Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2022 – 09:09 pm GMT

PDB ID	:	7B9Q
Title	:	The SERp optimized structure of Ribonucleotide reductase from Rhodobacter sphaeroides
Authors	:	Loderer, C.; Feiler, C.; Wilk, P.; Kabinger, F.
Deposited on	:	2020-12-14
Resolution	:	2.78 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:

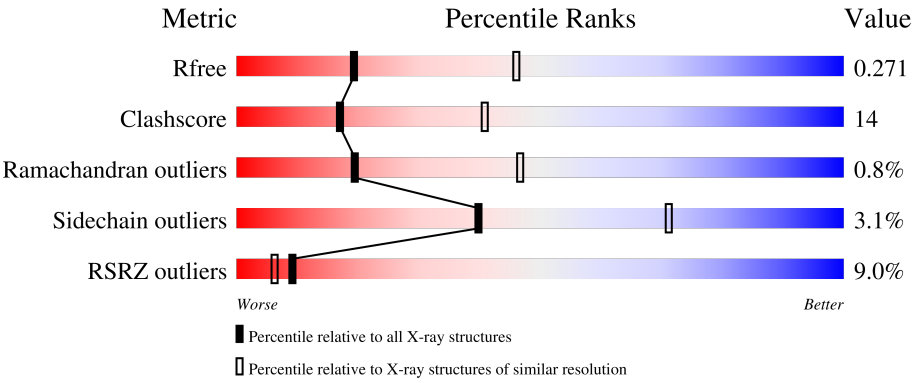
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.24
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.24

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 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	925	4% 77% 17% • 6%
1	B	925	13% 61% 30% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13460 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.

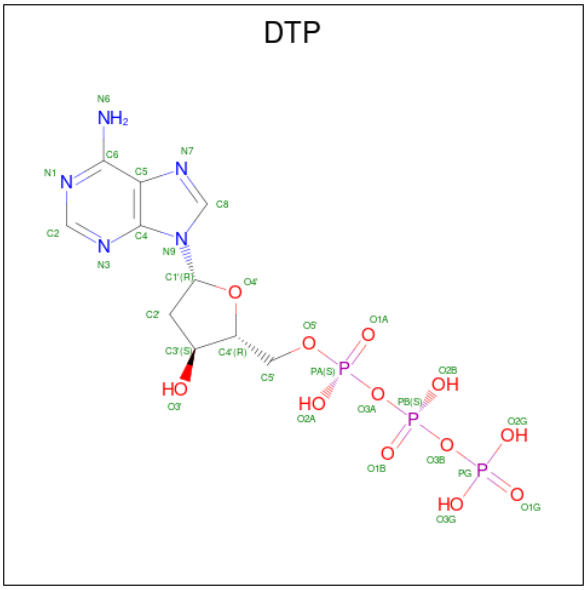
- Molecule 1 is a protein called Vitamin B12-dependent ribonucleotide reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	868	Total	C	N	O	S	0	1	0
			6625	4167	1167	1255	36			
1	B	860	Total	C	N	O	S	0	0	0
			6564	4130	1160	1239	35			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	ALA	GLU	engineered mutation	UNP A0A6H2IRA4
A	97	ALA	GLU	engineered mutation	UNP A0A6H2IRA4
A	98	ALA	GLU	engineered mutation	UNP A0A6H2IRA4
B	96	ALA	GLU	engineered mutation	UNP A0A6H2IRA4
B	97	ALA	GLU	engineered mutation	UNP A0A6H2IRA4
B	98	ALA	GLU	engineered mutation	UNP A0A6H2IRA4

- Molecule 2 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

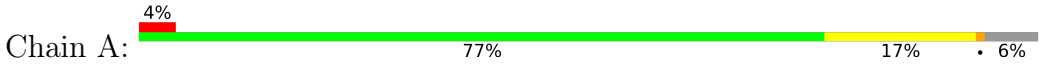
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	149	Total	O	0	0
			149	149		
4	B	60	Total	O	0	0
			60	60		

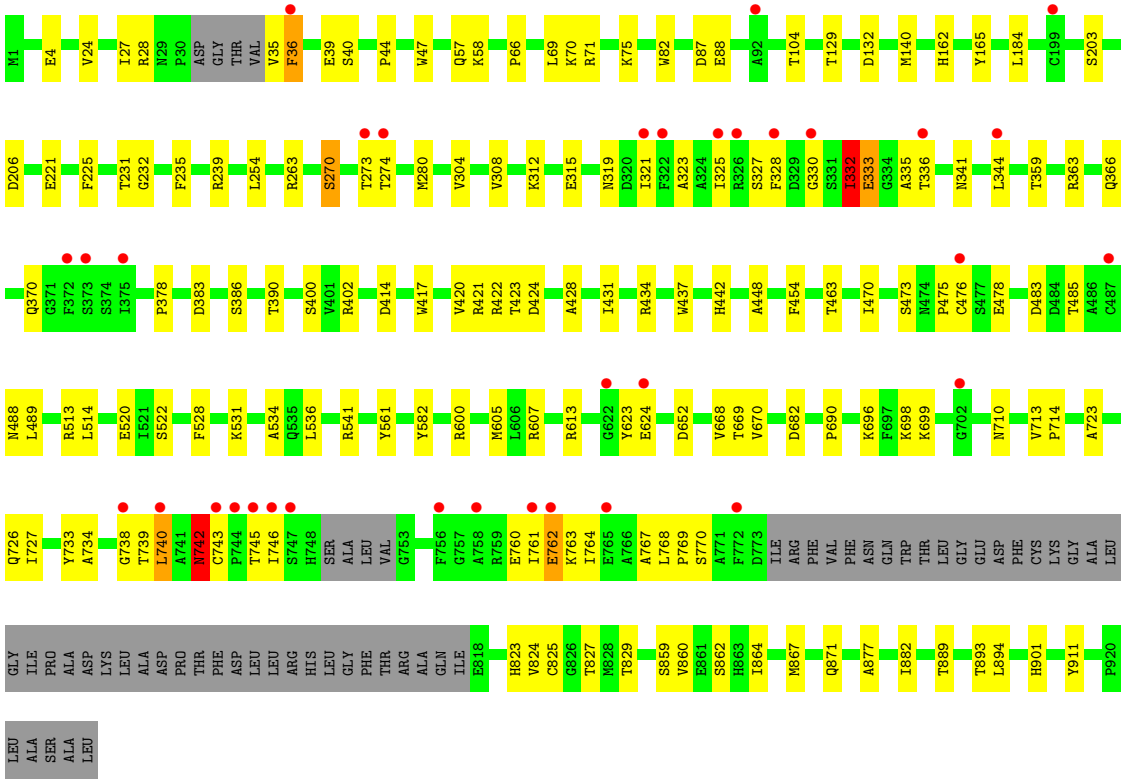
3 Residue-property plots (i)

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: Vitamin B12-dependent ribonucleotide reductase

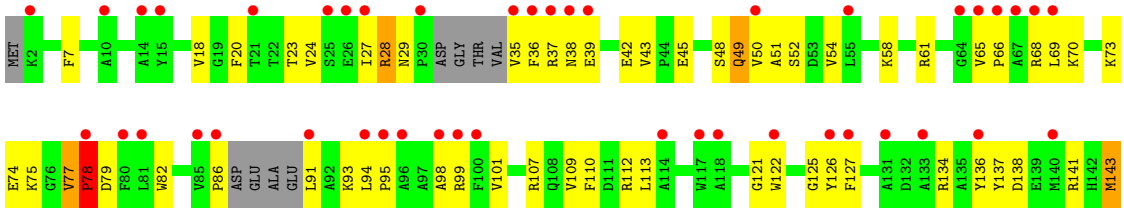
Chain A:

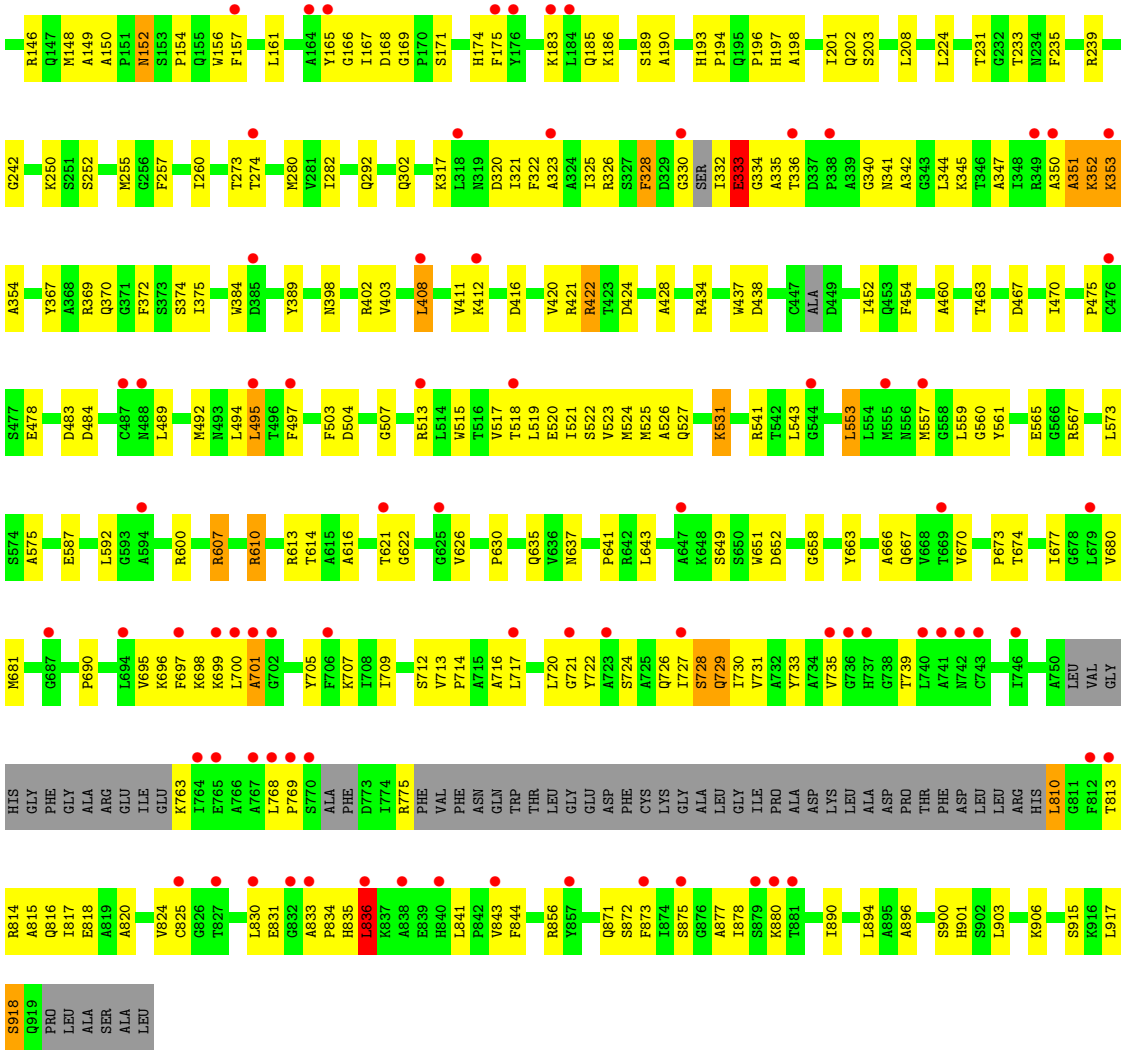




• Molecule 1: Vitamin B12-dependent ribonucleotide reductase

Chain B:




R146 Q147 M148 A149 A150 P151 N152 S153 P154 Q155 W156 F157 L161 A164 Y165 G166 I167 D168 G169 P170 S171 H174 F175 Y176 K183 L184 Q185 K186 S189 A190 H193 P194 Q195 P196 H197 A198 I201 Q202 S203 L208 L224 T231 G232 T233 N234 F235 R239
G242 K250 S251 S252 M255 G256 F257 I260 T273 T274 M280 V281 I282 Q292 Q302 K317 L318 N319 D320 I321 F322 A323 A324 I325 R326 S327 F328 D329 G330 SER I332 E333 G334 A335 T336 D337 P338 A339 G340 N341 A342 G343 L344 K345 T346 A347 I348 R349 A350 A351 K352 K353
A354 Y367 A368 R369 Q370 G371 F372 S373 S374 I375 W384 D385 Y389 N398 R402 V403 L408 V411 K412 D416 V420 R421 R422 T423 D424 A428 R434 W437 D438 C447 ALA D449 I452 Q453 F454 A460 T463 D467 I470 P475 C476
S477 E478 D483 D484 C487 N488 L489 M492 N493 L494 L495 T496 F497 F503 D504 G507 R513 L514 W515 T516 V517 T518 L519 E520 I521 S522 V523 M524 M525 A526 Q527 K531 R541 T542 L543 G544 L553 L554 M555 N556 M557 G558 L559 G560 Y561 E565 G566 R567 L573
S574 A575 E587 L592 G593 A594 R600 R607 R610 R613 T614 A615 A616 T621 G622 G625 V626 P630 Q635 V636 N637 P641 R642 L643 A647 K648 S649 S650 W651 D652 G658 Y663 A666 Q667 V668 T669 V670 P673 T674 I677 G678 L679 V680
M681 G687 P690 L694 V695 K696 F697 K698 K699 L700 A701 G702 Y705 F706 K707 I708 I709 S712 V713 P714 A715 A716 L717 L720 G721 Y722 A723 S724 A725 Q726 I727 S728 Q729 I730 V731 A732 Y733 A734 V735 G736 H737 G738 T739 L740 A741 N742 C743 T746 A750 LEU VAL GLY
HIS GLY PHE GLY ALA ARG GLU ILE GLU K763 I764 E765 A766 A767 L768 P769 S770 ALA PHE D773 I774 R775 PHE VAL PHE ASN GLN TRP THR LEU GLY GLU ASP PHE CYS LYS GLY ALA LEU GLY ILE PRO ALA ASP LYS LEU ALA ASP PRO THR PHE ASP LEU LEU ARG HIS L810 G811 F812 T813
R814 A815 Q816 I817 E818 A819 A820 V824 C825 G826 T827 L830 E831 G832 A833 P834 H835 L836 K837 A838 E839 H840 L841 P842 V843 F844 R856 Y857 Q871 S872 F873 I874 S875 G876 A877 I878 S879 K880 T881 I890 L894 A895 A896 S900 H901 S902 L903 K906 S915 K916 L917
S918 Q919 PRO LEU ALA SER ALA LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	161.59Å 161.59Å 97.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.59 – 2.78 47.12 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.59-2.78) 99.8 (47.12-2.78)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.220 , 0.271 0.220 , 0.271	Depositor DCC
R_{free} test set	2100 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å^2)	73.2	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13460	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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

5.1 Standard geometry

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

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	0.27	0/6778	0.45	1/9175 (0.0%)
1	B	0.30	0/6707	0.55	6/9074 (0.1%)
All	All	0.29	0/13485	0.50	7/18249 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	4
All	All	0	6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	77	VAL	C-N-CD	-14.27	89.21	120.60
1	B	78	PRO	N-CD-CG	-8.02	91.17	103.20
1	B	78	PRO	CA-N-CD	7.67	122.44	111.70
1	B	78	PRO	N-CA-C	6.73	129.59	112.10
1	A	742	ASN	C-N-CA	-6.04	106.61	121.70
1	B	836	LEU	CB-CG-CD1	-5.42	101.78	111.00
1	B	553	LEU	CA-CB-CG	5.37	127.65	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	332	ILE	Peptide
1	A	762	GLU	Peptide
1	B	333	GLU	Peptide
1	B	351	ALA	Peptide
1	B	408	LEU	Peptide
1	B	728	SER	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	6625	0	6435	113	2
1	B	6564	0	6387	256	2
2	A	30	0	12	1	0
2	B	30	0	12	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	149	0	0	6	0
4	B	60	0	0	10	0
All	All	13460	0	12846	365	2

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 14.

All (365) 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:77:VAL:CG2	1:B:78:PRO:HD2	1.52	1.37
1:B:77:VAL:HG22	1:B:78:PRO:CD	1.57	1.35
1:B:77:VAL:CG2	1:B:78:PRO:CD	2.18	1.15
1:B:408:LEU:HA	1:B:411:VAL:HG13	1.31	1.13
1:B:91:LEU:HB2	1:B:99:ARG:HD3	1.50	0.92
1:B:77:VAL:CG2	1:B:78:PRO:HD3	2.07	0.84
1:B:74:GLU:O	1:B:75:LYS:HD2	1.79	0.82
1:B:332:ILE:HG12	1:B:334:GLY:H	1.45	0.81
1:B:77:VAL:HG23	1:B:78:PRO:HD3	1.65	0.78
1:B:522:SER:HA	1:B:525:MET:HB3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:PHE:HD2	1:B:531:LYS:HB3	1.46	0.77
1:B:242:GLY:HA2	1:B:250:LYS:HD3	1.68	0.75
1:A:723:ALA:H	1:A:726:GLN:HE21	1.33	0.74
1:B:610:ARG:NH1	1:B:614:THR:OG1	2.21	0.74
1:B:408:LEU:CA	1:B:411:VAL:HG13	2.16	0.73
1:B:74:GLU:C	1:B:75:LYS:HD2	2.09	0.73
1:B:726:GLN:HG2	1:B:729:GLN:NE2	2.03	0.73
1:B:352:LYS:O	1:B:353:LYS:HB3	1.89	0.71
1:B:841:LEU:HD12	1:B:844:PHE:HD2	1.54	0.71
1:B:122:TRP:CE3	1:B:127:PHE:HB2	2.25	0.71
1:B:37:ARG:NH2	1:B:39:GLU:OE2	2.24	0.70
1:B:478:GLU:OE1	1:B:673:PRO:HD3	1.92	0.69
1:B:635:GLN:NE2	4:B:1204:HOH:O	2.24	0.69
1:B:497:PHE:HB2	1:B:503:PHE:CE1	2.28	0.69
1:A:239:ARG:HH11	1:A:423:THR:HG22	1.56	0.69
1:A:332:ILE:HA	1:A:335:ALA:HB3	1.73	0.69
1:B:523:VAL:HG11	1:B:541:ARG:HA	1.75	0.68
1:B:95:PRO:O	1:B:99:ARG:NE	2.27	0.68
1:A:760:GLU:HA	1:A:763:LYS:HE3	1.76	0.68
1:B:77:VAL:HG22	1:B:78:PRO:HD2	0.73	0.68
1:B:557:MET:HB3	1:B:559:LEU:CD2	2.23	0.67
1:A:370:GLN:HE22	1:B:890:ILE:H	1.42	0.67
1:B:43:VAL:HG21	1:B:52:SER:HB3	1.77	0.67
1:B:557:MET:HB3	1:B:559:LEU:HD23	1.76	0.67
1:A:280:MET:HB2	1:A:475:PRO:HA	1.75	0.66
1:B:495:LEU:HB2	1:B:553:LEU:HB3	1.77	0.66
1:B:610:ARG:NH2	1:B:622:GLY:O	2.28	0.66
1:B:478:GLU:OE1	1:B:673:PRO:CD	2.43	0.66
1:A:70:LYS:HD2	1:A:87:ASP:HA	1.77	0.66
2:B:1102:DTP:O5'	4:B:1201:HOH:O	2.15	0.65
1:B:717:LEU:HD23	1:B:720:LEU:HD13	1.77	0.65
1:A:4:GLU:OE2	4:A:1101:HOH:O	2.15	0.65
1:B:610:ARG:NH1	4:B:1209:HOH:O	2.28	0.64
1:A:827:THR:HG23	1:A:829:THR:H	1.62	0.64
1:B:23:THR:HG22	1:B:24:VAL:H	1.64	0.63
1:B:560:GLY:HA2	1:B:843:VAL:HA	1.81	0.63
1:B:728:SER:HA	1:B:731:VAL:HG12	1.79	0.63
1:B:630:PRO:HB2	1:B:872:SER:HB3	1.80	0.63
1:B:727:ILE:C	1:B:729:GLN:HB2	2.19	0.63
1:B:24:VAL:HG13	1:B:39:GLU:HA	1.80	0.63
1:B:816:GLN:C	1:B:818:GLU:OE2	2.37	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:739:THR:HG23	1:A:764:ILE:O	1.99	0.63
1:B:607:ARG:HH21	1:B:610:ARG:HD3	1.64	0.63
1:A:763:LYS:NZ	1:A:764:ILE:HB	2.13	0.63
1:B:613:ARG:HB3	1:B:651:TRP:HB3	1.80	0.63
1:B:411:VAL:HG23	1:B:412:LYS:CG	2.28	0.62
1:B:77:VAL:HG23	1:B:78:PRO:CD	2.18	0.62
1:A:221:GLU:HG2	1:A:231:THR:HG21	1.80	0.62
1:B:420:VAL:O	1:B:422:ARG:NH1	2.33	0.62
1:B:411:VAL:HG23	1:B:412:LYS:HG3	1.80	0.62
1:B:341:ASN:OD1	1:B:342:ALA:N	2.33	0.61
1:B:641:PRO:HD2	1:B:643:LEU:HD12	1.83	0.61
1:B:814:ARG:O	1:B:816:GLN:N	2.33	0.61
1:B:273:THR:HG22	1:B:274:THR:H	1.66	0.61
1:B:699:LYS:HA	1:B:705:TYR:H	1.64	0.61
1:B:138:ASP:OD1	1:B:141:ARG:NH2	2.34	0.61
1:A:739:THR:N	1:A:824:VAL:HG23	2.16	0.61
1:B:79:ASP:HA	1:B:82:TRP:CE2	2.35	0.61
1:B:421:ARG:HG3	1:B:428:ALA:HB2	1.82	0.61
1:A:488:ASN:HD22	1:A:522:SER:HB2	1.67	0.60
1:B:354:ALA:O	4:B:1202:HOH:O	2.16	0.60
1:B:816:GLN:HA	1:B:818:GLU:OE2	2.01	0.60
1:A:421:ARG:HG3	1:A:428:ALA:HB2	1.83	0.60
1:B:196:PRO:HG3	1:B:522:SER:HB2	1.83	0.60
1:A:323:ALA:O	1:A:327:SER:OG	2.17	0.60
1:A:333:GLU:HA	1:A:336:THR:HG23	1.83	0.60
1:B:65:VAL:HG13	1:B:101:VAL:HG13	1.84	0.59
1:B:402:ARG:NH1	1:B:470:ILE:O	2.35	0.59
1:B:49:GLN:NE2	1:B:700:LEU:HD12	2.17	0.59
1:B:317:LYS:HD2	1:B:350:ALA:O	2.01	0.59
1:A:363:ARG:NH2	1:B:915:SER:O	2.31	0.59
1:B:497:PHE:HB3	1:B:504:ASP:HB3	1.85	0.59
1:A:27:ILE:HG22	1:A:36:PHE:HD1	1.68	0.59
1:B:20:PHE:HE1	1:B:42:GLU:HB3	1.68	0.58
1:B:171:SER:HB2	1:B:190:ALA:HB2	1.84	0.58
1:A:402:ARG:NH2	4:A:1106:HOH:O	2.29	0.58
1:B:818:GLU:OE2	1:B:818:GLU:N	2.37	0.58
1:A:221:GLU:OE2	4:A:1102:HOH:O	2.17	0.58
1:B:150:ALA:HB1	1:B:156:TRP:HE1	1.68	0.58
1:A:463:THR:HB	1:A:605:MET:HE2	1.83	0.58
1:A:742:ASN:HB2	1:A:823:HIS:NE2	2.19	0.58
1:B:280:MET:HB2	1:B:475:PRO:HA	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASP:HA	1:B:82:TRP:CD2	2.39	0.58
1:B:613:ARG:HA	1:B:616:ALA:HB3	1.86	0.58
1:A:489:LEU:HD22	1:A:670:VAL:HG11	1.86	0.58
1:B:700:LEU:HG	1:B:701:ALA:H	1.68	0.58
1:A:864:ILE:HA	1:A:867:MET:HE2	1.85	0.57
1:B:698:LYS:HD2	1:B:699:LYS:H	1.69	0.57
1:A:273:THR:HG22	1:A:274:THR:H	1.69	0.57
1:A:768:LEU:N	1:A:769:PRO:HD2	2.20	0.57
1:A:239:ARG:HH21	2:A:1001:DTP:H5'1	1.69	0.57
1:A:733:TYR:CE2	1:A:827:THR:HG21	2.39	0.57
1:A:71:ARG:NH1	1:A:82:TRP:O	2.37	0.57
2:B:1102:DTP:H2'2	4:B:1201:HOH:O	2.04	0.57
1:A:668:VAL:HG13	1:A:669:THR:HG23	1.86	0.57
1:B:201:ILE:O	1:B:484:ASP:N	2.36	0.56
1:B:61:ARG:HB2	1:B:157:PHE:HE1	1.70	0.56
1:A:28:ARG:HG3	1:A:35:VAL:HG23	1.88	0.56
1:B:722:TYR:HB3	1:B:727:ILE:HD11	1.87	0.55
1:A:738:GLY:O	1:A:739:THR:OG1	2.20	0.55
1:B:156:TRP:NE1	1:B:677:ILE:HD11	2.20	0.55
1:A:304:VAL:O	1:A:308:VAL:HG23	2.06	0.55
1:B:152:ASN:HD22	1:B:154:PRO:HG2	1.72	0.55
1:B:707:LYS:NZ	1:B:768:LEU:HB3	2.21	0.55
1:B:841:LEU:HD12	1:B:844:PHE:CD2	2.39	0.55
1:A:184:LEU:HD21	1:A:531:LYS:HB3	1.88	0.55
1:B:18:VAL:HG13	1:B:45:GLU:HG2	1.87	0.54
1:A:745:THR:HG22	1:A:746:ILE:HG12	1.89	0.54
1:B:325:ILE:HG23	1:B:344:LEU:HD13	1.88	0.54
1:A:321:ILE:O	1:A:325:ILE:HG13	2.07	0.54
1:B:321:ILE:HG12	1:B:347:ALA:HB1	1.88	0.54
1:B:7:PHE:HZ	1:B:507:GLY:HA3	1.73	0.54
1:B:699:LYS:NZ	4:B:1216:HOH:O	2.39	0.53
1:B:834:PRO:HB2	1:B:835:HIS:ND1	2.23	0.53
1:B:729:GLN:HB3	1:B:730:ILE:HG13	1.90	0.53
1:A:520:GLU:OE2	1:A:541:ARG:NH1	2.41	0.53
1:A:417:TRP:N	1:A:431:ILE:O	2.40	0.53
1:A:613:ARG:NH1	1:A:652:ASP:OD1	2.42	0.53
1:B:136:TYR:OH	1:B:518:THR:HB	2.08	0.53
1:B:325:ILE:HA	1:B:341:ASN:HD21	1.74	0.53
1:B:820:ALA:O	1:B:824:VAL:HG12	2.08	0.53
1:A:414:ASP:HB2	1:A:434:ARG:HH21	1.73	0.53
1:A:383:ASP:HB2	1:A:386:SER:OG	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:ILE:C	1:B:27:ILE:HD12	2.29	0.52
1:B:77:VAL:CB	1:B:78:PRO:HD2	2.21	0.52
1:A:607:ARG:HG3	1:A:624:GLU:HB2	1.91	0.52
1:B:161:LEU:H	1:B:161:LEU:HD12	1.74	0.52
1:B:513:ARG:NH1	1:B:587:GLU:OE1	2.38	0.52
1:B:515:TRP:HA	1:B:518:THR:HG22	1.91	0.52
1:B:698:LYS:HD2	1:B:699:LYS:N	2.25	0.52
1:A:359:THR:HB	1:B:917:LEU:HD23	1.92	0.52
1:A:485:THR:HG22	1:A:536:LEU:HB3	1.92	0.52
1:B:48:SER:O	1:B:52:SER:OG	2.25	0.52
1:B:203:SER:HB3	1:B:483:ASP:HB3	1.92	0.52
1:B:54:VAL:O	1:B:58:LYS:HB2	2.10	0.51
1:B:374:SER:OG	1:B:375:ILE:N	2.41	0.51
1:B:519:LEU:HB3	1:B:543:LEU:HD22	1.93	0.51
1:B:134:ARG:HA	1:B:137:TYR:HB3	1.92	0.51
1:B:193:HIS:HB3	1:B:527:GLN:HB2	1.93	0.51
1:B:467:ASP:OD2	1:B:600:ARG:NH1	2.42	0.51
1:B:152:ASN:ND2	1:B:154:PRO:HG2	2.26	0.51
1:B:896:ALA:O	1:B:900:SER:OG	2.26	0.51
1:A:263:ARG:NH1	1:A:390:THR:O	2.37	0.51
1:B:332:ILE:HG12	1:B:334:GLY:N	2.21	0.51
1:A:4:GLU:H	1:A:4:GLU:CD	2.13	0.51
1:A:710:ASN:HB3	1:A:713:VAL:HG23	1.93	0.51
1:B:50:VAL:HG22	1:B:698:LYS:HE2	1.93	0.51
1:B:613:ARG:HB3	1:B:651:TRP:CB	2.41	0.51
1:A:476:CYS:HB2	1:A:478:GLU:OE1	2.11	0.51
1:B:49:GLN:NE2	1:B:700:LEU:HA	2.26	0.51
1:B:49:GLN:HB3	1:B:698:LYS:NZ	2.26	0.50
1:B:66:PRO:HG2	1:B:69:LEU:HD11	1.93	0.50
1:A:24:VAL:HG22	1:A:39:GLU:HA	1.93	0.50
1:B:66:PRO:HB2	1:B:69:LEU:HD11	1.93	0.50
1:A:203:SER:HB3	1:A:483:ASP:HB3	1.93	0.50
1:A:448:ALA:HB2	1:A:911:TYR:HD1	1.76	0.50
1:B:727:ILE:CA	1:B:729:GLN:HB2	2.42	0.50
1:B:168:ASP:OD1	1:B:169:GLY:N	2.45	0.50
1:B:454:PHE:CE1	1:B:901:HIS:HB2	2.47	0.50
1:A:763:LYS:HZ3	1:A:764:ILE:HB	1.76	0.50
1:B:478:GLU:OE1	1:B:673:PRO:HD2	2.11	0.50
1:A:66:PRO:HG2	1:A:69:LEU:HD21	1.94	0.50
1:A:129:THR:HG23	1:A:132:ASP:H	1.77	0.49
1:A:739:THR:CG2	1:A:764:ILE:HG12	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:SER:HB3	1:A:825:CYS:HB3	1.93	0.49
1:A:402:ARG:NH1	1:A:470:ILE:O	2.44	0.49
1:B:208:LEU:N	4:B:1201:HOH:O	2.45	0.49
1:A:437:TRP:CE2	1:A:894:LEU:HD22	2.47	0.49
1:B:49:GLN:H	1:B:698:LYS:HZ1	1.59	0.49
1:B:713:VAL:HA	1:B:716:ALA:HB3	1.93	0.49
1:B:122:TRP:HE3	1:B:127:PHE:HD2	1.59	0.49
1:B:437:TRP:CE2	1:B:894:LEU:HD22	2.47	0.49
1:B:637:ASN:OD1	4:B:1203:HOH:O	2.19	0.49
1:B:109:VAL:O	1:B:113:LEU:HG	2.13	0.49
1:B:112:ARG:NH1	1:B:157:PHE:O	2.44	0.49
1:A:698:LYS:HE3	1:A:699:LYS:O	2.12	0.49
1:B:816:GLN:CA	1:B:818:GLU:OE2	2.61	0.49
1:B:824:VAL:HG13	1:B:825:CYS:SG	2.53	0.49
1:A:488:ASN:ND2	1:A:522:SER:HB2	2.27	0.48
1:B:335:ALA:O	1:B:344:LEU:HD22	2.12	0.48
1:A:739:THR:HG23	1:A:764:ILE:CG1	2.43	0.48
1:A:739:THR:OG1	1:A:768:LEU:HD12	2.13	0.48
1:A:36:PHE:CE1	1:A:57:GLN:HG2	2.48	0.48
1:B:323:ALA:HA	1:B:326:ARG:NH2	2.29	0.48
1:B:833:ALA:HB3	1:B:836:LEU:HD22	1.94	0.48
1:B:39:GLU:CD	1:B:39:GLU:H	2.16	0.48
1:B:843:VAL:HG23	1:B:844:PHE:CE1	2.49	0.48
1:A:235:PHE:HB3	1:A:254:LEU:HD11	1.95	0.48
1:B:109:VAL:HA	1:B:112:ARG:HG2	1.95	0.48
1:A:698:LYS:HA	1:A:698:LYS:HD2	1.76	0.47
1:A:723:ALA:O	1:A:727:ILE:HG12	2.14	0.47
1:B:156:TRP:CD1	1:B:677:ILE:HD11	2.49	0.47
1:B:336:THR:HG21	1:B:369:ARG:HG3	1.96	0.47
1:A:162:HIS:HD2	4:A:1234:HOH:O	1.97	0.47
1:B:871:GLN:NE2	1:B:878:ILE:HG13	2.30	0.47
1:B:202:GLN:O	1:B:233:THR:HG23	2.15	0.47
1:B:398:ASN:ND2	4:B:1214:HOH:O	2.37	0.47
1:B:739:THR:N	1:B:824:VAL:HG23	2.29	0.47
1:B:154:PRO:HG3	1:B:198:ALA:HB2	1.96	0.47
1:B:50:VAL:H	1:B:698:LYS:HZ3	1.62	0.46
1:B:667:GLN:NE2	1:B:875:SER:HB3	2.31	0.46
1:A:75[B]:LYS:HA	1:A:75[B]:LYS:HD3	1.54	0.46
1:A:328:PHE:CD2	1:A:335:ALA:HB2	2.51	0.46
1:B:402:ARG:HH22	1:B:470:ILE:HG22	1.79	0.46
1:B:730:ILE:HG21	1:B:830:LEU:HG	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:ILE:HG13	1:A:762:GLU:N	2.31	0.46
1:B:94:LEU:HD22	1:B:98:ALA:HB1	1.97	0.46
1:A:40:SER:HB3	1:A:104:THR:OG1	2.14	0.46
1:B:122:TRP:HB2	1:B:127:PHE:CD2	2.51	0.46
1:B:27:ILE:HD12	1:B:35:VAL:N	2.30	0.46
1:B:27:ILE:CG1	1:B:36:PHE:HB3	2.45	0.46
1:B:841:LEU:CD1	1:B:844:PHE:HD2	2.27	0.46
1:B:517:VAL:O	1:B:521:ILE:HG13	2.16	0.46
1:B:713:VAL:HG12	1:B:714:PRO:HD3	1.98	0.46
1:A:859:SER:O	1:A:862:SER:OG	2.28	0.46
1:B:27:ILE:CD1	1:B:35:VAL:N	2.79	0.46
1:B:613:ARG:NH1	1:B:652:ASP:OD1	2.49	0.46
1:B:252:SER:OG	2:B:1102:DTP:H2	2.16	0.45
1:B:559:LEU:HB2	1:B:565:GLU:OE2	2.16	0.45
1:B:93:LYS:HA	1:B:93:LYS:HD3	1.75	0.45
1:B:525:MET:HB3	1:B:525:MET:HE2	1.79	0.45
1:B:411:VAL:HG23	1:B:412:LYS:HG2	1.99	0.45
1:B:875:SER:O	1:B:906:LYS:NZ	2.50	0.45
1:B:77:VAL:HG11	1:B:122:TRP:HB3	1.98	0.45
1:B:107:ARG:HA	1:B:110:PHE:HB2	1.97	0.45
1:A:44:PRO:HB2	1:A:47:TRP:CD1	2.52	0.45
1:A:225:PHE:O	1:A:270:SER:HA	2.17	0.45
1:B:328:PHE:HE2	1:B:340:GLY:O	1.99	0.45
1:B:322:PHE:O	1:B:326:ARG:HG2	2.17	0.45
1:B:709:ILE:HB	1:B:735:VAL:HG11	1.99	0.45
1:B:257:PHE:HA	1:B:260:ILE:HD12	1.99	0.45
1:A:478:GLU:HB2	1:A:670:VAL:HG22	1.99	0.45
1:B:48:SER:OG	1:B:49:GLN:N	2.50	0.45
1:A:70:LYS:NZ	1:A:88:GLU:OE2	2.45	0.45
1:A:206:ASP:OD2	1:A:239:ARG:HG3	2.17	0.45
1:B:408:LEU:HA	1:B:411:VAL:CG1	2.23	0.45
1:B:820:ALA:O	1:B:824:VAL:N	2.43	0.45
1:B:194:PRO:HD2	1:B:525:MET:HG3	1.99	0.44
1:B:224:LEU:HD23	1:B:231:THR:HB	1.98	0.44
1:B:325:ILE:HA	1:B:335:ALA:HB1	1.98	0.44
1:A:742:ASN:OD1	1:A:742:ASN:N	2.51	0.44
1:B:68:ARG:C	1:B:69:LEU:HD22	2.38	0.44
1:B:323:ALA:HA	1:B:326:ARG:CZ	2.48	0.44
1:B:370:GLN:HB2	1:B:372:PHE:HD2	1.82	0.44
1:B:560:GLY:CA	1:B:843:VAL:HA	2.46	0.44
1:B:280:MET:CG	1:B:282:ILE:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:HD2	1:A:165:TYR:HB3	1.99	0.44
1:A:454:PHE:CZ	1:A:901:HIS:HB2	2.53	0.44
1:B:411:VAL:HG23	1:B:412:LYS:N	2.32	0.44
1:B:122:TRP:O	1:B:125:GLY:N	2.50	0.44
1:B:489:LEU:CD2	1:B:670:VAL:HG21	2.48	0.44
1:B:658:GLY:HA3	1:B:663:TYR:CZ	2.52	0.44
1:A:315:GLU:HG2	1:A:319:ASN:HD21	1.83	0.44
1:B:48:SER:OG	1:B:698:LYS:CE	2.66	0.44
1:B:143:MET:HB3	1:B:148:MET:HB3	2.00	0.44
1:B:573:LEU:HD21	1:B:643:LEU:HD13	1.99	0.44
1:A:871:GLN:HE22	1:A:877:ALA:HA	1.83	0.44
1:B:49:GLN:HB3	1:B:698:LYS:HZ1	1.82	0.44
1:B:831:GLU:HA	1:B:841:LEU:HD21	1.99	0.44
1:A:488:ASN:OD1	1:A:488:ASN:N	2.41	0.44
1:B:161:LEU:HB3	1:B:167:ILE:HD12	1.99	0.44
1:A:341:ASN:HB3	1:A:344:LEU:HB3	2.00	0.43
1:B:50:VAL:N	1:B:698:LYS:HZ3	2.16	0.43
1:B:707:LYS:HZ3	1:B:768:LEU:HB3	1.82	0.43
1:A:528:PHE:HB2	1:A:534:ALA:HB2	1.99	0.43
1:A:733:TYR:O	1:A:827:THR:HG22	2.18	0.43
1:B:700:LEU:HG	1:B:701:ALA:N	2.31	0.43
1:B:813:THR:O	1:B:814:ARG:HG3	2.18	0.43
1:A:889:THR:O	1:A:893:THR:HG23	2.19	0.43
1:B:320:ASP:O	1:B:323:ALA:HB3	2.19	0.43
1:A:58:LYS:HA	1:A:58:LYS:HD3	1.86	0.43
1:A:232:GLY:HA3	1:A:473:SER:O	2.18	0.43
1:A:682:ASP:OD1	4:A:1103:HOH:O	2.21	0.43
1:B:330:GLY:O	1:B:332:ILE:HD12	2.19	0.43
1:B:434:ARG:O	1:B:438:ASP:N	2.50	0.43
1:A:370:GLN:NE2	1:B:890:ILE:H	2.12	0.43
1:A:740:LEU:O	1:A:764:ILE:HD11	2.19	0.43
1:A:561:TYR:CD1	1:A:690:PRO:HB3	2.54	0.43
1:A:739:THR:HA	1:A:767:ALA:HB3	2.01	0.43
1:B:575:ALA:HA	1:B:873:PHE:HB3	2.01	0.43
1:B:208:LEU:HB2	4:B:1201:HOH:O	2.18	0.43
1:B:559:LEU:HD12	1:B:565:GLU:HB2	2.00	0.43
1:B:122:TRP:O	1:B:122:TRP:CD1	2.72	0.43
1:B:350:ALA:HA	1:B:353:LYS:HD3	2.00	0.43
1:B:384:TRP:HA	1:B:389:TYR:CD2	2.53	0.43
1:B:621:THR:HG22	1:B:622:GLY:H	1.83	0.43
1:A:713:VAL:HB	1:A:714:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:860:VAL:HG13	1:A:882:ILE:HG21	2.00	0.42
1:B:39:GLU:OE2	1:B:39:GLU:N	2.52	0.42
1:B:48:SER:HG	1:B:50:VAL:HG22	1.84	0.42
1:B:833:ALA:HB3	1:B:836:LEU:CD2	2.48	0.42
1:B:48:SER:OG	1:B:50:VAL:HG22	2.20	0.42
1:B:126:TYR:CE1	1:B:592:LEU:HD12	2.53	0.42
1:B:196:PRO:HG2	1:B:197:HIS:CE1	2.54	0.42
1:B:325:ILE:HD12	1:B:326:ARG:N	2.34	0.42
1:B:403:VAL:HG11	1:B:452:ILE:HD11	2.01	0.42
1:A:454:PHE:CE1	1:A:901:HIS:HB2	2.54	0.42
1:B:77:VAL:HG21	1:B:122:TRP:CD2	2.54	0.42
1:B:183:LYS:HG3	1:B:185:GLN:HG2	2.01	0.42
1:B:255:MET:HG3	1:B:292:GLN:HB3	2.00	0.42
1:B:460:ALA:HB1	1:B:626:VAL:HA	2.00	0.42
1:B:494:LEU:HD23	1:B:494:LEU:HA	1.81	0.42
1:A:366:GLN:HE21	1:A:366:GLN:HB2	1.59	0.42
1:B:239:ARG:HA	1:B:422:ARG:HB2	2.00	0.42
1:B:557:MET:HB3	1:B:559:LEU:HD21	2.00	0.42
1:A:423:THR:OG1	1:A:424:ASP:N	2.53	0.42
1:B:121:GLY:HA2	1:B:521:ILE:HD13	2.01	0.42
1:B:489:LEU:HD22	1:B:670:VAL:HG21	2.02	0.42
1:A:308:VAL:HG12	1:A:312:LYS:HE3	2.01	0.42
1:B:86:PRO:HD3	1:B:166:GLY:HA3	2.02	0.42
1:B:122:TRP:C	1:B:125:GLY:H	2.23	0.42
1:B:375:ILE:HD12	1:B:375:ILE:HA	1.89	0.42
1:B:174:HIS:HB3	1:B:527:GLN:HG2	2.02	0.42
1:B:522:SER:O	1:B:526:ALA:HB2	2.20	0.42
1:B:384:TRP:HB3	1:B:918:SER:OG	2.20	0.41
1:B:877:ALA:HB2	1:B:906:LYS:HB2	2.02	0.41
1:A:420:VAL:O	1:A:422:ARG:NH2	2.35	0.41
1:A:437:TRP:NE1	1:A:894:LEU:HD22	2.34	0.41
1:A:824:VAL:HG13	1:A:825:CYS:SG	2.60	0.41
1:B:27:ILE:HG12	1:B:36:PHE:HB3	2.02	0.41
1:B:70:LYS:HA	1:B:70:LYS:HD3	1.81	0.41
1:A:140:MET:HE3	1:A:514:LEU:HB3	2.03	0.41
1:B:322:PHE:HE2	1:B:375:ILE:HB	1.85	0.41
1:B:677:ILE:O	1:B:681:MET:HG3	2.20	0.41
1:B:716:ALA:O	1:B:720:LEU:HD12	2.20	0.41
1:A:378:PRO:HD2	1:B:302:GLN:OE1	2.20	0.41
1:A:442:HIS:NE2	1:B:367:TYR:OH	2.42	0.41
1:B:49:GLN:HE22	1:B:700:LEU:HD12	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:695:VAL:C	1:B:696:LYS:HG3	2.41	0.41
1:B:817:ILE:N	1:B:818:GLU:OE2	2.53	0.41
1:B:51:ALA:HA	1:B:680:VAL:HA	2.03	0.41
1:A:734:ALA:HA	1:A:827:THR:HG22	2.03	0.41
1:B:351:ALA:C	1:B:352:LYS:O	2.58	0.41
1:B:389:TYR:OH	1:B:917:LEU:HB2	2.19	0.41
1:B:463:THR:HG21	1:B:666:ALA:O	2.21	0.41
1:B:193:HIS:O	1:B:527:GLN:NE2	2.54	0.41
1:B:233:THR:HB	1:B:235:PHE:CE1	2.56	0.41
1:A:88:GLU:CD	1:A:88:GLU:H	2.24	0.41
1:B:77:VAL:HG21	1:B:122:TRP:CG	2.56	0.41
1:A:4:GLU:OE1	1:A:4:GLU:N	2.52	0.41
1:B:561:TYR:CD2	1:B:690:PRO:HB3	2.56	0.41
1:B:643:LEU:HD23	1:B:643:LEU:HA	1.91	0.41
1:A:860:VAL:O	1:A:864:ILE:HG13	2.22	0.40
1:B:157:PHE:O	1:B:161:LEU:HD11	2.21	0.40
1:B:730:ILE:HA	1:B:733:TYR:HB3	2.03	0.40
1:B:27:ILE:HD12	1:B:28:ARG:N	2.36	0.40
1:B:65:VAL:HG23	1:B:165:TYR:HB3	2.03	0.40
1:A:600:ARG:NH2	4:A:1120:HOH:O	2.44	0.40
1:B:94:LEU:HD22	1:B:98:ALA:CB	2.51	0.40
1:B:175:PHE:CD2	1:B:531:LYS:HB3	2.39	0.40
1:B:674:THR:HB	1:B:677:ILE:HG22	2.03	0.40
1:B:810:LEU:HD23	1:B:810:LEU:HA	1.88	0.40
1:A:760:GLU:HG3	1:A:763:LYS:NZ	2.36	0.40
1:B:149:ALA:HA	1:B:492:MET:HA	2.03	0.40
1:B:726:GLN:HA	1:B:729:GLN:HG3	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:TYR:O	1:B:813:THR:OG1[2_545]	1.80	0.40
1:A:742:ASN:ND2	1:B:424:ASP:O[3_554]	2.03	0.17

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	861/925 (93%)	825 (96%)	32 (4%)	4 (0%)	29 58
1	B	844/925 (91%)	777 (92%)	58 (7%)	9 (1%)	14 38
All	All	1705/1850 (92%)	1602 (94%)	90 (5%)	13 (1%)	19 47

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	740	LEU
1	B	38	ASN
1	B	78	PRO
1	B	701	ALA
1	B	729	GLN
1	B	815	ALA
1	A	332	ILE
1	B	333	GLU
1	A	330	GLY
1	B	352	LYS
1	A	333	GLU
1	B	769	PRO
1	B	721	GLY

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	674/718 (94%)	666 (99%)	8 (1%)	71 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	669/718 (93%)	635 (95%)	34 (5%)	24 53
All	All	1343/1436 (94%)	1301 (97%)	42 (3%)	40 71

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	PHE
1	A	270	SER
1	A	400	SER
1	A	513	ARG
1	A	582	TYR
1	A	696	LYS
1	A	742	ASN
1	A	743	CYS
1	B	28	ARG
1	B	29	ASN
1	B	49	GLN
1	B	73	LYS
1	B	143	MET
1	B	146	ARG
1	B	152	ASN
1	B	186	LYS
1	B	189	SER
1	B	328	PHE
1	B	333	GLU
1	B	345	LYS
1	B	353	LYS
1	B	416	ASP
1	B	422	ARG
1	B	495	LEU
1	B	520	GLU
1	B	524	MET
1	B	531	LYS
1	B	567	ARG
1	B	607	ARG
1	B	610	ARG
1	B	649	SER
1	B	697	PHE
1	B	712	SER
1	B	724	SER
1	B	763	LYS
1	B	775	ARG

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Mol	Chain	Res	Type
1	B	810	LEU
1	B	836	LEU
1	B	856	ARG
1	B	880	LYS
1	B	903	LEU
1	B	918	SER

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

Mol	Chain	Res	Type
1	A	319	ASN
1	A	370	GLN
1	A	398	ASN
1	A	399	ASN
1	A	726	GLN
1	A	748	HIS
1	A	835	HIS
1	A	871	GLN
1	B	38	ASN
1	B	49	GLN
1	B	147	GLN
1	B	195	GLN
1	B	313	GLN
1	B	362	ASN
1	B	366	GLN
1	B	395	GLN
1	B	604	HIS
1	B	617	HIS
1	B	635	GLN
1	B	667	GLN
1	B	871	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	DTP	A	1001	3	26,32,32	0.66	0	30,50,50	0.80	1 (3%)
2	DTP	B	1102	3	26,32,32	0.68	0	30,50,50	0.78	1 (3%)

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	DTP	A	1001	3	-	2/18/34/34	0/3/3/3
2	DTP	B	1102	3	-	3/18/34/34	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1102	DTP	C5-C6-N6	2.31	123.86	120.35
2	A	1001	DTP	C5-C6-N6	2.27	123.80	120.35

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1102	DTP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	B	1102	DTP	C5'-O5'-PA-O3A
2	B	1102	DTP	C5'-O5'-PA-O2A
2	A	1001	DTP	PA-O3A-PB-O2B
2	A	1001	DTP	C5'-O5'-PA-O1A

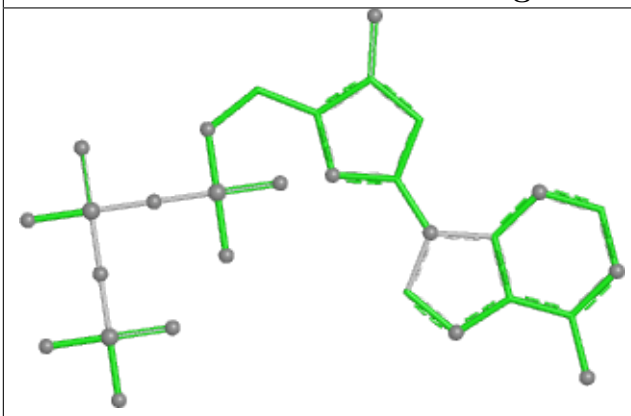
There are no ring outliers.

2 monomers are involved in 4 short contacts:

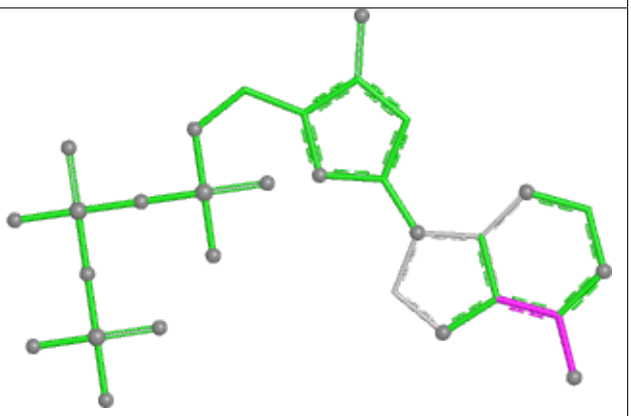
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	DTP	1	0
2	B	1102	DTP	3	0

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.

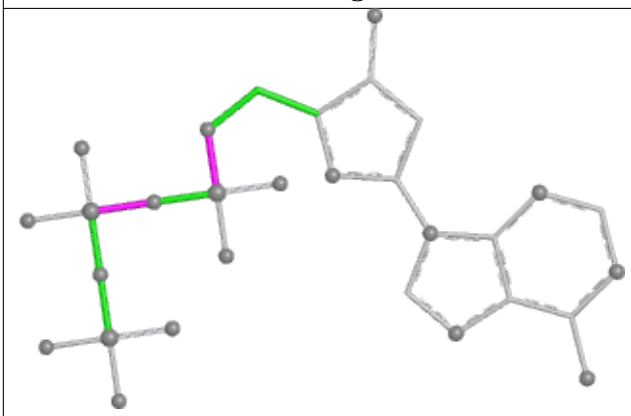
Ligand DTP A 1001



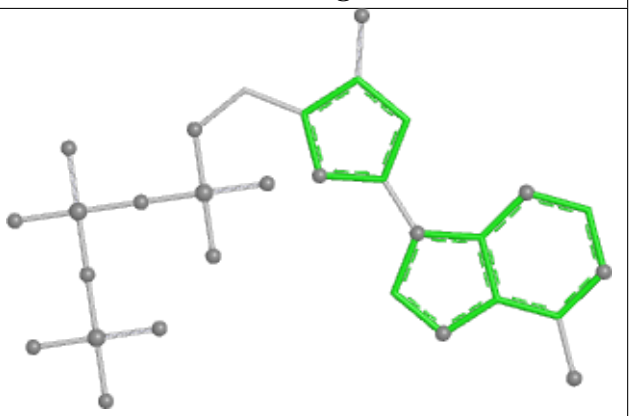
Bond lengths



Bond angles

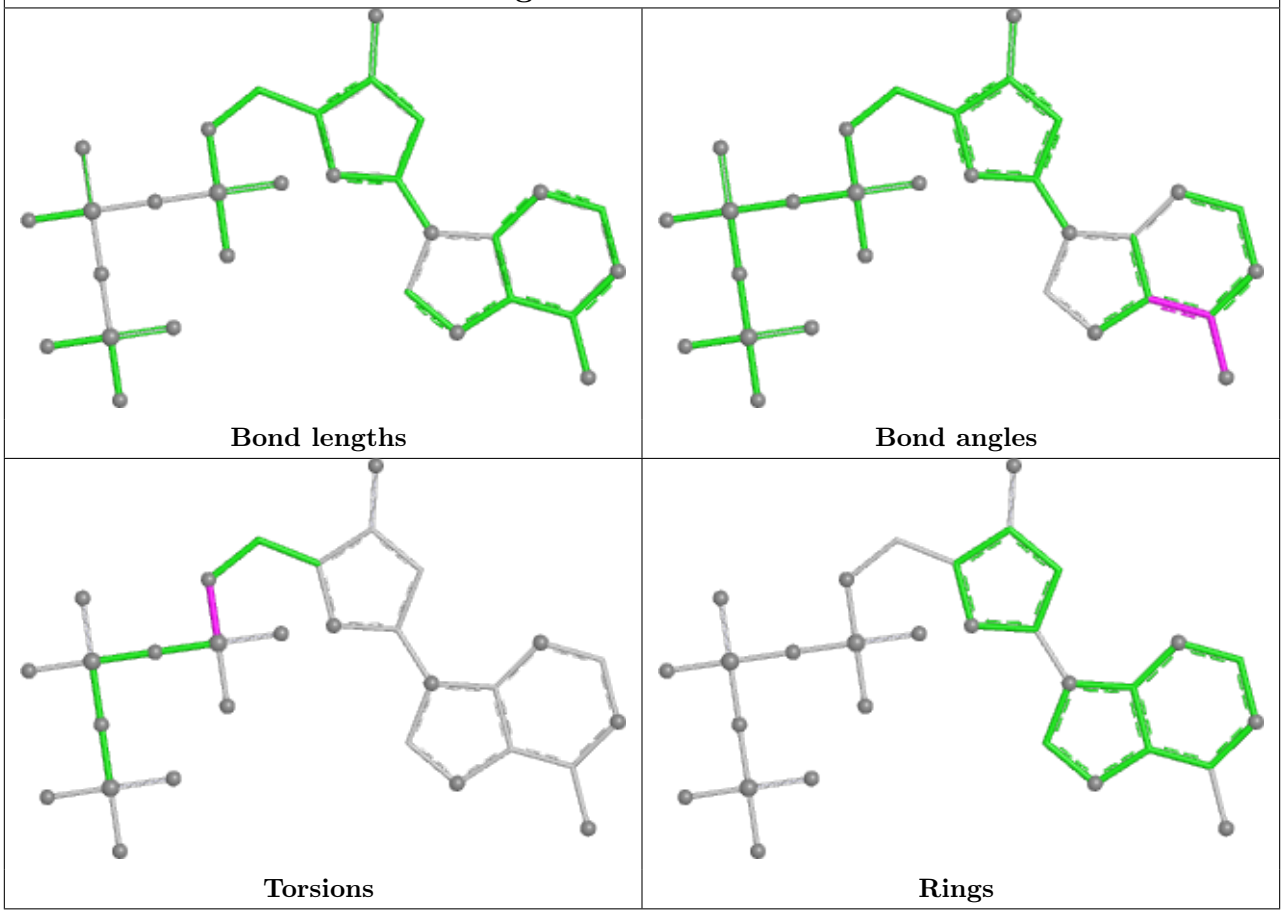


Torsions



Rings

Ligand DTP B 1102



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	868/925 (93%)	0.13	34 (3%) 39 34	37, 65, 139, 214	0
1	B	860/925 (92%)	0.73	122 (14%) 2 1	52, 115, 172, 216	0
All	All	1728/1850 (93%)	0.43	156 (9%) 9 6	37, 89, 163, 216	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	86	PRO	8.3
1	B	91	LEU	7.8
1	A	746	ILE	7.5
1	B	64	GLY	7.1
1	B	95	PRO	6.5
1	B	122	TRP	5.6
1	B	769	PRO	5.5
1	A	325	ILE	5.5
1	A	761	ILE	5.2
1	B	100	PHE	4.9
1	B	37	ARG	4.8
1	A	744	PRO	4.8
1	B	25	SER	4.7
1	B	14	ALA	4.7
1	B	740	LEU	4.6
1	A	765	GLU	4.3
1	B	36	PHE	4.3
1	B	721	GLY	4.2
1	B	55	LEU	4.1
1	B	812	PHE	4.0
1	B	476	CYS	4.0
1	B	118	ALA	4.0
1	B	2	LYS	3.8
1	B	706	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	98	ALA	3.8
1	B	35	VAL	3.7
1	B	38	ASN	3.6
1	A	624	GLU	3.5
1	B	133	ALA	3.5
1	B	99	ARG	3.5
1	B	21	THR	3.5
1	A	756	PHE	3.5
1	A	622	GLY	3.5
1	B	697	PHE	3.5
1	A	743	CYS	3.4
1	B	127	PHE	3.4
1	B	555	MET	3.4
1	B	832	GLY	3.4
1	A	336	THR	3.4
1	B	836	LEU	3.4
1	A	745	THR	3.3
1	B	727	ILE	3.3
1	A	758	ALA	3.3
1	B	857	TYR	3.2
1	B	165	TYR	3.2
1	A	740	LEU	3.2
1	B	743	CYS	3.2
1	A	373	SER	3.1
1	B	880	LYS	3.1
1	A	274	THR	3.1
1	A	199	CYS	3.1
1	B	67	ALA	3.1
1	B	717	LEU	3.1
1	B	701	ALA	3.0
1	B	830	LEU	3.0
1	B	50	VAL	3.0
1	A	92	ALA	3.0
1	A	738	GLY	3.0
1	B	136	TYR	2.9
1	B	621	THR	2.9
1	B	700	LEU	2.9
1	B	65	VAL	2.9
1	B	765	GLU	2.9
1	A	772	PHE	2.9
1	B	544	GLY	2.9
1	B	687	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	838	ALA	2.8
1	B	330	GLY	2.8
1	B	737	HIS	2.8
1	A	328	PHE	2.8
1	A	762	GLU	2.7
1	B	66	PRO	2.7
1	B	833	ALA	2.7
1	B	164	ALA	2.7
1	B	183	LYS	2.7
1	B	78	PRO	2.7
1	B	487	CYS	2.6
1	B	68	ARG	2.6
1	B	594	ALA	2.6
1	B	69	LEU	2.6
1	B	840	HIS	2.6
1	B	117	TRP	2.6
1	B	85	VAL	2.6
1	B	353	LYS	2.5
1	B	140	MET	2.5
1	B	131	ALA	2.5
1	B	175	PHE	2.5
1	B	26	GLU	2.5
1	B	157	PHE	2.5
1	B	879	SER	2.5
1	A	321	ILE	2.5
1	B	114	ALA	2.5
1	B	723	ALA	2.5
1	B	184	LEU	2.5
1	B	873	PHE	2.5
1	B	625	GLY	2.5
1	B	699	LYS	2.4
1	B	741	ALA	2.4
1	B	767	ALA	2.4
1	B	513	ARG	2.4
1	B	318	LEU	2.4
1	B	702	GLY	2.4
1	B	176	TYR	2.4
1	B	694	LEU	2.4
1	B	746	ILE	2.4
1	B	39	GLU	2.3
1	B	843	VAL	2.3
1	B	10	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	764	ILE	2.3
1	A	36	PHE	2.3
1	B	323	ALA	2.3
1	B	81	LEU	2.3
1	B	768	LEU	2.3
1	B	679	LEU	2.3
1	B	742	ASN	2.3
1	B	350	ALA	2.3
1	A	372	PHE	2.3
1	A	330	GLY	2.3
1	B	96	ALA	2.3
1	B	274	THR	2.3
1	B	412	LYS	2.3
1	A	747	SER	2.2
1	B	338	PRO	2.2
1	B	770	SER	2.2
1	B	80	PHE	2.2
1	A	375	ILE	2.2
1	A	476	CYS	2.2
1	B	488	ASN	2.2
1	B	15	TYR	2.2
1	A	273	THR	2.2
1	B	497	PHE	2.2
1	A	326	ARG	2.2
1	A	702	GLY	2.2
1	B	875	SER	2.2
1	B	736	GLY	2.2
1	B	349	ARG	2.1
1	B	495	LEU	2.1
1	B	518	THR	2.1
1	B	813	THR	2.1
1	A	487	CYS	2.1
1	B	336	THR	2.1
1	A	344	LEU	2.1
1	A	322	PHE	2.1
1	B	385	ASP	2.1
1	B	126	TYR	2.1
1	B	827	THR	2.1
1	B	408	LEU	2.1
1	B	27	ILE	2.1
1	B	825	CYS	2.1
1	B	669	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	30	PRO	2.0
1	B	94	LEU	2.0
1	B	735	VAL	2.0
1	B	881	THR	2.0
1	B	557	MET	2.0
1	B	647	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 monosaccharides in this entry.

6.4 Ligands (i)

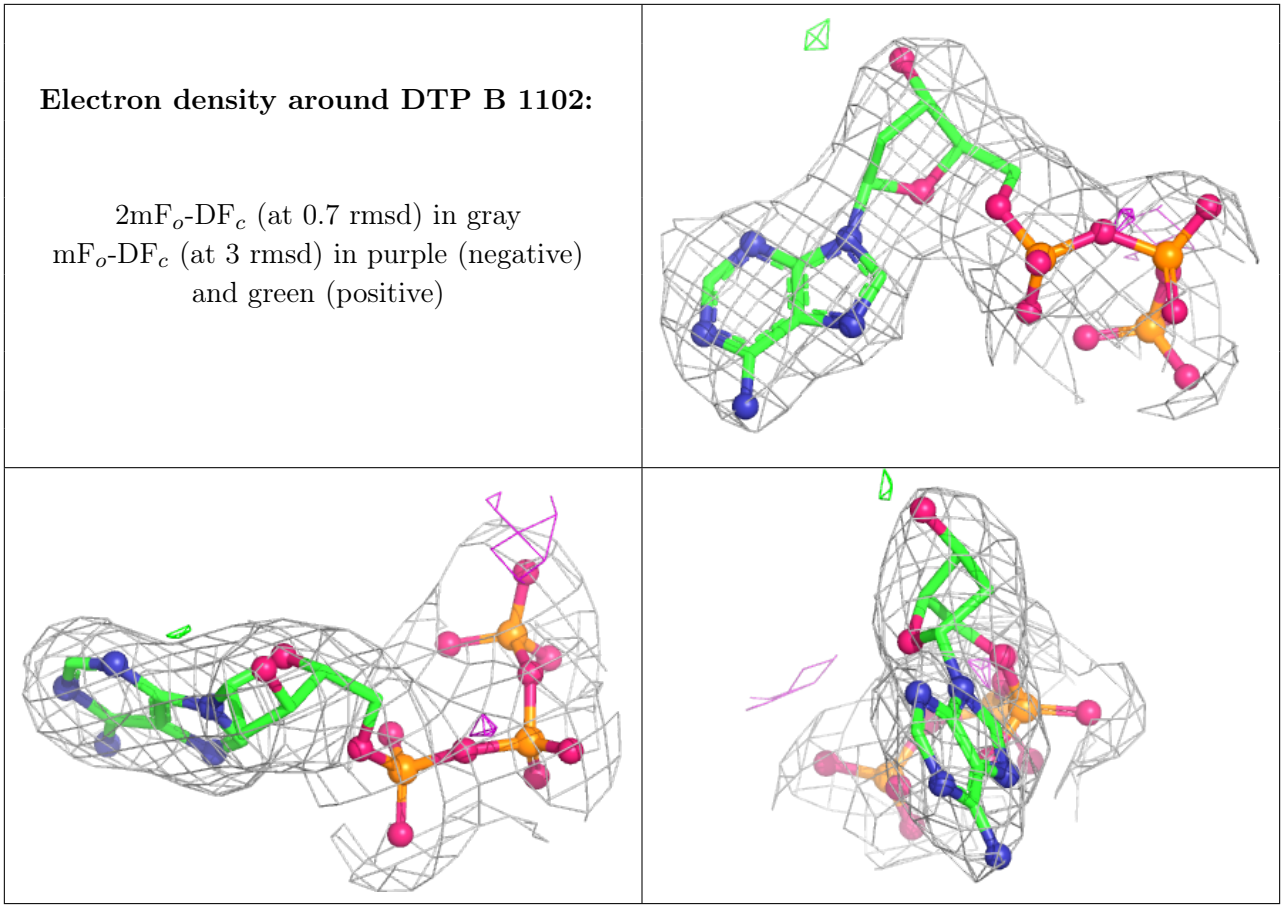
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DTP	B	1102	30/30	0.96	0.14	54,71,106,109	0
2	DTP	A	1001	30/30	0.97	0.15	49,74,101,106	0
3	MG	A	1002	1/1	0.98	0.18	39,39,39,39	0
3	MG	B	1101	1/1	0.99	0.14	49,49,49,49	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.

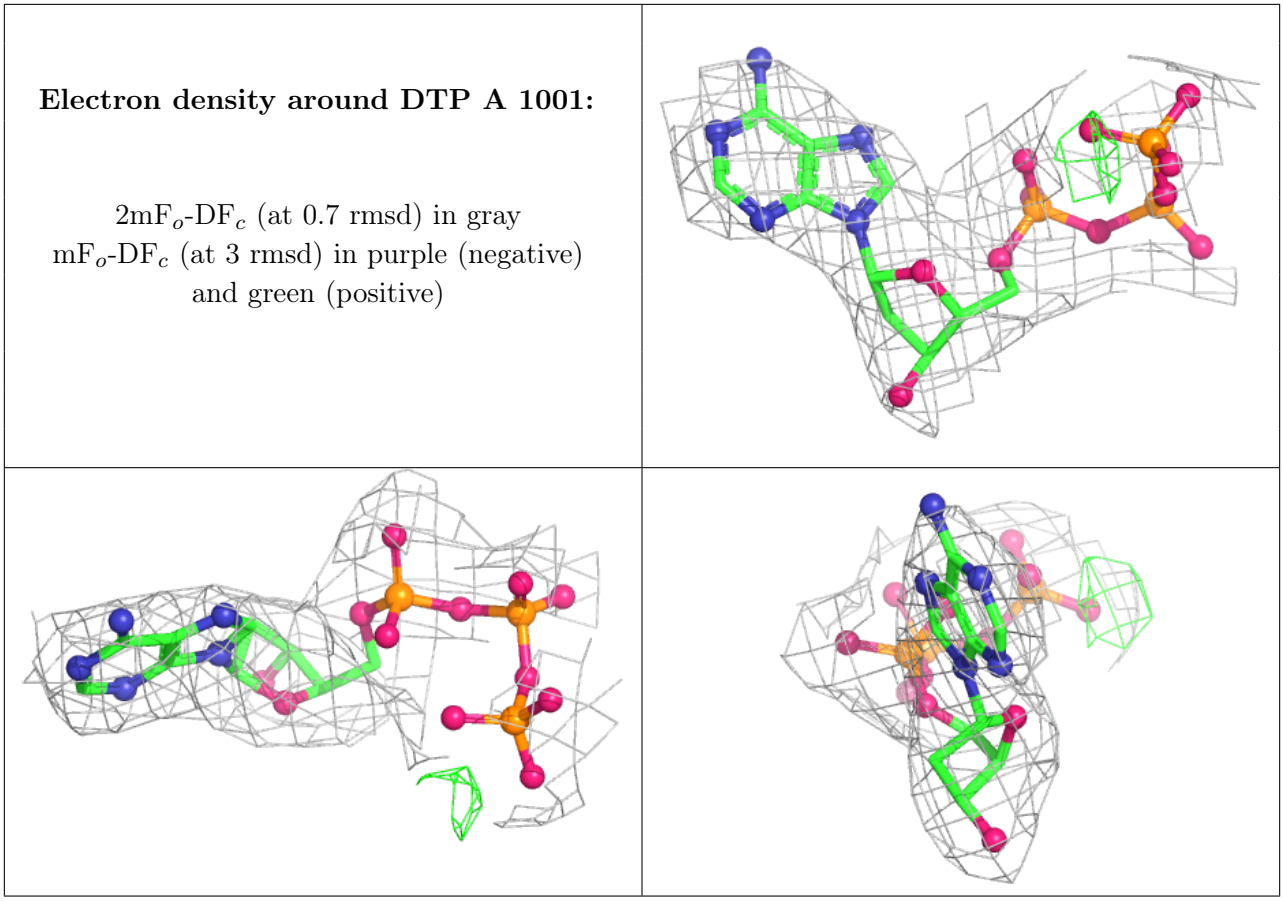
Electron density around DTP B 1102:

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



Electron density around DTP 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)



6.5 Other polymers

There are no such residues in this entry.