



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:09 am BST

PDB ID : 3FRK
Title : X-ray structure of QdtB from *T. thermosaccharolyticum* in complex with a P
LP:TDP-3-aminoquinovose aldimine
Authors : Thoden, J.B.; Holden, H.M.
Deposited on : 2009-01-08
Resolution : 2.15 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 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 : 2.11
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) : 2.11

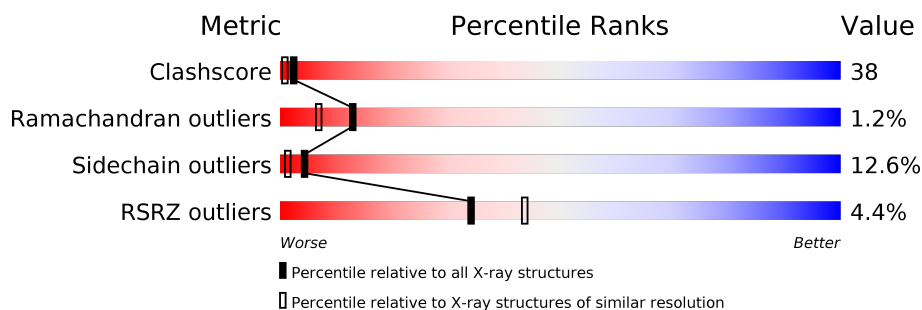
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	<div> <div>4%</div> <div>46%</div> <div>43%</div> <div>8%</div> <div>..</div> </div>
1	B	373	<div> <div>4%</div> <div>34%</div> <div>52%</div> <div>10%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6157 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.

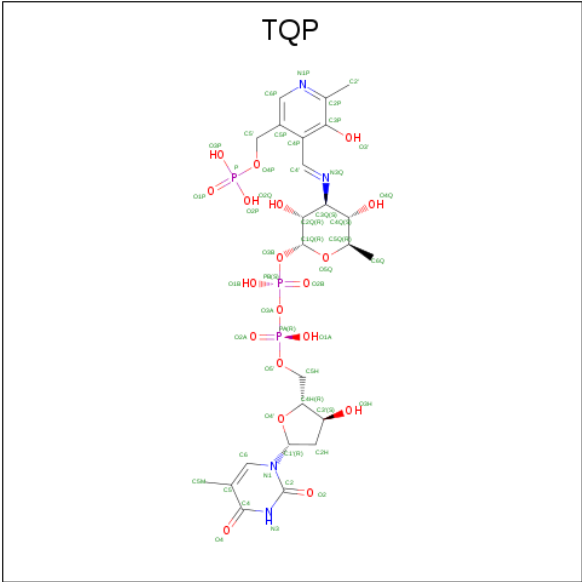
- Molecule 1 is a protein called QdtB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	3	0
			2953	1917	483	545	8			
1	B	364	Total	C	N	O	S	0	1	0
			2924	1895	480	541	8			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	366	LEU	-	EXPRESSION TAG	UNP Q6TFC4
A	367	GLU	-	EXPRESSION TAG	UNP Q6TFC4
A	368	HIS	-	EXPRESSION TAG	UNP Q6TFC4
A	369	HIS	-	EXPRESSION TAG	UNP Q6TFC4
A	370	HIS	-	EXPRESSION TAG	UNP Q6TFC4
A	371	HIS	-	EXPRESSION TAG	UNP Q6TFC4
A	372	HIS	-	EXPRESSION TAG	UNP Q6TFC4
A	373	HIS	-	EXPRESSION TAG	UNP Q6TFC4
B	366	LEU	-	EXPRESSION TAG	UNP Q6TFC4
B	367	GLU	-	EXPRESSION TAG	UNP Q6TFC4
B	368	HIS	-	EXPRESSION TAG	UNP Q6TFC4
B	369	HIS	-	EXPRESSION TAG	UNP Q6TFC4
B	370	HIS	-	EXPRESSION TAG	UNP Q6TFC4
B	371	HIS	-	EXPRESSION TAG	UNP Q6TFC4
B	372	HIS	-	EXPRESSION TAG	UNP Q6TFC4
B	373	HIS	-	EXPRESSION TAG	UNP Q6TFC4

- Molecule 2 is (2R,3R,4S,5S,6R)-3,5-dihydroxy-4-[(1E)-{3-hydroxy-2-methyl-5-[(phosphono oxy)methyl]pyridin-4-yl}methylidene]amino}-6-methyltetrahydro-2H-pyran-2-yl [(2R,3S,5R)-3-hydroxy-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-2-yl]methyl dihydrogen diphosphate (three-letter code: TQP) (formula: C₂₄H₃₅N₄O₁₉P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			50	24	4	19	3		
2	B	1	Total	C	N	O	P	0	0
			50	24	4	19	3		

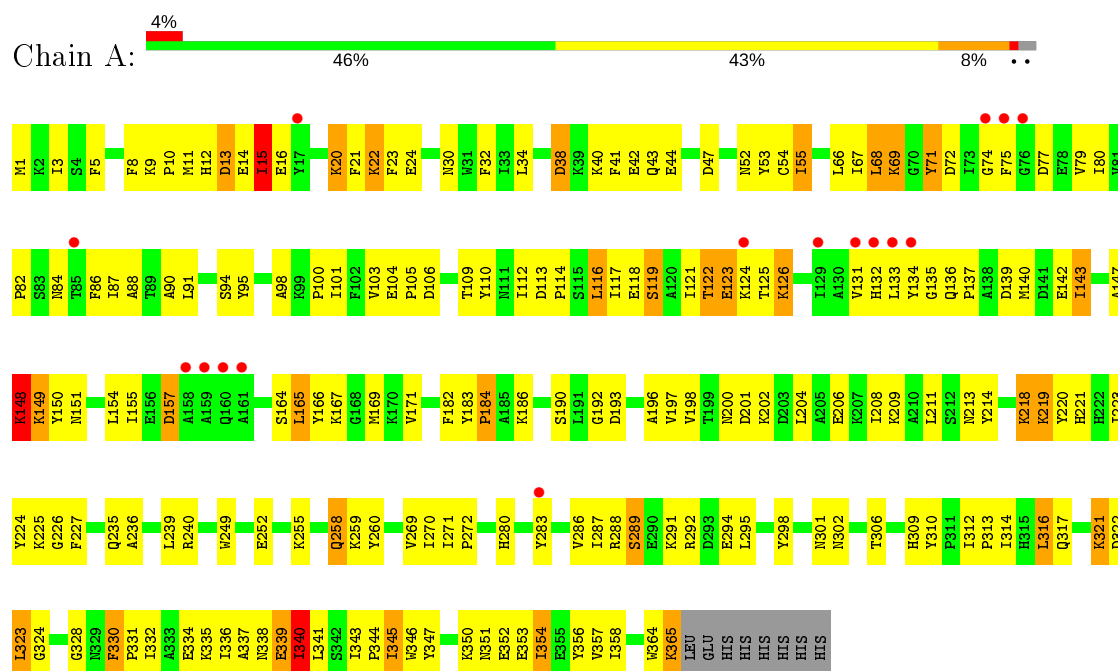
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	110	Total	O	0	0
			110	110		
3	B	70	Total	O	0	0
			70	70		

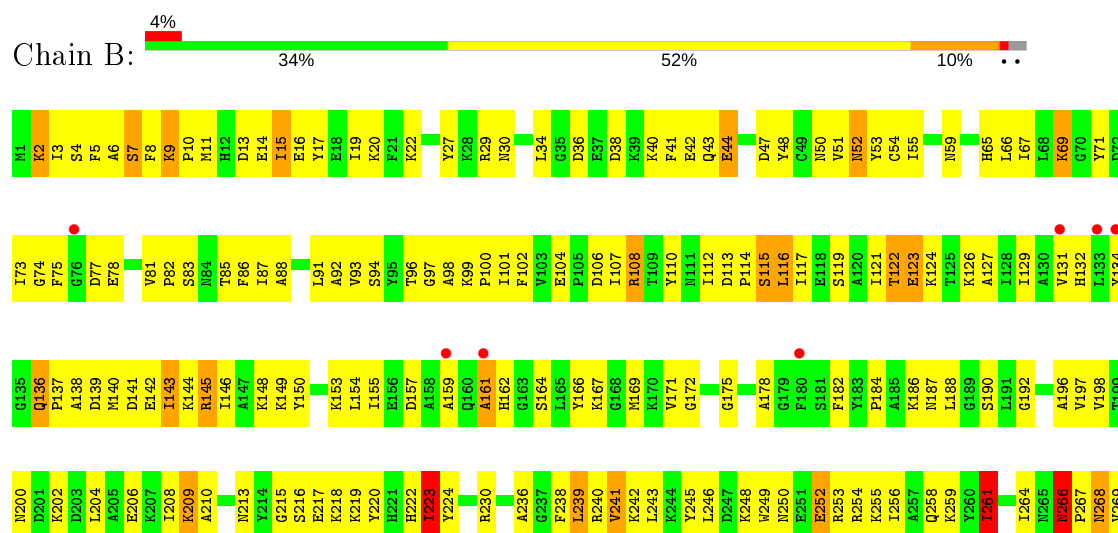
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: QdtB



• Molecule 1: QdtB





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	109.10 Å 109.10 Å 177.90 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.15 27.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.7 (30.00-2.15) 9.1 (27.85-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	TNT	Depositor
R, R_{free}	0.213 , 0.269 0.217 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 103.6	EDS
L-test for twinning ¹	$\langle L \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6157	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: (*Not available*)

¹Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: TQP

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	0.69	0/3037	1.37	20/4101 (0.5%)
1	B	0.67	0/2997	1.34	20/4048 (0.5%)
All	All	0.68	0/6034	1.35	40/8149 (0.5%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	330	PHE	C-N-CD	-11.13	96.11	120.60
1	A	13	ASP	CB-CG-OD2	9.63	126.96	118.30
1	B	239	LEU	CA-CB-CG	-9.07	94.44	115.30
1	A	165	LEU	CB-CG-CD2	-8.92	95.84	111.00
1	A	116	LEU	CB-CG-CD2	-7.83	97.69	111.00
1	B	141	ASP	CB-CG-OD1	-7.61	111.45	118.30
1	A	330	PHE	C-N-CD	-7.50	104.11	120.60
1	A	66	LEU	CA-CB-CG	-7.27	98.59	115.30
1	B	230	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	A	106	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	157	ASP	N-CA-C	-6.85	92.50	111.00
1	A	66	LEU	CB-CG-CD2	-6.80	99.44	111.00
1	B	261	ILE	CG1-CB-CG2	6.74	126.24	111.40
1	B	91	LEU	CB-CG-CD1	6.69	122.37	111.00
1	B	138	ALA	N-CA-C	-6.39	93.75	111.00
1	B	266	ASN	N-CA-C	-6.30	93.98	111.00
1	A	38	ASP	CB-CG-OD1	6.30	123.97	118.30
1	B	277	TYR	CB-CA-C	-6.25	97.89	110.40
1	B	223	ILE	CB-CA-C	-6.21	99.19	111.60
1	A	340	ILE	N-CA-C	5.97	127.12	111.00
1	A	68	LEU	CB-CG-CD1	-5.95	100.88	111.00
1	B	204	LEU	CB-CG-CD2	-5.94	100.90	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ILE	CG1-CB-CG2	5.89	124.37	111.40
1	A	323	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	B	161	ALA	N-CA-C	5.54	125.95	111.00
1	A	13	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	55	ILE	CB-CA-C	-5.44	100.72	111.60
1	B	66	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	B	13	ASP	N-CA-C	-5.40	96.43	111.00
1	B	15	ILE	CG1-CB-CG2	-5.37	99.59	111.40
1	A	316	LEU	CA-CB-CG	-5.36	102.97	115.30
1	B	54	CYS	CA-CB-SG	-5.26	104.53	114.00
1	A	15	ILE	CB-CA-C	-5.25	101.10	111.60
1	B	358	ILE	CB-CA-C	-5.25	101.09	111.60
1	A	154	LEU	CB-CG-CD2	-5.23	102.10	111.00
1	B	52	ASN	CB-CA-C	-5.22	99.96	110.40
1	B	241	VAL	CB-CA-C	-5.13	101.65	111.40
1	A	95	TYR	CA-CB-CG	5.13	123.14	113.40
1	A	165	LEU	CB-CG-CD1	-5.11	102.32	111.00
1	A	193	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2953	0	2931	174	0
1	B	2924	0	2904	277	0
2	A	50	0	30	4	0
2	B	50	0	30	4	0
3	A	110	0	0	6	0
3	B	70	0	0	3	0
All	All	6157	0	5895	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 38.

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:B:113:ASP:HB3	1:B:116:LEU:HG	1.16	1.14
1:B:122:THR:HG22	1:B:124:LYS:H	1.08	1.11
1:A:114:PRO:HA	1:A:117:ILE:HD12	1.32	1.10
1:A:292:ARG:NH2	1:A:337:ALA:O	1.88	1.06
1:B:114:PRO:HA	1:B:117:ILE:HD12	1.31	1.06
1:B:336:ILE:HG23	1:B:340:ILE:HD13	1.40	1.03
1:B:288:ARG:HG2	1:B:340:ILE:HD12	1.38	1.00
1:A:114:PRO:HA	1:A:117:ILE:CD1	1.92	1.00
1:A:149:LYS:HG2	1:A:150:TYR:CD2	1.99	0.97
1:B:113:ASP:CB	1:B:116:LEU:HG	1.95	0.97
1:B:292:ARG:NH2	1:B:337:ALA:O	1.99	0.96
1:B:320:TYR:O	1:B:323:LEU:HB2	1.65	0.95
1:B:116:LEU:HD23	1:B:116:LEU:N	1.83	0.93
1:B:113:ASP:HB3	1:B:116:LEU:CG	2.00	0.92
1:A:9:LYS:HB3	1:A:10:PRO:HD3	1.53	0.91
1:B:353:GLU:O	1:B:357:VAL:HG23	1.71	0.91
1:B:114:PRO:HA	1:B:117:ILE:CD1	2.00	0.91
1:B:259:LYS:HG2	1:B:354:ILE:HG21	1.50	0.90
1:B:16:GLU:O	1:B:20:LYS:HG3	1.72	0.88
1:B:267:PRO:HG2	1:B:268:ASN:HD21	1.39	0.87
1:B:149:LYS:HG2	1:B:150:TYR:CE2	2.10	0.86
1:B:356:TYR:CE2	1:B:360:LYS:HD2	2.10	0.85
1:A:149:LYS:HG2	1:A:150:TYR:CE2	2.11	0.84
1:B:104:GLU:OE2	1:B:332:ILE:HB	1.76	0.84
1:B:122:THR:HG22	1:B:124:LYS:N	1.92	0.84
1:A:149:LYS:HE2	1:A:150:TYR:CE2	2.13	0.84
1:A:1:MET:HB3	1:A:356:TYR:CE2	2.14	0.83
1:A:204:LEU:O	1:A:208:ILE:HG13	1.77	0.83
1:B:310:TYR:HB3	1:B:311:PRO:HD2	1.60	0.83
1:B:268:ASN:N	1:B:268:ASN:HD22	1.77	0.83
1:B:38:ASP:O	1:B:42:GLU:HG3	1.79	0.82
1:B:268:ASN:ND2	1:B:268:ASN:N	2.26	0.81
1:B:122:THR:CG2	1:B:124:LYS:H	1.93	0.81
1:A:271:ILE:HB	1:A:272:PRO:HD2	1.62	0.81
1:A:80:ILE:HD13	1:A:117:ILE:HG23	1.61	0.80
1:A:114:PRO:CA	1:A:117:ILE:HD12	2.10	0.80
1:B:16:GLU:HG2	1:B:17:TYR:HD1	1.46	0.80
1:B:93:VAL:CG1	1:B:100:PRO:HD3	2.12	0.79
1:B:104:GLU:HB3	1:B:332:ILE:HD12	1.64	0.79
1:A:77:ASP:OD1	1:A:126:LYS:HG2	1.84	0.78
1:A:74:GLY:O	1:A:77:ASP:HB2	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:O	1:A:24:GLU:HG3	1.85	0.76
1:A:100:PRO:O	1:A:101:ILE:HD13	1.85	0.76
1:B:3:ILE:HD12	1:B:353:GLU:HG2	1.65	0.76
1:A:259:LYS:HD3	1:A:354:ILE:HG21	1.66	0.76
1:B:256:ILE:O	1:B:259:LYS:HB3	1.85	0.76
1:A:184:PRO:HD3	1:A:192:GLY:O	1.85	0.75
1:B:250:ASN:O	1:B:254:ARG:HG3	1.86	0.75
1:B:266:ASN:OD1	1:B:268:ASN:ND2	2.20	0.74
1:A:148:LYS:O	1:A:151:ASN:N	2.21	0.74
1:B:52:ASN:HB2	1:B:53:TYR:CD2	2.23	0.73
1:B:267:PRO:HG2	1:B:268:ASN:ND2	2.04	0.73
1:A:220:TYR:CG	1:B:311:PRO:HG3	2.23	0.73
1:B:354:ILE:HG22	1:B:358:ILE:HD11	1.70	0.73
1:B:354:ILE:HG22	1:B:358:ILE:CD1	2.18	0.73
1:B:301:ASN:HD22	1:B:301:ASN:N	1.85	0.72
1:B:295:LEU:HB2	1:B:364:TRP:CZ2	2.25	0.72
1:A:321:LYS:O	1:A:324:GLY:N	2.19	0.72
1:B:132:HIS:CD2	1:B:171:VAL:HG23	2.25	0.72
1:B:184:PRO:HD3	1:B:192:GLY:O	1.90	0.72
1:B:258:GLN:O	1:B:261:ILE:HG22	1.89	0.71
1:A:236:ALA:O	1:A:240:ARG:HG3	1.90	0.71
1:B:274:GLU:HG2	1:B:274:GLU:O	1.91	0.71
1:B:202:LYS:O	1:B:206:GLU:HG3	1.90	0.71
1:A:354:ILE:O	1:A:358:ILE:HG13	1.90	0.71
1:A:86:PHE:CE2	1:A:88:ALA:HB2	2.26	0.70
1:B:268:ASN:H	1:B:268:ASN:HD22	1.39	0.69
1:B:55:ILE:HG23	1:B:209:LYS:HG3	1.73	0.69
1:B:41:PHE:HA	1:B:44:GLU:HG3	1.73	0.68
1:A:202:LYS:O	1:A:206:GLU:HG3	1.93	0.68
1:A:136:GLN:HB3	1:A:280:HIS:CD2	2.29	0.68
1:A:271:ILE:C	1:A:271:ILE:HD12	2.14	0.68
1:B:11:MET:O	1:B:14:GLU:HB3	1.93	0.68
1:B:314:ILE:O	1:B:317:GLN:HB2	1.94	0.68
1:B:182:PHE:CE2	1:B:196:ALA:HB2	2.30	0.67
1:B:106:ASP:OD1	1:B:108:ARG:HB2	1.94	0.67
1:B:271:ILE:HG23	1:B:272:PRO:HD2	1.76	0.67
1:A:118:GLU:HB2	3:A:415:HOH:O	1.93	0.67
1:A:113:ASP:HB3	1:A:116:LEU:HD12	1.76	0.67
1:B:121:ILE:HD13	1:B:150:TYR:CG	2.30	0.67
1:A:123:GLU:CD	1:A:123:GLU:H	1.99	0.66
1:A:219:LYS:O	1:A:220:TYR:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LYS:O	1:B:220:TYR:HB2	1.93	0.66
1:A:113:ASP:O	1:A:116:LEU:HB2	1.95	0.66
1:B:223:ILE:HG13	1:B:224:TYR:CG	2.30	0.66
1:B:93:VAL:HG11	1:B:100:PRO:HD3	1.77	0.66
1:A:218:LYS:HG2	1:A:221:HIS:HB2	1.78	0.65
1:B:140:MET:HA	1:B:143:ILE:HG13	1.77	0.65
1:B:266:ASN:CG	1:B:267:PRO:HD2	2.17	0.65
1:B:116:LEU:HD23	1:B:116:LEU:H	1.62	0.65
1:B:5:PHE:CE2	1:B:307:LEU:HB2	2.32	0.65
1:B:74:GLY:O	1:B:77:ASP:HB2	1.96	0.65
1:B:19:ILE:HG22	1:B:20:LYS:N	2.11	0.65
1:B:295:LEU:HB2	1:B:364:TRP:CH2	2.31	0.65
1:B:116:LEU:CD2	1:B:116:LEU:N	2.58	0.64
1:A:119:SER:OG	3:A:414:HOH:O	2.14	0.64
1:B:264:ILE:HB	1:B:271:ILE:HD11	1.79	0.64
1:B:272:PRO:HD3	1:B:285:PHE:CE2	2.32	0.64
1:B:137:PRO:HD3	1:B:164:SER:OG	1.97	0.64
1:B:288:ARG:CG	1:B:340:ILE:HD12	2.21	0.64
1:A:184:PRO:HB2	2:A:374:TQP:H5MA	1.81	0.63
1:B:313:PRO:O	1:B:314:ILE:C	2.34	0.63
1:B:336:ILE:CG2	1:B:340:ILE:HD13	2.21	0.62
1:A:69:LYS:O	1:A:72:ASP:N	2.29	0.62
1:B:6:ALA:O	1:B:7:SER:HB2	2.00	0.62
1:B:122:THR:CG2	1:B:123:GLU:N	2.63	0.62
1:A:38:ASP:O	1:A:42:GLU:HG3	1.99	0.62
1:B:122:THR:CG2	1:B:124:LYS:HB2	2.30	0.62
1:B:295:LEU:O	1:B:298:TYR:HB3	1.99	0.62
1:B:2:LYS:C	1:B:3:ILE:HD13	2.19	0.62
1:B:93:VAL:HG12	1:B:100:PRO:HD3	1.80	0.62
1:B:261:ILE:HD12	1:B:285:PHE:HE1	1.65	0.61
1:B:167:LYS:HG3	1:B:277:TYR:HB2	1.81	0.61
1:B:358:ILE:HG22	1:B:362:ASN:ND2	2.15	0.61
1:B:277:TYR:CD2	1:B:277:TYR:C	2.73	0.61
1:B:117:ILE:HD13	1:B:143:ILE:HG23	1.83	0.61
1:B:326:LYS:O	1:B:329:ASN:HB2	2.00	0.61
1:B:197:VAL:HG12	1:B:198:VAL:N	2.16	0.61
1:A:235:GLN:O	1:A:239:LEU:HG	2.01	0.60
1:B:139:ASP:O	1:B:143:ILE:HG13	2.01	0.60
1:B:5:PHE:CD1	1:B:306:THR:HA	2.36	0.60
1:A:87:ILE:HA	1:A:314:ILE:HD11	1.84	0.60
1:A:86:PHE:HD2	1:A:88:ALA:HB3	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:TRP:HD1	1:B:347:TYR:CE2	2.19	0.59
1:A:271:ILE:CB	1:A:272:PRO:HD2	2.27	0.59
1:B:261:ILE:CD1	1:B:285:PHE:HE1	2.15	0.59
1:B:252:GLU:HA	1:B:255:LYS:HG3	1.83	0.59
1:A:40:LYS:O	1:A:44:GLU:HG3	2.03	0.59
1:B:341:LEU:HG	1:B:342:SER:N	2.17	0.59
1:A:331:PRO:HA	1:A:334:GLU:HB2	1.84	0.59
1:B:149:LYS:HG2	1:B:150:TYR:CD2	2.37	0.58
1:A:139:ASP:O	1:A:143:ILE:HG13	2.04	0.58
1:A:113:ASP:HB3	1:A:116:LEU:CD1	2.33	0.58
2:A:374:TQP:O2A	3:A:426:HOH:O	2.16	0.58
1:A:183:TYR:HB3	1:A:186:LYS:HE3	1.85	0.57
1:B:53:TYR:HE2	1:B:200:ASN:O	1.87	0.57
1:A:298:TYR:O	1:A:302:ASN:ND2	2.37	0.57
1:A:75:PHE:HZ	1:B:75:PHE:CZ	2.22	0.57
1:B:115:SER:HB2	1:B:116:LEU:HD23	1.85	0.57
1:B:266:ASN:OD1	1:B:269:VAL:HG23	2.04	0.57
1:A:86:PHE:CD2	1:A:88:ALA:CB	2.87	0.57
1:B:87:ILE:HA	1:B:314:ILE:HD11	1.87	0.57
1:A:335:LYS:O	1:A:338:ASN:HB2	2.03	0.57
1:B:164:SER:HA	1:B:281:VAL:HG13	1.85	0.57
1:A:147:ALA:O	1:A:151:ASN:N	2.36	0.57
1:A:12:HIS:ND1	1:B:30:ASN:OD1	2.26	0.57
1:B:161:ALA:O	1:B:171:VAL:HG11	2.05	0.57
1:B:3:ILE:CD1	1:B:353:GLU:HG2	2.34	0.57
1:B:139:ASP:HA	1:B:166:TYR:HE1	1.69	0.56
1:A:105:PRO:HA	1:A:112:ILE:HA	1.86	0.56
1:B:122:THR:HG21	1:B:124:LYS:HB2	1.87	0.56
1:B:261:ILE:HD12	1:B:285:PHE:CE1	2.41	0.56
1:B:356:TYR:CZ	1:B:360:LYS:HD2	2.40	0.56
1:A:86:PHE:CD2	1:A:88:ALA:HB3	2.40	0.56
1:B:245:TYR:HA	3:B:397:HOH:O	2.04	0.56
1:B:249:TRP:CD1	1:B:347:TYR:CE2	2.93	0.56
1:B:142:GLU:O	1:B:146:ILE:HG13	2.05	0.56
1:A:149:LYS:HE2	1:A:150:TYR:CZ	2.41	0.55
1:A:44:GLU:O	1:A:47:ASP:HB2	2.06	0.55
1:A:330:PHE:N	1:A:331:PRO:HD3	2.21	0.55
1:B:334:GLU:O	1:B:338:ASN:ND2	2.38	0.55
1:B:114:PRO:CA	1:B:117:ILE:HD12	2.22	0.55
1:B:272:PRO:CD	1:B:285:PHE:CE2	2.90	0.55
1:A:8:PHE:O	1:A:9:LYS:C	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:TYR:O	1:A:72:ASP:HB2	2.07	0.55
1:B:166:TYR:CZ	1:B:167:LYS:HE3	2.41	0.55
1:A:86:PHE:HE2	1:A:88:ALA:HB2	1.72	0.55
1:A:43:GLN:O	1:A:43:GLN:NE2	2.38	0.54
1:B:272:PRO:CD	1:B:285:PHE:CZ	2.89	0.54
1:B:301:ASN:ND2	1:B:301:ASN:N	2.51	0.54
1:A:149:LYS:HE2	1:A:150:TYR:HE2	1.69	0.54
1:A:252:GLU:HG2	1:A:347:TYR:CD2	2.43	0.54
1:B:142:GLU:O	1:B:145:ARG:HB2	2.07	0.54
1:B:331:PRO:N	1:B:334:GLU:OE2	2.39	0.54
1:B:346:TRP:O	1:B:347:TYR:C	2.44	0.54
1:A:351:ASN:HA	1:A:354:ILE:HG13	1.89	0.54
1:B:354:ILE:O	1:B:358:ILE:HD12	2.08	0.54
1:B:71:TYR:CB	1:B:73:ILE:HD12	2.38	0.54
1:A:353:GLU:O	1:A:356:TYR:HB3	2.07	0.54
1:B:148:LYS:O	1:B:149:LYS:C	2.46	0.54
1:A:109:THR:O	1:A:110:TYR:HB2	2.07	0.53
1:A:9:LYS:HG3	1:A:13:ASP:OD2	2.07	0.53
1:B:182:PHE:HE2	1:B:196:ALA:HB2	1.69	0.53
1:A:166:TYR:CZ	1:A:167:LYS:HD2	2.43	0.53
2:A:374:TQP:O2B	2:A:374:TQP:O5'	2.25	0.53
1:A:182:PHE:HE2	1:A:196:ALA:HB2	1.74	0.53
1:B:15:ILE:O	1:B:16:GLU:C	2.45	0.53
1:B:122:THR:HG23	1:B:123:GLU:N	2.23	0.53
1:B:272:PRO:HG3	1:B:285:PHE:CE2	2.43	0.53
1:B:357:VAL:O	1:B:361:ILE:HG12	2.08	0.53
1:B:9:LYS:HB3	1:B:10:PRO:HD3	1.90	0.53
1:A:82:PRO:HA	1:A:103:VAL:O	2.09	0.53
1:B:242:LYS:O	1:B:243:LEU:C	2.47	0.53
1:A:306:THR:HB	1:A:341:LEU:HD11	1.90	0.53
1:B:8:PHE:N	1:B:8:PHE:CD1	2.76	0.53
1:B:113:ASP:HB3	1:B:116:LEU:CD1	2.38	0.53
1:B:223:ILE:HG13	1:B:224:TYR:CD1	2.44	0.53
1:B:65:HIS:HD2	1:B:96:THR:HG22	1.74	0.53
1:B:357:VAL:O	1:B:361:ILE:CG1	2.56	0.53
1:B:107:ILE:HD11	1:B:288:ARG:NE	2.24	0.52
1:B:107:ILE:HG13	1:B:107:ILE:O	2.09	0.52
1:B:197:VAL:CG1	1:B:198:VAL:N	2.72	0.52
1:B:236:ALA:O	1:B:240:ARG:HG3	2.09	0.52
2:B:374:TQP:O3'	2:B:374:TQP:N3Q	2.39	0.52
1:A:272:PRO:HD3	1:A:286:VAL:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:TRP:HD1	1:A:347:TYR:CE2	2.27	0.52
1:A:22:LYS:HE2	1:A:22:LYS:HA	1.91	0.52
1:A:223:ILE:HG13	1:A:224:TYR:CE2	2.45	0.52
1:B:223:ILE:CG1	1:B:224:TYR:N	2.72	0.52
1:B:171:VAL:HG13	3:B:403:HOH:O	2.08	0.52
1:A:75:PHE:CZ	1:B:75:PHE:CZ	2.98	0.52
1:A:121:ILE:HG22	1:A:122:THR:N	2.24	0.52
1:A:166:TYR:CE2	1:A:167:LYS:HD2	2.43	0.52
1:A:41:PHE:CE1	1:A:239:LEU:HB3	2.45	0.52
1:A:5:PHE:HA	1:A:344:PRO:HG3	1.91	0.52
1:A:103:VAL:HG11	1:A:117:ILE:HG13	1.92	0.51
1:A:213:ASN:O	1:A:214:TYR:HB2	2.10	0.51
1:A:269:VAL:HG13	1:A:287:ILE:HB	1.93	0.51
1:B:104:GLU:CD	1:B:332:ILE:HB	2.30	0.51
1:B:190:SER:HB3	1:B:239:LEU:HD11	1.93	0.51
1:B:310:TYR:CB	1:B:311:PRO:HD2	2.37	0.51
1:A:289:SER:O	1:A:339:GLU:HB3	2.09	0.51
1:B:255:LYS:O	1:B:256:ILE:C	2.49	0.51
1:B:100:PRO:O	1:B:101:ILE:HD13	2.11	0.51
1:B:136:GLN:HE22	1:B:274:GLU:HA	1.76	0.51
1:A:21:PHE:HD2	3:A:402:HOH:O	1.93	0.50
1:B:132:HIS:CD2	1:B:171:VAL:CG2	2.93	0.50
1:B:308:ILE:HG12	1:B:341:LEU:HD12	1.92	0.50
1:B:52:ASN:CB	1:B:53:TYR:CD2	2.93	0.50
1:A:103:VAL:HB	1:A:112:ILE:HD11	1.93	0.50
1:B:144:LYS:O	1:B:148:LYS:HG3	2.12	0.50
1:A:317:GLN:NE2	1:B:222:HIS:HD2	2.08	0.50
1:A:9:LYS:HB3	1:A:10:PRO:CD	2.32	0.50
1:B:40:LYS:O	1:B:44:GLU:CG	2.59	0.50
1:A:55:ILE:N	1:A:55:ILE:HD12	2.26	0.50
1:A:22:LYS:HA	1:A:22:LYS:CE	2.42	0.50
1:A:331:PRO:CA	1:A:334:GLU:HB2	2.42	0.50
1:B:139:ASP:O	1:B:143:ILE:CG1	2.60	0.50
1:B:52:ASN:CB	1:B:53:TYR:CE2	2.95	0.50
1:B:52:ASN:HB2	1:B:53:TYR:CE2	2.47	0.49
1:A:211:LEU:CD2	1:A:226:GLY:HA2	2.42	0.49
1:A:249:TRP:CD1	1:A:347:TYR:CE2	3.01	0.49
1:A:90:ALA:O	1:A:91:LEU:C	2.50	0.49
1:B:78:GLU:OE1	1:B:122:THR:HB	2.12	0.49
1:B:71:TYR:CZ	1:B:153:LYS:HD2	2.47	0.49
1:A:270:ILE:HD13	1:A:288:ARG:CZ	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ASP:OD2	1:B:116:LEU:HD21	2.13	0.49
1:B:323:LEU:HD23	1:B:323:LEU:N	2.18	0.49
1:B:71:TYR:HB3	1:B:73:ILE:HD12	1.94	0.49
1:B:81:VAL:HG12	1:B:129:ILE:HB	1.94	0.49
1:A:350:LYS:HB2	1:A:353:GLU:HG3	1.94	0.49
1:B:2:LYS:O	1:B:3:ILE:HD13	2.13	0.49
1:A:295:LEU:HD13	1:A:364:TRP:CD2	2.48	0.48
1:B:139:ASP:OD1	1:B:166:TYR:OH	2.26	0.48
1:A:220:TYR:CD2	1:B:311:PRO:HG3	2.48	0.48
1:B:113:ASP:CG	1:B:116:LEU:HD21	2.34	0.48
1:B:277:TYR:HD2	1:B:277:TYR:C	2.17	0.48
1:A:271:ILE:HB	1:A:272:PRO:CD	2.40	0.48
1:B:354:ILE:HG22	1:B:358:ILE:HD12	1.93	0.48
1:B:298:TYR:CD2	1:B:299:LEU:N	2.82	0.48
1:A:23:PHE:O	1:A:24:GLU:C	2.50	0.48
1:B:115:SER:CB	1:B:116:LEU:HD23	2.43	0.48
1:B:93:VAL:HG11	1:B:100:PRO:CD	2.44	0.48
1:A:271:ILE:CB	1:A:272:PRO:CD	2.91	0.48
1:B:161:ALA:O	1:B:162:HIS:C	2.51	0.48
1:B:272:PRO:CG	1:B:285:PHE:CE2	2.97	0.48
1:B:75:PHE:HA	1:B:97:GLY:O	2.14	0.48
1:B:36[B]:ASP:OD2	1:B:40:LYS:HE3	2.13	0.48
1:B:83:SER:OG	1:B:104:GLU:HA	2.12	0.48
2:B:374:TQP:O4Q	2:B:374:TQP:H4'	2.14	0.48
1:B:106:ASP:O	1:B:110:TYR:N	2.47	0.48
1:B:328:GLY:H	1:B:334:GLU:CD	2.17	0.48
1:B:360:LYS:O	1:B:361:ILE:C	2.50	0.48
1:B:48:TYR:CZ	1:B:246:LEU:HD23	2.48	0.48
1:B:40:LYS:O	1:B:44:GLU:HG2	2.14	0.47
1:B:85:THR:HG23	1:B:86:PHE:O	2.13	0.47
1:B:159:ALA:O	1:B:186:LYS:HE3	2.14	0.47
1:B:249:TRP:CD1	1:B:347:TYR:CZ	3.03	0.47
1:B:127:ALA:HB2	1:B:153:LYS:HB2	1.96	0.47
1:B:51:VAL:HB	1:B:200:ASN:OD1	2.14	0.47
1:B:272:PRO:CG	1:B:285:PHE:CZ	2.97	0.47
1:A:139:ASP:O	1:A:143:ILE:CG1	2.63	0.47
1:B:283:TYR:CD2	1:B:284:THR:OG1	2.67	0.47
1:A:52:ASN:HB2	1:A:200:ASN:HA	1.97	0.47
1:A:87:ILE:HA	1:A:314:ILE:CD1	2.45	0.47
1:B:51:VAL:HG21	1:B:198:VAL:HB	1.96	0.47
1:A:113:ASP:HB3	1:A:116:LEU:CG	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:GLY:H	1:A:334:GLU:CD	2.18	0.47
1:A:183:TYR:CZ	2:A:374:TQP:H6QB	2.50	0.47
1:B:172:GLY:HA2	1:B:178:ALA:CB	2.45	0.47
1:A:211:LEU:HD22	1:A:226:GLY:HA2	1.96	0.47
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.56	0.47
1:A:316:LEU:HD23	1:A:316:LEU:HA	1.52	0.47
1:B:323:LEU:HD13	1:B:325:PHE:HE2	1.80	0.47
1:B:142:GLU:O	1:B:145:ARG:CB	2.63	0.46
1:B:69:LYS:HD2	1:B:69:LYS:HA	1.81	0.46
1:A:131:VAL:HG22	1:A:157:ASP:HB3	1.95	0.46
1:A:271:ILE:O	1:A:271:ILE:HD12	2.15	0.46
1:B:238:PHE:O	1:B:241:VAL:HB	2.15	0.46
1:B:309:HIS:HA	1:B:310:TYR:CG	2.50	0.46
1:A:104:GLU:OE1	1:A:331:PRO:HD2	2.15	0.46
1:A:69:LYS:HD2	1:A:69:LYS:HA	1.45	0.46
2:B:374:TQP:H5H	2:B:374:TQP:O2B	2.15	0.46
1:B:92:ALA:O	1:B:96:THR:HG23	2.15	0.46
1:A:165:LEU:HA	1:A:169:MET:O	2.15	0.46
1:B:52:ASN:N	1:B:200:ASN:OD1	2.47	0.46
1:B:261:ILE:CD1	1:B:285:PHE:CE1	2.97	0.46
1:A:309:HIS:HA	1:A:310:TYR:CD2	2.51	0.46
1:A:104:GLU:CD	1:A:332:ILE:HB	2.35	0.46
1:A:30:ASN:HA	1:A:32:PHE:CE2	2.51	0.46
1:B:166:TYR:O	1:B:167:LYS:C	2.54	0.46
1:B:52:ASN:HB2	1:B:200:ASN:HA	1.98	0.46
1:B:223:ILE:HG12	1:B:224:TYR:N	2.31	0.46
1:B:252:GLU:O	1:B:253:ARG:C	2.54	0.46
1:B:5:PHE:CZ	1:B:307:LEU:HB2	2.51	0.46
1:A:134:TYR:O	1:A:283:TYR:N	2.49	0.46
1:A:312:ILE:HA	1:A:313:PRO:HD3	1.54	0.46
1:A:69:LYS:C	1:A:72:ASP:H	2.16	0.46
1:B:317:GLN:HA	1:B:317:GLN:OE1	2.15	0.46
1:A:331:PRO:O	1:A:334:GLU:HB2	2.16	0.45
1:B:29:ARG:O	1:B:30:ASN:C	2.54	0.45
1:A:249:TRP:CD1	1:A:347:TYR:CZ	3.05	0.45
1:A:86:PHE:CE2	1:A:88:ALA:CB	2.98	0.45
1:B:285:PHE:CD2	1:B:285:PHE:C	2.90	0.45
1:B:332:ILE:O	1:B:336:ILE:HG13	2.16	0.45
1:B:74:GLY:O	1:B:98:ALA:HA	2.16	0.45
1:B:213:ASN:ND2	1:B:216:SER:HB3	2.32	0.45
1:A:330:PHE:N	1:A:331:PRO:CD	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:LYS:CD	1:B:240:ARG:NH2	2.79	0.45
1:B:266:ASN:OD1	1:B:267:PRO:HD2	2.16	0.45
1:A:271:ILE:C	1:A:271:ILE:CD1	2.80	0.45
1:A:140:MET:HA	1:A:143:ILE:HG13	1.98	0.45
1:A:164:SER:HB3	1:A:171:VAL:HG21	1.99	0.45
1:B:309:HIS:HA	1:B:310:TYR:CD2	2.51	0.45
1:A:1:MET:HE3	1:A:352:GLU:OE2	2.16	0.45
1:A:3:ILE:HD12	1:A:353:GLU:HB3	1.99	0.45
1:B:40:LYS:HB3	1:B:240:ARG:NH2	2.32	0.45
1:B:71:TYR:HB2	1:B:73:ILE:HD12	1.98	0.45
1:B:99:LYS:HA	1:B:100:PRO:HD2	1.65	0.45
1:B:75:PHE:CZ	1:B:97:GLY:HA3	2.52	0.45
1:A:10:PRO:O	1:A:14:GLU:HB2	2.16	0.44
1:B:123:GLU:H	1:B:123:GLU:HG3	1.26	0.44
1:B:354:ILE:CG2	1:B:358:ILE:HD11	2.42	0.44
1:B:307:LEU:HD12	2:B:374:TQP:O2B	2.16	0.44
1:B:313:PRO:HD2	1:B:316:LEU:HB2	1.98	0.44
1:B:82:PRO:HG3	1:B:112:ILE:HB	1.99	0.44
1:B:16:GLU:HG2	1:B:17:TYR:N	2.31	0.44
1:A:137:PRO:HD3	1:A:164:SER:OG	2.17	0.44
1:A:16[B]:GLU:HG3	1:B:27:TYR:HE2	1.82	0.44
1:B:8:PHE:HD1	1:B:8:PHE:N	2.15	0.44
1:A:121:ILE:CG2	1:A:122:THR:N	2.80	0.44
1:B:188:LEU:HD11	1:B:242:LYS:CB	2.48	0.44
1:A:80:ILE:CD1	1:A:117:ILE:HG23	2.39	0.44
1:B:19:ILE:O	1:B:22:LYS:HB3	2.18	0.44
1:B:314:ILE:HG22	1:B:315:HIS:N	2.24	0.44
1:B:77:ASP:OD1	1:B:126:LYS:HG3	2.17	0.44
1:A:112:ILE:O	1:A:112:ILE:HG23	2.18	0.44
1:A:271:ILE:HD13	3:A:404:HOH:O	2.18	0.44
1:B:248:LYS:O	1:B:248:LYS:HG3	2.18	0.44
1:B:313:PRO:O	1:B:316:LEU:N	2.50	0.44
1:B:223:ILE:HD11	1:B:224:TYR:CE2	2.53	0.43
1:B:252:GLU:O	1:B:256:ILE:HG13	2.18	0.43
1:B:266:ASN:HA	1:B:267:PRO:HD3	1.81	0.43
1:B:239:LEU:HA	1:B:239:LEU:HD23	1.67	0.43
1:B:4:SER:HB2	1:B:6:ALA:O	2.18	0.43
1:B:10:PRO:O	1:B:14:GLU:HB2	2.18	0.43
1:B:210:ALA:O	1:B:215:GLY:CA	2.66	0.43
1:B:210:ALA:O	1:B:215:GLY:N	2.52	0.43
1:B:358:ILE:CG2	1:B:362:ASN:ND2	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:139:ASP:HA	1:B:166:TYR:CE1	2.53	0.43
1:B:270:ILE:HD13	1:B:288:ARG:NH2	2.34	0.43
1:A:104:GLU:OE1	1:A:332:ILE:HD12	2.19	0.43
1:A:67:ILE:HG21	1:A:155:ILE:HD13	2.00	0.43
1:A:79:VAL:O	1:A:100:PRO:HA	2.18	0.43
1:B:102:PHE:HE1	1:B:323:LEU:HD12	1.83	0.43
1:B:286:VAL:O	1:B:286:VAL:HG23	2.18	0.43
1:A:201:ASP:OD1	1:A:201:ASP:C	2.58	0.43
1:B:122:THR:HG22	1:B:124:LYS:HB2	2.01	0.43
1:B:40:LYS:O	1:B:44:GLU:HG3	2.19	0.43
1:A:148:LYS:O	1:A:150:TYR:N	2.51	0.42
1:A:259:LYS:HE2	1:A:351:ASN:OD1	2.19	0.42
1:A:69:LYS:C	1:A:71:TYR:N	2.72	0.42
1:B:250:ASN:O	1:B:253:ARG:HB2	2.19	0.42
1:B:358:ILE:HG22	1:B:358:ILE:O	2.18	0.42
1:B:77:ASP:OD1	1:B:126:LYS:NZ	2.34	0.42
1:A:197:VAL:HG12	1:A:198:VAL:N	2.33	0.42
1:A:260:TYR:CZ	1:A:343:ILE:HD12	2.54	0.42
1:A:291:LYS:HA	1:A:291:LYS:HD2	1.90	0.42
1:B:318:GLN:HB2	3:B:401:HOH:O	2.19	0.42
1:B:292:ARG:HB2	1:B:339:GLU:HA	2.02	0.42
1:B:43:GLN:HG2	1:B:44:GLU:N	2.34	0.42
1:A:353:GLU:O	1:A:357:VAL:HG23	2.19	0.42
1:A:365:LYS:HE2	1:A:365:LYS:HB3	1.38	0.42
1:B:353:GLU:O	1:B:354:ILE:C	2.58	0.42
1:A:114:PRO:O	1:A:117:ILE:HD12	2.20	0.42
1:B:41:PHE:CA	1:B:44:GLU:HG3	2.46	0.42
1:A:321:LYS:HD3	3:A:431:HOH:O	2.18	0.42
1:A:67:ILE:CG2	1:A:155:ILE:HD13	2.49	0.42
1:B:187:ASN:HD21	1:B:253:ARG:HD2	1.85	0.42
1:B:294:GLU:HG2	1:B:294:GLU:H	1.53	0.42
1:B:316:LEU:HA	1:B:316:LEU:HD23	1.58	0.42
1:B:346:TRP:O	1:B:349:MET:HG3	2.19	0.42
1:B:113:ASP:HA	1:B:114:PRO:HD3	1.84	0.42
1:B:144:LYS:O	1:B:145:ARG:C	2.58	0.42
1:B:218:LYS:O	1:B:219:LYS:C	2.57	0.42
1:A:336:ILE:O	1:A:340:ILE:HB	2.20	0.42
1:B:150:TYR:N	1:B:150:TYR:CD2	2.88	0.42
1:B:134:TYR:CD1	1:B:284:THR:HB	2.55	0.42
1:A:166:TYR:CE2	1:A:167:LYS:CD	3.03	0.41
1:B:131:VAL:HG22	1:B:157:ASP:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:PHE:CE2	1:B:88:ALA:HB2	2.55	0.41
1:B:100:PRO:C	1:B:101:ILE:HD13	2.39	0.41
1:B:154:LEU:HG	1:B:175:GLY:HA3	2.02	0.41
1:A:133:LEU:C	1:A:135:GLY:H	2.24	0.41
1:A:301:ASN:HD22	1:A:301:ASN:HA	1.59	0.41
1:A:91:LEU:O	1:A:94:SER:N	2.54	0.41
1:B:153:LYS:HD3	1:B:153:LYS:HA	1.61	0.41
1:B:286:VAL:O	1:B:286:VAL:CG2	2.68	0.41
1:B:331:PRO:HA	1:B:334:GLU:OE2	2.21	0.41
1:B:67:ILE:HA	1:B:208:ILE:HD11	2.02	0.41
1:B:306:THR:HB	1:B:342:SER:O	2.21	0.41
1:A:294:GLU:O	1:A:295:LEU:C	2.58	0.41
1:A:68:LEU:HA	1:A:68:LEU:HD23	1.80	0.41
1:B:107:ILE:HG13	1:B:288:ARG:NH1	2.36	0.41
1:A:125:THR:HG22	1:A:126:LYS:N	2.35	0.41
1:A:53:TYR:OH	1:A:202:LYS:HB2	2.20	0.41
1:B:34:LEU:HA	1:B:34:LEU:HD23	1.77	0.41
1:A:84:ASN:CG	1:A:105:PRO:HG3	2.41	0.41
1:A:331:PRO:C	1:A:334:GLU:HB2	2.42	0.41
1:B:113:ASP:CG	1:B:116:LEU:HG	2.39	0.41
1:B:172:GLY:HA2	1:B:178:ALA:HB2	2.02	0.41
1:B:182:PHE:CZ	1:B:196:ALA:HB2	2.55	0.41
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.57	0.41
1:B:188:LEU:HD11	1:B:242:LYS:HB3	2.02	0.41
1:A:132:HIS:CD2	1:A:171:VAL:HG13	2.56	0.40
1:A:142:GLU:H	1:A:142:GLU:HG2	1.44	0.40
1:A:190:SER:OG	1:A:192:GLY:N	2.49	0.40
1:B:166:TYR:O	1:B:169:MET:N	2.41	0.40
1:B:323:LEU:HA	1:B:323:LEU:HD22	1.38	0.40
1:A:149:LYS:CE	1:A:150:TYR:CE2	2.94	0.40
1:A:182:PHE:CE2	1:A:196:ALA:HB2	2.54	0.40
1:A:54:CYS:HA	1:A:197:VAL:O	2.22	0.40
1:A:323:LEU:HD23	1:A:323:LEU:HA	1.57	0.40
1:A:105:PRO:HA	1:A:112:ILE:CA	2.50	0.40
1:B:312:ILE:HA	1:B:313:PRO:HD3	1.65	0.40
1:B:292:ARG:HH22	1:B:338:ASN:HA	1.87	0.40
1:B:361:ILE:O	1:B:362:ASN:C	2.57	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	366/373 (98%)	326 (89%)	36 (10%)	4 (1%)	14	8
1	B	363/373 (97%)	320 (88%)	38 (10%)	5 (1%)	11	5
All	All	729/746 (98%)	646 (89%)	74 (10%)	9 (1%)	13	7

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	345	ILE
1	B	345	ILE
1	A	149	LYS
1	B	7	SER
1	B	275	ALA
1	A	98	ALA
1	A	148	LYS
1	B	331	PRO
1	B	9	LYS

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	310/316 (98%)	279 (90%)	31 (10%)	7	4
1	B	306/316 (97%)	259 (85%)	47 (15%)	2	1
All	All	616/632 (98%)	538 (87%)	78 (13%)	4	1

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	MET
1	A	15	ILE
1	A	20	LYS
1	A	22	LYS
1	A	69	LYS
1	A	71	TYR
1	A	119	SER
1	A	122	THR
1	A	123	GLU
1	A	124	LYS
1	A	126	LYS
1	A	143	ILE
1	A	148	LYS
1	A	184	PRO
1	A	209	LYS
1	A	218	LYS
1	A	219	LYS
1	A	225	LYS
1	A	227	PHE
1	A	255	LYS
1	A	258[A]	GLN
1	A	258[B]	GLN
1	A	289	SER
1	A	321	LYS
1	A	322	ASP
1	A	339	GLU
1	A	340	ILE
1	A	345	ILE
1	A	346	TRP
1	A	354	ILE
1	A	365	LYS
1	B	2	LYS
1	B	44	GLU
1	B	47	ASP
1	B	50	ASN
1	B	59	ASN
1	B	69	LYS
1	B	94	SER
1	B	108	ARG
1	B	115	SER
1	B	116	LEU
1	B	119	SER

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Mol	Chain	Res	Type
1	B	122	THR
1	B	123	GLU
1	B	136	GLN
1	B	143	ILE
1	B	145	ARG
1	B	209	LYS
1	B	217	GLU
1	B	223	ILE
1	B	252	GLU
1	B	261	ILE
1	B	266	ASN
1	B	268	ASN
1	B	271	ILE
1	B	274	GLU
1	B	284	THR
1	B	286	VAL
1	B	287	ILE
1	B	291	LYS
1	B	292	ARG
1	B	294	GLU
1	B	301	ASN
1	B	307	LEU
1	B	314	ILE
1	B	321	LYS
1	B	322	ASP
1	B	323	LEU
1	B	327	THR
1	B	329	ASN
1	B	331	PRO
1	B	335	LYS
1	B	339	GLU
1	B	340	ILE
1	B	342	SER
1	B	345	ILE
1	B	352	GLU
1	B	360	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	ASN
1	B	65	HIS

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Mol	Chain	Res	Type
1	B	136	GLN
1	B	213	ASN
1	B	222	HIS
1	B	265	ASN
1	B	268	ASN
1	B	301	ASN
1	B	338	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TQP	B	374	-	47,53,53	1.06	2 (4%)	61,81,81	1.99	14 (22%)
2	TQP	A	374	-	47,53,53	1.12	2 (4%)	61,81,81	2.18	12 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TQP	B	374	-	-	6/29/64/64	0/4/4/4
2	TQP	A	374	-	-	9/29/64/64	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	374	TQP	PA-O2A	3.45	1.63	1.50
2	A	374	TQP	PA-O2A	3.36	1.62	1.50
2	B	374	TQP	PB-O2B	2.76	1.60	1.50
2	A	374	TQP	PB-O2B	2.16	1.58	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	374	TQP	C3Q-N3Q-C4'	7.40	131.12	117.99
2	A	374	TQP	O5'-C5H-C4H	6.80	132.39	108.99
2	B	374	TQP	C4-N3-C2	6.01	120.22	115.14
2	B	374	TQP	C4P-C4'-N3Q	-5.97	109.75	123.01
2	A	374	TQP	C4-N3-C2	5.34	119.65	115.14
2	A	374	TQP	PB-O3A-PA	-5.19	115.01	132.83
2	B	374	TQP	C3Q-N3Q-C4'	4.45	125.89	117.99
2	B	374	TQP	PB-O3A-PA	-4.30	118.06	132.83
2	A	374	TQP	C1Q-O5Q-C5Q	-4.21	106.44	113.67
2	B	374	TQP	C1Q-O5Q-C5Q	-4.21	106.44	113.67
2	A	374	TQP	O3A-PB-O3B	4.14	110.84	102.48
2	B	374	TQP	C6Q-C5Q-C4Q	-4.03	105.62	113.07
2	A	374	TQP	O5Q-C5Q-C6Q	3.66	114.59	106.70
2	B	374	TQP	O5'-C5H-C4H	-3.58	96.68	108.99
2	A	374	TQP	C5-C6-N1	-3.53	118.39	122.19
2	B	374	TQP	O5Q-C1Q-O3B	2.76	114.97	111.36
2	B	374	TQP	C5-C6-N1	-2.76	119.22	122.19
2	B	374	TQP	PB-O3B-C1Q	-2.59	109.73	119.74
2	A	374	TQP	PB-O3B-C1Q	-2.56	109.83	119.74
2	B	374	TQP	O3B-C1Q-C2Q	2.49	112.95	108.38
2	A	374	TQP	O4'-C4H-C5H	-2.40	101.47	109.37
2	A	374	TQP	O3P-P-O4P	2.19	112.56	106.73
2	B	374	TQP	O1A-PA-O5'	-2.18	97.63	107.75
2	B	374	TQP	O3B-PB-O2B	2.07	117.24	109.47
2	A	374	TQP	O4P-C5'-C5P	2.06	113.27	109.35
2	B	374	TQP	C2H-C3'-C4H	2.02	106.98	102.76

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	374	TQP	C5H-O5'-PA-O2A
2	B	374	TQP	C4Q-C3Q-N3Q-C4'
2	A	374	TQP	C4H-C5H-O5'-PA
2	A	374	TQP	C5H-O5'-PA-O2A
2	A	374	TQP	C4Q-C3Q-N3Q-C4'
2	A	374	TQP	C4P-C4'-N3Q-C3Q
2	A	374	TQP	O4'-C4H-C5H-O5'
2	A	374	TQP	C3'-C4H-C5H-O5'
2	B	374	TQP	C2Q-C1Q-O3B-PB
2	B	374	TQP	C1Q-O3B-PB-O2B
2	B	374	TQP	C5'-O4P-P-O1P
2	A	374	TQP	PB-O3A-PA-O5'
2	A	374	TQP	C2Q-C1Q-O3B-PB
2	B	374	TQP	C5'-O4P-P-O2P
2	A	374	TQP	PA-O3A-PB-O2B

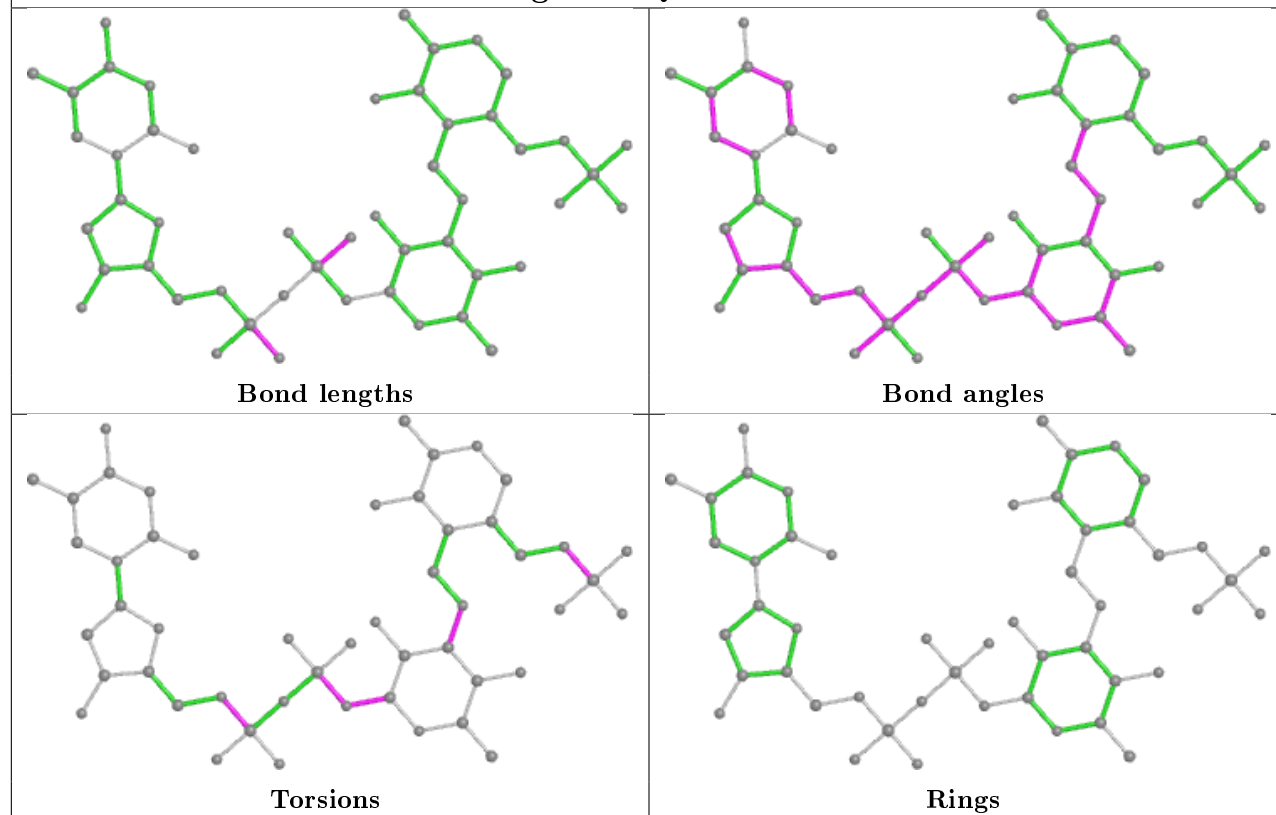
There are no ring outliers.

2 monomers are involved in 8 short contacts:

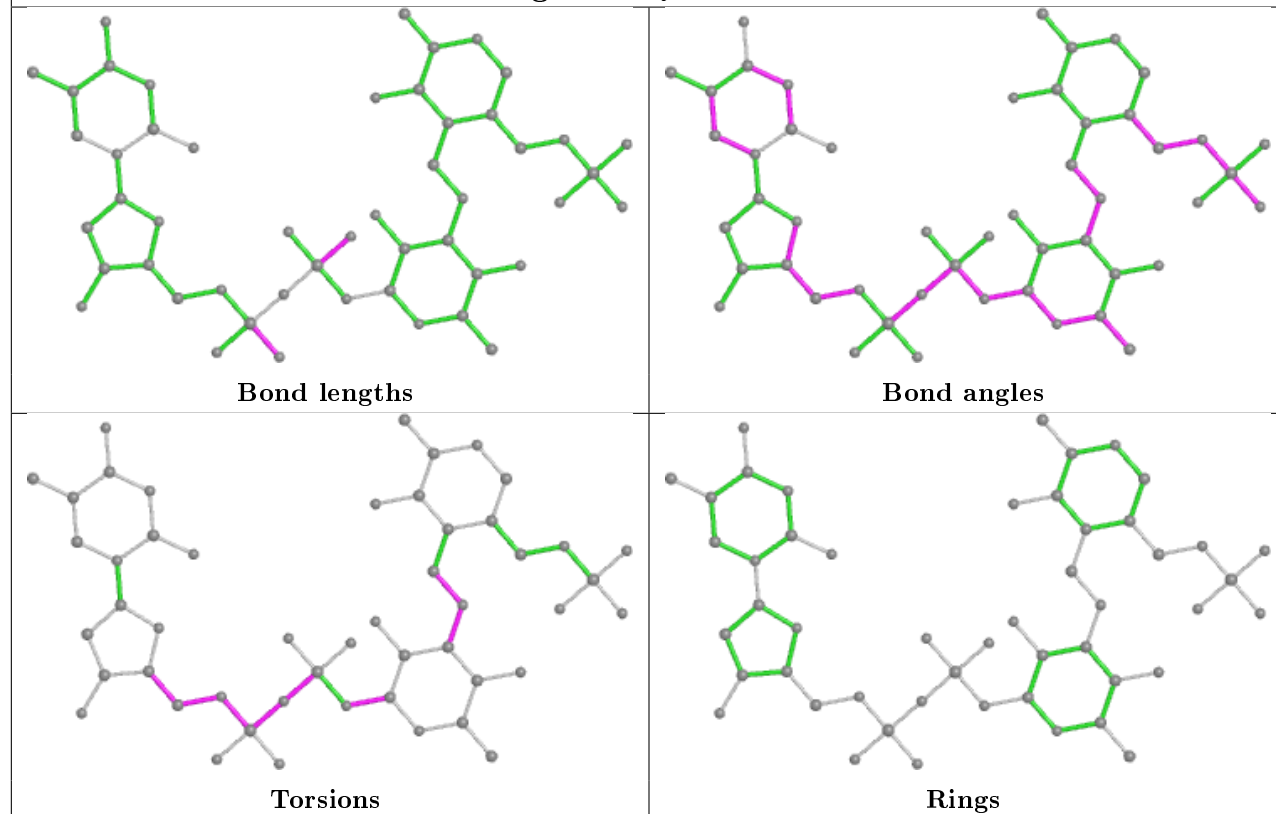
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	374	TQP	4	0
2	A	374	TQP	4	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand TQP B 374



Ligand TQP A 374



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	365/373 (97%)	-0.18	16 (4%) 34 43	24, 44, 72, 88	0
1	B	364/373 (97%)	-0.05	16 (4%) 34 43	25, 52, 77, 97	0
All	All	729/746 (97%)	-0.12	32 (4%) 34 43	24, 48, 75, 97	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	17[A]	TYR	4.8
1	A	133	LEU	4.4
1	A	283	TYR	3.3
1	B	283	TYR	3.2
1	A	131	VAL	3.0
1	B	159	ALA	2.9
1	A	76	GLY	2.8
1	A	159	ALA	2.8
1	B	131	VAL	2.7
1	A	75	PHE	2.6
1	A	134	TYR	2.6
1	B	327	THR	2.5
1	B	324	GLY	2.5
1	B	134	TYR	2.5
1	A	132	HIS	2.5
1	A	129	ILE	2.5
1	A	74	GLY	2.5
1	B	285	PHE	2.5
1	B	133	LEU	2.4
1	B	284	THR	2.4
1	A	158	ALA	2.3
1	A	161	ALA	2.3
1	A	160	GLN	2.2
1	A	124	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	328	GLY	2.2
1	A	85	THR	2.1
1	B	161	ALA	2.1
1	B	286	VAL	2.1
1	B	180	PHE	2.1
1	B	325	PHE	2.1
1	B	76	GLY	2.0
1	B	275	ALA	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 carbohydrates in this entry.

6.4 Ligands [i](#)

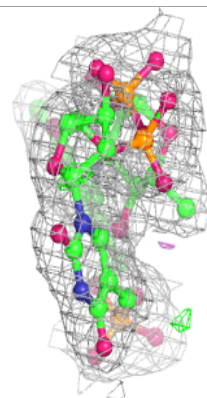
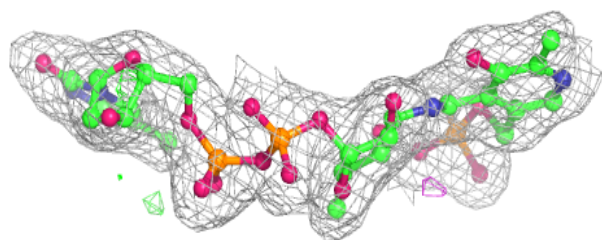
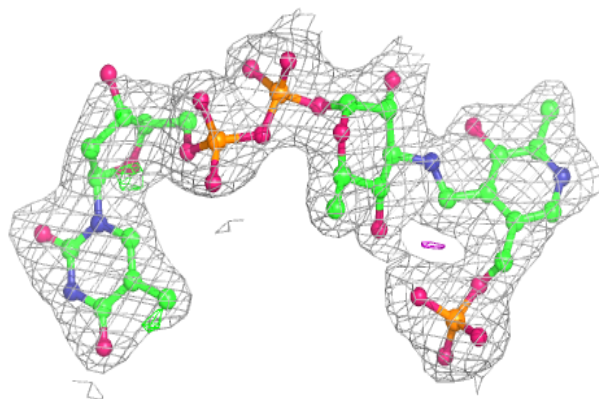
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	TQP	B	374	50/50	0.97	0.12	21,48,100,100	0
2	TQP	A	374	50/50	0.98	0.11	18,36,72,86	0

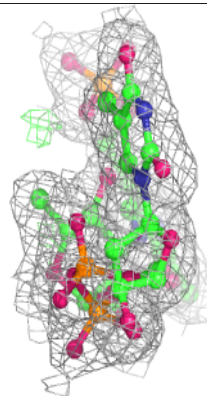
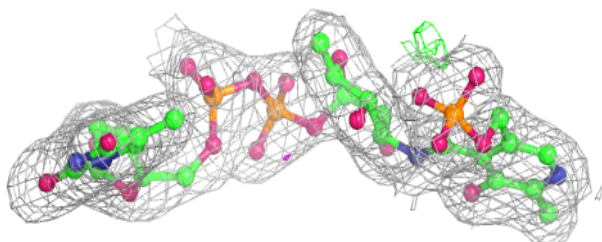
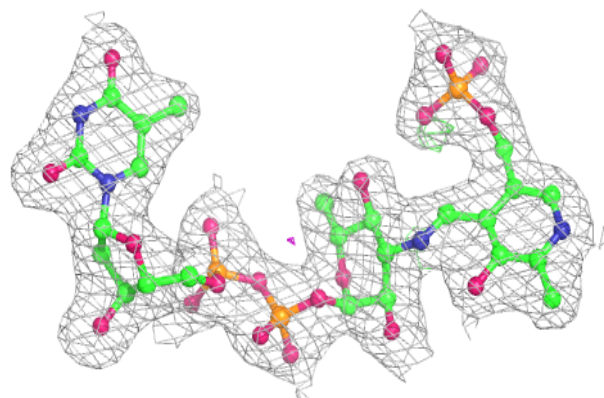
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TQP B 374:

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

**Electron density around TQP A 374:**

$2mF_o-DF_c$ (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.