D:531:THR:HG22	1:D:534:ARG:HH22	1.77	0.50
1:B:314:THR:HG23	1:B:324:VAL:HB	1.94	0.49
1:C:68:SER:HA	4:C:2050:HOH:O	2.11	0.49
1:A:359:VAL:HG23	1:A:515:THR:HG21	1.94	0.49
1:A:510:VAL:HG21	1:A:521:LEU:CD2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ASN:ND2	1:C:121:ASP:HB3	2.28	0.49
1:A:302:LYS:N	1:D:304:LYS:NZ	2.59	0.49
1:D:200:VAL:O	1:D:204:VAL:HG23	2.13	0.49
1:D:381:GLY:O	1:D:436:LYS:HG3	2.12	0.49
1:A:393:PHE:HE2	1:A:476:ILE:CD1	2.18	0.49
1:C:24:GLY:HA3	1:C:71:ILE:O	2.12	0.49
1:C:73:THR:HG22	4:C:2051:HOH:O	2.12	0.49
1:A:562:LYS:HG2	1:A:563:ASN:H	1.78	0.49
1:B:359:VAL:HG23	1:B:515:THR:HG21	1.95	0.48
1:C:246:PRO:HB2	1:C:410:VAL:HG21	1.93	0.48
1:B:141:ASP:CG	1:D:135:THR:HG23	2.38	0.48
1:C:31:LEU:HD11	1:D:477:GLU:HG3	1.95	0.48
1:C:514:THR:OG1	1:C:517:GLU:HG3	2.13	0.48
1:D:552:GLN:O	1:D:556:THR:HG23	2.12	0.48
1:B:135:THR:HG22	1:B:136:THR:H	1.78	0.48
1:A:314:THR:HG22	1:A:324:VAL:O	2.14	0.47
1:C:202:GLU:HG2	4:C:2198:HOH:O	2.15	0.47
1:D:386:THR:HG21	1:D:395:ILE:HB	1.96	0.47
1:D:92:HIS:CD2	1:D:288:LEU:CD1	2.97	0.47
1:A:17:VAL:HG12	1:A:187:LEU:HD11	1.97	0.47
1:A:483:GLU:HG3	1:A:543:MET:HE2	1.95	0.47
1:B:314:THR:HG22	1:B:324:VAL:O	2.14	0.47
1:C:389:GLY:HA2	1:C:476:ILE:HG21	1.97	0.47
1:C:473:GLY:HA2	1:C:490:ILE:HG12	1.96	0.47
1:D:205:LEU:HD11	1:D:336:LYS:HB2	1.96	0.47
1:B:411:LEU:O	1:B:411:LEU:HD23	2.14	0.47
1:B:560:ASN:OD1	1:B:560:ASN:N	2.48	0.47
2:C:600:TPP:H7'1	1:D:27:GLY:HA2	1.97	0.47
1:D:135:THR:HG22	1:D:136:THR:H	1.80	0.47
1:A:101:VAL:HB	1:A:102:PRO:CD	2.45	0.46
1:B:135:THR:HG21	1:B:151:ARG:NH1	2.24	0.46
1:C:244:VAL:HG21	1:C:249:LYS:HA	1.98	0.46
1:A:471:ASN:O	1:A:542:THR:HB	2.16	0.46
1:C:293:ASN:HB2	1:D:113:LEU:HB3	1.96	0.46
1:D:154:ARG:NH2	1:D:188:SER:O	2.49	0.46
1:A:510:VAL:HG21	1:A:521:LEU:HD22	1.97	0.46
1:D:385:ILE:HG12	1:D:407:ILE:HB	1.98	0.46
1:A:498:LEU:HD12	1:B:501:THR:CG2	2.46	0.46
1:B:310:HIS:O	1:B:326:MET:HB2	2.16	0.46
1:D:344:TYR:CE2	1:D:346:PRO:HA	2.51	0.46
1:B:73:THR:HG22	4:B:2037:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:LYS:HB2	1:A:436:LYS:HE2	1.74	0.45
1:A:562:LYS:CG	1:A:563:ASN:H	2.29	0.45
1:B:387:GLU:HG2	1:B:446:SER:CB	2.46	0.45
1:D:139:ILE:HG22	1:D:171:LEU:HD12	1.98	0.45
1:D:87:GLY:HA2	1:D:412:TRP:CG	2.52	0.45
1:D:154:ARG:NE	1:D:186:ASP:O	2.43	0.45
1:D:310:HIS:O	1:D:326:MET:HB2	2.16	0.45
1:A:3:GLU:HG2	1:A:177:PRO:HA	1.98	0.45
1:C:90:ALA:HB1	1:C:411:LEU:CD2	2.47	0.45
1:C:135:THR:CG2	1:C:151:ARG:HH12	2.22	0.45
1:C:247:MET:HE3	1:C:411:LEU:HB2	1.99	0.45
1:D:64:LEU:HD21	1:D:383:VAL:HG21	1.97	0.45
1:B:303:THR:HG21	1:B:305:ASN:HB2	1.99	0.45
1:C:145:ALA:HB3	1:C:146:PRO:HD3	1.99	0.45
1:D:459:ARG:NH2	4:D:2233:HOH:O	2.48	0.45
1:B:103:SER:C	1:B:105:SER:H	2.25	0.45
1:B:168:PRO:HB2	1:B:171:LEU:HD23	1.99	0.45
1:C:225:HIS:HB2	1:C:326:MET:CE	2.46	0.45
1:C:109:LYS:HB3	1:C:109:LYS:HE3	1.63	0.44
1:B:103:SER:CB	1:B:170:ASN:OD1	2.66	0.44
1:C:154:ARG:NH2	1:C:188:SER:O	2.50	0.44
1:C:314:THR:HG23	1:C:324:VAL:O	2.17	0.44
1:D:314:THR:HG22	1:D:324:VAL:O	2.17	0.44
1:A:40:VAL:HB	1:A:43:MET:HG3	2.00	0.44
1:A:435:LYS:HD2	1:A:435:LYS:HA	1.78	0.44
1:A:3:GLU:HB3	1:A:175:THR:HB	2.00	0.44
1:B:463:LYS:N	1:B:464:PRO:CD	2.81	0.44
1:A:314:THR:HG23	1:A:324:VAL:HB	2.00	0.44
1:D:247:MET:HE3	1:D:247:MET:H	1.82	0.44
1:D:554:GLN:HG3	4:D:2304:HOH:O	2.17	0.44
1:D:469:LEU:HD13	1:D:540:LEU:CD1	2.47	0.43
1:B:71:ILE:HA	1:B:98:VAL:O	2.18	0.43
1:B:89:TYR:O	1:B:161:ARG:HD3	2.17	0.43
1:C:288:LEU:CD1	1:C:411:LEU:CD1	2.96	0.43
1:C:551:LYS:O	1:C:555:LEU:HB3	2.18	0.43
1:B:290:SER:HB2	4:B:2157:HOH:O	2.18	0.43
1:C:555:LEU:C	1:C:557:ALA:H	2.26	0.43
1:D:40:VAL:HB	1:D:43:MET:HG3	1.99	0.43
1:D:312:ASP:OD2	1:D:312:ASP:N	2.50	0.43
1:C:244:VAL:HG23	1:C:262:VAL:HB	2.00	0.43
1:A:312:ASP:HB3	1:A:313:TYR:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:CG1	1:B:167:LEU:HD22	2.49	0.43
1:B:372:THR:HB	4:B:2220:HOH:O	2.19	0.43
1:B:381:GLY:O	1:B:436:LYS:HG3	2.19	0.43
1:C:472:ASP:HB3	1:C:542:THR:HG22	2.00	0.43
1:D:267:LEU:HD13	1:D:393:PHE:CE1	2.54	0.43
1:D:135:THR:HG21	1:D:151:ARG:NH1	2.31	0.43
1:A:12:GLU:O	1:A:16:GLN:HG3	2.19	0.42
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.78	0.42
1:A:101:VAL:HB	1:A:102:PRO:HD2	2.00	0.42
1:D:107:GLN:N	1:D:107:GLN:OE1	2.52	0.42
1:A:135:THR:CG2	1:C:141:ASP:OD2	2.67	0.42
1:A:426:ALA:HA	1:A:438:VAL:HG21	1.99	0.42
1:C:120:GLY:HA2	4:C:2072:HOH:O	2.19	0.42
1:C:347:VAL:HA	1:C:348:PRO:HD2	1.90	0.42
1:A:82:LEU:HD12	1:A:82:LEU:HA	1.95	0.42
1:C:459:ARG:NH1	4:C:2291:HOH:O	2.53	0.42
1:A:160:GLN:O	1:A:161:ARG:HG2	2.19	0.42
1:A:289:LEU:HD23	1:A:289:LEU:O	2.20	0.42
1:A:309:PHE:HB3	1:A:326:MET:HG3	2.02	0.42
1:C:294:THR:HG22	1:C:295:GLY:N	2.35	0.41
1:A:386:THR:HG21	1:A:395:ILE:CB	2.46	0.41
1:A:541:PRO:HB2	1:A:544:ASP:HB2	2.02	0.41
1:C:253:ASP:HB3	1:C:402:ASN:OD1	2.20	0.41
1:D:372:THR:HG21	4:D:2165:HOH:O	2.20	0.41
1:B:71:ILE:HG12	1:B:98:VAL:HB	2.03	0.41
1:C:371:TRP:CD1	1:C:394:GLY:HA3	2.55	0.41
1:D:135:THR:HG22	1:D:136:THR:N	2.35	0.41
1:A:244:VAL:HG23	1:A:262:VAL:HB	2.03	0.41
1:A:345:LYS:HA	1:A:346:PRO:HD3	1.72	0.41
1:A:563:ASN:OD1	1:B:106:SER:HB2	2.20	0.41
1:B:380:GLU:HG2	1:B:402:ASN:O	2.21	0.41
1:D:289:LEU:HD22	1:D:411:LEU:HD21	2.02	0.41
1:D:415:ILE:HB	1:D:446:SER:OG	2.20	0.41
1:A:167:LEU:HD12	1:A:167:LEU:HA	1.93	0.41
1:B:24:GLY:HA3	1:B:71:ILE:O	2.20	0.41
1:B:345:LYS:O	1:B:346:PRO:O	2.39	0.41
1:A:267:LEU:CD1	1:A:297:PHE:HB3	2.47	0.41
1:B:233:LYS:HE3	1:B:237:LEU:HD21	2.03	0.41
1:B:294:THR:CG2	1:B:296:SER:H	2.06	0.41
1:B:116:THR:HG23	1:B:118:GLY:H	1.86	0.41
1:B:469:LEU:HB3	1:B:540:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:ALA:HA	1:D:420:GLY:O	2.21	0.41
1:D:314:THR:HG23	1:D:324:VAL:HB	2.02	0.41
1:D:472:ASP:HB3	1:D:542:THR:HG22	2.03	0.41
1:B:183:THR:HA	1:B:184:PRO:HD3	1.97	0.40
1:B:197:GLU:OE2	1:B:332:LYS:HD3	2.21	0.40
1:B:136:THR:HA	1:B:164:TYR:O	2.21	0.40
1:D:71:ILE:HA	1:D:98:VAL:O	2.21	0.40
1:B:95:VAL:O	1:B:162:PRO:HA	2.22	0.40
1:B:386:THR:HG21	1:B:395:ILE:HB	2.03	0.40
1:B:389:GLY:HA2	1:B:476:ILE:HG21	2.03	0.40
1:D:119:ASN:ND2	4:D:2061:HOH:O	2.29	0.40
1:D:160:GLN:O	1:D:161:ARG:HG2	2.21	0.40
1:A:345:LYS:HA	1:A:345:LYS:HD3	1.91	0.40
1:D:303:THR:HG22	1:D:305:ASN:CA	2.48	0.40
1:D:303:THR:CG2	1:D:304:LYS:N	2.84	0.40
1:B:415:ILE:HG13	1:B:449:LEU:HD22	2.03	0.40
1:B:463:LYS:HD2	1:B:530:ASN:O	2.22	0.40
1:C:535:LEU:C	1:C:535:LEU:HD23	2.47	0.40
1:D:253:ASP:HB3	1:D:402:ASN:OD1	2.22	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	556/563 (99%)	527 (95%)	24 (4%)	5 (1%)	14	6
1	B	553/563 (98%)	538 (97%)	11 (2%)	4 (1%)	18	10
1	C	551/563 (98%)	535 (97%)	14 (2%)	2 (0%)	30	21
1	D	556/563 (99%)	539 (97%)	17 (3%)	0	100	100
All	All	2216/2252 (98%)	2139 (96%)	66 (3%)	11 (0%)	24	16

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	301	TYR
1	B	346	PRO
1	B	347	VAL
1	B	559	THR
1	C	109	LYS
1	A	291	ASP
1	A	300	SER
1	A	290	SER
1	B	104	VAL
1	C	291	ASP
1	A	346	PRO

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	471/474 (99%)	432 (92%)	39 (8%)	10	3
1	B	468/474 (99%)	437 (93%)	31 (7%)	15	5
1	C	467/474 (98%)	440 (94%)	27 (6%)	18	7
1	D	471/474 (99%)	440 (93%)	31 (7%)	15	5
All	All	1877/1896 (99%)	1749 (93%)	128 (7%)	14	5

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ILE
1	A	82	LEU
1	A	104	VAL
1	A	107	GLN
1	A	109	LYS
1	A	111	LEU
1	A	135	THR
1	A	139	ILE
1	A	149	ILE

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Mol	Chain	Res	Type
1	A	158	VAL
1	A	161	ARG
1	A	167	LEU
1	A	172	VAL
1	A	174	LEU
1	A	190	LYS
1	A	217	LEU
1	A	224	ARG
1	A	233	LYS
1	A	262	VAL
1	A	264	VAL
1	A	283	LEU
1	A	291	ASP
1	A	296	SER
1	A	297	PHE
1	A	302	LYS
1	A	306	ILE
1	A	314	THR
1	A	330	LEU
1	A	333	LEU
1	A	339	ASP
1	A	459	ARG
1	A	463	LYS
1	A	477	GLU
1	A	479	LEU
1	A	480	ILE
1	A	498	LEU
1	A	515	THR
1	A	542	THR
1	A	549	LEU
1	B	105	SER
1	B	115	HIS
1	B	161	ARG
1	B	165	LEU
1	B	167	LEU
1	B	171	LEU
1	B	172	VAL
1	B	174	LEU
1	B	190	LYS
1	B	202	GLU
1	B	207	LEU
1	B	262	VAL

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Mol	Chain	Res	Type
1	B	283	LEU
1	B	288	LEU
1	B	291	ASP
1	B	294	THR
1	B	305	ASN
1	B	314	THR
1	B	346	PRO
1	B	359	VAL
1	B	370	VAL
1	B	372	THR
1	B	459	ARG
1	B	469	LEU
1	B	477	GLU
1	B	515	THR
1	B	521	LEU
1	B	551	LYS
1	B	552	GLN
1	B	555	LEU
1	B	560	ASN
1	C	82	LEU
1	C	109	LYS
1	C	110	GLN
1	C	112	LEU
1	C	135	THR
1	C	161	ARG
1	C	171	LEU
1	C	172	VAL
1	C	190	LYS
1	C	207	LEU
1	C	217	LEU
1	C	262	VAL
1	C	266	THR
1	C	288	LEU
1	C	291	ASP
1	C	300	SER
1	C	315	LYS
1	C	366	LYS
1	C	447	LEU
1	C	469	LEU
1	C	515	THR
1	C	525	GLU
1	C	531	THR

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Mol	Chain	Res	Type
1	C	549	LEU
1	C	555	LEU
1	C	556	THR
1	C	560	ASN
1	D	82	LEU
1	D	109	LYS
1	D	112	LEU
1	D	138	MET
1	D	161	ARG
1	D	171	LEU
1	D	174	LEU
1	D	190	LYS
1	D	201	ILE
1	D	207	LEU
1	D	212	LYS
1	D	217	LEU
1	D	264	VAL
1	D	266	THR
1	D	289	LEU
1	D	302	LYS
1	D	314	THR
1	D	333	LEU
1	D	337	VAL
1	D	342	LYS
1	D	354	GLU
1	D	357	GLU
1	D	459	ARG
1	D	469	LEU
1	D	477	GLU
1	D	479	LEU
1	D	515	THR
1	D	520	LYS
1	D	551	LYS
1	D	554	GLN
1	D	562	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	A	110	GLN
1	A	160	GLN

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Mol	Chain	Res	Type
1	A	206	GLN
1	A	213	ASN
1	A	448	GLN
1	A	492	ASN
1	A	528	GLN
1	B	36	ASN
1	B	114	HIS
1	B	143	ASN
1	B	206	GLN
1	B	325	GLN
1	C	239	GLN
1	C	293	ASN
1	C	397	GLN
1	C	528	GLN
1	D	107	GLN
1	D	206	GLN
1	D	448	GLN
1	D	492	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	2.03	9 (34%)	38,40,40	2.09	11 (28%)
2	TPP	D	600	3	26,27,27	1.93	7 (26%)	38,40,40	2.01	12 (31%)
2	TPP	A	600	3	26,27,27	1.73	9 (34%)	38,40,40	1.93	13 (34%)
2	TPP	C	600	3	26,27,27	1.92	9 (34%)	38,40,40	1.79	12 (31%)

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	-	2/17/17/17	0/2/2/2
2	TPP	D	600	3	-	3/17/17/17	0/2/2/2
2	TPP	A	600	3	-	2/17/17/17	0/2/2/2
2	TPP	C	600	3	-	3/17/17/17	0/2/2/2

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	TPP	C6'-N1'	4.64	1.43	1.34
2	D	600	TPP	C2-N3	4.40	1.43	1.32
2	C	600	TPP	C5-S1	-4.12	1.62	1.72
2	A	600	TPP	C5-S1	-4.07	1.62	1.72
2	C	600	TPP	C4'-N3'	3.73	1.40	1.35
2	D	600	TPP	PA-O3A	3.73	1.63	1.59
2	B	600	TPP	C2'-N1'	3.63	1.39	1.34
2	B	600	TPP	C2-N3	3.53	1.41	1.32
2	B	600	TPP	C5-C4	3.50	1.42	1.35
2	D	600	TPP	C5-S1	-3.27	1.64	1.72
2	C	600	TPP	C2-N3	3.11	1.39	1.32
2	D	600	TPP	C4'-N3'	3.10	1.39	1.35
2	B	600	TPP	C5-S1	-3.01	1.64	1.72
2	A	600	TPP	C6'-N1'	2.99	1.40	1.34
2	D	600	TPP	C2'-N1'	2.97	1.38	1.34
2	B	600	TPP	C2'-N3'	2.93	1.39	1.34
2	D	600	TPP	C5-C4	2.90	1.41	1.35
2	C	600	TPP	C5-C4	2.84	1.41	1.35
2	D	600	TPP	C6'-N1'	2.79	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	TPP	C2'-N3'	2.78	1.38	1.34
2	A	600	TPP	C2'-N3'	2.76	1.38	1.34
2	B	600	TPP	C4'-N3'	2.69	1.38	1.35
2	A	600	TPP	C2-N3	2.63	1.38	1.32
2	C	600	TPP	PA-O3A	2.61	1.62	1.59
2	A	600	TPP	C5-C4	2.54	1.40	1.35
2	C	600	TPP	C5'-C4'	-2.46	1.38	1.42
2	B	600	TPP	PA-O3A	2.44	1.62	1.59
2	C	600	TPP	C2'-N1'	2.25	1.37	1.34
2	A	600	TPP	PB-O2B	-2.24	1.46	1.54
2	B	600	TPP	C6'-C5'	2.24	1.42	1.37
2	C	600	TPP	C6-C5	2.21	1.55	1.50
2	A	600	TPP	C2'-N1'	2.19	1.37	1.34
2	A	600	TPP	C2-S1	-2.04	1.62	1.69
2	A	600	TPP	C4'-N3'	2.02	1.37	1.35

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	TPP	CM2-C2'-N1'	5.96	123.55	117.20
2	B	600	TPP	C2-N3-C4	-5.50	106.63	114.06
2	B	600	TPP	CM2-C2'-N1'	5.32	122.86	117.20
2	B	600	TPP	S1-C2-N3	4.44	117.91	112.30
2	D	600	TPP	C2-N3-C4	-4.27	108.30	114.06
2	C	600	TPP	C2-N3-C4	-4.24	108.33	114.06
2	B	600	TPP	C2-S1-C5	-4.13	88.48	91.22
2	A	600	TPP	N1'-C2'-N3'	-4.03	118.82	125.53
2	A	600	TPP	C6'-N1'-C2'	3.81	122.33	116.07
2	D	600	TPP	N1'-C2'-N3'	-3.68	119.41	125.53
2	A	600	TPP	C6'-C5'-C4'	3.67	120.06	115.55
2	A	600	TPP	C5'-C6'-N1'	-3.66	117.87	123.83
2	A	600	TPP	C2-N3-C4	-3.64	109.14	114.06
2	C	600	TPP	N1'-C2'-N3'	-3.42	119.84	125.53
2	D	600	TPP	C4-C5-S1	3.36	115.80	110.56
2	B	600	TPP	C5'-C6'-N1'	-3.25	118.55	123.83
2	C	600	TPP	C6'-C5'-C4'	3.23	119.52	115.55
2	D	600	TPP	S1-C2-N3	3.18	116.32	112.30
2	C	600	TPP	C6'-N1'-C2'	3.06	121.09	116.07
2	B	600	TPP	C4-C5-S1	3.00	115.24	110.56
2	B	600	TPP	C6'-C5'-C4'	2.99	119.22	115.55
2	A	600	TPP	CM2-C2'-N1'	2.88	120.27	117.20
2	C	600	TPP	CM4-C4-N3	2.60	126.56	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	TPP	C2'-N3'-C4'	2.59	122.07	118.10
2	C	600	TPP	O3A-PA-O1A	2.58	118.47	110.70
2	C	600	TPP	C5'-C6'-N1'	-2.58	119.64	123.83
2	D	600	TPP	C2-S1-C5	-2.58	89.51	91.22
2	C	600	TPP	CM2-C2'-N1'	2.54	119.91	117.20
2	C	600	TPP	C4-C5-S1	2.53	114.50	110.56
2	A	600	TPP	CM2-C2'-N3'	2.53	120.91	117.13
2	D	600	TPP	C6'-C5'-C4'	2.51	118.64	115.55
2	B	600	TPP	C6-C5-S1	-2.49	115.07	120.90
2	A	600	TPP	O3A-PA-O1A	2.44	118.03	110.70
2	B	600	TPP	N1'-C2'-N3'	-2.41	121.51	125.53
2	A	600	TPP	C6-C5-S1	-2.41	115.25	120.90
2	D	600	TPP	C6'-N1'-C2'	2.40	120.01	116.07
2	B	600	TPP	C7'-C5'-C4'	-2.32	118.13	122.36
2	A	600	TPP	S1-C2-N3	2.31	115.22	112.30
2	D	600	TPP	C6-C5-S1	-2.28	115.57	120.90
2	B	600	TPP	C6'-N1'-C2'	2.21	119.70	116.07
2	A	600	TPP	C2'-N3'-C4'	2.18	121.45	118.10
2	A	600	TPP	C4-C5-S1	2.18	113.96	110.56
2	C	600	TPP	CM4-C4-C5	-2.11	122.33	127.75
2	C	600	TPP	CM2-C2'-N3'	2.09	120.26	117.13
2	C	600	TPP	S1-C2-N3	2.08	114.93	112.30
2	D	600	TPP	N4'-C4'-N3'	2.04	119.78	117.03
2	D	600	TPP	CM4-C4-N3	2.02	125.23	120.57
2	A	600	TPP	C7'-N3-C4	2.02	127.71	122.36

There are no chirality outliers.

All (10) torsion outliers are listed below:

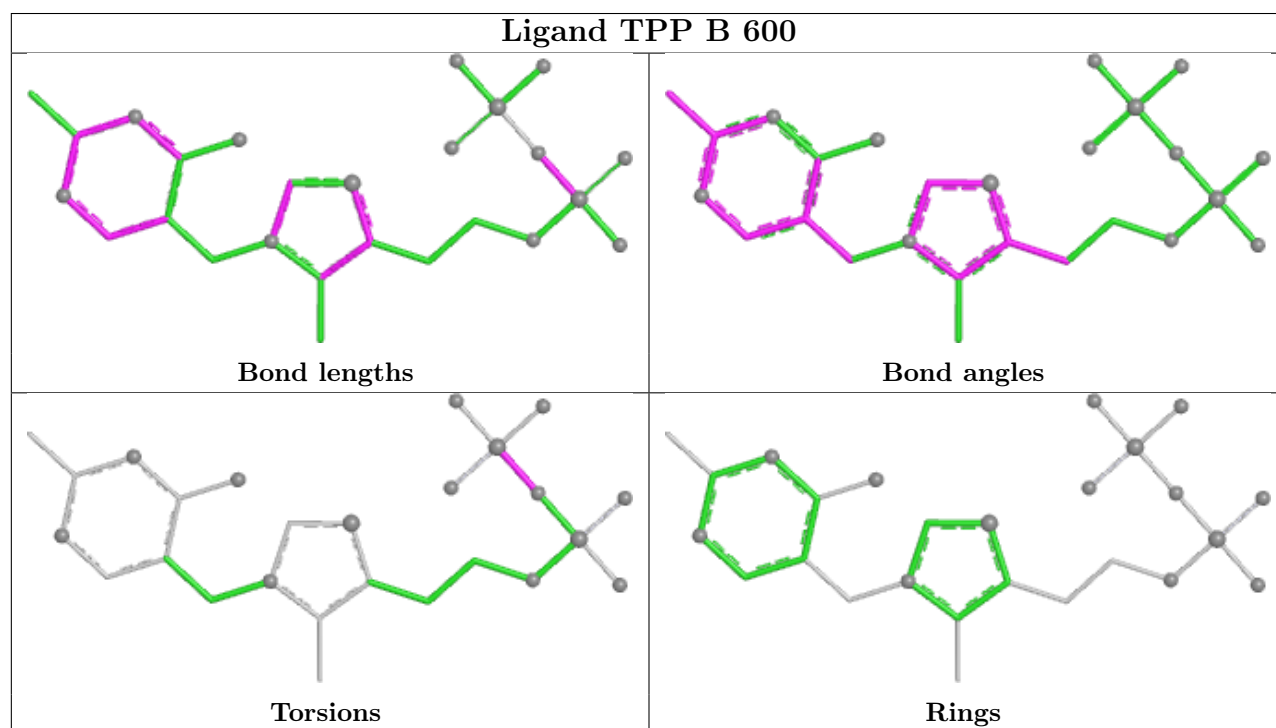
Mol	Chain	Res	Type	Atoms
2	A	600	TPP	PA-O3A-PB-O3B
2	B	600	TPP	PA-O3A-PB-O3B
2	C	600	TPP	PA-O3A-PB-O3B
2	D	600	TPP	PA-O3A-PB-O3B
2	B	600	TPP	PA-O3A-PB-O1B
2	A	600	TPP	PA-O3A-PB-O2B
2	C	600	TPP	PA-O3A-PB-O2B
2	D	600	TPP	PA-O3A-PB-O2B
2	D	600	TPP	C5-C6-C7-O7
2	C	600	TPP	PA-O3A-PB-O1B

There are no ring outliers.

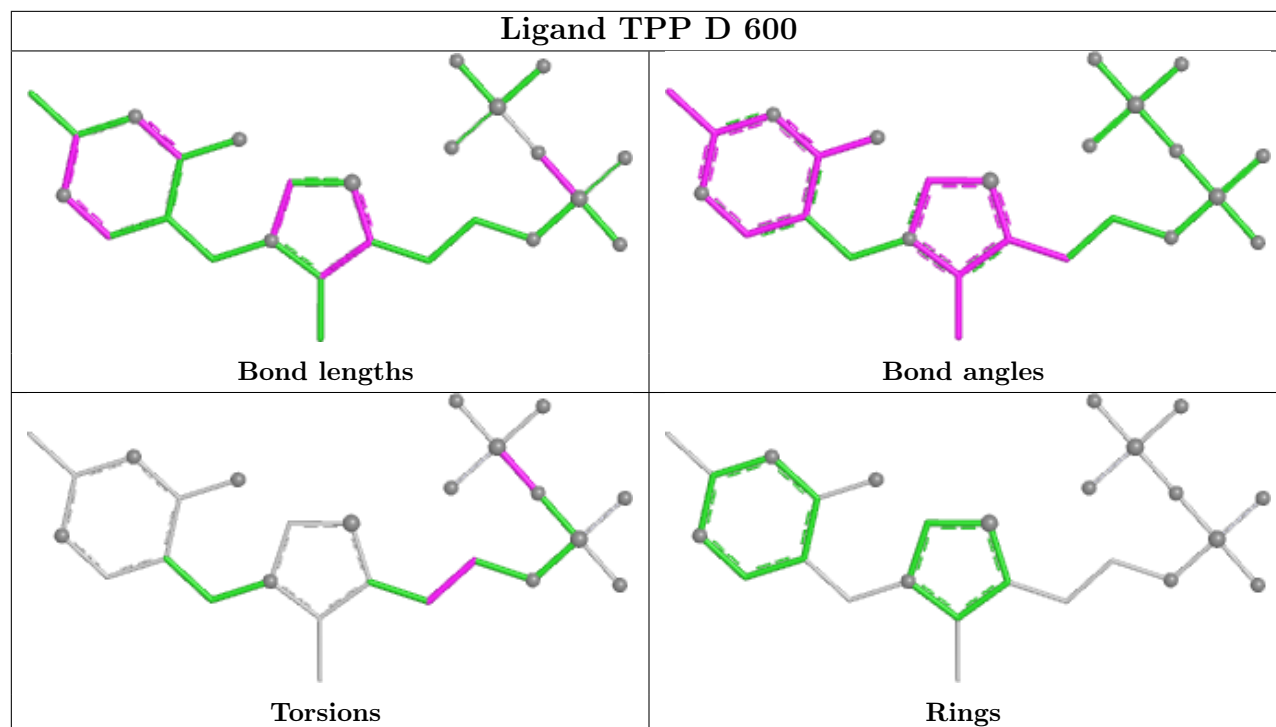
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	TPP	1	0
2	C	600	TPP	1	0

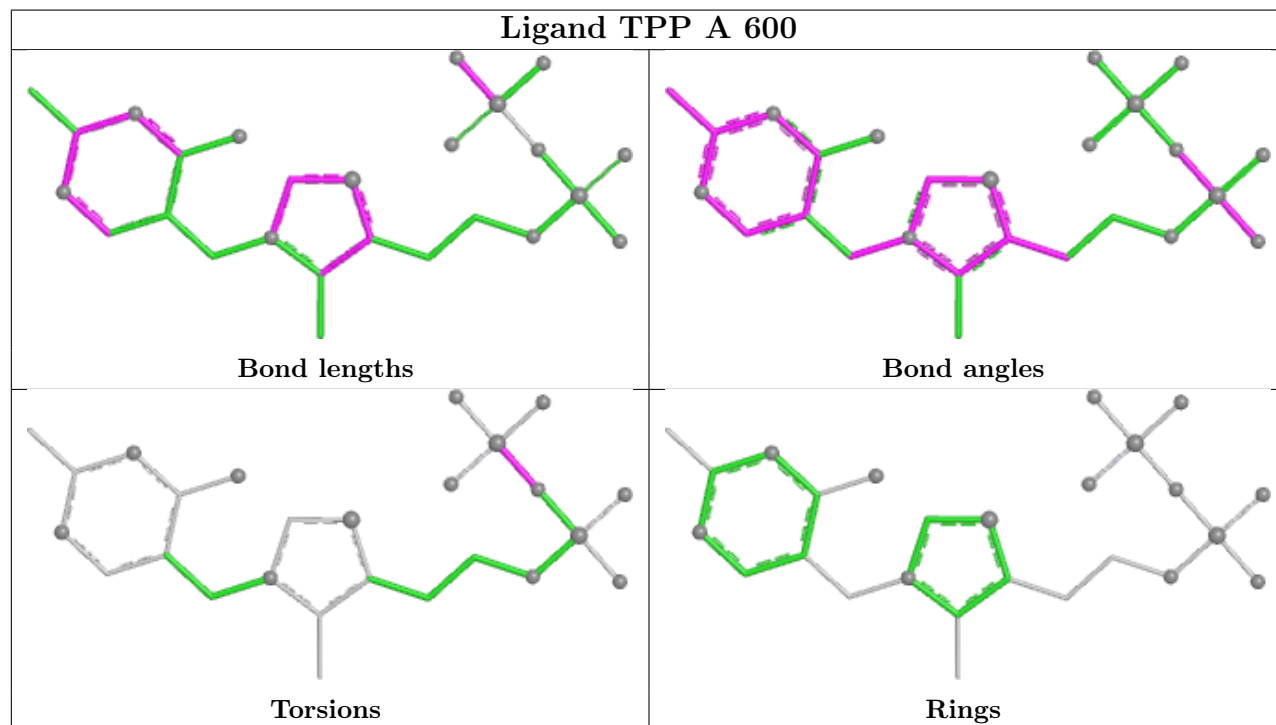
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

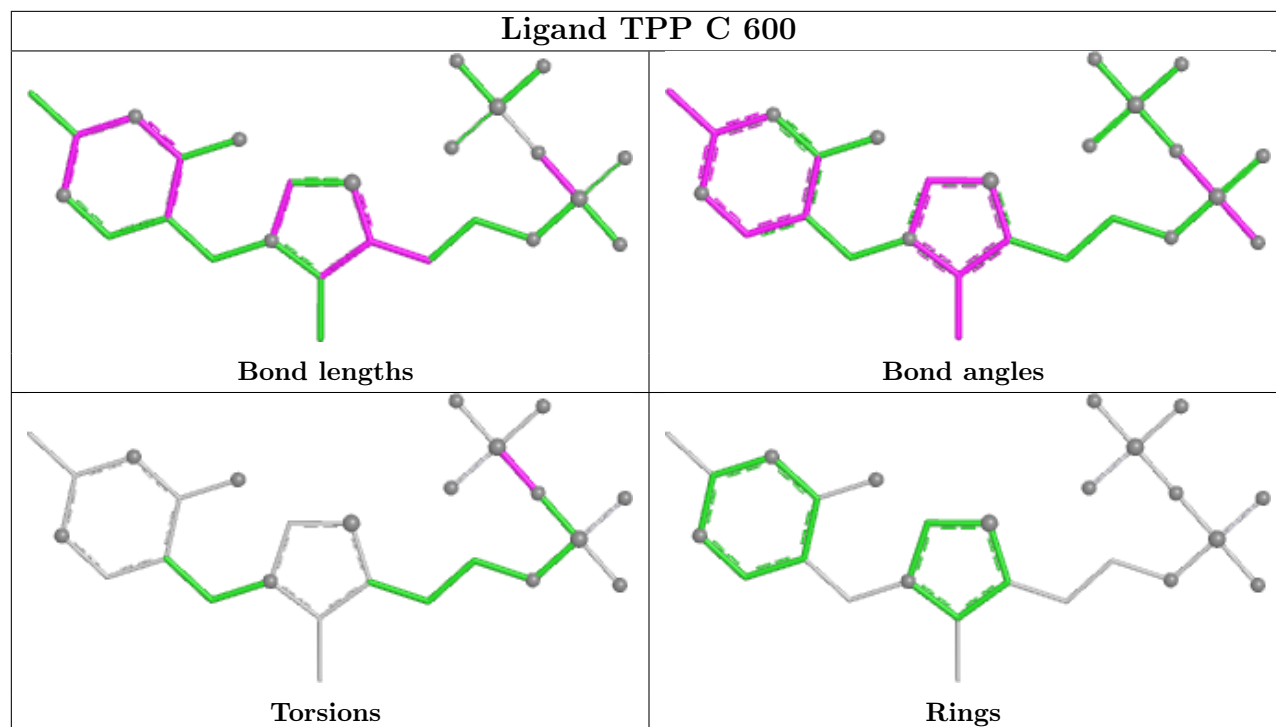


Ligand TPP D 600



Ligand TPP A 600





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	560/563 (99%)	-0.04	27 (4%)	35	41	9, 21, 44, 74	0
1	B	557/563 (98%)	-0.09	21 (3%)	44	50	9, 20, 37, 79	0
1	C	555/563 (98%)	-0.23	29 (5%)	33	38	8, 17, 41, 81	0
1	D	560/563 (99%)	-0.09	23 (4%)	41	48	8, 20, 42, 68	0
All	All	2232/2252 (99%)	-0.11	100 (4%)	38	44	8, 19, 42, 81	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	113	LEU	6.2
1	D	111	LEU	6.0
1	A	292	PHE	6.0
1	B	108	ALA	5.9
1	A	297	PHE	5.8
1	B	561	ALA	5.6
1	A	301	TYR	5.3
1	C	108	ALA	5.2
1	C	559	THR	5.1
1	A	299	TYR	5.1
1	B	558	ALA	5.0
1	C	557	ALA	4.9
1	C	290	SER	4.8
1	A	289	LEU	4.7
1	C	558	ALA	4.6
1	B	112	LEU	4.6
1	D	108	ALA	4.5
1	A	294	THR	4.5
1	D	112	LEU	4.4
1	A	108	ALA	4.4
1	D	113	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	107	GLN	4.2
1	A	563	ASN	4.0
1	B	559	THR	3.9
1	C	556	THR	3.9
1	B	560	ASN	3.9
1	D	117	LEU	3.9
1	B	557	ALA	3.8
1	B	104	VAL	3.8
1	B	105	SER	3.8
1	B	114	HIS	3.8
1	D	104	VAL	3.7
1	A	296	SER	3.6
1	C	560	ASN	3.6
1	C	347	VAL	3.5
1	B	556	THR	3.4
1	C	299	TYR	3.4
1	B	347	VAL	3.4
1	C	291	ASP	3.3
1	C	555	LEU	3.3
1	A	300	SER	3.3
1	C	111	LEU	3.2
1	D	116	THR	3.2
1	A	295	GLY	3.2
1	C	110	GLN	3.2
1	C	348	PRO	3.1
1	A	104	VAL	3.1
1	D	294	THR	3.1
1	C	288	LEU	3.0
1	A	556	THR	3.0
1	A	298	SER	3.0
1	A	288	LEU	3.0
1	A	107	GLN	3.0
1	B	115	HIS	2.9
1	D	347	VAL	2.9
1	D	114	HIS	2.9
1	B	555	LEU	2.9
1	C	312	ASP	2.9
1	A	557	ALA	2.9
1	A	303	THR	2.8
1	A	293	ASN	2.8
1	A	291	ASP	2.8
1	C	112	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	106	SER	2.7
1	D	300	SER	2.7
1	B	107	GLN	2.6
1	D	122	PHE	2.6
1	C	294	THR	2.6
1	C	298	SER	2.6
1	D	558	ALA	2.6
1	B	295	GLY	2.6
1	C	292	PHE	2.5
1	A	120	GLY	2.4
1	C	289	LEU	2.4
1	C	113	LEU	2.4
1	D	288	LEU	2.4
1	D	348	PRO	2.4
1	B	289	LEU	2.3
1	C	266	THR	2.3
1	D	119	ASN	2.3
1	C	120	GLY	2.3
1	A	225	HIS	2.3
1	A	558	ALA	2.2
1	C	103	SER	2.2
1	A	111	LEU	2.2
1	A	109	LYS	2.2
1	D	563	ASN	2.2
1	A	113	LEU	2.2
1	D	557	ALA	2.2
1	D	110	GLN	2.2
1	D	118	GLY	2.2
1	C	109	LYS	2.2
1	C	297	PHE	2.1
1	C	118	GLY	2.1
1	C	295	GLY	2.1
1	D	109	LYS	2.1
1	B	28	ASP	2.1
1	A	118	GLY	2.0
1	D	293	ASN	2.0
1	B	291	ASP	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](#)

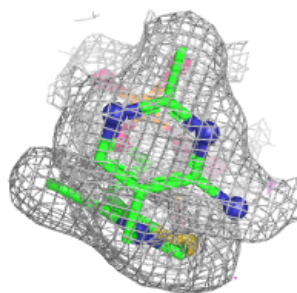
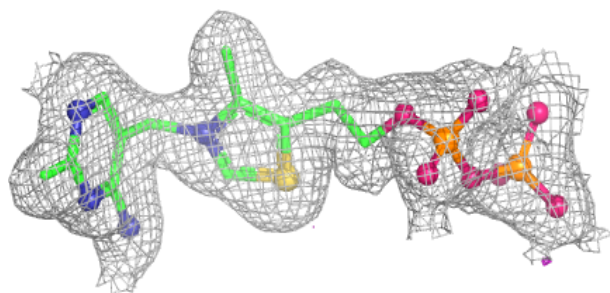
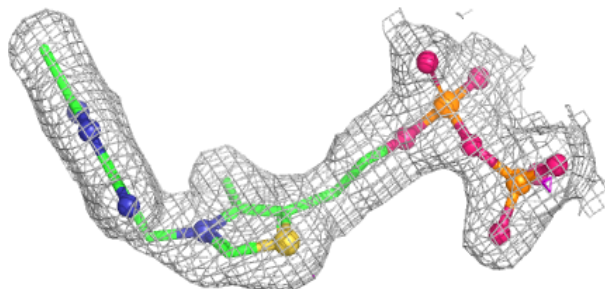
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	MG	B	601	1/1	0.97	0.04	17,17,17,17	0
3	MG	D	601	1/1	0.97	0.08	20,20,20,20	0
3	MG	A	601	1/1	0.98	0.03	15,15,15,15	0
2	TPP	A	600	26/26	0.98	0.05	10,13,15,16	0
3	MG	C	601	1/1	0.98	0.02	12,12,12,12	0
2	TPP	B	600	26/26	0.98	0.04	9,12,15,15	0
2	TPP	C	600	26/26	0.99	0.04	7,10,12,14	0
2	TPP	D	600	26/26	0.99	0.04	8,14,17,18	0

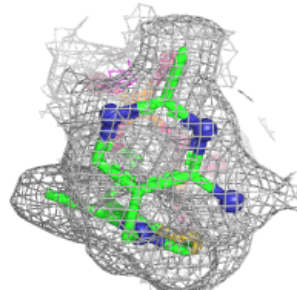
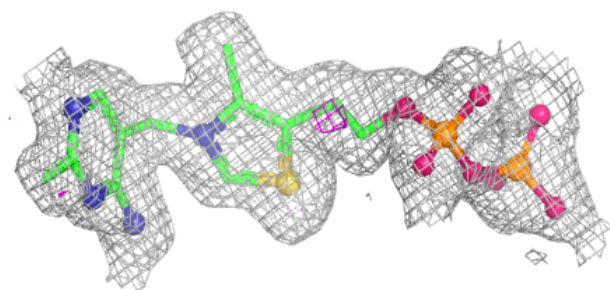
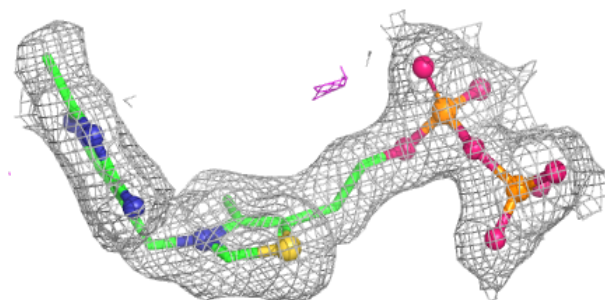
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 600:

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

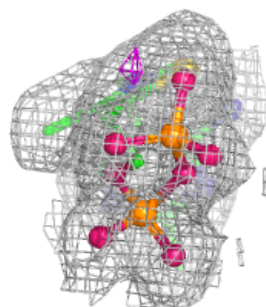
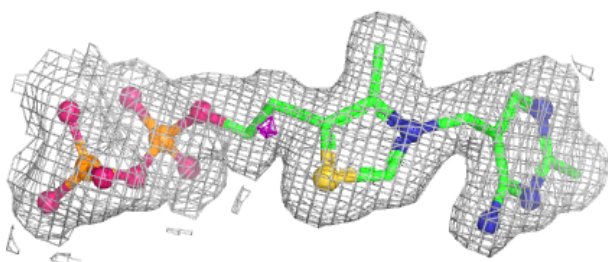
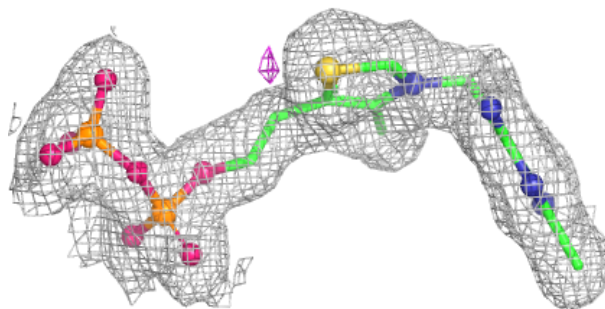
**Electron density around TPP B 600:**

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

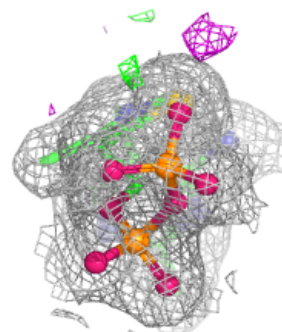
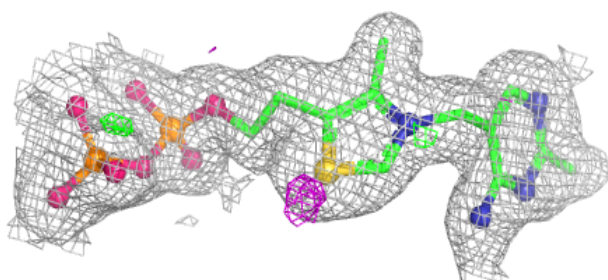
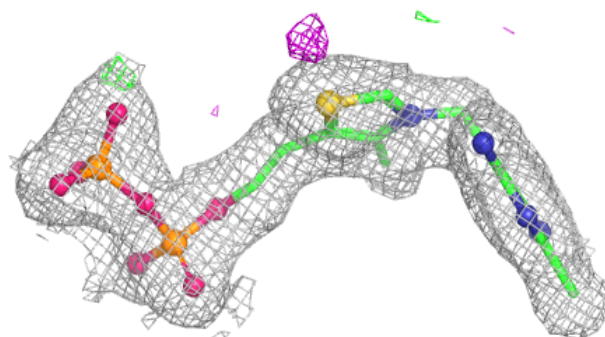


Electron density around TPP C 600:

$2mF_o-DF_c$ (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.