Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 01:00 PM EDT

PDB ID	:	2O1X
Title	:	1-deoxy-D-xylulose 5-phosphate synthase (DXS) from Deinococcus radiodurans
Authors	:	Xiang, S.; Usunow, G.; Lange, G.; Busch, M.; Tong, L.
Deposited on	:	2006-11-29
Resolution	:	2.90 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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

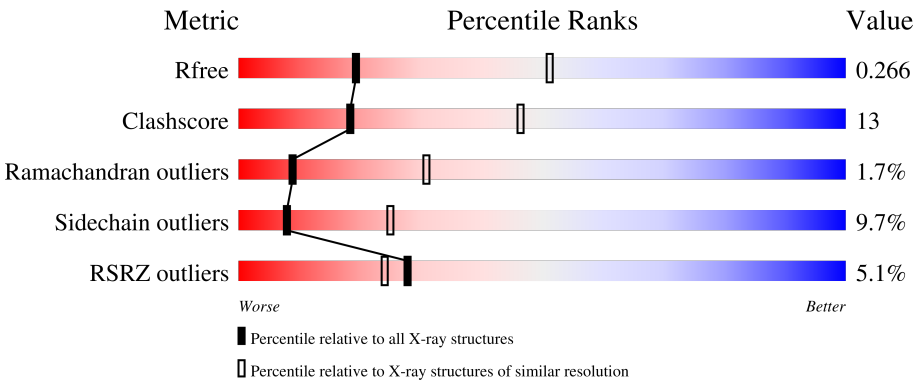
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	629	% 65% 23% • 8%
1	B	629	% 64% 22% 5% • 8%
1	C	629	8% 58% 23% • 14%
1	D	629	8% 58% 24% • 16%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16910 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 1-deoxy-D-xylulose-5-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	578	4362	2753	771	821	17	0	0	0
1	B	579	4376	2761	775	823	17	0	0	0
1	C	538	4063	2558	724	766	15	0	0	0
1	D	530	4001	2521	715	750	15	0	0	0

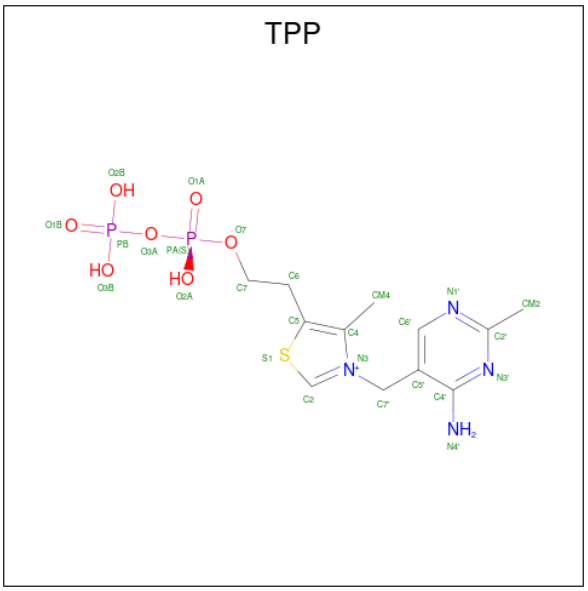
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	130	THR	ALA	engineered mutation	UNP Q9RUB5
B	130	THR	ALA	engineered mutation	UNP Q9RUB5
C	130	THR	ALA	engineered mutation	UNP Q9RUB5
D	130	THR	ALA	engineered mutation	UNP Q9RUB5

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



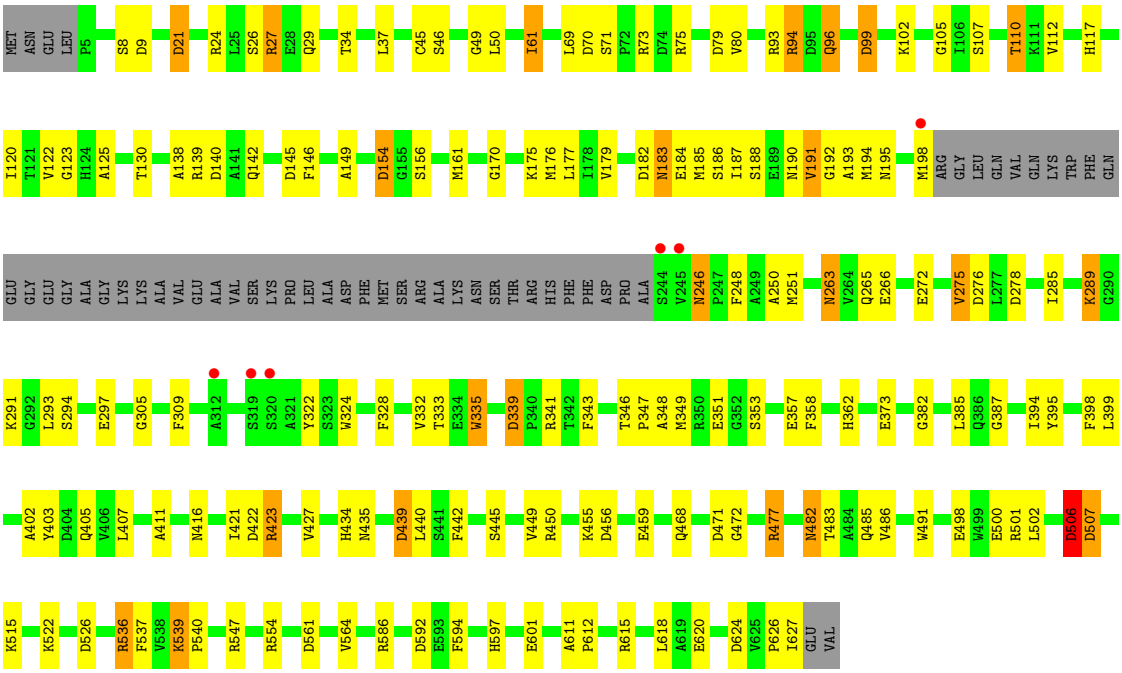
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	26	12	4	7	2	1	0	0
			Total	C	N	O	P	S		
3	B	1	26	12	4	7	2	1	0	0
			Total	C	N	O	P	S		
3	C	1	26	12	4	7	2	1	0	0
			Total	C	N	O	P	S		
3	D	1	26	12	4	7	2	1	0	0

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.

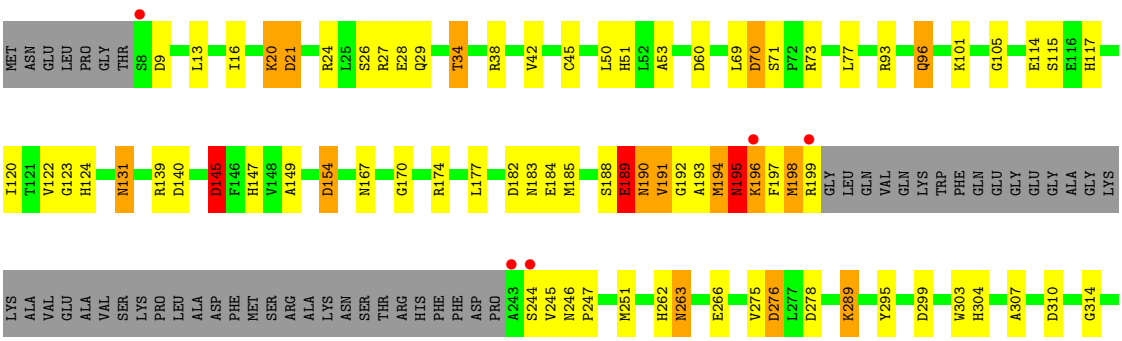
- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

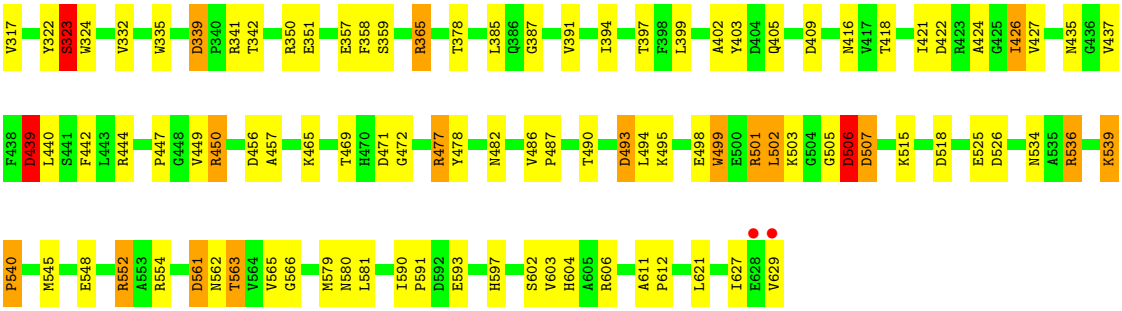
Chain A:



- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

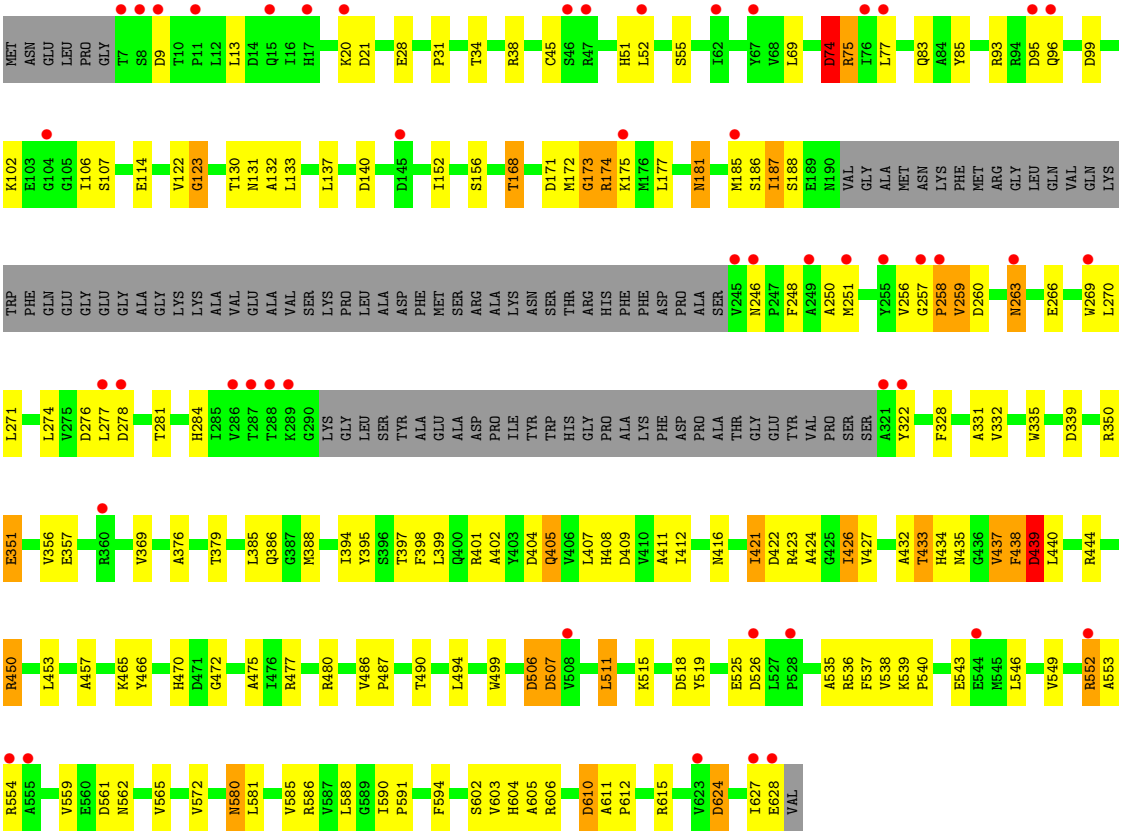
Chain B:





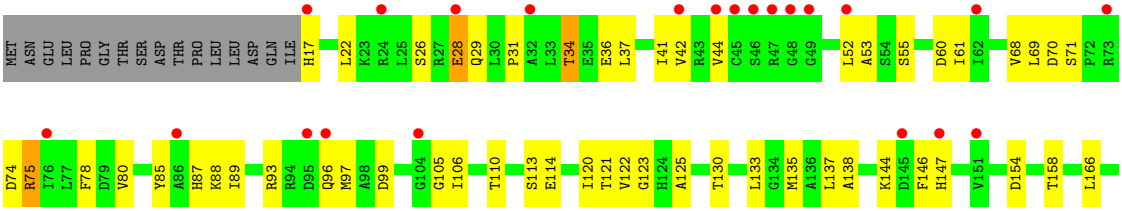
- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

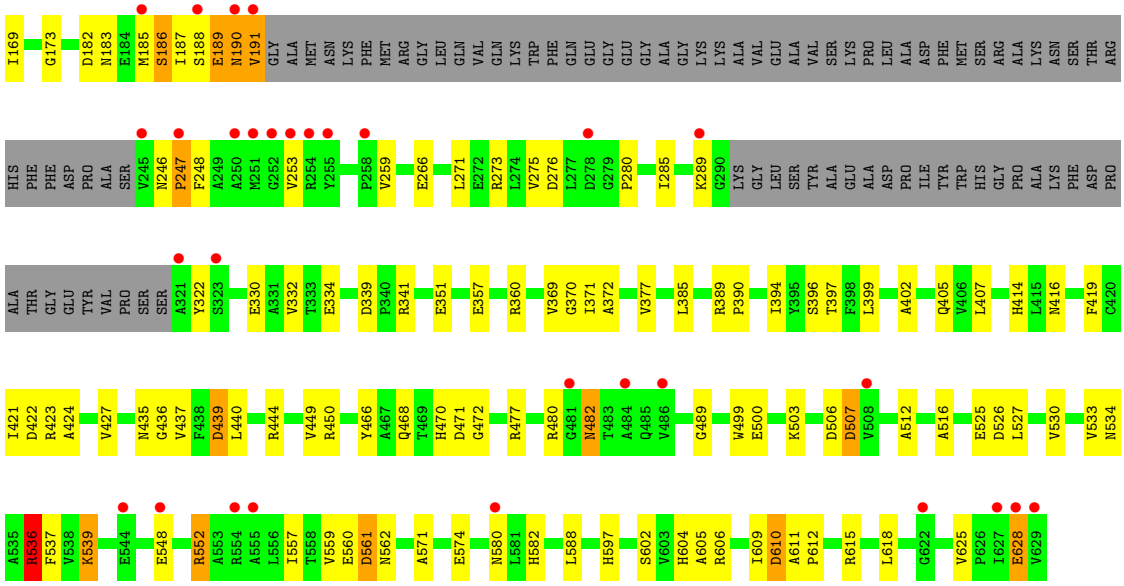
Chain C:



- Molecule 1: 1-deoxy-D-xylulose-5-phosphate synthase

Chain D:




I169 G173 D182 N183 E184 M185 S186 I187 S188 E189 N190 V191 GLY ALA MET ASN LYS PHE MET ARG GLY LEU GLN VAL GLN LYS TRP PHE GLN GLU GLY GLU GLY ALA GLY LYS LYS ALA VAL GLU ALA VAL SER LYS PRO LEU ALA ASP PHE MET SER ARG ALA LYS ASN SER THR ARG
HIS PHE PHE ASP PRO ALA SER V245 N246 P247 F248 A249 A250 M251 G252 V253 R254 Y255 P258 V259 E266 L271 E272 R273 L274 V275 D276 L277 D278 G279 P280 I285 K289 G290 LYS GLY LEU SER TYR ALA GLU ALA ASP PRO ILE TYR TRP HIS GLY PRO ALA LYS PHE ASP PRO
ALA THR GLY GLU TYR VAL PRO SER SER A321 Y322 S323 E330 A331 V332 T333 E334 D339 P340 R341 E351 E357 R360 V369 G370 I371 A372 V377 L385 R389 P390 I394 Y395 S396 T397 F398 L399 A402 Q405 V406 L407 H414 L415 N416 F419 C420
I421 D422 R423 A424 V427 N435 G436 V437 F438 D439 L440 R444 V449 R450 Y466 A467 Q468 T469 H470 D471 G472 R477 R480 G481 N482 T483 A484 Q485 V486 G489 W499 E500 K503 D506 D507 V508 A512 A516 E525 D526 L527 V530 V533 N534
A535 R536 F537 V538 K539 E544 E548 R552 A553 R554 A555 L556 I557 T558 V559 E560 D561 N562 A571 E574 N580 L581 H582 L588 H597 S602 V603 H604 A605 R606 I609 D610 A611 P612 R615 L618 G622 V625 P626 I627 E628 V629

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.26Å 154.06Å 124.88Å 90.00° 98.91° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 29.25 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.4 (30.00-2.90) 97.4 (29.25-2.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.44 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.209 , 0.272 0.207 , 0.266	Depositor DCC
R_{free} test set	3206 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	40.7	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16910	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 7.83% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]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 (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	0.53	0/4452	0.85	19/6049 (0.3%)
1	B	0.53	0/4465	0.87	16/6066 (0.3%)
1	C	0.43	0/4139	0.80	18/5621 (0.3%)
1	D	0.83	6/4076 (0.1%)	0.80	15/5534 (0.3%)
All	All	0.60	6/17132 (0.0%)	0.83	68/23270 (0.3%)

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	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	36	GLU	CD-OE2	28.08	1.56	1.25
1	D	628	GLU	CD-OE1	23.04	1.50	1.25
1	D	628	GLU	CD-OE2	18.05	1.45	1.25
1	D	36	GLU	CD-OE1	16.34	1.43	1.25
1	D	28	GLU	CD-OE2	9.40	1.35	1.25
1	D	28	GLU	CD-OE1	7.49	1.33	1.25

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	182	ASP	CB-CG-OD2	7.46	125.02	118.30
1	D	561	ASP	CB-CG-OD2	7.41	124.97	118.30
1	B	310	ASP	CB-CG-OD2	7.27	124.84	118.30
1	A	154	ASP	CB-CG-OD2	7.21	124.79	118.30
1	C	422	ASP	CB-CG-OD2	7.20	124.78	118.30
1	A	182	ASP	CB-CG-OD2	7.19	124.77	118.30
1	A	439	ASP	CB-CG-OD2	6.92	124.52	118.30
1	C	518	ASP	CB-CG-OD2	6.81	124.43	118.30
1	D	422	ASP	CB-CG-OD2	6.81	124.43	118.30
1	B	422	ASP	CB-CG-OD2	6.64	124.28	118.30
1	B	154	ASP	CB-CG-OD2	6.53	124.18	118.30
1	B	278	ASP	CB-CG-OD2	6.49	124.14	118.30
1	B	561	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	493	ASP	CB-CG-OD2	6.25	123.92	118.30
1	D	182	ASP	CB-CG-OD2	6.22	123.90	118.30
1	C	409	ASP	CB-CG-OD2	6.21	123.89	118.30
1	A	21	ASP	CB-CG-OD2	6.08	123.77	118.30
1	B	540	PRO	N-CD-CG	-6.07	94.09	103.20
1	A	276	ASP	CB-CG-OD2	6.07	123.76	118.30
1	A	145	ASP	CB-CG-OD2	6.07	123.76	118.30
1	C	278	ASP	CB-CG-OD2	6.07	123.76	118.30
1	D	339	ASP	CB-CG-OD2	5.97	123.68	118.30
1	A	278	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	79	ASP	CB-CG-OD2	5.95	123.66	118.30
1	C	404	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	339	ASP	CB-CG-OD2	5.90	123.61	118.30
1	D	154	ASP	CB-CG-OD2	5.87	123.59	118.30
1	A	624	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	9	ASP	CB-CG-OD2	5.75	123.48	118.30
1	A	140	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	507	ASP	CB-CG-OD2	5.72	123.45	118.30
1	B	145	ASP	CB-CG-OD2	5.72	123.44	118.30
1	C	506	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	60	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	422	ASP	CB-CG-OD2	5.61	123.35	118.30
1	D	36	GLU	CG-CD-OE2	-5.61	107.08	118.30
1	D	276	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	99	ASP	CB-CG-OD2	5.58	123.33	118.30
1	B	21	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	506	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	74	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	561	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	95	ASP	CB-CG-OD2	5.45	123.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	561	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	339	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	70	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	592	ASP	CB-CG-OD2	5.38	123.15	118.30
1	C	624	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	21	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	339	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	260	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	526	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	610	ASP	CB-CG-OD2	5.27	123.05	118.30
1	D	36	GLU	OE1-CD-OE2	5.26	129.62	123.30
1	C	171	ASP	CB-CG-OD2	5.23	123.00	118.30
1	C	9	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	518	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	456	ASP	CB-CG-OD2	5.18	122.97	118.30
1	C	276	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	70	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	276	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	506	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	507	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	70	ASP	CB-CG-OD2	5.08	122.87	118.30
1	A	526	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	74	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	99	ASP	CB-CG-OD2	5.05	122.85	118.30
1	D	506	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	191	VAL	Peptide
1	B	539	LYS	Peptide
1	C	438	PHE	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	4362	0	4337	101	0
1	B	4376	0	4352	140	0
1	C	4063	0	4054	115	0
1	D	4001	0	3997	106	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	0	16	2	0
3	B	26	0	16	4	0
3	C	26	0	16	0	0
3	D	26	0	16	1	0
All	All	16910	0	16804	449	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 13.

All (449) 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:439:ASP:OD2	1:D:477:ARG:HD2	1.47	1.11
1:C:75:ARG:HG3	1:C:75:ARG:HH11	0.93	1.09
1:B:440:LEU:HD21	1:B:477:ARG:HD3	1.34	1.08
1:B:365:ARG:HG3	1:B:365:ARG:HH11	1.19	1.02
1:C:423:ARG:HD2	1:C:480:ARG:HG3	1.44	0.99
1:C:552:ARG:HG3	1:C:552:ARG:HH11	1.24	0.99
1:B:486:VAL:HG12	1:B:487:PRO:HD2	1.45	0.97
1:C:402:ALA:HA	1:C:405:GLN:NE2	1.78	0.97
1:D:552:ARG:HG2	1:D:552:ARG:HH11	1.30	0.96
1:C:75:ARG:HG3	1:C:75:ARG:NH1	1.73	0.95
1:B:198:MET:HG2	1:B:198:MET:O	1.66	0.95
1:B:139:ARG:HD3	1:B:145:ASP:HA	1.47	0.94
1:C:486:VAL:HG12	1:C:487:PRO:HD2	1.49	0.94
1:A:110:THR:HG22	1:A:120:ILE:O	1.68	0.93
1:C:250:ALA:H	1:D:247:PRO:HG2	1.30	0.93
1:B:71:SER:OG	1:B:117:HIS:HD2	1.50	0.92
1:A:187:ILE:HD12	1:A:349:MET:HE1	1.55	0.88
1:A:61:ILE:CD1	1:A:179:VAL:HG11	2.04	0.87
1:C:34:THR:HG22	1:C:38:ARG:HH12	1.41	0.84
1:A:138:ALA:O	1:A:142:GLN:HG3	1.79	0.83
1:B:21:ASP:HA	1:B:24:ARG:NH1	1.94	0.82
1:A:61:ILE:HD12	1:A:179:VAL:HG11	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:SER:H	1:B:29:GLN:NE2	1.80	0.80
1:C:602:SER:HB2	1:C:606:ARG:HH12	1.46	0.80
1:A:93:ARG:HA	1:A:96:GLN:HE21	1.47	0.79
1:A:427:VAL:H	1:A:435:ASN:HD22	1.29	0.79
1:D:499:TRP:HB2	1:D:534:ASN:O	1.83	0.79
1:B:38:ARG:O	1:B:42:VAL:HG23	1.83	0.78
1:A:416:ASN:HD21	1:A:471:ASP:HA	1.45	0.77
1:B:439:ASP:OD1	1:B:477:ARG:HD2	1.84	0.77
1:B:427:VAL:H	1:B:435:ASN:ND2	1.83	0.77
1:B:402:ALA:HA	1:B:405:GLN:NE2	1.99	0.77
1:B:440:LEU:CD2	1:B:477:ARG:HD3	2.14	0.77
1:B:427:VAL:H	1:B:435:ASN:HD22	1.34	0.75
1:B:402:ALA:HA	1:B:405:GLN:HE21	1.50	0.75
1:A:139:ARG:HB2	1:A:146:PHE:CZ	2.21	0.75
1:C:423:ARG:HD2	1:C:480:ARG:CG	2.17	0.75
1:A:26:SER:H	1:A:29:GLN:NE2	1.84	0.74
1:A:335:TRP:CZ3	1:A:468:GLN:HG2	2.23	0.73
1:B:611:ALA:HB3	1:B:612:PRO:HD3	1.69	0.73
1:C:552:ARG:HG3	1:C:552:ARG:NH1	1.98	0.73
1:D:440:LEU:HD21	1:D:477:ARG:HD3	1.71	0.73
3:B:1002:TPP:HN42	3:B:1002:TPP:C2	2.02	0.73
1:C:75:ARG:HH11	1:C:75:ARG:CG	1.85	0.73
1:C:402:ALA:HA	1:C:405:GLN:HE22	1.52	0.72
1:B:323:SER:HA	1:B:482:ASN:HA	1.70	0.72
1:B:26:SER:H	1:B:29:GLN:HE21	1.36	0.72
1:B:139:ARG:NH1	1:B:140:ASP:OD1	2.23	0.71
1:A:485:GLN:HG3	1:A:486:VAL:H	1.54	0.71
1:C:486:VAL:CG1	1:C:487:PRO:HD2	2.20	0.70
1:D:402:ALA:HA	1:D:405:GLN:HE21	1.56	0.70
1:A:21:ASP:HA	1:A:24:ARG:HH11	1.55	0.70
1:B:498:GLU:O	1:B:536:ARG:NH1	2.24	0.70
1:B:365:ARG:HG3	1:B:365:ARG:NH1	1.93	0.70
1:A:440:LEU:HD21	1:A:477:ARG:HD3	1.72	0.69
1:B:486:VAL:HG12	1:B:487:PRO:CD	2.21	0.69
1:D:439:ASP:HB3	1:D:477:ARG:NH1	2.08	0.69
1:B:105:GLY:O	1:B:597:HIS:HE1	1.75	0.69
1:C:96:GLN:HG3	1:C:106:ILE:HD11	1.72	0.69
1:D:186:SER:OG	1:D:189:GLU:O	2.11	0.68
1:A:110:THR:CG2	1:A:120:ILE:O	2.40	0.68
1:C:437:VAL:HG22	1:C:562:ASN:HA	1.76	0.68
1:A:69:LEU:HD21	1:A:275:VAL:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:426:ILE:CD1	1:B:590:ILE:HG12	2.25	0.67
1:B:499:TRP:HB2	1:B:534:ASN:O	1.93	0.67
1:D:322:TYR:O	1:D:482:ASN:HB3	1.94	0.67
1:C:274:LEU:HD22	1:C:281:THR:HG21	1.77	0.66
1:C:174:ARG:HE	1:C:174:ARG:N	1.92	0.66
1:C:535:ALA:O	1:C:537:PHE:N	2.25	0.66
1:C:590:ILE:HD12	1:C:590:ILE:N	2.11	0.66
1:C:402:ALA:CA	1:C:405:GLN:NE2	2.56	0.66
1:D:31:PRO:O	1:D:34:THR:HG22	1.96	0.66
1:B:71:SER:OG	1:B:117:HIS:CD2	2.42	0.65
1:A:594:PHE:CE2	1:B:447:PRO:HG2	2.32	0.65
1:D:246:ASN:O	1:D:248:PHE:N	2.30	0.64
1:D:402:ALA:HA	1:D:405:GLN:NE2	2.12	0.64
1:A:26:SER:H	1:A:29:GLN:HE21	1.42	0.64
1:A:93:ARG:HA	1:A:96:GLN:NE2	2.12	0.64
1:C:457:ALA:HB3	1:C:486:VAL:HG23	1.78	0.64
1:A:21:ASP:HA	1:A:24:ARG:NH1	2.13	0.64
1:A:439:ASP:OD2	1:A:477:ARG:NH1	2.30	0.63
1:C:427:VAL:H	1:C:435:ASN:HD22	1.45	0.63
1:B:339:ASP:O	1:B:365:ARG:NH2	2.32	0.63
1:B:597:HIS:H	1:B:597:HIS:CD2	2.14	0.63
1:D:44:VAL:HG12	1:D:44:VAL:O	1.99	0.63
1:C:466:TYR:O	1:C:470:HIS:HD2	1.82	0.63
1:D:449:VAL:O	1:D:539:LYS:HG2	1.99	0.62
1:D:602:SER:HB2	1:D:606:ARG:HH12	1.64	0.62
1:D:503:LYS:HD3	1:D:530:VAL:O	1.99	0.62
1:C:586:ARG:HH22	1:D:580:ASN:HD21	1.46	0.62
1:D:93:ARG:NH1	1:D:114:GLU:OE2	2.32	0.62
1:A:586:ARG:NH2	1:A:620:GLU:OE1	2.33	0.62
1:D:466:TYR:O	1:D:470:HIS:HD2	1.83	0.62
1:A:611:ALA:HB3	1:A:612:PRO:HD3	1.81	0.61
1:A:394:ILE:O	1:A:421:ILE:HA	2.00	0.61
1:A:246:ASN:ND2	1:A:248:PHE:H	1.98	0.61
1:C:602:SER:HB2	1:C:606:ARG:NH1	2.16	0.61
1:D:75:ARG:HG2	1:D:75:ARG:HH11	1.66	0.60
1:D:450:ARG:HH22	1:D:472:GLY:HA3	1.65	0.60
1:A:187:ILE:HD12	1:A:349:MET:CE	2.29	0.60
1:C:611:ALA:HB3	1:C:612:PRO:HD3	1.83	0.60
1:A:615:ARG:HH12	1:A:626:PRO:HD2	1.66	0.60
1:B:494:LEU:O	1:B:494:LEU:HD12	2.01	0.60
1:B:194:MET:O	1:B:196:LYS:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:GLN:HG3	1:A:486:VAL:N	2.16	0.60
1:B:563:THR:HG23	1:B:565:VAL:H	1.67	0.59
1:C:427:VAL:H	1:C:435:ASN:ND2	2.00	0.59
1:A:27:ARG:NH2	1:A:272:GLU:OE1	2.35	0.59
1:D:423:ARG:HD2	1:D:480:ARG:HB2	1.83	0.59
1:D:444:ARG:HH22	1:D:574:GLU:CD	2.06	0.59
1:C:172:MET:HB2	1:C:174:ARG:CZ	2.32	0.59
1:D:611:ALA:HB3	1:D:612:PRO:CD	2.33	0.59
1:B:322:TYR:O	1:B:323:SER:HB3	2.01	0.58
1:A:105:GLY:O	1:A:597:HIS:HE1	1.85	0.58
1:A:335:TRP:CZ3	1:A:468:GLN:CG	2.86	0.58
1:B:322:TYR:O	1:B:323:SER:CB	2.52	0.58
1:B:502:LEU:HD22	1:B:534:ASN:HB2	1.85	0.58
1:B:548:GLU:HG2	1:B:552:ARG:NH1	2.18	0.58
1:B:170:GLY:HA3	1:B:251:MET:O	2.03	0.58
1:D:552:ARG:HG2	1:D:552:ARG:NH1	2.07	0.58
1:D:512:ALA:HB2	1:D:559:VAL:HB	1.84	0.58
1:B:426:ILE:HG12	1:B:603:VAL:HG11	1.86	0.58
1:B:554:ARG:NH2	1:B:621:LEU:O	2.36	0.58
1:C:605:ALA:HA	1:C:610:ASP:HB2	1.86	0.58
1:C:45:CYS:SG	1:C:52:LEU:HA	2.44	0.58
1:C:55:SER:HB3	1:C:85:TYR:HB2	1.84	0.58
1:C:106:ILE:HG23	1:C:114:GLU:OE2	2.03	0.58
1:C:440:LEU:O	1:C:444:ARG:HB2	2.04	0.58
1:B:335:TRP:HD1	1:B:342:THR:HG1	1.52	0.57
1:C:432:ALA:HB1	1:C:594:PHE:HB3	1.86	0.57
1:B:506:ASP:O	1:B:507:ASP:CB	2.53	0.57
1:B:563:THR:CG2	1:B:565:VAL:H	2.17	0.57
1:D:560:GLU:OE2	1:D:562:ASN:HB3	2.04	0.57
1:B:486:VAL:CG1	1:B:487:PRO:HD2	2.27	0.57
1:C:426:ILE:HD11	1:C:590:ILE:HG12	1.88	0.56
1:D:396:SER:HB3	1:D:436:GLY:HA3	1.87	0.56
1:D:61:ILE:HD13	1:D:285:ILE:HD13	1.87	0.56
1:B:350:ARG:HD2	1:B:359:SER:OG	2.05	0.56
1:B:365:ARG:NH1	1:B:365:ARG:CG	2.67	0.56
1:D:394:ILE:O	1:D:421:ILE:HA	2.05	0.56
1:A:94:ARG:HH11	1:A:94:ARG:CG	2.18	0.56
1:A:322:TYR:O	1:A:482:ASN:HB3	2.06	0.56
1:B:416:ASN:HD21	1:B:471:ASP:HA	1.71	0.56
1:C:258:PRO:HA	1:C:284:HIS:HB3	1.86	0.56
1:D:158:THR:HG21	1:D:191:VAL:HG21	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:552:ARG:HH11	1:D:552:ARG:CG	2.13	0.56
1:D:75:ARG:HH11	1:D:75:ARG:CG	2.18	0.56
1:A:71:SER:OG	1:A:117:HIS:HD2	1.89	0.55
1:C:256:VAL:HG21	1:C:274:LEU:HD21	1.88	0.55
1:C:328:PHE:O	1:C:331:ALA:N	2.38	0.55
1:C:439:ASP:OD1	1:C:477:ARG:HD2	2.07	0.55
1:D:548:GLU:HG2	1:D:552:ARG:HH12	1.72	0.55
1:D:527:LEU:HD11	1:D:625:VAL:HG22	1.88	0.55
1:B:590:ILE:N	1:B:590:ILE:HD12	2.20	0.55
1:C:424:ALA:HB1	1:C:477:ARG:NE	2.22	0.55
1:B:26:SER:N	1:B:29:GLN:HE21	2.02	0.55
1:D:588:LEU:HB3	1:D:609:ILE:HG22	1.89	0.55
1:C:590:ILE:HD12	1:C:590:ILE:H	1.70	0.55
1:B:477:ARG:NH2	1:B:561:ASP:O	2.39	0.54
1:B:439:ASP:CG	1:B:477:ARG:HH11	2.10	0.54
1:B:21:ASP:OD1	1:B:24:ARG:NH1	2.37	0.54
1:B:140:ASP:OD2	1:B:174:ARG:HD2	2.08	0.54
1:B:197:PHE:O	1:B:198:MET:HB3	2.07	0.54
1:A:27:ARG:HH22	1:A:272:GLU:CD	2.11	0.54
1:A:416:ASN:ND2	1:A:471:ASP:HA	2.21	0.54
1:A:440:LEU:CD2	1:A:477:ARG:HD3	2.38	0.53
1:D:414:HIS:CE1	1:D:450:ARG:NH2	2.77	0.53
1:A:506:ASP:O	1:A:507:ASP:HB2	2.08	0.53
1:C:437:VAL:HG22	1:C:562:ASN:CA	2.39	0.53
1:A:450:ARG:HH22	1:A:472:GLY:HA3	1.73	0.53
1:D:377:VAL:HG22	1:D:419:PHE:HE2	1.74	0.53
1:D:516:ALA:HB1	1:D:559:VAL:HG12	1.90	0.53
1:A:193:ALA:HB3	1:B:167:ASN:OD1	2.08	0.53
1:C:77:LEU:HD22	1:C:132:ALA:HB2	1.91	0.53
1:C:177:LEU:HD21	1:C:271:LEU:HD22	1.90	0.53
1:C:440:LEU:HD12	1:C:562:ASN:HB2	1.91	0.53
1:A:250:ALA:HB3	1:B:196:LYS:HG2	1.89	0.52
1:C:440:LEU:HD22	1:C:538:VAL:HG21	1.91	0.52
1:D:439:ASP:HB3	1:D:477:ARG:HH11	1.73	0.52
1:C:31:PRO:O	1:C:34:THR:HB	2.09	0.52
1:D:499:TRP:CD1	1:D:533:VAL:CG1	2.92	0.52
3:A:1001:TPP:HN42	3:A:1001:TPP:C2	2.22	0.52
1:A:183:ASN:ND2	1:A:185:MET:H	2.06	0.52
1:C:133:LEU:HD13	1:C:174:ARG:HH22	1.74	0.52
1:D:424:ALA:HB1	1:D:477:ARG:CZ	2.39	0.52
1:C:457:ALA:HB3	1:C:486:VAL:CG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:ASN:C	1:D:248:PHE:H	2.13	0.52
1:D:499:TRP:CD1	1:D:533:VAL:HG11	2.44	0.52
1:A:506:ASP:O	1:A:507:ASP:CB	2.57	0.52
1:B:506:ASP:O	1:B:507:ASP:HB3	2.09	0.52
1:B:465:LYS:HE2	1:B:493:ASP:OD2	2.09	0.52
1:C:536:ARG:HD3	1:C:537:PHE:CE1	2.45	0.52
1:D:53:ALA:HB1	1:D:289:LYS:HG2	1.92	0.52
1:D:394:ILE:HG21	1:D:399:LEU:HD13	1.90	0.52
1:B:394:ILE:O	1:B:421:ILE:HA	2.10	0.51
1:B:194:MET:HB2	1:B:198:MET:HB3	1.92	0.51
1:A:427:VAL:H	1:A:435:ASN:ND2	2.05	0.51
1:C:274:LEU:HD23	1:C:277:LEU:HD12	1.93	0.51
1:A:341:ARG:HD2	1:A:387:GLY:O	2.09	0.51
1:B:457:ALA:HB3	1:B:486:VAL:HG23	1.92	0.51
1:D:246:ASN:C	1:D:248:PHE:N	2.64	0.51
1:D:500:GLU:CD	1:D:536:ARG:HH21	2.13	0.51
1:D:526:ASP:HB2	1:D:615:ARG:HH22	1.74	0.51
1:D:88:LYS:HD2	1:D:106:ILE:HD11	1.93	0.51
1:C:335:TRP:CZ3	1:C:465:LYS:HG3	2.45	0.51
1:A:402:ALA:HA	1:A:405:GLN:NE2	2.25	0.51
1:B:192:GLY:O	1:B:193:ALA:HB3	2.10	0.51
1:D:557:ILE:HG23	1:D:588:LEU:HD23	1.92	0.51
1:C:402:ALA:CA	1:C:405:GLN:HE21	2.23	0.51
1:B:154:ASP:HB2	1:B:197:PHE:CZ	2.46	0.51
1:A:395:TYR:CE2	1:A:423:ARG:HG2	2.46	0.50
1:C:627:ILE:O	1:C:628:GLU:HG2	2.11	0.50
1:A:405:GLN:NE2	1:A:405:GLN:H	2.09	0.50
1:D:444:ARG:NH2	1:D:571:ALA:HA	2.27	0.50
1:B:21:ASP:HA	1:B:24:ARG:HH12	1.74	0.50
1:C:416:ASN:ND2	1:C:472:GLY:H	2.10	0.50
1:D:105:GLY:O	1:D:597:HIS:HE1	1.94	0.50
1:A:50:LEU:O	1:A:305:GLY:HA2	2.11	0.50
1:C:351:GLU:HA	1:C:356:VAL:HG23	1.94	0.50
1:C:432:ALA:CB	1:C:594:PHE:HB3	2.41	0.50
1:C:75:ARG:NH1	1:C:75:ARG:CG	2.56	0.50
1:C:399:LEU:HD22	1:C:421:ILE:HD13	1.93	0.50
1:A:250:ALA:CB	1:B:196:LYS:HG2	2.42	0.49
1:B:426:ILE:HD12	1:B:437:VAL:HG21	1.94	0.49
1:B:469:THR:O	1:B:469:THR:CG2	2.60	0.49
1:D:615:ARG:HA	1:D:618:LEU:HD12	1.94	0.49
1:C:140:ASP:OD2	1:C:174:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:ASN:C	1:B:263:ASN:HD22	2.14	0.49
1:C:93:ARG:HB3	1:C:106:ILE:HD11	1.94	0.49
1:D:183:ASN:ND2	3:D:1004:TPP:O2B	2.42	0.49
1:C:525:GLU:HB2	1:C:615:ARG:HH21	1.77	0.49
1:B:295:TYR:CD2	1:B:314:GLY:HA3	2.47	0.49
1:B:402:ALA:CA	1:B:405:GLN:HE21	2.21	0.49
1:B:499:TRP:CD1	1:B:545:MET:SD	3.05	0.49
1:C:440:LEU:HD21	1:C:477:ARG:HD3	1.95	0.49
1:A:395:TYR:CD2	1:A:423:ARG:HG2	2.47	0.49
1:B:440:LEU:O	1:B:444:ARG:HB2	2.12	0.49
1:C:440:LEU:HD12	1:C:562:ASN:CB	2.42	0.49
1:A:289:LYS:HE3	3:A:1001:TPP:O1B	2.12	0.49
1:B:53:ALA:HB1	1:B:289:LYS:HD3	1.94	0.49
1:C:590:ILE:H	1:C:590:ILE:CD1	2.25	0.49
1:D:37:LEU:O	1:D:41:ILE:HD12	2.11	0.49
1:B:561:ASP:OD2	1:B:604:HIS:HE1	1.96	0.49
1:A:263:ASN:HD21	1:A:265:GLN:HB2	1.77	0.49
1:B:469:THR:O	1:B:469:THR:HG22	2.12	0.49
1:D:611:ALA:HB3	1:D:612:PRO:HD2	1.94	0.49
1:B:51:HIS:HA	1:B:304:HIS:O	2.13	0.48
1:B:149:ALA:HA	1:B:177:LEU:O	2.13	0.48
1:B:444:ARG:NH1	1:B:566:GLY:O	2.45	0.48
1:D:133:LEU:O	1:D:137:LEU:HB2	2.13	0.48
1:B:154:ASP:O	1:B:195:ASN:ND2	2.47	0.48
1:C:499:TRP:CD1	1:C:535:ALA:O	2.66	0.48
1:D:183:ASN:HD22	1:D:289:LYS:HB2	1.78	0.48
1:C:407:LEU:O	1:C:411:ALA:HB3	2.13	0.48
1:D:42:VAL:HA	1:D:52:LEU:HD21	1.95	0.48
1:B:501:ARG:NH2	1:B:505:GLY:O	2.46	0.48
1:C:186:SER:O	1:C:187:ILE:C	2.51	0.48
1:D:416:ASN:HD21	1:D:471:ASP:HA	1.78	0.48
1:C:28:GLU:CD	1:C:28:GLU:H	2.16	0.48
1:C:426:ILE:HG12	1:C:603:VAL:HG11	1.94	0.48
1:C:486:VAL:HG11	1:C:490:THR:HG21	1.96	0.48
1:A:149:ALA:HA	1:A:177:LEU:O	2.14	0.48
1:D:605:ALA:HA	1:D:610:ASP:HB2	1.96	0.48
1:A:175:LYS:O	1:A:176:MET:HG3	2.14	0.48
1:A:407:LEU:O	1:A:411:ALA:HB3	2.14	0.48
1:A:263:ASN:C	1:A:263:ASN:HD22	2.15	0.48
1:A:138:ALA:O	1:A:142:GLN:CG	2.59	0.47
1:A:449:VAL:O	1:A:539:LYS:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:LEU:HD22	1:C:74:ASP:OD2	2.14	0.47
1:B:183:ASN:ND2	3:B:1002:TPP:O3B	2.48	0.47
1:B:193:ALA:O	1:B:194:MET:C	2.53	0.47
1:D:499:TRP:HZ3	1:D:537:PHE:O	1.98	0.47
1:A:373:GLU:HG2	1:A:398:PHE:O	2.14	0.47
1:B:69:LEU:HD21	1:B:275:VAL:HG21	1.97	0.47
1:D:477:ARG:NH2	1:D:561:ASP:O	2.47	0.47
1:B:579:MET:HE3	1:B:581:LEU:HD12	1.97	0.47
1:B:499:TRP:HD1	1:B:545:MET:SD	2.37	0.47
1:D:80:VAL:HG22	1:D:125:ALA:HA	1.97	0.47
1:D:110:THR:HG22	1:D:120:ILE:O	2.15	0.47
1:D:253:VAL:HG13	1:D:280:PRO:HB2	1.96	0.47
1:D:341:ARG:NE	1:D:389:ARG:HE	2.12	0.47
1:A:26:SER:N	1:A:29:GLN:HE21	2.10	0.47
1:A:61:ILE:HD12	1:A:285:ILE:HD13	1.96	0.47
1:A:539:LYS:HA	1:A:540:PRO:HA	1.81	0.47
1:B:195:ASN:O	1:B:196:LYS:HG3	2.14	0.47
1:B:439:ASP:CB	1:B:477:ARG:HH11	2.28	0.47
1:A:170:GLY:HA3	1:A:251:MET:O	2.15	0.47
1:C:34:THR:CG2	1:C:38:ARG:HH12	2.20	0.47
1:C:106:ILE:HG22	1:C:107:SER:O	2.15	0.47
1:C:270:LEU:O	1:C:274:LEU:N	2.48	0.47
1:C:612:PRO:HA	1:C:615:ARG:HB2	1.97	0.47
1:D:582:HIS:ND1	1:D:582:HIS:N	2.62	0.47
1:C:386:GLN:HG2	1:D:135:MET:HG3	1.97	0.46
1:D:341:ARG:HE	1:D:389:ARG:HE	1.63	0.46
1:D:44:VAL:O	1:D:44:VAL:CG1	2.63	0.46
1:D:561:ASP:OD2	1:D:604:HIS:HE1	1.97	0.46
1:B:50:LEU:HD23	1:B:101:LYS:HD3	1.98	0.46
1:C:123:GLY:HA3	1:C:433:THR:OG1	2.15	0.46
1:D:75:ARG:CG	1:D:75:ARG:NH1	2.78	0.46
1:A:130:THR:HG21	1:A:161:MET:HE2	1.98	0.46
1:A:427:VAL:HG21	1:A:434:HIS:HB3	1.97	0.46
1:A:291:LYS:HA	1:A:297:GLU:OE2	2.15	0.46
1:A:601:GLU:H	1:A:601:GLU:CD	2.19	0.46
1:C:395:TYR:HB2	1:C:398:PHE:CD2	2.51	0.46
1:D:444:ARG:NE	1:D:571:ALA:HB2	2.30	0.46
1:D:552:ARG:NH1	1:D:552:ARG:CG	2.77	0.46
1:B:105:GLY:O	1:B:597:HIS:CE1	2.63	0.46
3:B:1002:TPP:HN42	3:B:1002:TPP:H2	1.80	0.46
1:B:341:ARG:HD2	1:B:387:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ARG:O	1:B:96:GLN:HG2	2.16	0.46
1:A:498:GLU:O	1:A:536:ARG:NH1	2.35	0.46
1:B:20:LYS:HE2	1:B:20:LYS:HB2	1.77	0.46
1:B:188:SER:HB3	1:B:351:GLU:OE1	2.16	0.46
1:D:466:TYR:O	1:D:470:HIS:CD2	2.68	0.46
1:B:196:LYS:HD3	1:B:247:PRO:O	2.15	0.46
1:B:437:VAL:O	1:B:437:VAL:HG13	2.15	0.46
1:B:486:VAL:HG11	1:B:490:THR:HG21	1.97	0.46
1:B:26:SER:N	1:B:29:GLN:NE2	2.58	0.45
1:B:449:VAL:O	1:B:539:LYS:HD3	2.16	0.45
1:C:511:LEU:HD23	1:C:511:LEU:N	2.31	0.45
1:D:147:HIS:ND1	1:D:275:VAL:O	2.50	0.45
1:D:189:GLU:HB3	1:D:190:ASN:H	1.50	0.45
1:A:594:PHE:CZ	1:B:447:PRO:HG2	2.51	0.45
1:B:437:VAL:O	1:B:437:VAL:CG1	2.63	0.45
1:D:173:GLY:HA2	1:D:280:PRO:HD3	1.99	0.45
1:B:124:HIS:NE2	1:B:397:THR:HB	2.32	0.45
1:B:378:THR:HG23	1:B:409:ASP:HB3	1.98	0.45
1:B:590:ILE:HA	1:B:591:PRO:HD2	1.81	0.45
1:C:133:LEU:CD1	1:C:174:ARG:HH12	2.28	0.45
1:C:398:PHE:O	1:C:401:ARG:HB2	2.15	0.45
1:B:324:TRP:HB3	1:B:478:TYR:CD1	2.51	0.45
1:C:438:PHE:CD2	1:D:407:LEU:HD11	2.51	0.45
1:A:46:SER:HA	1:A:309:PHE:CE2	2.51	0.45
1:A:291:LYS:HD2	1:A:297:GLU:OE2	2.16	0.45
1:B:120:ILE:HG13	1:B:122:VAL:HG13	1.99	0.45
1:C:439:ASP:HB3	1:C:440:LEU:H	1.48	0.45
1:D:477:ARG:O	1:D:477:ARG:HG3	2.15	0.45
1:B:45:CYS:HA	1:B:50:LEU:HD12	1.99	0.45
1:B:194:MET:HB2	1:B:197:PHE:O	2.17	0.45
1:C:257:GLY:HA2	1:C:259:VAL:HG22	1.99	0.45
1:C:450:ARG:HH22	1:C:472:GLY:HA3	1.82	0.45
1:A:358:PHE:CD2	1:A:358:PHE:C	2.90	0.44
1:A:80:VAL:HG22	1:A:125:ALA:HA	1.98	0.44
1:B:358:PHE:C	1:B:358:PHE:CD2	2.91	0.44
1:C:246:ASN:ND2	1:C:248:PHE:H	2.15	0.44
1:C:539:LYS:HA	1:C:540:PRO:HA	1.81	0.44
1:A:382:GLY:CA	1:B:131:ASN:HD22	2.29	0.44
1:B:190:ASN:ND2	1:B:191:VAL:H	2.15	0.44
1:C:394:ILE:O	1:C:421:ILE:HA	2.18	0.44
1:D:341:ARG:HE	1:D:389:ARG:HH21	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:THR:O	1:D:121:THR:HA	2.18	0.44
1:D:468:GLN:OE1	1:D:468:GLN:HA	2.16	0.44
1:A:427:VAL:N	1:A:435:ASN:HD22	2.06	0.44
1:A:502:LEU:HD12	1:A:502:LEU:HA	1.77	0.44
1:B:16:ILE:HA	1:B:21:ASP:CB	2.48	0.44
1:B:426:ILE:HD12	1:B:437:VAL:CG2	2.48	0.44
1:B:486:VAL:CG1	1:B:487:PRO:CD	2.91	0.44
1:B:60:ASP:OD2	1:B:262:HIS:HA	2.18	0.44
1:D:68:VAL:HG21	1:D:271:LEU:HB2	1.99	0.44
1:C:369:VAL:HG21	1:C:376:ALA:HB2	1.99	0.43
1:D:427:VAL:H	1:D:435:ASN:ND2	2.15	0.43
1:A:250:ALA:HB1	1:B:196:LYS:HA	2.00	0.43
1:B:424:ALA:HB1	1:B:477:ARG:CZ	2.48	0.43
1:C:590:ILE:HA	1:C:591:PRO:HD2	1.83	0.43
1:A:192:GLY:HA2	1:A:195:ASN:HB3	2.01	0.43
1:C:99:ASP:HA	1:C:102:LYS:HD2	2.01	0.43
1:C:173:GLY:C	1:C:174:ARG:HE	2.20	0.43
1:C:408:HIS:HA	1:C:412:ILE:HD12	2.00	0.43
1:A:394:ILE:HD13	1:A:399:LEU:HA	2.00	0.43
1:B:147:HIS:NE2	1:B:275:VAL:HG13	2.34	0.43
1:B:391:VAL:HG22	1:B:418:THR:HB	2.00	0.43
1:A:439:ASP:OD1	1:A:477:ARG:HD2	2.17	0.43
1:B:53:ALA:CB	1:B:289:LYS:HD3	2.49	0.43
1:A:536:ARG:HG2	1:A:537:PHE:CD1	2.54	0.43
1:B:185:MET:HA	1:B:189:GLU:HA	2.01	0.43
1:C:424:ALA:HB1	1:C:477:ARG:CZ	2.49	0.43
1:D:246:ASN:O	1:D:247:PRO:C	2.56	0.43
1:A:333:THR:O	1:A:362:HIS:HE1	2.01	0.43
1:B:34:THR:HG23	1:B:38:ARG:NH1	2.33	0.43
1:C:152:ILE:HG13	1:C:156:SER:HB2	2.01	0.43
1:C:168:THR:HG21	1:D:369:VAL:HA	2.01	0.43
1:A:335:TRP:HD1	1:A:491:TRP:CH2	2.37	0.42
1:A:402:ALA:HA	1:A:405:GLN:HE21	1.83	0.42
1:B:394:ILE:HG21	1:B:399:LEU:HD13	2.01	0.42
1:B:590:ILE:HD12	1:B:590:ILE:H	1.83	0.42
1:C:187:ILE:HD12	1:C:188:SER:N	2.35	0.42
1:C:379:THR:HA	1:D:130:THR:O	2.19	0.42
1:B:561:ASP:OD2	1:B:604:HIS:CE1	2.72	0.42
1:A:335:TRP:CD1	1:A:491:TRP:CH2	3.08	0.42
1:C:402:ALA:C	1:C:405:GLN:NE2	2.73	0.42
1:D:423:ARG:HB3	1:D:427:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ALA:HB2	1:C:477:ARG:HB2	2.02	0.42
1:B:21:ASP:HA	1:B:24:ARG:HH11	1.78	0.42
1:C:559:VAL:HA	1:C:588:LEU:O	2.19	0.42
1:D:500:GLU:HG3	1:D:534:ASN:HB3	2.02	0.42
1:D:611:ALA:CB	1:D:612:PRO:CD	2.97	0.42
1:D:370:GLY:O	1:D:372:ALA:N	2.47	0.42
1:A:500:GLU:OE1	1:A:500:GLU:HA	2.20	0.42
1:A:335:TRP:HZ3	1:A:339:ASP:OD1	2.03	0.42
1:B:450:ARG:HH22	1:B:472:GLY:HA3	1.85	0.42
1:C:405:GLN:NE2	1:C:405:GLN:H	2.17	0.42
1:C:519:TYR:HE1	1:C:604:HIS:CD2	2.37	0.42
1:D:44:VAL:HG11	1:D:97:MET:HB3	2.01	0.42
1:C:440:LEU:HD21	1:C:453:LEU:HD11	2.01	0.42
1:D:89:ILE:HG12	1:D:97:MET:HG3	2.02	0.42
1:A:346:THR:HA	1:A:347:PRO:HD3	1.93	0.41
1:B:194:MET:HB3	1:B:197:PHE:CE1	2.55	0.41
1:C:174:ARG:N	1:C:174:ARG:NE	2.64	0.41
1:C:546:LEU:HD11	1:C:572:VAL:HG13	2.02	0.41
1:A:45:CYS:HA	1:A:50:LEU:HD12	2.02	0.41
1:B:195:ASN:HD22	1:B:197:PHE:HE2	1.68	0.41
1:B:502:LEU:HD12	1:B:502:LEU:HA	1.80	0.41
1:D:55:SER:HB3	1:D:85:TYR:HB2	2.02	0.41
1:A:348:ALA:O	1:A:349:MET:HE3	2.20	0.41
1:A:407:LEU:HD23	1:A:407:LEU:C	2.41	0.41
1:A:154:ASP:OD1	1:A:184:GLU:HA	2.21	0.41
1:C:421:ILE:HD11	1:C:475:ALA:HB1	2.03	0.41
1:C:549:VAL:O	1:C:553:ALA:HB3	2.21	0.41
1:D:69:LEU:HD21	1:D:275:VAL:HG11	2.02	0.41
1:D:390:PRO:HD2	1:D:416:ASN:O	2.20	0.41
1:B:77:LEU:HD23	1:B:120:ILE:HD13	2.01	0.41
1:A:293:LEU:O	1:A:294:SER:C	2.59	0.41
1:B:263:ASN:C	1:B:263:ASN:ND2	2.74	0.41
1:A:94:ARG:HH11	1:A:94:ARG:HG2	1.85	0.41
1:A:99:ASP:O	1:A:102:LYS:HB2	2.21	0.41
1:A:403:TYR:HH	1:B:442:PHE:HD2	1.66	0.41
1:A:455:LYS:HG2	1:A:459:GLU:OE1	2.21	0.41
1:A:615:ARG:HA	1:A:618:LEU:HD12	2.02	0.41
1:B:289:LYS:HE3	3:B:1002:TPP:O2B	2.20	0.41
1:B:450:ARG:NH2	1:B:472:GLY:HA3	2.35	0.41
1:C:263:ASN:OD1	1:C:266:GLU:HB2	2.21	0.41
1:D:78:PHE:HE1	1:D:87:HIS:ND1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:HIS:CG	1:D:275:VAL:HG13	2.56	0.41
1:D:437:VAL:HG12	1:D:437:VAL:O	2.21	0.41
1:A:442:PHE:HD2	1:B:403:TYR:HH	1.66	0.41
1:B:16:ILE:HA	1:B:21:ASP:HB3	2.02	0.41
1:C:188:SER:OG	1:C:350:ARG:NH1	2.50	0.40
1:C:388:MET:HG2	1:D:138:ALA:HB1	2.03	0.40
1:A:324:TRP:CH2	1:A:456:ASP:HA	2.56	0.40
1:B:426:ILE:HD11	1:B:590:ILE:HG12	2.02	0.40
1:B:93:ARG:NH1	1:B:114:GLU:OE2	2.46	0.40
1:B:299:ASP:O	1:B:303:TRP:HD1	2.05	0.40
1:C:181:ASN:C	1:C:181:ASN:HD22	2.25	0.40
1:B:307:ALA:O	1:B:317:VAL:HB	2.22	0.40
1:B:602:SER:HB2	1:B:606:ARG:NH1	2.35	0.40
1:C:552:ARG:NH1	1:C:552:ARG:CG	2.74	0.40
1:D:26:SER:H	1:D:29:GLN:HE21	1.69	0.40
1:D:166:LEU:HA	1:D:169:ILE:HB	2.03	0.40
1:D:334:GLU:OE1	1:D:489:GLY:N	2.55	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	574/629 (91%)	536 (93%)	34 (6%)	4 (1%)	22 54
1	B	575/629 (91%)	531 (92%)	32 (6%)	12 (2%)	7 26
1	C	532/629 (85%)	473 (89%)	48 (9%)	11 (2%)	7 26
1	D	524/629 (83%)	470 (90%)	44 (8%)	10 (2%)	8 28
All	All	2205/2516 (88%)	2010 (91%)	158 (7%)	37 (2%)	9 31

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	507	ASP
1	B	194	MET
1	B	195	ASN
1	B	244	SER
1	B	439	ASP
1	B	540	PRO
1	C	439	ASP
1	D	247	PRO
1	D	439	ASP
1	D	536	ARG
1	D	628	GLU
1	A	49	GLY
1	B	507	ASP
1	C	187	ILE
1	C	322	TYR
1	B	323	SER
1	C	175	LYS
1	C	506	ASP
1	D	189	GLU
1	D	371	ILE
1	D	525	GLU
1	B	189	GLU
1	B	196	LYS
1	B	525	GLU
1	C	123	GLY
1	C	173	GLY
1	D	188	SER
1	A	328	PHE
1	C	51	HIS
1	C	507	ASP
1	C	580	ASN
1	B	246	ASN
1	B	123	GLY
1	D	123	GLY
1	D	187	ILE
1	A	123	GLY
1	C	258	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	452/493 (92%)	404 (89%)	48 (11%)	6	20
1	B	453/493 (92%)	404 (89%)	49 (11%)	6	20
1	C	422/493 (86%)	380 (90%)	42 (10%)	7	23
1	D	414/493 (84%)	384 (93%)	30 (7%)	14	39
All	All	1741/1972 (88%)	1572 (90%)	169 (10%)	8	25

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	27	ARG
1	A	34	THR
1	A	37	LEU
1	A	61	ILE
1	A	73	ARG
1	A	75	ARG
1	A	94	ARG
1	A	96	GLN
1	A	107	SER
1	A	110	THR
1	A	112	VAL
1	A	122	VAL
1	A	156	SER
1	A	183	ASN
1	A	186	SER
1	A	188	SER
1	A	190	ASN
1	A	191	VAL
1	A	194	MET
1	A	198	MET
1	A	246	ASN
1	A	263	ASN
1	A	266	GLU
1	A	275	VAL
1	A	289	LYS
1	A	332	VAL
1	A	335	TRP
1	A	343	PHE
1	A	351	GLU

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Mol	Chain	Res	Type
1	A	353	SER
1	A	357	GLU
1	A	385	LEU
1	A	423	ARG
1	A	445	SER
1	A	477	ARG
1	A	482	ASN
1	A	483	THR
1	A	501	ARG
1	A	506	ASP
1	A	515	LYS
1	A	522	LYS
1	A	536	ARG
1	A	539	LYS
1	A	547	ARG
1	A	554	ARG
1	A	564	VAL
1	A	627	ILE
1	B	9	ASP
1	B	13	LEU
1	B	20	LYS
1	B	27	ARG
1	B	28	GLU
1	B	34	THR
1	B	70	ASP
1	B	73	ARG
1	B	96	GLN
1	B	115	SER
1	B	131	ASN
1	B	145	ASP
1	B	184	GLU
1	B	189	GLU
1	B	190	ASN
1	B	191	VAL
1	B	195	ASN
1	B	198	MET
1	B	199	ARG
1	B	245	VAL
1	B	263	ASN
1	B	266	GLU
1	B	276	ASP
1	B	289	LYS

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Mol	Chain	Res	Type
1	B	323	SER
1	B	332	VAL
1	B	357	GLU
1	B	365	ARG
1	B	385	LEU
1	B	426	ILE
1	B	439	ASP
1	B	450	ARG
1	B	477	ARG
1	B	495	LYS
1	B	499	TRP
1	B	501	ARG
1	B	502	LEU
1	B	503	LYS
1	B	506	ASP
1	B	515	LYS
1	B	526	ASP
1	B	536	ARG
1	B	552	ARG
1	B	562	ASN
1	B	563	THR
1	B	580	ASN
1	B	593	GLU
1	B	627	ILE
1	B	629	VAL
1	C	13	LEU
1	C	20	LYS
1	C	74	ASP
1	C	75	ARG
1	C	83	GLN
1	C	122	VAL
1	C	130	THR
1	C	131	ASN
1	C	137	LEU
1	C	168	THR
1	C	174	ARG
1	C	181	ASN
1	C	185	MET
1	C	251	MET
1	C	259	VAL
1	C	263	ASN
1	C	269	TRP

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Mol	Chain	Res	Type
1	C	332	VAL
1	C	351	GLU
1	C	357	GLU
1	C	385	LEU
1	C	397	THR
1	C	405	GLN
1	C	421	ILE
1	C	426	ILE
1	C	433	THR
1	C	434	HIS
1	C	437	VAL
1	C	439	ASP
1	C	450	ARG
1	C	494	LEU
1	C	511	LEU
1	C	515	LYS
1	C	543	GLU
1	C	552	ARG
1	C	554	ARG
1	C	565	VAL
1	C	580	ASN
1	C	581	LEU
1	C	585	VAL
1	C	610	ASP
1	C	624	ASP
1	D	17	HIS
1	D	22	LEU
1	D	28	GLU
1	D	34	THR
1	D	71	SER
1	D	75	ARG
1	D	96	GLN
1	D	113	SER
1	D	122	VAL
1	D	144	LYS
1	D	146	PHE
1	D	185	MET
1	D	186	SER
1	D	190	ASN
1	D	191	VAL
1	D	259	VAL
1	D	266	GLU

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Mol	Chain	Res	Type
1	D	273	ARG
1	D	330	GLU
1	D	332	VAL
1	D	351	GLU
1	D	357	GLU
1	D	360	ARG
1	D	385	LEU
1	D	397	THR
1	D	482	ASN
1	D	507	ASP
1	D	536	ARG
1	D	539	LYS
1	D	552	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	96	GLN
1	A	117	HIS
1	A	131	ASN
1	A	167	ASN
1	A	183	ASN
1	A	190	ASN
1	A	246	ASN
1	A	263	ASN
1	A	304	HIS
1	A	362	HIS
1	A	405	GLN
1	A	416	ASN
1	A	435	ASN
1	A	577	ASN
1	A	597	HIS
1	A	604	HIS
1	B	15	GLN
1	B	29	GLN
1	B	117	HIS
1	B	131	ASN
1	B	190	ASN
1	B	195	ASN
1	B	263	ASN
1	B	304	HIS

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Mol	Chain	Res	Type
1	B	405	GLN
1	B	416	ASN
1	B	435	ASN
1	B	470	HIS
1	B	595	GLN
1	B	597	HIS
1	B	604	HIS
1	C	29	GLN
1	C	117	HIS
1	C	131	ASN
1	C	181	ASN
1	C	246	ASN
1	C	362	HIS
1	C	405	GLN
1	C	416	ASN
1	C	435	ASN
1	C	470	HIS
1	C	580	ASN
1	C	604	HIS
1	D	29	GLN
1	D	96	GLN
1	D	131	ASN
1	D	362	HIS
1	D	400	GLN
1	D	405	GLN
1	D	416	ASN
1	D	435	ASN
1	D	470	HIS
1	D	577	ASN
1	D	580	ASN
1	D	595	GLN
1	D	597	HIS
1	D	604	HIS

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 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	$\#\|Z\| > 2$
3	TPP	D	1004	2	22,27,27	2.24	5 (22%)	29,40,40	1.92	11 (37%)
3	TPP	A	1001	2	22,27,27	1.82	5 (22%)	29,40,40	1.91	10 (34%)
3	TPP	B	1002	2	22,27,27	1.46	3 (13%)	29,40,40	1.81	8 (27%)
3	TPP	C	1003	2	22,27,27	2.95	7 (31%)	29,40,40	2.03	8 (27%)

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	D	1004	2	-	3/16/17/17	0/2/2/2
3	TPP	A	1001	2	-	3/16/17/17	0/2/2/2
3	TPP	B	1002	2	-	5/16/17/17	0/2/2/2
3	TPP	C	1003	2	-	4/16/17/17	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1003	TPP	C6-C5	11.51	1.56	1.50
3	D	1004	TPP	C6-C5	7.33	1.54	1.50
3	A	1001	TPP	PB-O1B	4.51	1.65	1.50
3	D	1004	TPP	PB-O1B	4.20	1.64	1.50
3	B	1002	TPP	C4-N3	-4.18	1.36	1.39
3	C	1003	TPP	PB-O1B	3.92	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1001	TPP	PA-O1A	3.85	1.64	1.50
3	A	1001	TPP	C4-N3	-3.11	1.37	1.39
3	D	1004	TPP	C4-N3	-3.06	1.37	1.39
3	C	1003	TPP	PA-O1A	2.95	1.61	1.50
3	B	1002	TPP	PB-O3B	2.81	1.65	1.54
3	A	1001	TPP	PB-O2B	2.53	1.64	1.54
3	D	1004	TPP	CM4-C4	2.38	1.54	1.49
3	C	1003	TPP	C4-N3	-2.30	1.37	1.39
3	D	1004	TPP	C7'-C5'	2.27	1.56	1.51
3	C	1003	TPP	CM4-C4	2.27	1.54	1.49
3	C	1003	TPP	C7'-C5'	2.19	1.55	1.51
3	A	1001	TPP	PB-O3B	-2.05	1.46	1.54
3	B	1002	TPP	C5'-C4'	-2.04	1.39	1.42
3	C	1003	TPP	PB-O2B	2.02	1.62	1.54

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1003	TPP	C6-C5-C4	4.80	131.28	127.43
3	C	1003	TPP	C5-C4-N3	3.96	115.50	107.57
3	B	1002	TPP	CM2-C2'-N1'	3.86	121.38	117.14
3	B	1002	TPP	C5-C4-N3	3.62	114.83	107.57
3	C	1003	TPP	C7'-N3-C2	-3.61	118.83	125.35
3	D	1004	TPP	CM2-C2'-N1'	3.60	121.10	117.14
3	A	1001	TPP	CM4-C4-C5	-3.55	119.83	127.60
3	A	1001	TPP	C5-C4-N3	3.53	114.63	107.57
3	D	1004	TPP	C5-C4-N3	3.40	114.38	107.57
3	B	1002	TPP	N1'-C2'-N3'	-3.29	119.88	125.54
3	D	1004	TPP	PA-O3A-PB	-3.21	121.80	132.83
3	A	1001	TPP	N1'-C2'-N3'	-3.19	120.05	125.54
3	D	1004	TPP	C6-C5-C4	3.16	129.97	127.43
3	C	1003	TPP	CM4-C4-C5	-3.12	120.78	127.60
3	B	1002	TPP	C6'-N1'-C2'	3.08	121.20	115.96
3	D	1004	TPP	N1'-C2'-N3'	-3.08	120.24	125.54
3	C	1003	TPP	N1'-C2'-N3'	-2.91	120.53	125.54
3	C	1003	TPP	O3B-PB-O3A	2.86	114.23	104.64
3	C	1003	TPP	C6'-N1'-C2'	2.77	120.67	115.96
3	A	1001	TPP	C7'-C5'-C6'	-2.76	115.42	120.69
3	A	1001	TPP	C6-C5-C4	2.71	129.61	127.43
3	D	1004	TPP	C7'-N3-C2	-2.69	120.49	125.35
3	D	1004	TPP	CM4-C4-C5	-2.68	121.75	127.60
3	C	1003	TPP	CM2-C2'-N1'	2.67	120.07	117.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1001	TPP	C6'-N1'-C2'	2.67	120.50	115.96
3	B	1002	TPP	CM4-C4-C5	-2.62	121.86	127.60
3	D	1004	TPP	O3B-PB-O3A	2.58	113.27	104.64
3	A	1001	TPP	C7'-N3-C2	-2.57	120.70	125.35
3	B	1002	TPP	C6-C5-C4	2.53	129.47	127.43
3	B	1002	TPP	PA-O3A-PB	-2.44	124.45	132.83
3	D	1004	TPP	C2'-N3'-C4'	2.37	121.78	118.08
3	A	1001	TPP	C2'-N3'-C4'	2.37	121.78	118.08
3	D	1004	TPP	C6'-N1'-C2'	2.37	120.00	115.96
3	A	1001	TPP	CM4-C4-N3	2.36	125.54	122.53
3	A	1001	TPP	CM2-C2'-N3'	2.23	120.64	117.15
3	B	1002	TPP	C7'-C5'-C6'	-2.06	116.76	120.69
3	D	1004	TPP	O2B-PB-O1B	-2.06	102.63	110.68

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1001	TPP	C4'-C5'-C7'-N3
3	B	1002	TPP	C4'-C5'-C7'-N3
3	C	1003	TPP	C4'-C5'-C7'-N3
3	D	1004	TPP	C4'-C5'-C7'-N3
3	D	1004	TPP	C5-C6-C7-O7
3	D	1004	TPP	PA-O3A-PB-O2B
3	C	1003	TPP	C5-C6-C7-O7
3	C	1003	TPP	PA-O3A-PB-O2B
3	B	1002	TPP	PB-O3A-PA-O2A
3	A	1001	TPP	C6'-C5'-C7'-N3
3	B	1002	TPP	C6'-C5'-C7'-N3
3	A	1001	TPP	C4-C5-C6-C7
3	B	1002	TPP	PB-O3A-PA-O1A
3	B	1002	TPP	C7-O7-PA-O1A
3	C	1003	TPP	C6'-C5'-C7'-N3

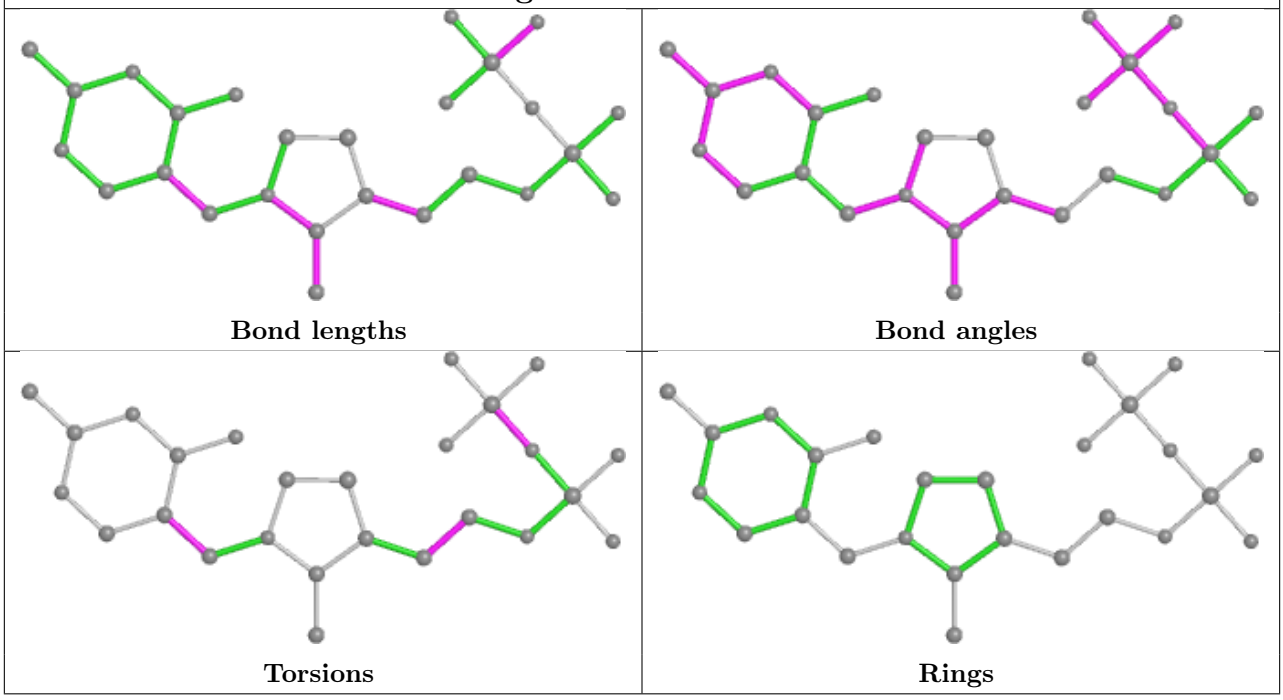
There are no ring outliers.

3 monomers are involved in 7 short contacts:

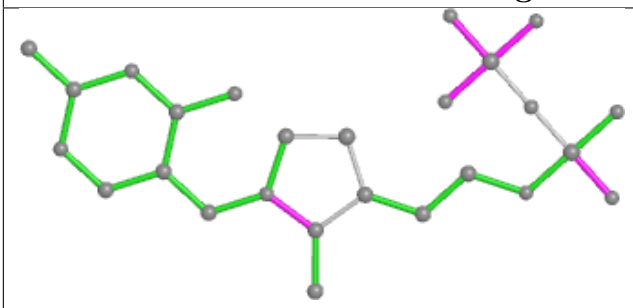
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1004	TPP	1	0
3	A	1001	TPP	2	0
3	B	1002	TPP	4	0

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.

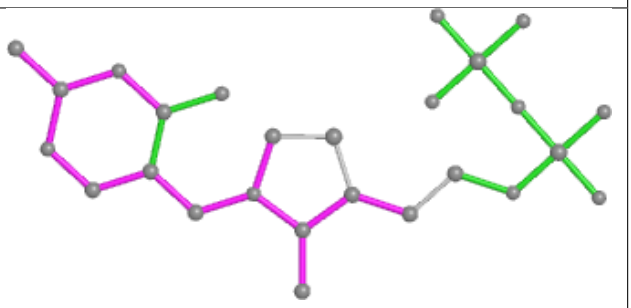
Ligand TPP D 1004



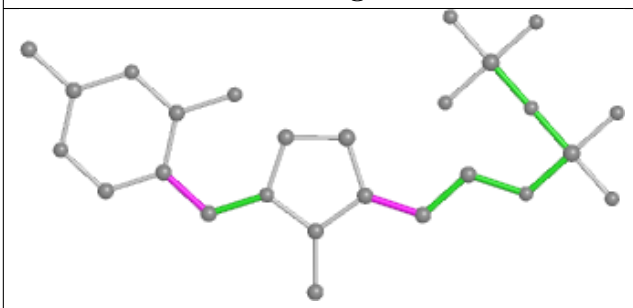
Ligand TPP A 1001



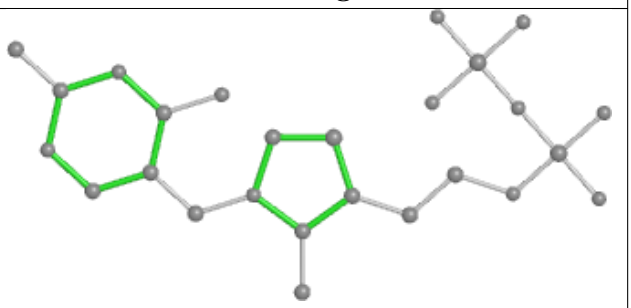
Bond lengths



Bond angles

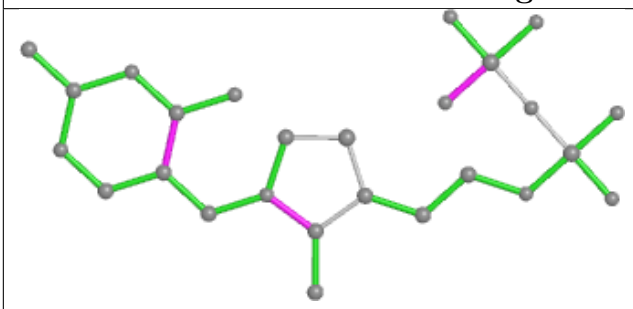


Torsions

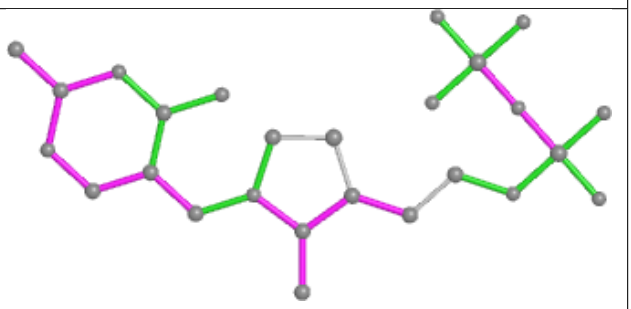


Rings

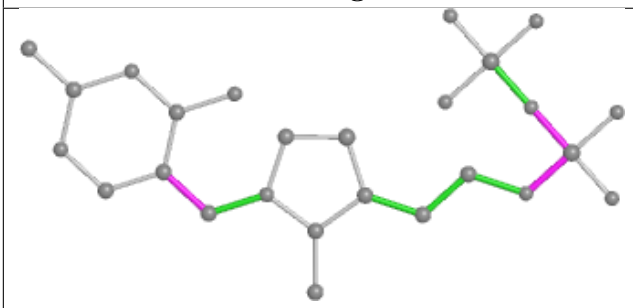
Ligand TPP B 1002



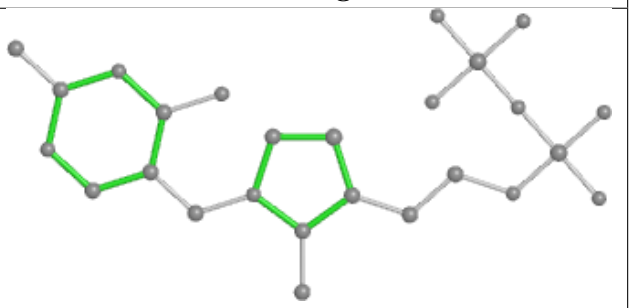
Bond lengths



Bond angles

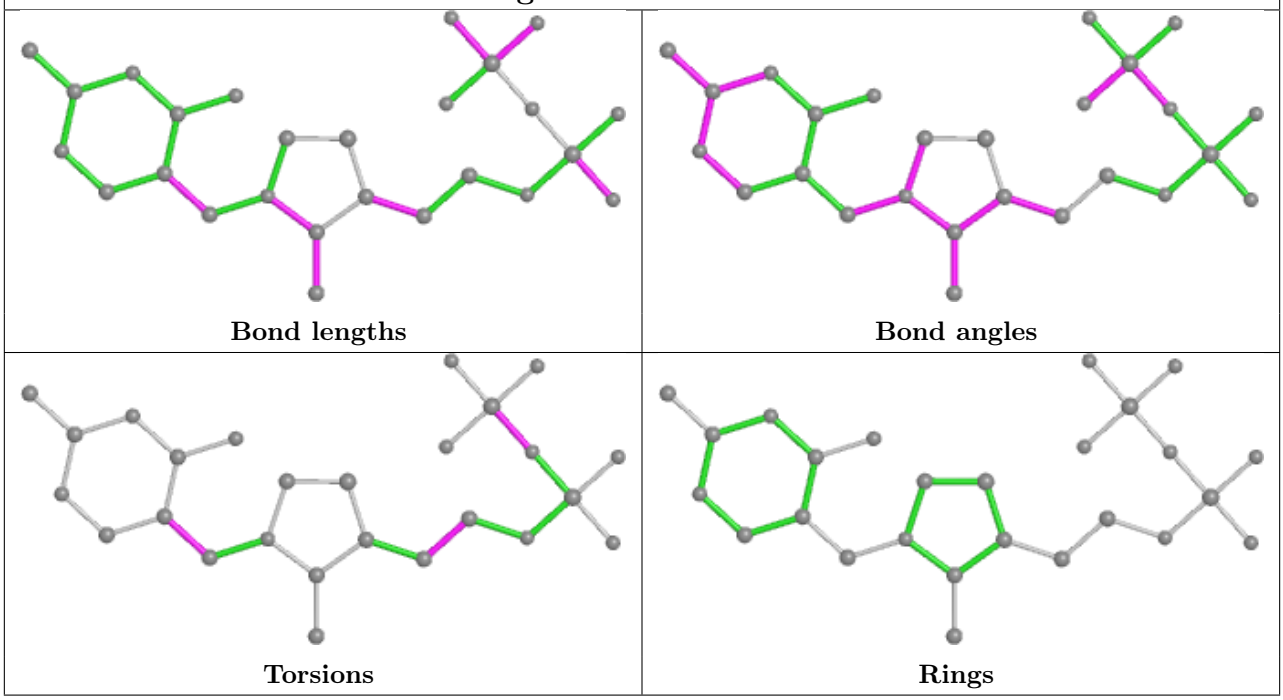


Torsions



Rings

Ligand TPP C 1003



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	578/629 (91%)	-0.48	6 (1%)	82	82	-5, 10, 34, 53	0
1	B	579/629 (92%)	-0.49	7 (1%)	79	79	-3, 11, 39, 75	0
1	C	538/629 (85%)	0.37	48 (8%)	9	7	6, 65, 139, 191	0
1	D	530/629 (84%)	0.35	52 (9%)	7	5	7, 60, 133, 175	0
All	All	2225/2516 (88%)	-0.08	113 (5%)	28	24	-5, 24, 121, 191	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	15	GLN	6.1
1	D	46	SER	6.1
1	D	49	GLY	5.6
1	C	321	ALA	5.5
1	C	8	SER	5.5
1	C	628	GLU	5.5
1	D	45	CYS	5.4
1	C	104	GLY	4.7
1	D	147	HIS	4.7
1	B	244	SER	4.7
1	B	629	VAL	4.6
1	D	42	VAL	4.4
1	C	627	ILE	4.3
1	C	544	GLU	4.2
1	D	48	GLY	4.2
1	C	7	THR	4.1
1	C	251	MET	4.0
1	C	9	ASP	3.9
1	B	628	GLU	3.8
1	D	185	MET	3.8
1	D	247	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	627	ILE	3.7
1	D	245	VAL	3.5
1	C	47	ARG	3.5
1	C	67	TYR	3.5
1	C	360	ARG	3.4
1	D	24	ARG	3.4
1	C	508	VAL	3.4
1	C	145	ASP	3.4
1	C	11	PRO	3.4
1	C	263	ASN	3.3
1	D	47	ARG	3.3
1	B	243	ALA	3.3
1	A	320	SER	3.3
1	C	95	ASP	3.2
1	C	17	HIS	3.2
1	C	46	SER	3.1
1	A	319	SER	3.1
1	A	244	SER	3.1
1	B	196	LYS	3.1
1	D	254	ARG	3.1
1	C	269	TRP	3.0
1	D	555	ALA	3.0
1	C	277	LEU	3.0
1	D	554	ARG	2.9
1	A	245	VAL	2.9
1	C	555	ALA	2.9
1	C	249	ALA	2.9
1	D	622	GLY	2.9
1	C	246	ASN	2.9
1	D	32	ALA	2.9
1	D	628	GLU	2.8
1	C	257	GLY	2.8
1	D	44	VAL	2.8
1	C	245	VAL	2.8
1	D	96	GLN	2.7
1	D	508	VAL	2.7
1	C	528	PRO	2.7
1	D	481	GLY	2.7
1	B	199	ARG	2.7
1	D	191	VAL	2.7
1	C	322	TYR	2.6
1	C	62	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	52	LEU	2.6
1	D	188	SER	2.6
1	D	62	ILE	2.6
1	D	278	ASP	2.6
1	C	175	LYS	2.5
1	D	255	TYR	2.5
1	C	526	ASP	2.5
1	D	52	LEU	2.5
1	C	286	VAL	2.5
1	C	20	LYS	2.5
1	D	258	PRO	2.4
1	D	252	GLY	2.4
1	D	76	ILE	2.4
1	D	580	ASN	2.4
1	D	544	GLU	2.4
1	D	95	ASP	2.3
1	C	76	ILE	2.3
1	D	73	ARG	2.3
1	D	321	ALA	2.3
1	D	145	ASP	2.3
1	D	28	GLU	2.3
1	C	255	TYR	2.3
1	C	258	PRO	2.3
1	D	190	ASN	2.2
1	D	629	VAL	2.2
1	D	484	ALA	2.2
1	C	287	THR	2.2
1	C	77	LEU	2.2
1	D	250	ALA	2.2
1	D	548	GLU	2.2
1	D	251	MET	2.2
1	D	289	LYS	2.2
1	C	278	ASP	2.2
1	C	289	LYS	2.2
1	C	185	MET	2.2
1	C	552	ARG	2.2
1	D	17	HIS	2.1
1	C	96	GLN	2.1
1	D	486	VAL	2.1
1	C	554	ARG	2.1
1	A	312	ALA	2.1
1	B	8	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	623	VAL	2.1
1	C	288	THR	2.0
1	A	198	MET	2.0
1	D	323	SER	2.0
1	D	86	ALA	2.0
1	D	104	GLY	2.0
1	D	151	VAL	2.0
1	D	253	VAL	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)

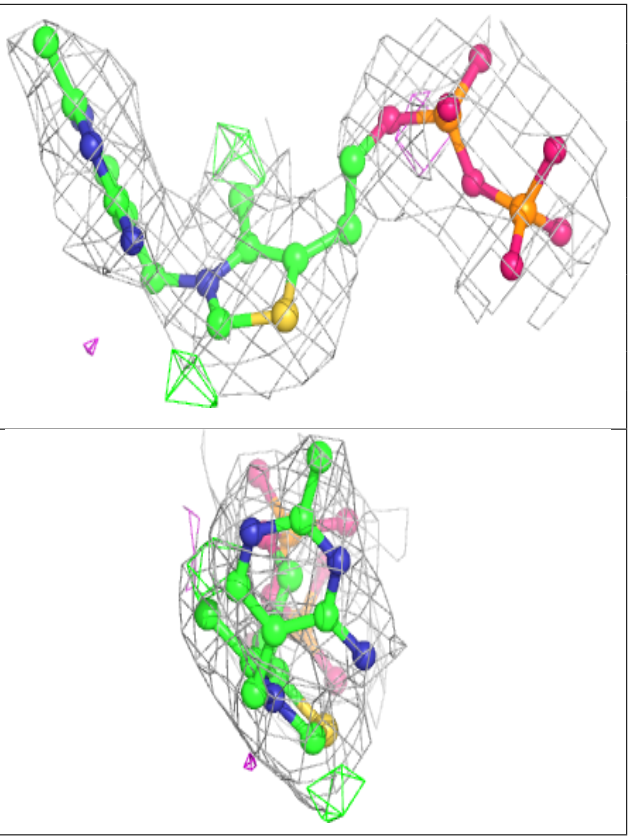
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

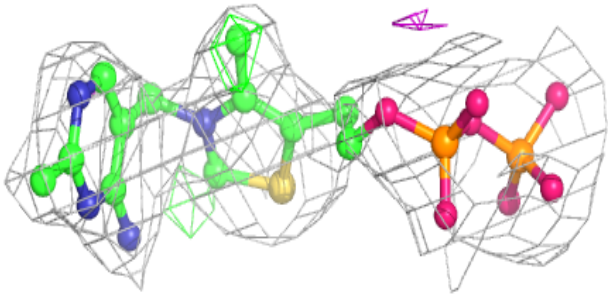
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TPP	D	1004	26/26	0.92	0.16	40,44,48,48	0
2	MG	C	2003	1/1	0.93	0.12	33,33,33,33	0
2	MG	D	2004	1/1	0.93	0.12	35,35,35,35	0
3	TPP	C	1003	26/26	0.93	0.16	50,50,52,53	0
2	MG	B	2002	1/1	0.93	0.21	8,8,8,8	0
2	MG	A	2001	1/1	0.97	0.21	9,9,9,9	0
3	TPP	A	1001	26/26	0.98	0.11	2,2,4,5	0
3	TPP	B	1002	26/26	0.98	0.13	2,3,4,6	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 D 1004:

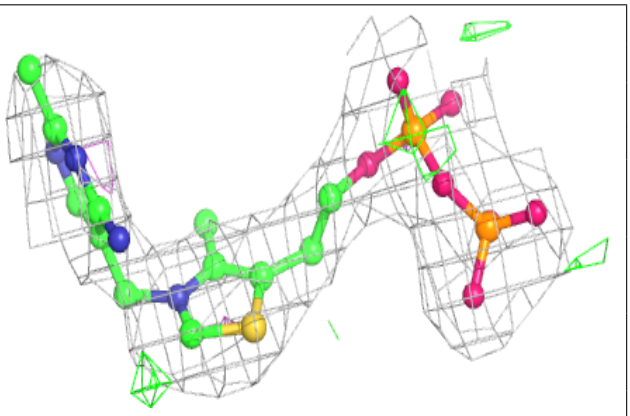
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

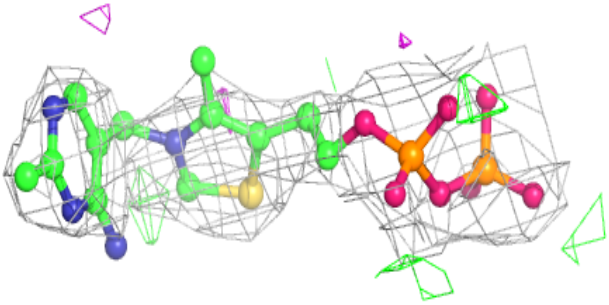


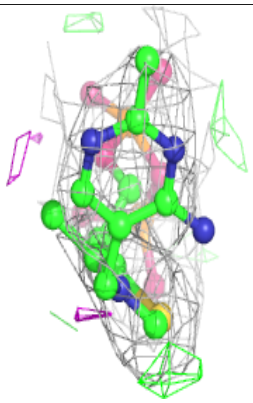


Electron density around TPP C 1003:

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

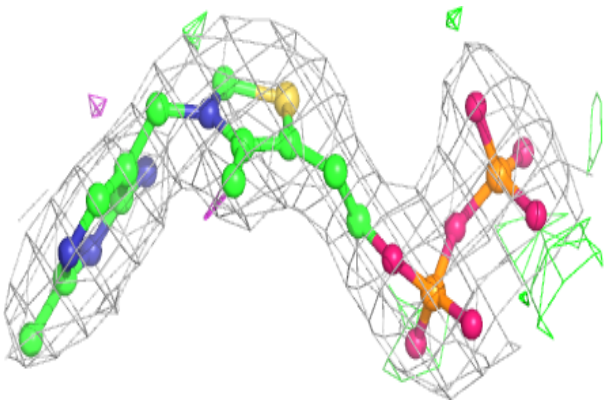


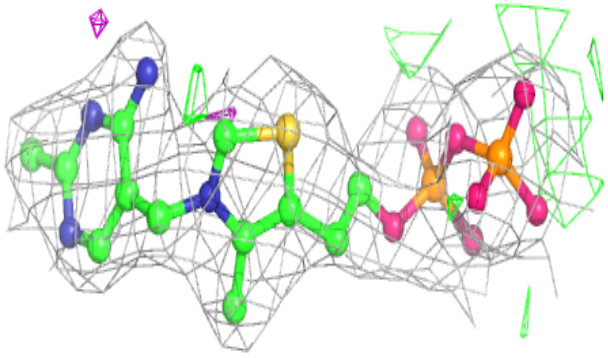


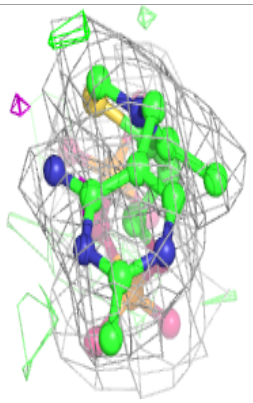


Electron density around TPP A 1001:

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

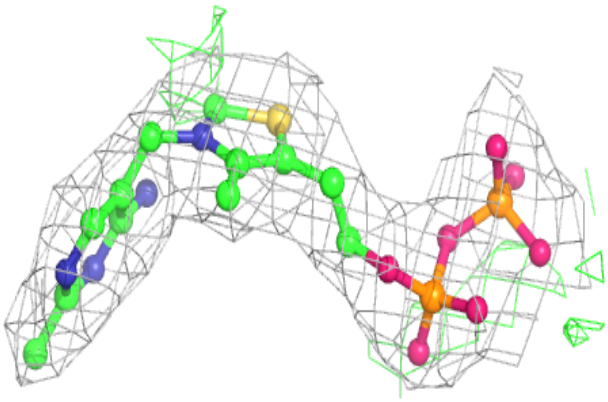


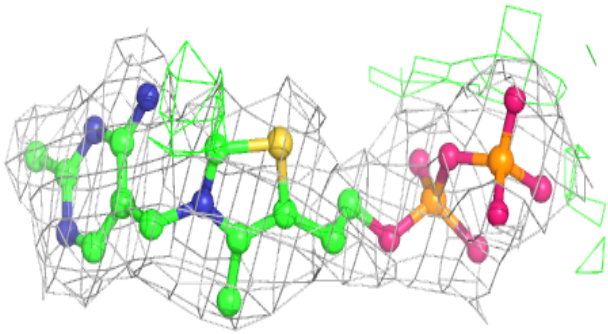


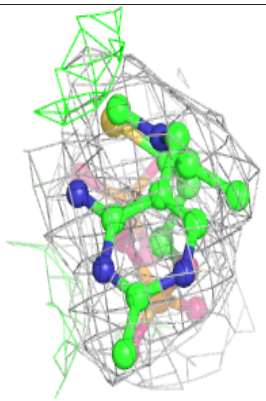


Electron density around TPP B 1002:

$2mF_o$-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.