Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 11:29 AM EST

PDB ID	:	1PVD
Title	:	CRYSTAL STRUCTURE OF THE THIAMIN DIPHOSPHATE DEPENDENT ENZYME PYRUVATE DECARBOXYLASE FROM THE YEAST SACCHAROMYCES CEREVISIAE AT 2.3 ANGSTROMS RESOLUTION
Authors	:	Furey, W.; Arjunan, P.
Deposited on	:	1995-04-20
Resolution	:	2.30 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:

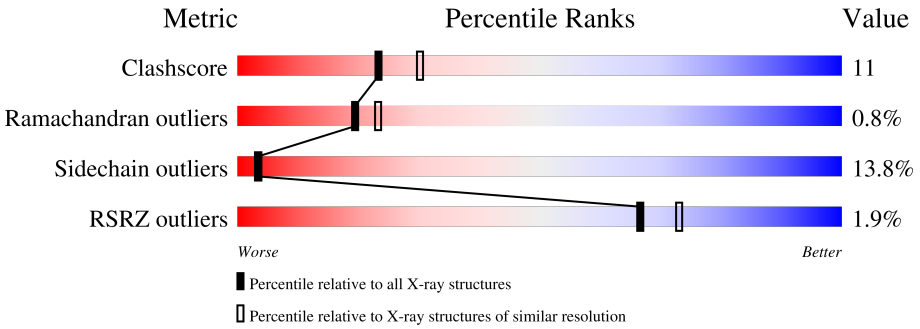
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	555	2% 60% 25% 11%
1	B	555	% 59% 26% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8753 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	537	Total	C	N	O	S	0	0	0
			4130	2638	694	782	16			
1	B	537	Total	C	N	O	S	0	0	0
			4130	2638	694	782	16			

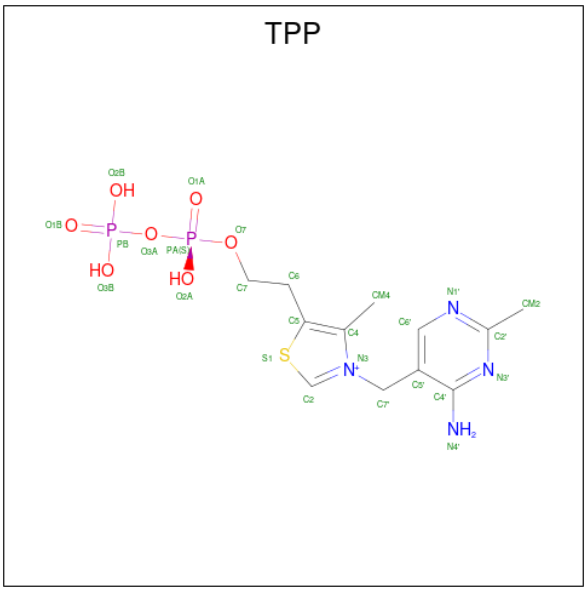
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ALA	ARG	conflict	UNP P06169
A	143	ALA	CYS	conflict	UNP P06169
A	206	ALA	VAL	conflict	UNP P06169
A	208	VAL	ALA	conflict	UNP P06169
A	538	ILE	VAL	conflict	UNP P06169
A	551	LYS	GLU	conflict	UNP P06169
B	55	ALA	ARG	conflict	UNP P06169
B	143	ALA	CYS	conflict	UNP P06169
B	206	ALA	VAL	conflict	UNP P06169
B	208	VAL	ALA	conflict	UNP P06169
B	538	ILE	VAL	conflict	UNP P06169
B	551	LYS	GLU	conflict	UNP P06169

- Molecule 2 is MAGNESIUM ION (three-letter code: 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 (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



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

- Molecule 4 is water.

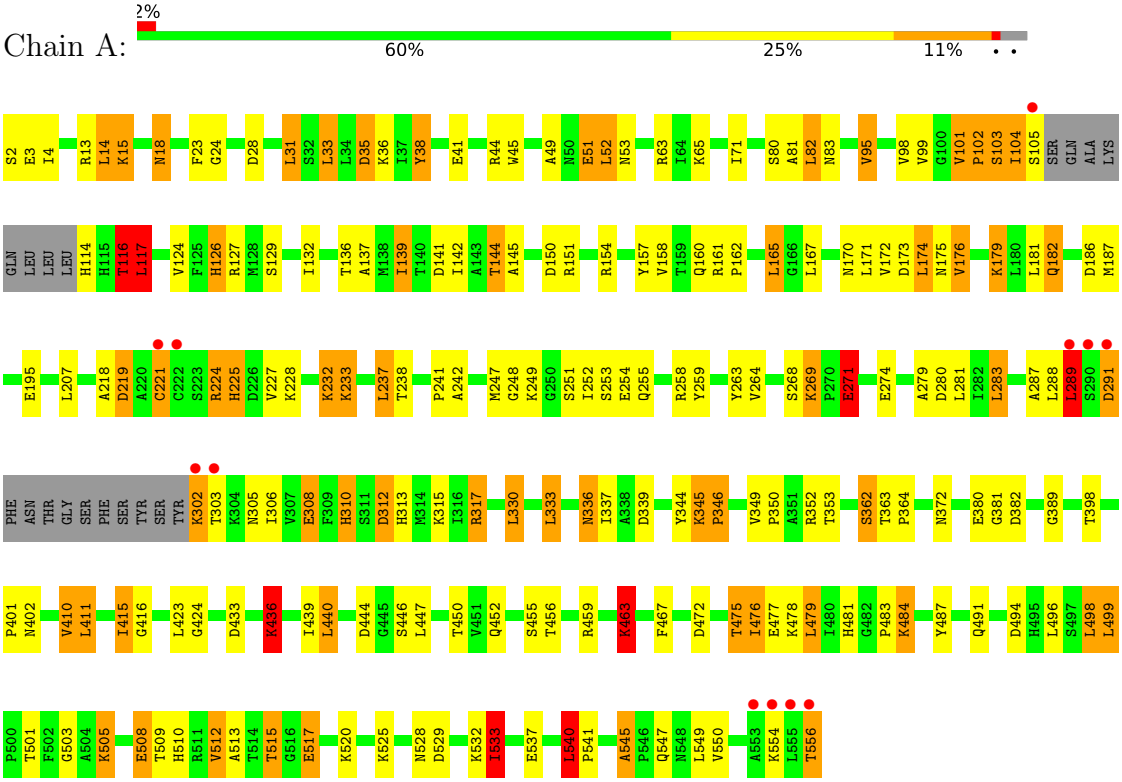
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	235	Total	O	0	0
			235	235		
4	B	204	Total	O	0	0
			204	204		

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.

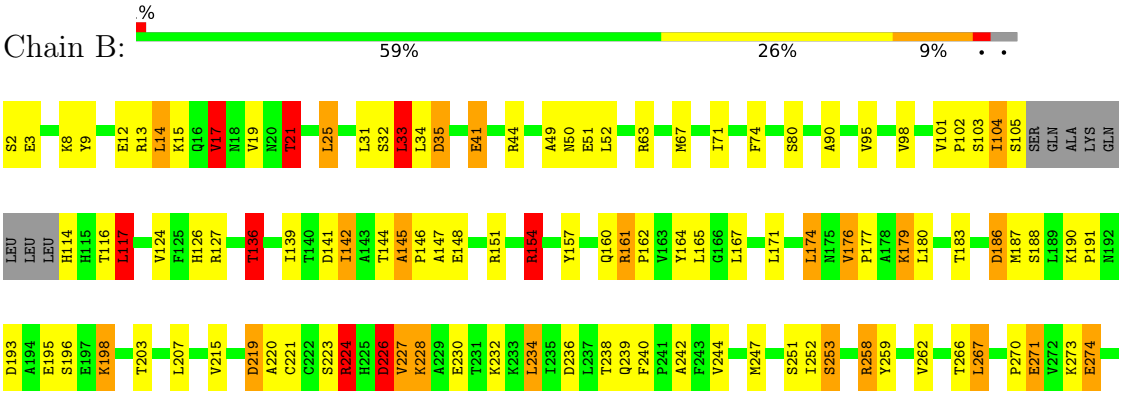
• Molecule 1: PYRUVATE DECARBOXYLASE

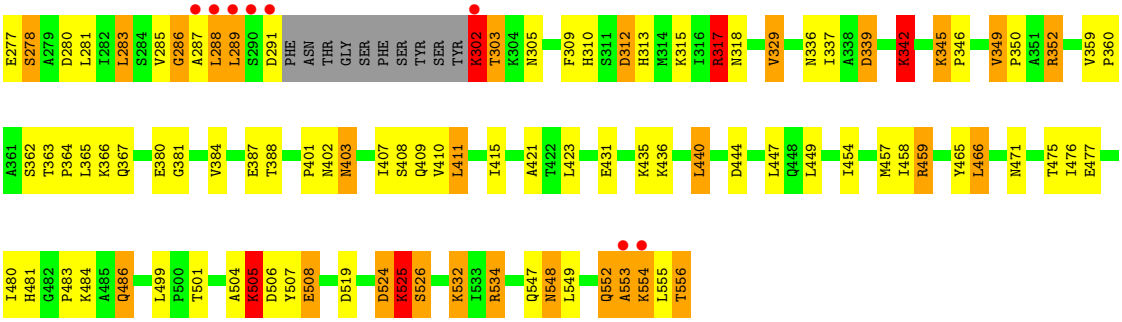
Chain A:



• Molecule 1: PYRUVATE DECARBOXYLASE

Chain B:




E277 S278 A279 D280 L281 I282 L283 S284 V285 G286 A287 L288 L289 S290 D291 PHE ASN THR GLY SER PHE SER TYR SER TYR K302 T303 K304 N305 F309 H310 S311 D312 H313 M314 K315 I316 R317 N318 V329 N336 I337 A338 D339 K342 K345 P346 V349 P350 A351 R352 V359 P360
A361 S362 T363 P364 L365 K366 Q367 E380 G381 V384 E387 T388 P401 N402 N403 I407 S408 Q409 V410 L411 I415 A421 T422 L423 E431 K435 K436 L440 D444 L447 Q448 L449 I454 M457 I458 R459 Y465 L466 N471 T475 I476 E477
I480 H481 G482 P483 K484 A485 Q486 L499 P500 T501 A504 K505 D506 Y507 E508 D519 D524 K525 S526 K532 I533 R534 Q547 N548 L549 Q552 A553 K554 L555 T556

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.06Å 74.75Å 120.32Å 90.00° 116.58° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 32.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.8 (10.00-2.30) 93.0 (32.21-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	GPRLSA, X-PLOR	Depositor
R, R_{free}	0.165 , (Not available) 0.153 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 63.7	EDS
L-test for twinning[1]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8753	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ 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	1.07	4/4215 (0.1%)	2.08	141/5728 (2.5%)
1	B	1.05	3/4215 (0.1%)	2.12	126/5728 (2.2%)
All	All	1.06	7/8430 (0.1%)	2.10	267/11456 (2.3%)

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	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	SER	CB-OG	7.96	1.52	1.42
1	B	471	ASN	CB-CG	7.40	1.68	1.51
1	A	416	GLY	N-CA	6.45	1.55	1.46
1	B	459	ARG	CZ-NH1	5.20	1.39	1.33
1	A	415	ILE	C-O	5.18	1.33	1.23
1	A	254	GLU	CD-OE1	-5.18	1.20	1.25
1	A	537	GLU	CD-OE1	-5.17	1.20	1.25

All (267) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	258	ARG	NE-CZ-NH2	-22.95	108.83	120.30
1	B	459	ARG	NE-CZ-NH1	20.68	130.64	120.30
1	B	534	ARG	NE-CZ-NH1	-20.26	110.17	120.30
1	A	317	ARG	NE-CZ-NH2	-19.94	110.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	317	ARG	NE-CZ-NH1	19.18	129.89	120.30
1	B	459	ARG	CD-NE-CZ	19.14	150.40	123.60
1	B	151	ARG	NE-CZ-NH2	-18.61	111.00	120.30
1	A	258	ARG	NE-CZ-NH1	17.82	129.21	120.30
1	B	258	ARG	NE-CZ-NH1	16.55	128.57	120.30
1	B	161	ARG	NE-CZ-NH2	-16.49	112.05	120.30
1	B	459	ARG	NE-CZ-NH2	-16.36	112.12	120.30
1	A	494	ASP	CB-CG-OD2	16.10	132.79	118.30
1	B	151	ARG	NE-CZ-NH1	15.69	128.15	120.30
1	A	312	ASP	CB-CG-OD1	14.28	131.15	118.30
1	A	224	ARG	NE-CZ-NH1	13.64	127.12	120.30
1	A	352	ARG	NE-CZ-NH1	13.30	126.95	120.30
1	B	161	ARG	NE-CZ-NH1	12.72	126.66	120.30
1	B	63	ARG	NE-CZ-NH1	12.60	126.60	120.30
1	B	127	ARG	NE-CZ-NH2	12.52	126.56	120.30
1	B	352	ARG	NE-CZ-NH1	12.45	126.52	120.30
1	B	459	ARG	CA-CB-CG	12.39	140.66	113.40
1	A	154	ARG	NE-CZ-NH1	-12.22	114.19	120.30
1	A	13	ARG	NE-CZ-NH2	-12.12	114.24	120.30
1	A	339	ASP	CB-CG-OD1	12.11	129.20	118.30
1	B	534	ARG	NE-CZ-NH2	11.92	126.26	120.30
1	B	17	VAL	CA-CB-CG1	11.90	128.75	110.90
1	B	25	LEU	CA-CB-CG	11.86	142.58	115.30
1	A	433	ASP	CB-CG-OD2	-11.75	107.73	118.30
1	B	477	GLU	OE1-CD-OE2	11.73	137.37	123.30
1	A	151	ARG	NE-CZ-NH2	11.23	125.92	120.30
1	A	459	ARG	NE-CZ-NH2	-11.23	114.69	120.30
1	B	277	GLU	OE1-CD-OE2	-11.16	109.91	123.30
1	A	317	ARG	CD-NE-CZ	10.54	138.35	123.60
1	A	433	ASP	CB-CG-OD1	10.52	127.77	118.30
1	B	280	ASP	CB-CG-OD1	10.40	127.66	118.30
1	A	114	HIS	CA-CB-CG	10.16	130.87	113.60
1	A	150	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	A	501	THR	CA-CB-CG2	9.65	125.91	112.40
1	B	342	LYS	N-CA-CB	9.51	127.73	110.60
1	A	352	ARG	NE-CZ-NH2	-9.51	115.55	120.30
1	A	280	ASP	CB-CG-OD1	9.24	126.62	118.30
1	A	127	ARG	CD-NE-CZ	-9.20	110.72	123.60
1	A	494	ASP	OD1-CG-OD2	-9.05	106.09	123.30
1	B	164	TYR	CB-CG-CD1	8.89	126.33	121.00
1	B	519	ASP	CB-CG-OD1	8.81	126.23	118.30
1	A	280	ASP	CB-CG-OD2	-8.81	110.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	336	ASN	CB-CA-C	-8.72	92.96	110.40
1	A	151	ARG	NH1-CZ-NH2	-8.67	109.87	119.40
1	A	415	ILE	CA-C-N	8.54	133.29	116.20
1	B	524	ASP	CB-CG-OD2	-8.45	110.69	118.30
1	A	533	ILE	CB-CA-C	-8.39	94.82	111.60
1	A	533	ILE	CA-CB-CG2	8.32	127.54	110.90
1	A	44	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	B	524	ASP	CB-CG-OD1	8.28	125.75	118.30
1	B	258	ARG	CD-NE-CZ	8.27	135.18	123.60
1	A	459	ARG	NH1-CZ-NH2	8.21	128.43	119.40
1	A	102	PRO	C-N-CA	8.19	142.16	121.70
1	B	154	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	B	227	VAL	CG1-CB-CG2	8.12	123.89	110.90
1	A	515	THR	N-CA-CB	-8.12	94.88	110.30
1	B	151	ARG	CD-NE-CZ	8.05	134.88	123.60
1	B	317	ARG	NE-CZ-NH1	-8.01	116.29	120.30
1	B	444	ASP	CB-CG-OD1	7.95	125.45	118.30
1	B	291	ASP	CB-CG-OD1	7.94	125.45	118.30
1	B	274	GLU	CA-CB-CG	7.90	130.78	113.40
1	A	151	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	219	ASP	CB-CG-OD2	-7.82	111.27	118.30
1	B	342	LYS	CA-CB-CG	7.75	130.45	113.40
1	A	237	LEU	CB-CA-C	7.74	124.91	110.20
1	B	403	ASN	N-CA-CB	-7.71	96.73	110.60
1	B	280	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	B	136	THR	N-CA-CB	-7.62	95.81	110.30
1	A	161	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	35	ASP	CB-CG-OD1	7.49	125.04	118.30
1	A	127	ARG	NE-CZ-NH2	7.48	124.04	120.30
1	A	499	LEU	CB-CA-C	7.45	124.36	110.20
1	A	477	GLU	OE1-CD-OE2	7.44	132.22	123.30
1	A	33	LEU	CA-CB-CG	7.43	132.39	115.30
1	A	176	VAL	N-CA-CB	-7.35	95.33	111.50
1	B	526	SER	CA-CB-OG	-7.34	91.39	111.20
1	B	21	THR	CA-CB-CG2	7.33	122.66	112.40
1	B	230	GLU	OE1-CD-OE2	-7.28	114.56	123.30
1	B	285	VAL	CA-C-O	7.28	135.38	120.10
1	B	403	ASN	OD1-CG-ND2	7.22	138.50	121.90
1	B	35	ASP	CB-CG-OD2	-7.09	111.91	118.30
1	B	164	TYR	CB-CG-CD2	-7.06	116.77	121.00
1	A	35	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	B	310	HIS	N-CA-CB	7.00	123.20	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	459	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	A	237	LEU	N-CA-CB	-6.91	96.58	110.40
1	A	444	ASP	CB-CG-OD2	6.89	124.50	118.30
1	A	436	LYS	CD-CE-NZ	-6.89	95.86	111.70
1	A	312	ASP	OD1-CG-OD2	-6.84	110.31	123.30
1	B	167	LEU	CB-CG-CD2	-6.80	99.44	111.00
1	B	227	VAL	N-CA-CB	-6.79	96.57	111.50
1	B	384	VAL	CG1-CB-CG2	-6.79	100.04	110.90
1	B	259	TYR	CB-CG-CD2	6.77	125.06	121.00
1	B	17	VAL	N-CA-CB	-6.75	96.64	111.50
1	B	286	GLY	O-C-N	6.75	133.50	122.70
1	B	145	ALA	CB-CA-C	6.74	120.22	110.10
1	B	525	LYS	CB-CG-CD	6.71	129.05	111.60
1	A	515	THR	OG1-CB-CG2	6.62	125.24	110.00
1	A	150	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	330	LEU	CA-CB-CG	6.58	130.43	115.30
1	B	148	GLU	OE1-CD-OE2	-6.55	115.44	123.30
1	B	17	VAL	CB-CA-C	6.54	123.83	111.40
1	A	258	ARG	NH1-CZ-NH2	-6.52	112.23	119.40
1	B	227	VAL	CB-CA-C	6.51	123.78	111.40
1	A	238	THR	CA-CB-CG2	6.51	121.51	112.40
1	A	479	LEU	CA-CB-CG	6.51	130.26	115.30
1	B	283	LEU	CA-CB-CG	6.50	130.25	115.30
1	A	186	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	63	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	A	28	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	329	VAL	CA-CB-CG1	6.47	120.61	110.90
1	B	215	VAL	CA-CB-CG1	6.39	120.49	110.90
1	B	339	ASP	CB-CA-C	6.38	123.16	110.40
1	A	382	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	193	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	424	GLY	CA-C-O	-6.34	109.19	120.60
1	A	23	PHE	CB-CG-CD2	-6.33	116.37	120.80
1	B	251	SER	CB-CA-C	-6.33	98.08	110.10
1	B	154	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	A	141	ASP	CB-CG-OD1	6.31	123.98	118.30
1	A	533	ILE	N-CA-CB	6.27	125.21	110.80
1	B	312	ASP	CB-CG-OD1	6.26	123.93	118.30
1	B	471	ASN	N-CA-CB	6.24	121.84	110.60
1	B	74	PHE	CB-CG-CD1	-6.21	116.45	120.80
1	A	137	ALA	N-CA-CB	6.20	118.78	110.10
1	A	362	SER	CB-CA-C	-6.20	98.31	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264	VAL	N-CA-C	-6.19	94.28	111.00
1	A	144	THR	CA-CB-CG2	6.16	121.02	112.40
1	A	49	ALA	CB-CA-C	6.13	119.30	110.10
1	A	472	ASP	N-CA-CB	-6.12	99.59	110.60
1	A	271	GLU	CA-CB-CG	6.09	126.80	113.40
1	A	467	PHE	CB-CG-CD1	-6.09	116.54	120.80
1	A	503	GLY	CA-C-O	-6.06	109.69	120.60
1	A	116	THR	OG1-CB-CG2	-6.06	96.06	110.00
1	A	31	LEU	CB-CG-CD1	6.05	121.29	111.00
1	A	95	VAL	O-C-N	6.04	132.36	122.70
1	B	285	VAL	N-CA-C	-6.01	94.78	111.00
1	A	81	ALA	N-CA-CB	-5.99	101.72	110.10
1	A	161	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	13	ARG	NH1-CZ-NH2	5.98	125.98	119.40
1	A	291	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	317	ARG	CA-CB-CG	5.97	126.54	113.40
1	A	545	ALA	N-CA-CB	-5.96	101.76	110.10
1	B	136	THR	OG1-CB-CG2	5.94	123.66	110.00
1	A	99	VAL	CA-CB-CG2	5.94	119.80	110.90
1	B	302	LYS	CA-CB-CG	5.92	126.42	113.40
1	A	287	ALA	C-N-CA	5.89	136.42	121.70
1	B	116	THR	N-CA-CB	5.89	121.48	110.30
1	A	529	ASP	N-CA-CB	-5.88	100.01	110.60
1	B	180	LEU	CA-CB-CG	5.88	128.83	115.30
1	B	236	ASP	O-C-N	5.87	132.09	122.70
1	A	436	LYS	N-CA-CB	-5.87	100.04	110.60
1	A	444	ASP	OD1-CG-OD2	-5.86	112.17	123.30
1	A	263	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	A	289	LEU	N-CA-C	5.81	126.70	111.00
1	A	463	LYS	CB-CG-CD	5.81	126.71	111.60
1	A	18	ASN	N-CA-C	5.80	126.66	111.00
1	B	352	ARG	NH1-CZ-NH2	-5.80	113.03	119.40
1	A	44	ARG	NH1-CZ-NH2	-5.79	113.03	119.40
1	B	224	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	415	ILE	CA-C-O	-5.78	107.96	120.10
1	A	176	VAL	CG1-CB-CG2	5.78	120.15	110.90
1	A	513	ALA	CB-CA-C	-5.75	101.47	110.10
1	B	219	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	B	484	LYS	CB-CA-C	5.72	121.83	110.40
1	A	227	VAL	N-CA-CB	-5.71	98.93	111.50
1	A	339	ASP	OD1-CG-OD2	-5.71	112.45	123.30
1	B	234	LEU	CA-CB-CG	5.68	128.35	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	TYR	CB-CG-CD1	5.67	124.40	121.00
1	A	176	VAL	CB-CA-C	5.67	122.17	111.40
1	B	366	LYS	N-CA-CB	5.66	120.78	110.60
1	B	259	TYR	CB-CG-CD1	-5.65	117.61	121.00
1	A	173	ASP	O-C-N	5.65	131.73	122.70
1	A	476	ILE	CG1-CB-CG2	5.63	123.78	111.40
1	B	141	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	B	147	ALA	CB-CA-C	5.58	118.47	110.10
1	A	141	ASP	CA-C-O	-5.58	108.39	120.10
1	A	508	GLU	N-CA-CB	5.57	120.63	110.60
1	A	308	GLU	OE1-CD-OE2	5.56	129.97	123.30
1	A	333	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	226	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	227	VAL	CB-CA-C	5.54	121.92	111.40
1	A	195	GLU	CA-CB-CG	5.53	125.57	113.40
1	A	259	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	B	475	THR	N-CA-CB	5.51	120.78	110.30
1	B	186	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	503	GLY	O-C-N	5.49	131.49	122.70
1	B	486	GLN	CB-CG-CD	5.49	125.87	111.60
1	B	277	GLU	CB-CA-C	5.48	121.36	110.40
1	B	407	ILE	C-N-CA	5.48	135.40	121.70
1	B	33	LEU	CB-CG-CD2	5.48	120.31	111.00
1	A	505	LYS	CB-CG-CD	5.47	125.83	111.60
1	A	444	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	289	LEU	CB-CA-C	5.46	120.58	110.20
1	A	219	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	349	VAL	N-CA-CB	-5.46	99.50	111.50
1	A	289	LEU	N-CA-CB	-5.42	99.55	110.40
1	A	224	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	528	ASN	CA-CB-CG	-5.42	101.48	113.40
1	B	440	LEU	CA-CB-CG	5.40	127.73	115.30
1	A	456	THR	CA-CB-OG1	-5.40	97.66	109.00
1	B	19	VAL	N-CA-C	-5.38	96.47	111.00
1	A	439	ILE	CA-CB-CG2	5.37	121.63	110.90
1	B	14	LEU	CB-CG-CD1	5.37	120.12	111.00
1	A	3	GLU	CG-CD-OE1	5.35	129.00	118.30
1	B	167	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	101	VAL	N-CA-CB	-5.34	99.74	111.50
1	A	440	LEU	CA-CB-CG	5.34	127.59	115.30
1	A	310	HIS	N-CA-CB	5.29	120.13	110.60
1	A	51	GLU	OE1-CD-OE2	5.29	129.65	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	529	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	549	LEU	CB-CA-C	5.26	120.20	110.20
1	B	117	LEU	CB-CG-CD2	-5.26	102.05	111.00
1	A	167	LEU	N-CA-CB	-5.26	99.88	110.40
1	A	95	VAL	CA-C-O	-5.26	109.06	120.10
1	B	117	LEU	CB-CG-CD1	5.26	119.94	111.00
1	A	175	ASN	O-C-N	5.25	131.11	122.70
1	B	309	PHE	O-C-N	5.25	131.10	122.70
1	B	174	LEU	CB-CA-C	5.25	120.17	110.20
1	A	28	ASP	CB-CG-OD1	5.22	123.00	118.30
1	B	144	THR	CA-CB-OG1	-5.22	98.04	109.00
1	B	401	PRO	N-CA-C	-5.21	98.56	112.10
1	A	525	LYS	O-C-N	5.20	131.03	122.70
1	B	532	LYS	CB-CG-CD	5.20	125.13	111.60
1	A	105	SER	CB-CA-C	5.20	119.98	110.10
1	B	466	LEU	CB-CG-CD1	5.19	119.83	111.00
1	B	114	HIS	N-CA-CB	5.19	119.94	110.60
1	B	525	LYS	CG-CD-CE	5.19	127.47	111.90
1	B	203	THR	CA-CB-OG1	-5.18	98.12	109.00
1	B	401	PRO	N-CD-CG	-5.18	95.44	103.20
1	A	410	VAL	CA-CB-CG2	-5.17	103.14	110.90
1	B	176	VAL	N-CA-CB	-5.17	100.12	111.50
1	B	342	LYS	CB-CG-CD	5.17	125.03	111.60
1	B	409	GLN	CB-CA-C	5.16	120.73	110.40
1	A	283	LEU	CA-CB-CG	5.16	127.17	115.30
1	B	154	ARG	CG-CD-NE	-5.16	100.97	111.80
1	B	367	GLN	O-C-N	-5.15	114.46	122.70
1	A	117	LEU	CB-CG-CD1	5.13	119.72	111.00
1	B	465	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	B	9	TYR	CB-CG-CD2	5.12	124.07	121.00
1	B	380	GLU	CB-CA-C	-5.11	100.18	110.40
1	A	38	TYR	CB-CG-CD2	5.10	124.06	121.00
1	B	13	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	A	487	TYR	CB-CG-CD2	5.10	124.06	121.00
1	B	421	ALA	CB-CA-C	5.09	117.73	110.10
1	B	63	ARG	CD-NE-CZ	-5.08	116.49	123.60
1	A	45	TRP	O-C-N	5.08	130.82	122.70
1	B	349	VAL	CB-CA-C	5.07	121.04	111.40
1	A	517	GLU	CG-CD-OE1	5.06	128.41	118.30
1	A	154	ARG	CD-NE-CZ	5.05	130.68	123.60
1	B	183	THR	CA-CB-CG2	5.04	119.46	112.40
1	A	14	LEU	CB-CG-CD1	5.04	119.56	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	32	SER	N-CA-CB	5.03	118.05	110.50
1	A	540	LEU	N-CA-CB	-5.03	100.34	110.40
1	A	160	GLN	N-CA-CB	5.02	119.64	110.60
1	B	339	ASP	CB-CG-OD1	5.02	122.82	118.30
1	B	508	GLU	O-C-N	5.02	130.74	122.70
1	A	127	ARG	O-C-N	5.02	130.73	122.70
1	B	33	LEU	CA-CB-CG	5.02	126.85	115.30
1	A	38	TYR	CB-CG-CD1	-5.02	117.99	121.00
1	B	505	LYS	N-CA-CB	-5.01	101.58	110.60
1	A	237	LEU	CA-CB-CG	5.01	126.82	115.30
1	A	411	LEU	CB-CA-C	5.00	119.71	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	154	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	4130	0	4150	87	0
1	B	4130	0	4151	107	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	16	1	0
3	B	26	0	16	0	0
4	A	235	0	0	8	0
4	B	204	0	0	5	0
All	All	8753	0	8333	188	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 11.

All (188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LYS:HD3	1:B:228:LYS:H	1.17	1.09
1:A:303:THR:HG22	1:A:306:ILE:HD11	1.47	0.96
1:B:505:LYS:HE2	1:B:506:ASP:H	1.31	0.91
1:A:116:THR:HG22	4:A:935:HOH:O	1.73	0.88
1:A:496:LEU:HD22	1:A:509:THR:HB	1.56	0.85
1:A:157:TYR:HD2	1:A:187:MET:HE2	1.43	0.83
1:A:475:THR:HG22	4:A:834:HOH:O	1.77	0.83
1:A:241:PRO:HB3	1:A:349:VAL:HG12	1.62	0.82
1:B:476:ILE:HG22	4:B:861:HOH:O	1.86	0.74
1:B:266:THR:HA	1:B:273:LYS:HE2	1.69	0.73
1:A:158:VAL:HG23	1:A:187:MET:CE	2.18	0.73
1:A:380:GLU:HG2	1:A:401:PRO:HB2	1.71	0.73
1:B:228:LYS:H	1:B:228:LYS:CD	2.01	0.71
1:A:415:ILE:O	1:A:446:SER:HB3	1.92	0.70
1:B:219:ASP:HB3	1:B:286:GLY:HA2	1.72	0.70
1:B:553:ALA:HA	1:B:556:THR:HG22	1.73	0.69
1:A:158:VAL:HG23	1:A:187:MET:HE3	1.73	0.69
1:A:157:TYR:HB3	1:A:187:MET:HE1	1.73	0.69
1:B:228:LYS:HD3	1:B:228:LYS:N	1.99	0.68
1:B:525:LYS:H	1:B:525:LYS:HE2	1.58	0.68
1:B:154:ARG:NH2	1:B:188:SER:O	2.27	0.67
1:B:345:LYS:HE3	1:B:346:PRO:HD2	1.77	0.67
1:B:476:ILE:O	1:B:480:ILE:HD12	1.95	0.66
1:B:287:ALA:HB1	1:B:288:LEU:HD12	1.78	0.66
1:B:303:THR:HB	1:B:305:ASN:H	1.61	0.65
1:B:274:GLU:O	1:B:278:SER:HB2	1.96	0.65
1:B:267:LEU:HD11	1:B:552:GLN:HA	1.77	0.65
1:B:387:GLU:HG3	1:B:388:THR:N	2.11	0.64
1:A:499:LEU:HD22	1:A:533:ILE:HD12	1.80	0.64
1:A:508:GLU:HG3	1:A:532:LYS:HD2	1.81	0.63
1:B:524:ASP:HA	1:B:525:LYS:HE2	1.81	0.62
1:A:171:LEU:HA	1:A:174:LEU:HD22	1.82	0.62
1:B:139:ILE:HG22	1:B:171:LEU:HD12	1.81	0.61
1:B:505:LYS:H	1:B:505:LYS:CD	2.14	0.60
1:A:71:ILE:HG12	1:A:98:VAL:HB	1.83	0.60
1:A:139:ILE:HG21	1:A:145:ALA:HB2	1.83	0.60
1:B:95:VAL:O	1:B:162:PRO:HA	2.01	0.60
1:B:342:LYS:HD2	1:B:342:LYS:O	2.01	0.60
1:B:554:LYS:HD2	1:B:555:LEU:HG	1.84	0.60
1:B:247:MET:HG3	1:B:410:VAL:HB	1.84	0.59
1:B:359:VAL:HB	1:B:360:PRO:HD2	1.85	0.59
1:A:219:ASP:HB2	4:A:965:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:VAL:HG22	1:A:517:GLU:HB3	1.85	0.58
1:A:126:HIS:HE1	1:A:136:THR:OG1	1.85	0.58
1:B:476:ILE:HG13	1:B:549:LEU:HD21	1.85	0.58
1:A:95:VAL:O	1:A:162:PRO:HA	2.04	0.57
1:B:15:LYS:HE3	1:B:41:GLU:O	2.03	0.57
1:A:478:LYS:HB3	1:A:483:PRO:HA	1.85	0.57
1:B:142:ILE:HG21	1:B:174:LEU:HB3	1.86	0.57
1:A:247:MET:CG	1:A:410:VAL:HB	2.35	0.57
1:A:271:GLU:HB3	1:A:350:PRO:HB3	1.86	0.56
1:A:228:LYS:O	1:A:232:LYS:HG3	2.06	0.56
1:A:269:LYS:HE3	4:A:667:HOH:O	2.06	0.56
1:B:33:LEU:HD13	1:B:71:ILE:HD13	1.87	0.56
1:A:157:TYR:HD2	1:A:187:MET:CE	2.18	0.56
1:B:552:GLN:OE1	1:B:553:ALA:N	2.39	0.56
1:A:101:VAL:HG13	1:A:102:PRO:HD2	1.88	0.56
1:B:160:GLN:O	1:B:161:ARG:HG3	2.06	0.55
1:B:177:PRO:HB3	1:B:179:LYS:HE2	1.89	0.55
1:A:389:GLY:HA2	1:A:476:ILE:HG21	1.89	0.55
1:B:525:LYS:H	1:B:525:LYS:CD	2.20	0.55
1:B:302:LYS:O	1:B:303:THR:OG1	2.23	0.55
1:A:463:LYS:NZ	4:A:798:HOH:O	2.38	0.55
1:A:104:ILE:O	1:A:104:ILE:HG22	2.07	0.55
1:A:4:ILE:HD11	1:A:181:LEU:HD11	1.89	0.55
1:B:267:LEU:HD21	1:B:552:GLN:HB2	1.89	0.55
1:B:525:LYS:H	1:B:525:LYS:CE	2.19	0.55
1:B:49:ALA:O	1:B:50:ASN:HB3	2.07	0.54
1:B:228:LYS:HE2	4:B:966:HOH:O	2.07	0.54
1:A:484:LYS:HB2	1:A:484:LYS:NZ	2.22	0.54
1:B:126:HIS:HE1	1:B:136:THR:CG2	2.20	0.54
1:B:288:LEU:HD12	1:B:288:LEU:H	1.71	0.54
1:B:98:VAL:HG22	1:B:165:LEU:HD23	1.90	0.53
1:B:271:GLU:HB2	1:B:350:PRO:HB3	1.91	0.53
1:B:508:GLU:HB2	1:B:534:ARG:HG2	1.91	0.52
1:A:247:MET:HG3	1:A:410:VAL:HB	1.91	0.52
1:A:233:LYS:O	1:A:237:LEU:HB2	2.09	0.52
1:A:253:SER:HB3	1:A:402:ASN:OD1	2.10	0.52
1:B:21:THR:HB	1:B:44:ARG:HG3	1.92	0.52
1:A:345:LYS:H	1:A:345:LYS:CD	2.24	0.51
1:A:281:LEU:HD13	1:A:305:ASN:HB3	1.93	0.50
1:B:458:ILE:HG23	1:B:505:LYS:HZ3	1.77	0.50
1:A:481:HIS:HE1	1:B:35:ASP:OD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:LYS:HE3	4:B:941:HOH:O	2.10	0.49
1:A:52:LEU:HD21	1:A:83:ASN:HB3	1.94	0.49
1:B:190:LYS:HG2	1:B:191:PRO:HD2	1.94	0.49
1:B:504:ALA:HA	1:B:505:LYS:HZ3	1.77	0.49
1:B:154:ARG:HG3	1:B:186:ASP:O	2.12	0.49
1:A:224:ARG:NH1	4:A:854:HOH:O	2.42	0.48
1:B:505:LYS:H	1:B:505:LYS:CE	2.26	0.48
1:A:15:LYS:HG2	4:A:895:HOH:O	2.14	0.48
1:B:21:THR:HG22	1:B:431:GLU:OE2	2.14	0.48
1:A:179:LYS:O	1:A:182:GLN:HG2	2.14	0.48
1:B:126:HIS:HE1	1:B:136:THR:HG23	1.78	0.47
1:B:548:ASN:O	1:B:552:GLN:HB2	2.14	0.47
1:B:126:HIS:CE1	1:B:136:THR:HG23	2.49	0.47
1:A:139:ILE:HD11	1:A:165:LEU:HD21	1.96	0.47
1:A:233:LYS:HD3	1:A:233:LYS:HA	1.86	0.47
1:B:226:ASP:HB3	4:B:936:HOH:O	2.15	0.47
1:A:554:LYS:O	1:A:554:LYS:HD2	2.15	0.47
1:B:483:PRO:HG3	4:B:605:HOH:O	2.14	0.47
1:A:117:LEU:HD22	1:A:124:VAL:HG11	1.97	0.47
1:A:344:TYR:CE2	1:A:346:PRO:HA	2.50	0.47
1:B:317:ARG:NH1	1:B:317:ARG:HG2	2.29	0.47
1:A:53:ASN:OD1	1:A:450:THR:HG22	2.16	0.46
1:A:248:GLY:O	1:A:251:SER:HB2	2.16	0.46
1:B:157:TYR:CG	1:B:187:MET:HE3	2.52	0.45
1:A:249:LYS:NZ	1:A:398:THR:O	2.36	0.45
1:B:17:VAL:HG22	1:B:187:MET:HE2	1.98	0.45
1:A:218:ALA:HB2	1:A:252:ILE:HD11	1.98	0.45
1:A:279:ALA:O	1:A:302:LYS:NZ	2.49	0.45
1:A:508:GLU:OE1	1:A:510:HIS:NE2	2.31	0.45
1:B:238:THR:HB	1:B:240:PHE:CE1	2.52	0.45
1:A:38:TYR:OH	1:B:486:GLN:HB3	2.16	0.45
1:A:255:GLN:HB2	1:A:402:ASN:OD1	2.17	0.45
1:A:308:GLU:HB3	1:A:310:HIS:NE2	2.31	0.45
1:A:336:ASN:ND2	1:A:336:ASN:N	2.64	0.45
1:B:190:LYS:HG2	1:B:191:PRO:CD	2.47	0.45
1:B:381:GLY:O	1:B:436:LYS:HG3	2.17	0.45
1:B:145:ALA:HB3	1:B:146:PRO:HD3	1.98	0.45
1:A:232:LYS:HZ1	1:A:252:ILE:HG23	1.82	0.45
1:B:238:THR:CG2	1:B:337:ILE:HG12	2.46	0.45
1:B:315:LYS:HE2	1:B:317:ARG:O	2.17	0.45
1:B:317:ARG:HB3	1:B:318:ASN:H	1.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:LEU:HA	1:B:174:LEU:HD22	1.98	0.44
1:B:171:LEU:O	1:B:174:LEU:HB2	2.17	0.44
1:B:312:ASP:O	1:B:313:HIS:HB3	2.17	0.44
1:B:8:LYS:NZ	1:B:12:GLU:OE2	2.47	0.44
1:B:221:CYS:HA	1:B:224:ARG:HB2	2.00	0.44
1:A:312:ASP:O	1:A:313:HIS:HB3	2.18	0.44
1:A:104:ILE:HD12	1:A:170:ASN:OD1	2.18	0.44
1:A:481:HIS:HB3	1:B:31:LEU:HD13	1.99	0.44
1:B:51:GLU:HB2	1:B:80:SER:HB2	1.99	0.43
1:B:499:LEU:HD13	1:B:507:TYR:HB2	1.99	0.43
1:B:534:ARG:HH11	1:B:534:ARG:HD2	1.50	0.43
1:A:344:TYR:CD1	1:A:345:LYS:HE3	2.53	0.43
1:A:498:LEU:HD13	1:B:501:THR:HG21	2.00	0.43
1:B:117:LEU:HD22	1:B:124:VAL:HG11	1.99	0.43
1:B:239:GLN:O	1:B:258:ARG:HD3	2.18	0.43
1:B:449:LEU:HD12	1:B:449:LEU:N	2.33	0.43
1:A:232:LYS:NZ	1:A:252:ILE:HG23	2.33	0.43
1:A:491:GLN:H	1:B:459:ARG:NH1	2.15	0.43
1:A:101:VAL:HA	1:A:102:PRO:HD3	1.91	0.43
1:A:82:LEU:HG	1:A:132:ILE:HD11	2.00	0.43
1:A:545:ALA:HB3	1:A:550:VAL:HG23	2.01	0.43
1:B:253:SER:HB3	1:B:402:ASN:OD1	2.18	0.43
1:A:15:LYS:HE3	1:A:41:GLU:O	2.18	0.43
1:A:308:GLU:HB3	1:A:310:HIS:HE2	1.84	0.43
1:B:454:ILE:O	1:B:457:MET:HB2	2.19	0.43
1:A:139:ILE:HG21	1:A:145:ALA:CB	2.46	0.43
1:B:505:LYS:H	1:B:505:LYS:HD3	1.84	0.43
1:B:101:VAL:HB	1:B:102:PRO:CD	2.49	0.42
1:B:242:ALA:HB1	1:B:252:ILE:HD13	2.01	0.42
1:B:90:ALA:HB1	1:B:411:LEU:HD13	2.01	0.42
1:B:104:ILE:O	1:B:105:SER:CB	2.67	0.42
1:B:480:ILE:CG1	1:B:553:ALA:HB1	2.48	0.42
1:A:540:LEU:HA	1:A:541:PRO:HD3	1.88	0.42
1:B:244:VAL:O	1:B:262:VAL:HA	2.19	0.42
1:A:308:GLU:HB2	1:A:315:LYS:HB3	2.01	0.42
1:A:554:LYS:C	1:A:556:THR:H	2.23	0.42
1:A:363:THR:HA	1:A:364:PRO:HD3	1.83	0.42
1:B:302:LYS:HB3	1:B:303:THR:H	1.70	0.42
1:A:333:LEU:HD22	1:A:337:ILE:HD13	2.01	0.42
1:A:51:GLU:HB2	1:A:80:SER:HB2	2.02	0.41
1:A:242:ALA:HB1	1:A:252:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:458:ILE:HG23	1:B:505:LYS:NZ	2.34	0.41
1:A:221:CYS:O	1:A:225:HIS:HB2	2.21	0.41
1:A:269:LYS:N	1:A:269:LYS:HD3	2.34	0.41
1:A:35:ASP:OD2	1:B:481:HIS:HE1	2.03	0.41
1:B:176:VAL:HA	1:B:177:PRO:HD3	1.81	0.41
1:B:352:ARG:N	1:B:352:ARG:HD2	2.36	0.41
1:A:157:TYR:CD2	1:A:187:MET:HE2	2.36	0.41
1:B:21:THR:CG2	1:B:44:ARG:HE	2.33	0.41
1:B:302:LYS:C	1:B:303:THR:OG1	2.59	0.41
1:B:198:LYS:HD3	1:B:198:LYS:HA	1.62	0.41
1:B:363:THR:HA	1:B:364:PRO:HD3	1.82	0.41
1:A:24:GLY:HA3	1:A:71:ILE:O	2.20	0.41
3:A:557:TPP:N1'	1:B:51:GLU:OE2	2.54	0.41
1:B:552:GLN:O	1:B:554:LYS:N	2.54	0.41
1:A:381:GLY:O	1:A:436:LYS:HG3	2.21	0.41
1:A:452:GLN:O	1:A:455:SER:HB3	2.21	0.41
1:B:126:HIS:CE1	1:B:136:THR:CG2	3.03	0.41
1:B:480:ILE:HD11	1:B:553:ALA:HB1	2.03	0.41
1:A:302:LYS:HE3	1:A:302:LYS:HB3	1.81	0.40
1:B:552:GLN:HB3	1:B:553:ALA:H	1.73	0.40
1:A:158:VAL:HG11	4:A:723:HOH:O	2.21	0.40
1:B:388:THR:HB	1:B:415:ILE:HG22	2.02	0.40
1:B:238:THR:O	1:B:239:GLN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	531/555 (96%)	503 (95%)	25 (5%)	3 (1%)	25 31
1	B	531/555 (96%)	501 (94%)	25 (5%)	5 (1%)	17 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1062/1110 (96%)	1004 (94%)	50 (5%)	8 (1%)	19 23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	SER
1	B	553	ALA
1	A	289	LEU
1	B	226	ASP
1	B	552	GLN
1	B	220	ALA
1	A	104	ILE
1	B	104	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	447/463 (96%)	383 (86%)	64 (14%)	3 3
1	B	447/463 (96%)	388 (87%)	59 (13%)	4 4
All	All	894/926 (96%)	771 (86%)	123 (14%)	3 3

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	14	LEU
1	A	15	LYS
1	A	18	ASN
1	A	31	LEU
1	A	33	LEU
1	A	36	LYS
1	A	52	LEU
1	A	65	LYS
1	A	82	LEU

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Mol	Chain	Res	Type
1	A	103	SER
1	A	116	THR
1	A	117	LEU
1	A	126	HIS
1	A	129	SER
1	A	139	ILE
1	A	142	ILE
1	A	144	THR
1	A	165	LEU
1	A	172	VAL
1	A	174	LEU
1	A	176	VAL
1	A	179	LYS
1	A	182	GLN
1	A	207	LEU
1	A	221	CYS
1	A	225	HIS
1	A	232	LYS
1	A	233	LYS
1	A	268	SER
1	A	269	LYS
1	A	271	GLU
1	A	274	GLU
1	A	283	LEU
1	A	288	LEU
1	A	289	LEU
1	A	291	ASP
1	A	302	LYS
1	A	317	ARG
1	A	330	LEU
1	A	336	ASN
1	A	345	LYS
1	A	346	PRO
1	A	353	THR
1	A	362	SER
1	A	372	ASN
1	A	411	LEU
1	A	423	LEU
1	A	436	LYS
1	A	440	LEU
1	A	447	LEU
1	A	463	LYS

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Mol	Chain	Res	Type
1	A	475	THR
1	A	479	LEU
1	A	484	LYS
1	A	498	LEU
1	A	505	LYS
1	A	512	VAL
1	A	515	THR
1	A	520	LYS
1	A	533	ILE
1	A	540	LEU
1	A	547	GLN
1	A	556	THR
1	B	2	SER
1	B	3	GLU
1	B	14	LEU
1	B	17	VAL
1	B	21	THR
1	B	25	LEU
1	B	33	LEU
1	B	34	LEU
1	B	41	GLU
1	B	52	LEU
1	B	67	MET
1	B	103	SER
1	B	117	LEU
1	B	136	THR
1	B	142	ILE
1	B	179	LYS
1	B	195	GLU
1	B	196	SER
1	B	198	LYS
1	B	207	LEU
1	B	223	SER
1	B	224	ARG
1	B	227	VAL
1	B	228	LYS
1	B	234	LEU
1	B	267	LEU
1	B	270	PRO
1	B	271	GLU
1	B	278	SER
1	B	281	LEU

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Mol	Chain	Res	Type
1	B	283	LEU
1	B	288	LEU
1	B	289	LEU
1	B	302	LYS
1	B	303	THR
1	B	317	ARG
1	B	329	VAL
1	B	339	ASP
1	B	342	LYS
1	B	345	LYS
1	B	349	VAL
1	B	362	SER
1	B	365	LEU
1	B	403	ASN
1	B	408	SER
1	B	411	LEU
1	B	423	LEU
1	B	435	LYS
1	B	440	LEU
1	B	447	LEU
1	B	466	LEU
1	B	505	LYS
1	B	525	LYS
1	B	526	SER
1	B	532	LYS
1	B	547	GLN
1	B	548	ASN
1	B	554	LYS
1	B	556	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	126	HIS
1	A	372	ASN
1	A	481	HIS
1	A	523	GLN
1	A	547	GLN
1	B	20	ASN
1	B	83	ASN
1	B	92	HIS

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Mol	Chain	Res	Type
1	B	114	HIS
1	B	126	HIS
1	B	175	ASN
1	B	225	HIS
1	B	397	GLN
1	B	481	HIS
1	B	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	557	2	22,27,27	1.78	6 (27%)	29,40,40	2.11	10 (34%)
3	TPP	A	557	2	22,27,27	1.45	4 (18%)	29,40,40	1.33	4 (13%)

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	B	557	2	-	4/16/17/17	0/2/2/2
3	TPP	A	557	2	-	4/16/17/17	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	557	TPP	C7'-N3	3.83	1.55	1.48
3	B	557	TPP	C7'-N3	3.43	1.54	1.48
3	B	557	TPP	C4'-N3'	3.35	1.39	1.35
3	B	557	TPP	C6-C5	-3.33	1.49	1.50
3	B	557	TPP	PB-O2B	-3.13	1.42	1.54
3	A	557	TPP	C2-N3	-2.94	1.29	1.36
3	A	557	TPP	C4'-N3'	2.86	1.39	1.35
3	B	557	TPP	PB-O1B	2.45	1.58	1.50
3	A	557	TPP	PB-O3B	-2.27	1.46	1.54
3	B	557	TPP	C2-N3	-2.16	1.31	1.36

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	557	TPP	C6-C5-C4	5.68	131.99	127.43
3	B	557	TPP	C7'-N3-C2	-4.01	118.10	125.35
3	A	557	TPP	CM2-C2'-N1'	3.99	121.53	117.14
3	B	557	TPP	O3B-PB-O2B	3.44	120.80	107.64
3	B	557	TPP	C5-C4-N3	3.14	113.85	107.57
3	B	557	TPP	O2B-PB-O1B	2.70	121.23	110.68
3	B	557	TPP	O3A-PB-O1B	-2.60	96.77	111.19
3	B	557	TPP	O3B-PB-O1B	-2.57	100.61	110.68
3	A	557	TPP	PA-O3A-PB	2.38	141.00	132.83
3	B	557	TPP	O2A-PA-O1A	2.36	123.92	112.24
3	B	557	TPP	PA-O3A-PB	-2.26	125.06	132.83
3	A	557	TPP	C6-C5-C4	2.14	129.15	127.43
3	A	557	TPP	C5'-C4'-N4'	2.09	125.15	122.19
3	B	557	TPP	C6'-N1'-C2'	2.02	119.40	115.96

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	557	TPP	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	A	557	TPP	PA-O3A-PB-O3B
3	B	557	TPP	PA-O3A-PB-O3B
3	B	557	TPP	C4-C5-C6-C7
3	B	557	TPP	PA-O3A-PB-O1B
3	A	557	TPP	PA-O3A-PB-O2B
3	B	557	TPP	PA-O3A-PB-O2B
3	A	557	TPP	PA-O3A-PB-O1B

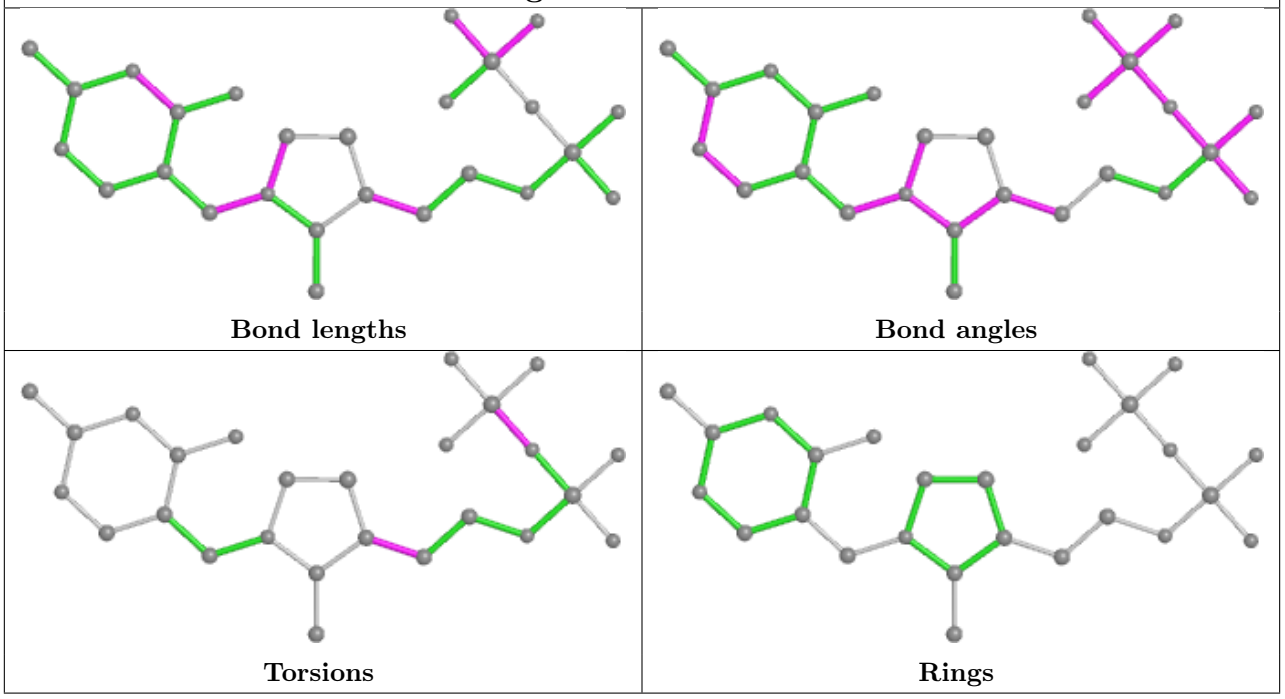
There are no ring outliers.

1 monomer is involved in 1 short contact:

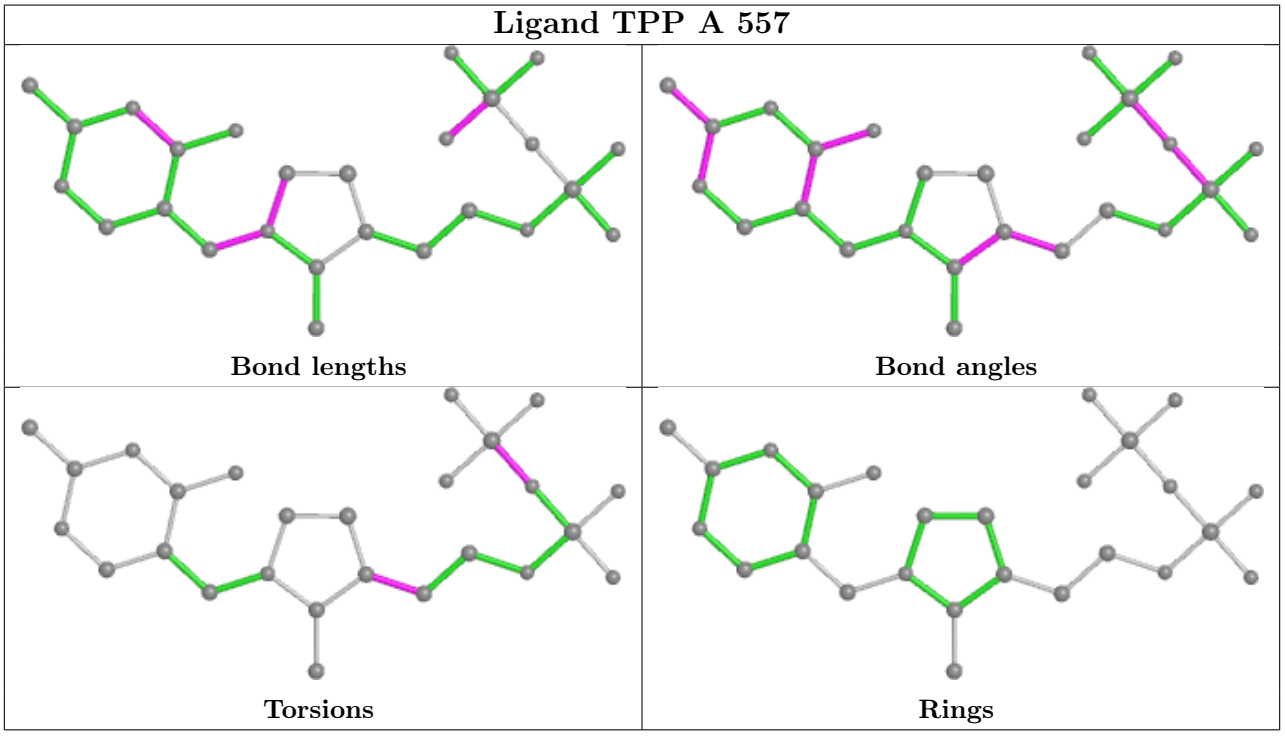
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	557	TPP	1	0

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 then 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 557



Ligand TPP A 557



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, 95^{th} 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	537/555 (96%)	-0.49	12 (2%) 62 69	3, 13, 33, 58	0
1	B	537/555 (96%)	-0.41	8 (1%) 73 79	3, 13, 32, 58	0
All	All	1074/1110 (96%)	-0.45	20 (1%) 66 73	3, 13, 33, 58	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	289	LEU	6.5
1	B	290	SER	5.8
1	A	555	LEU	5.3
1	B	553	ALA	4.7
1	B	288	LEU	4.7
1	A	221	CYS	4.5
1	A	289	LEU	4.2
1	A	290	SER	3.9
1	A	553	ALA	3.9
1	A	554	LYS	3.3
1	B	287	ALA	3.2
1	A	303	THR	2.9
1	A	556	THR	2.9
1	B	554	LYS	2.8
1	A	302	LYS	2.8
1	B	291	ASP	2.5
1	A	291	ASP	2.4
1	B	302	LYS	2.4
1	A	222	CYS	2.2
1	A	105	SER	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 monosaccharides in this entry.

6.4 Ligands (i)

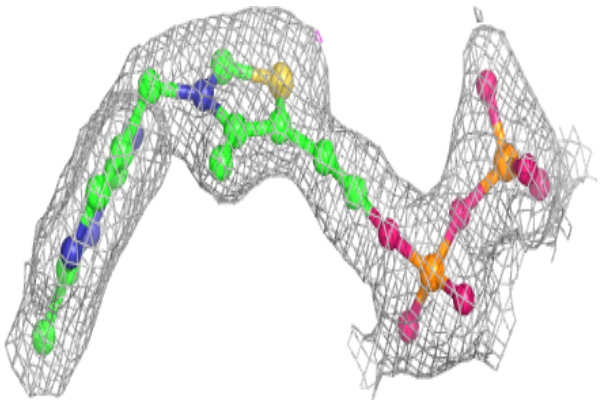
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

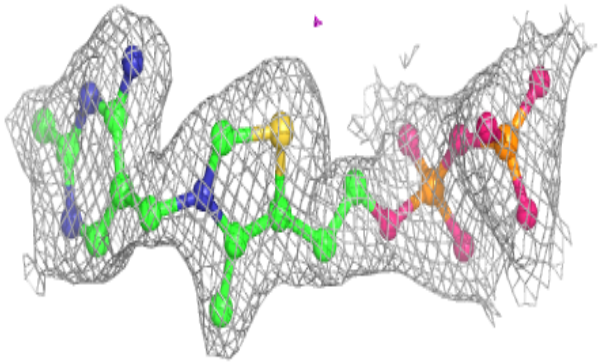
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	558	1/1	0.97	0.12	19,19,19,19	0
2	MG	B	558	1/1	0.97	0.11	13,13,13,13	0
3	TPP	A	557	26/26	0.99	0.06	2,6,8,11	0
3	TPP	B	557	26/26	0.99	0.06	2,5,10,11	0

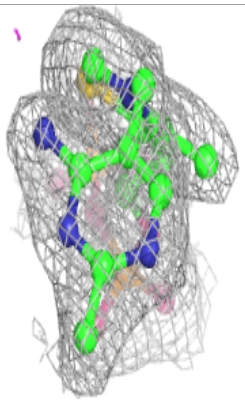
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP A 557:

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

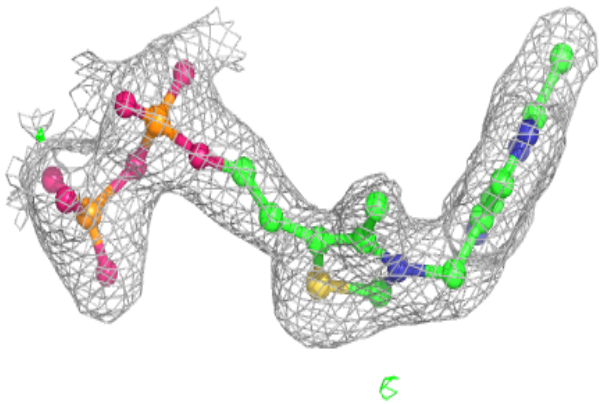


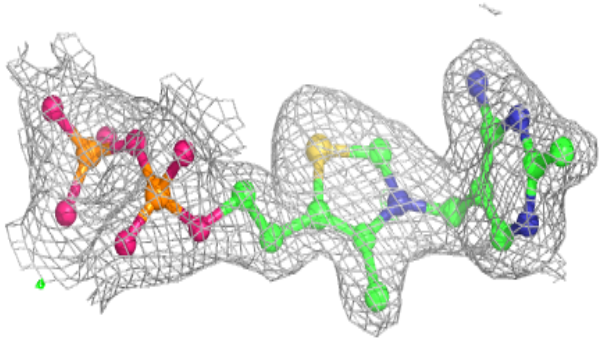


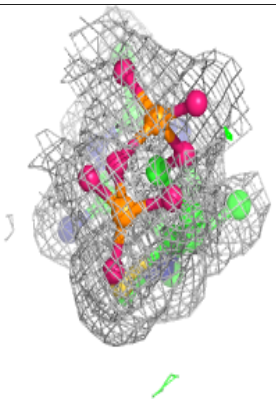


Electron density around TPP B 557:

$2mF_o$-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.