Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 06:46 AM EDT

PDB ID	:	3HNE
Title	:	Crystal structure of human ribonucleotide reductase 1 bound to the effectors TTP and ATP
Authors	:	Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.
Deposited on	:	2009-05-31
Resolution	:	3.11 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

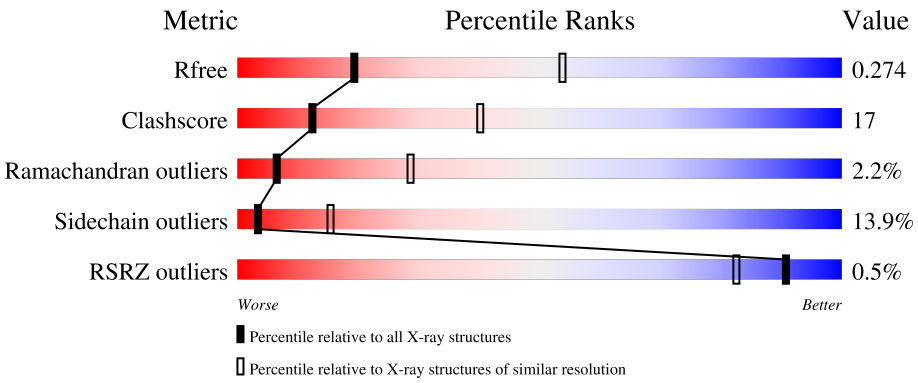
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.11 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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	792	61% 24% 5% • 10%
1	B	792	% 51% 33% 8% 9%

2 Entry composition (i)

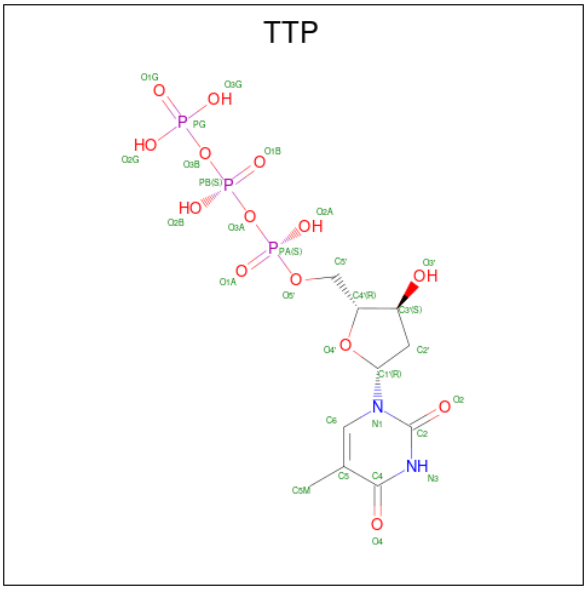
There are 6 unique types of molecules in this entry. The entry contains 11380 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	715	5568	3557	927	1051	33	6	1	0
1	B	724	5644	3593	955	1062	34	0	0	0

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).

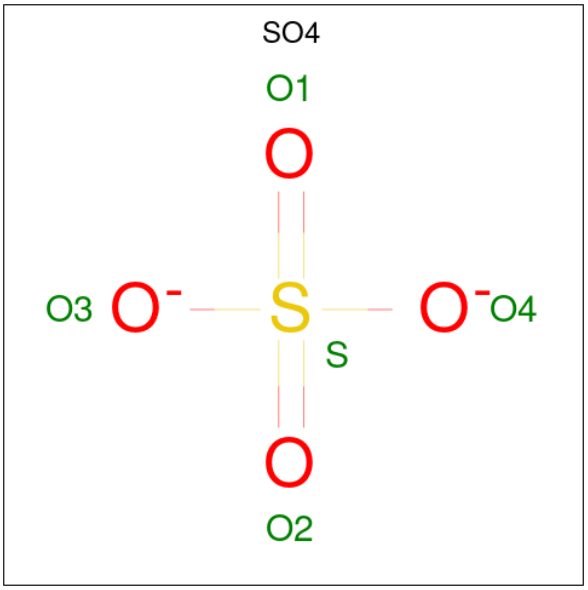


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	29	10	2	14	3	0	0
2	B	1	29	10	2	14	3	0	0

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

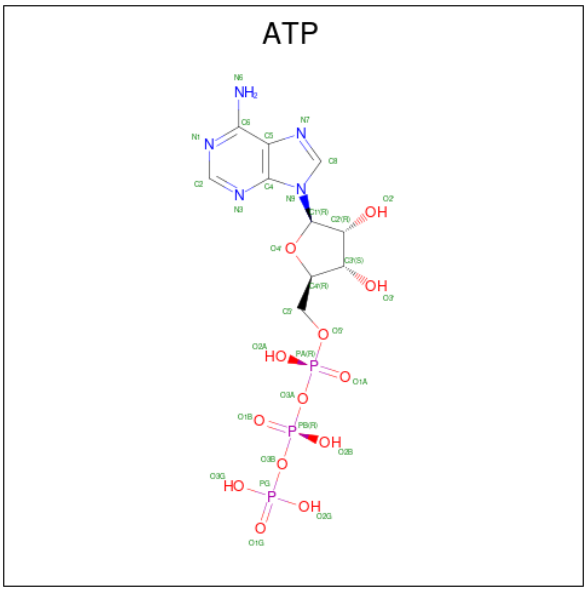
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	3	Total Mg 3 3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	B	1	31	10	5	13	3	0	0

- Molecule 6 is water.

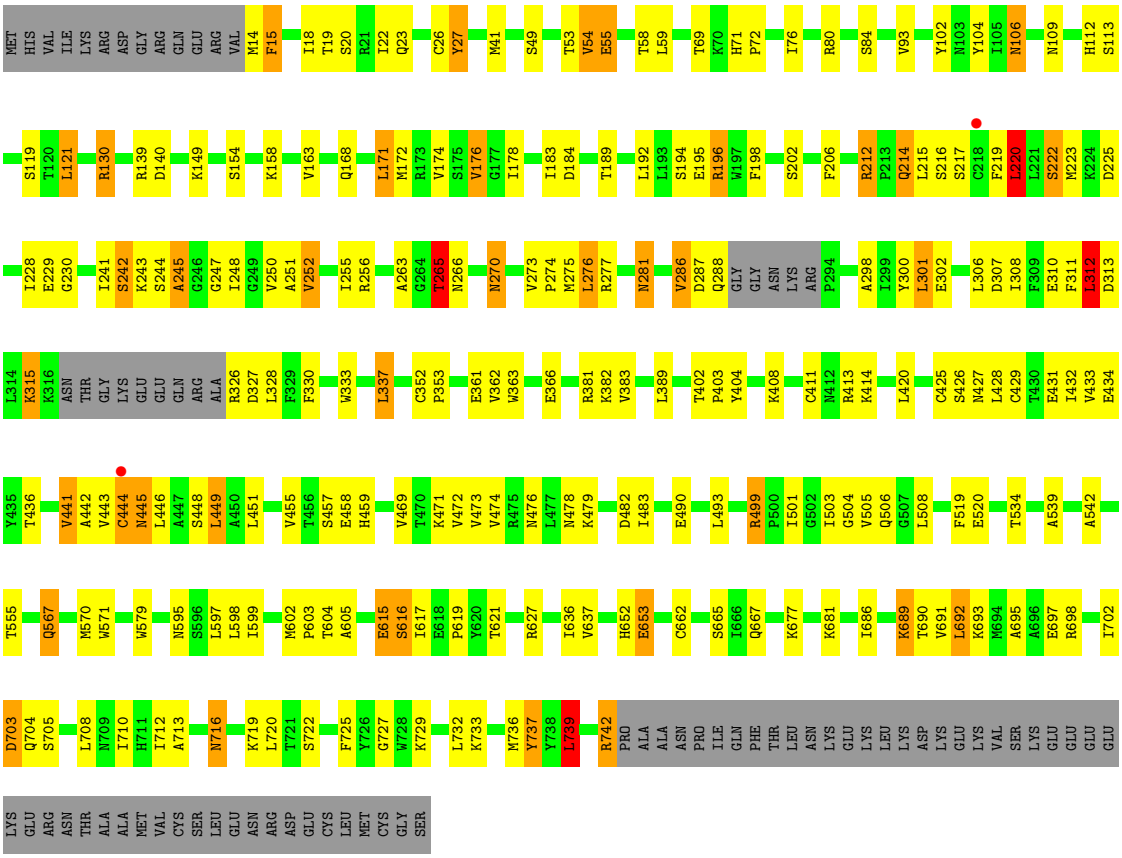
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	27	27	27	0	0
			Total	O		
6	B	18	18	18	0	0

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.

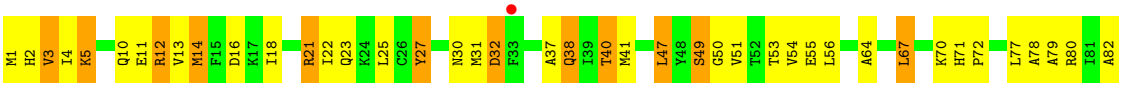
• Molecule 1: Ribonucleoside-diphosphate reductase large subunit

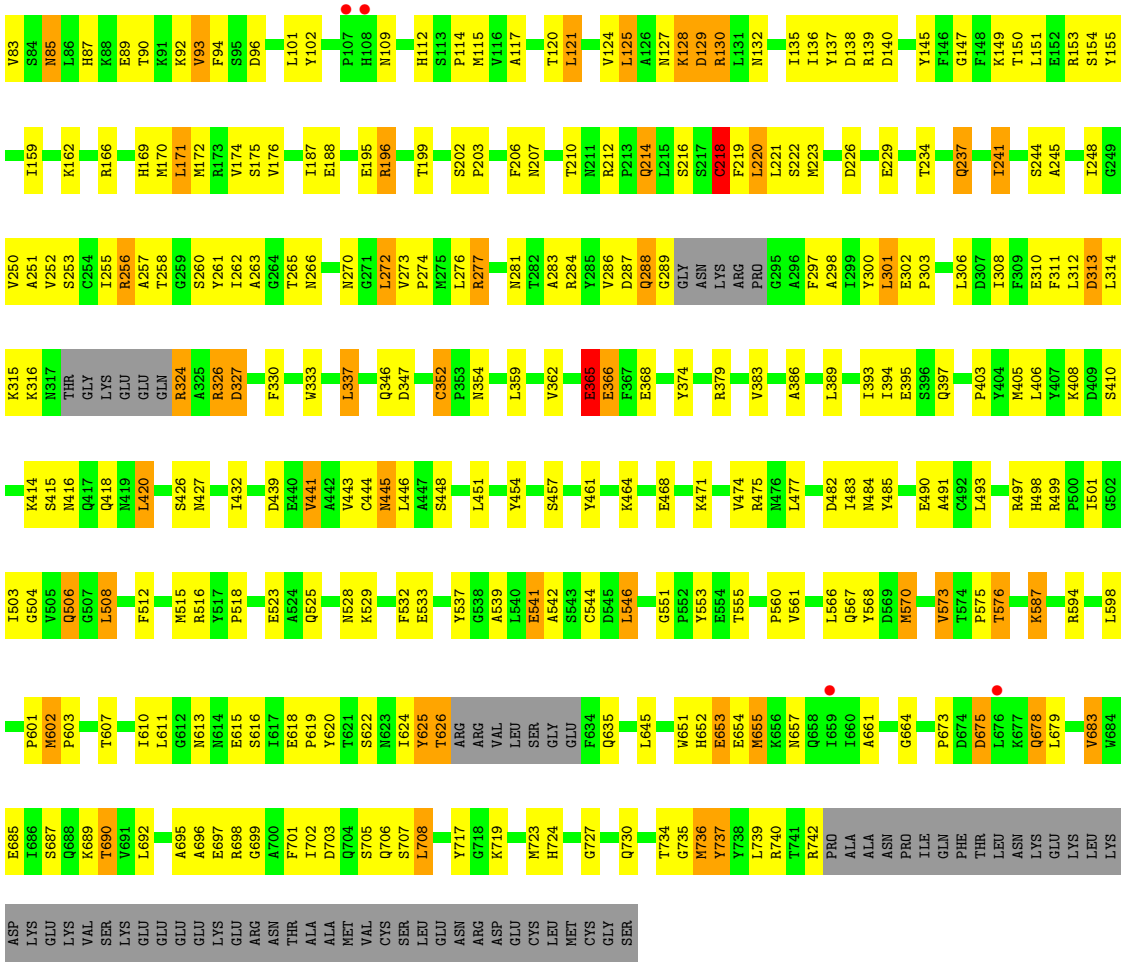
Chain A: 61% 24% 5% • 10%



• Molecule 1: Ribonucleoside-diphosphate reductase large subunit

Chain B: % 51% 33% 8% 9%




V83 S84 N85 L86 H87 K88 E89 T90 K91 K92 V93 F94 S95 D96 L101 Y102 P107 H108 N109 H112 S113 P114 M115 V116 A117 T120 L121 V124 L125 A126 N127 K128 D129 R130 L131 N132 I135 I136 Y137 D138 R139 D140 Y145 F146 G147 F148 K149 T150 L151 E152 R153 S154 Y155
I159 K162 R166 H169 M170 L171 M172 R173 V174 S175 V176 I187 E188 E195 R196 T199 S202 P203 F206 N207 T210 N211 R212 P213 Q214 L215 S216 S217 C218 F219 L220 L221 S222 M223 D226 E229 T234 Q237 I241 S244 A245 I248 G249
V250 A251 V252 S253 C254 I255 R256 A257 T258 G259 S260 Y261 I262 A263 G264 T265 N266 N270 G271 L272 V273 P274 M275 L276 R277 N281 T282 A283 R284 Y285 V286 D287 Q288 G289 GLY ASN LYS ARG PRO G295 A296 F297 A298 I299 Y300 L301 E302 P303 L306 D307 I308 F309 E310 F311 L312 D313 L314
K315 K316 N317 THR GLY LYS GLU GLU GLN R324 A325 R326 D327 F330 W333 L337 Q346 D347 C352 P353 N354 L359 V362 E365 E366 F367 E368 Y374 R379 V383 A386 L389 I393 I394 E395 S396 Q397 P403 Y404 M405 L406 Y407 K408 D409 S410
K414 S415 N416 Q417 Q418 M419 L420 S426 N427 I432 D439 E440 V441 A442 V443 C444 N445 L446 A447 S448 L451 Y454 S457 Y461 K464 E468 K471 V474 R475 N476 L477 D482 I483 N484 Y485 E490 A491 C492 L493 R497 H498 R499 P500 I501 G502
I503 G504 Y505 Q506 G507 L508 F512 M515 R516 Y517 P518 E523 A524 Q525 N528 K529 F532 E533 Y537 G538 A539 L540 E541 A542 S543 C544 D545 L546 G551 P552 Y553 E554 T555 P560 V561 L566 Q567 Y568 D569 M570 V573 T574 P575 T576 K587 R594 L598
P601 M602 P603 T607 I610 L611 G612 N613 H614 E615 S616 I617 E618 P619 Y620 T621 S622 N623 I624 Y625 T626 ARG ARG VAL LEU SER GLY GLU F634 Q635 L645 W651 H652 E653 E654 M655 K656 N657 Q658 I659 I660 A661 G664 P673 D674 D675 L676 K677 Q678 L679 V683 W684
E685 I686 S687 Q688 K689 T690 V691 L692 A695 A696 E697 R698 G699 A700 F701 I702 D703 Q704 S705 Q706 S707 L708 Y717 G718 K719 M723 H724 G727 Q730 T734 G735 M736 Y737 Y738 L739 R740 T741 R742 PRO ALA ALA ASN PRO ILE GLN PHE THR LEU ASN LYS GLU LYS LEU LYS
ASP LYS GLU LYS VAL SER LYS GLU GLU GLU GLU GLU LYS GLU ARG ASN THR ALA ALA MET VAL CYS SER LEU GLU ASN ARG ASP GLU CYS LEU MET CYS GLY SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.15Å 114.37Å 222.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.07 – 3.11 44.07 – 3.11	Depositor EDS
% Data completeness (in resolution range)	88.5 (44.07-3.11) 88.5 (44.07-3.11)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.275 0.188 , 0.274	Depositor DCC
R_{free} test set	1440 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	69.4	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11380	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: SO4, TTP, MG, ATP

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	0.74	3/5696 (0.1%)	0.78	4/7749 (0.1%)
1	B	0.71	2/5767 (0.0%)	0.80	1/7840 (0.0%)
All	All	0.72	5/11463 (0.0%)	0.79	5/15589 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	615	GLU	CB-CG	6.68	1.64	1.52
1	B	218	CYS	CB-SG	-6.52	1.71	1.82
1	A	662	CYS	CB-SG	-6.20	1.71	1.82
1	A	615	GLU	CG-CD	5.86	1.60	1.51
1	B	365	GLU	CB-CG	5.49	1.62	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	449	LEU	CA-CB-CG	7.33	132.16	115.30
1	A	312	LEU	CA-CB-CG	6.74	130.81	115.30
1	A	220	LEU	CA-CB-CG	5.58	128.14	115.30
1	A	739	LEU	CA-CB-CG	5.36	127.62	115.30
1	B	221	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

There are no planarity outliers.

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	5568	0	5368	166	0
1	B	5644	0	5448	208	0
2	A	29	0	13	1	0
2	B	29	0	13	4	0
3	A	1	0	0	0	0
3	B	3	0	0	0	0
4	A	15	0	0	2	0
4	B	15	0	0	1	0
5	B	31	0	12	3	0
6	A	27	0	0	3	0
6	B	18	0	0	3	0
All	All	11380	0	10854	374	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 17.

All (374) 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:A:445:ASN:C	1:A:446:LEU:HD23	1.34	1.44
1:A:445:ASN:O	1:A:446:LEU:HD23	1.50	1.11
1:A:130:ARG:HG2	1:A:130:ARG:HH11	1.18	1.01
1:A:443:VAL:HG12	1:A:444:CYS:H	1.23	0.99
1:A:445:ASN:C	1:A:446:LEU:CD2	2.30	0.98
1:A:567:GLN:HA	1:A:567:GLN:HE21	1.27	0.95
1:B:256:ARG:HD3	2:B:805:TTP:H4'	1.49	0.95
1:B:506:GLN:HA	1:B:616:SER:HA	1.46	0.94
1:A:443:VAL:HG12	1:A:444:CYS:N	1.80	0.94
1:A:446:LEU:HD23	1:A:446:LEU:N	1.67	0.94
1:B:256:ARG:CD	2:B:805:TTP:H4'	1.97	0.94
1:B:568:TYR:HB2	1:B:573:VAL:HG12	1.54	0.87
1:A:534:THR:HG23	1:A:579:TRP:CZ2	2.13	0.84
5:B:807:ATP:H5'2	5:B:807:ATP:O1B	1.80	0.82
1:A:130:ARG:HG2	1:A:130:ARG:NH1	1.93	0.82
1:A:273:VAL:HG23	1:A:274:PRO:HD3	1.63	0.81
1:A:616:SER:OG	1:A:617:ILE:N	2.14	0.80
1:B:619:PRO:HG2	1:B:683:VAL:HG23	1.63	0.80
1:A:742:ARG:HA	1:A:742:ARG:NE	1.95	0.80
1:A:277:ARG:NH2	1:B:277:ARG:HH22	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:742:ARG:HA	1:A:742:ARG:HE	1.47	0.80
1:B:82:ALA:HA	1:B:85:ASN:OD1	1.81	0.80
1:B:337:LEU:HG	1:B:368:GLU:HG2	1.63	0.79
1:A:445:ASN:O	1:A:446:LEU:CD2	2.30	0.79
1:B:30:ASN:OD1	1:B:32:ASP:HB2	1.83	0.78
1:A:443:VAL:CG1	1:A:444:CYS:H	1.96	0.78
1:B:695:ALA:HB1	1:B:708:LEU:HD11	1.64	0.78
1:A:534:THR:HG23	1:A:579:TRP:HZ2	1.48	0.78
1:B:270:ASN:HB3	1:B:274:PRO:HG2	1.65	0.77
1:A:567:GLN:HA	1:A:567:GLN:NE2	2.00	0.77
1:A:736:MET:SD	1:A:739:LEU:HB2	2.25	0.77
1:B:482:ASP:OD2	1:B:499:ARG:NH2	2.17	0.76
1:A:414:LYS:HG2	1:A:570:MET:HB3	1.66	0.76
1:B:416:ASN:OD1	1:B:561:VAL:HG12	1.85	0.75
1:A:273:VAL:CG2	1:A:274:PRO:HD3	2.18	0.74
1:B:172:MET:O	1:B:176:VAL:HG23	1.89	0.73
1:A:310:GLU:H	1:A:310:GLU:CD	1.90	0.73
1:A:597:LEU:HA	1:A:703:ASP:OD2	1.89	0.72
1:B:482:ASP:CG	1:B:499:ARG:HH22	1.93	0.72
1:A:140:ASP:OD2	1:A:168:GLN:HG2	1.90	0.72
1:B:147:GLY:O	1:B:150:THR:HB	1.90	0.71
1:B:533:GLU:OE2	1:B:576:THR:HG23	1.90	0.71
1:A:245:ALA:HB2	1:A:288:GLN:O	1.90	0.71
1:A:306:LEU:HD13	1:A:381:ARG:HB3	1.73	0.70
1:B:71:HIS:CG	1:B:72:PRO:HD2	2.27	0.70
1:B:71:HIS:CD2	1:B:72:PRO:HD2	2.27	0.70
1:B:420:LEU:HD22	1:B:498:HIS:HE1	1.55	0.69
1:A:474:VAL:HG22	1:A:503:ILE:HD11	1.74	0.69
1:A:14:MET:HE3	1:A:15:PHE:HB3	1.73	0.69
1:B:261:TYR:CE1	1:B:263:ALA:HA	2.28	0.69
1:A:302:GLU:HG2	1:A:333:TRP:HB3	1.74	0.68
1:A:652[B]:HIS:CD2	1:A:653:GLU:H	2.11	0.68
1:B:260:SER:OG	1:B:352:CYS:SG	2.50	0.68
1:A:599:ILE:HG22	1:A:702:ILE:HG23	1.75	0.68
1:B:248:ILE:CD1	1:B:297:PHE:HE2	2.07	0.68
1:A:478:ASN:ND2	1:A:595:ASN:OD1	2.27	0.68
1:B:362:VAL:CG2	1:B:366:GLU:HB3	2.24	0.67
1:B:397:GLN:HG3	1:B:403:PRO:HD2	1.76	0.67
1:A:265:THR:O	1:A:266:ASN:HB2	1.95	0.67
1:A:270:ASN:HB2	1:A:274:PRO:HG2	1.75	0.67
1:B:284:ARG:NH2	1:B:324:ARG:HB3	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:SER:O	1:B:418:GLN:HB2	1.95	0.67
1:B:170:MET:O	1:B:174:VAL:HG23	1.95	0.67
1:B:386:ALA:HB3	6:B:933:HOH:O	1.94	0.66
1:B:475:ARG:HG2	1:B:546:LEU:HD11	1.78	0.66
1:B:374:TYR:HE2	1:B:379:ARG:NH2	1.93	0.66
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.77	0.65
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.62	0.65
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.79	0.65
1:A:26:CYS:O	1:A:27:TYR:C	2.35	0.64
1:A:298:ALA:HB2	1:A:428:LEU:HA	1.80	0.63
1:B:533:GLU:HG2	1:B:701:PHE:CZ	2.34	0.63
1:A:742:ARG:HE	1:A:742:ARG:CA	2.12	0.63
1:B:568:TYR:HB2	1:B:573:VAL:CG1	2.29	0.62
1:A:652[B]:HIS:CG	1:A:653:GLU:H	2.17	0.62
1:A:71:HIS:CE1	1:A:72:PRO:HD2	2.34	0.62
1:A:241:ILE:CG2	1:A:248:ILE:HD11	2.30	0.62
1:A:420:LEU:HD21	1:A:555:THR:HB	1.82	0.62
1:B:121:LEU:HD22	1:B:125:LEU:HD12	1.82	0.62
1:B:93:VAL:HG13	1:B:96:ASP:HB2	1.81	0.61
1:B:315:LYS:HD2	1:B:326:ARG:HG2	1.82	0.61
1:B:689:LYS:HB2	4:B:810:SO4:O3	2.01	0.61
1:A:429:CYS:HB2	1:A:431:GLU:OE2	2.01	0.60
1:B:302:GLU:HG2	1:B:333:TRP:HB3	1.84	0.60
1:A:71:HIS:ND1	1:A:72:PRO:HD2	2.17	0.60
1:B:493:LEU:HD11	1:B:497:ARG:NH1	2.17	0.60
1:B:308:ILE:O	1:B:311:PHE:HB3	2.02	0.60
1:A:446:LEU:HB3	1:A:602:MET:HE2	1.83	0.60
1:B:94:PHE:CE1	1:B:172:MET:HB3	2.37	0.59
1:B:206:PHE:HB3	1:B:207:ASN:HD22	1.67	0.59
1:B:394:ILE:HD12	1:B:395:GLU:N	2.17	0.59
1:B:89:GLU:O	1:B:90:THR:HB	2.02	0.59
1:A:474:VAL:HG21	1:A:539:ALA:HA	1.84	0.59
1:A:270:ASN:H	1:A:270:ASN:ND2	2.00	0.59
1:B:37:ALA:O	1:B:41:MET:HG2	2.03	0.59
1:A:251:ALA:HB2	1:A:425:CYS:HB3	1.85	0.59
1:B:248:ILE:HD13	1:B:297:PHE:CE2	2.39	0.58
1:A:225:ASP:HB3	1:A:230:GLY:HA3	1.85	0.58
1:A:219:PHE:N	1:A:247:GLY:O	2.35	0.58
1:A:352:CYS:HB3	1:A:381:ARG:NH2	2.18	0.58
1:A:501:ILE:HG13	1:A:598:LEU:HA	1.84	0.57
1:A:214:GLN:HG3	1:A:244:SER:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:PHE:CB	1:B:207:ASN:HD22	2.17	0.57
1:B:408:LYS:HD3	6:B:924:HOH:O	2.04	0.57
5:B:807:ATP:O1B	5:B:807:ATP:C5'	2.52	0.57
1:A:14:MET:CE	1:A:15:PHE:HB3	2.33	0.57
1:A:698:ARG:O	1:A:702:ILE:HG13	2.04	0.57
1:B:117:ALA:H	1:B:210:THR:HA	1.69	0.57
1:A:315:LYS:HZ1	1:A:326:ARG:HA	1.70	0.57
1:B:248:ILE:HD13	1:B:297:PHE:HE2	1.70	0.57
1:B:553:TYR:HB3	1:B:594:ARG:O	2.04	0.57
1:B:218:CYS:O	1:B:443:VAL:HA	2.05	0.57
1:A:426:SER:OG	1:A:427:ASN:N	2.38	0.56
1:B:346:GLN:HG3	1:B:347:ASP:H	1.69	0.56
1:A:433:VAL:H	1:A:704:GLN:HB3	1.71	0.56
1:A:18:ILE:O	1:A:22:ILE:HG12	2.06	0.56
1:A:76:ILE:O	1:A:80:ARG:HG3	2.06	0.56
1:A:222:SER:OG	1:A:436:THR:OG1	2.22	0.56
1:A:441:VAL:HG13	1:A:490:GLU:HB3	1.86	0.56
1:B:83:VAL:HG11	1:B:140:ASP:HB3	1.86	0.55
1:B:18:ILE:HB	1:B:40:THR:HG23	1.87	0.55
1:B:673:PRO:HB2	1:B:675:ASP:OD1	2.06	0.55
1:A:219:PHE:CE2	1:A:443:VAL:HG22	2.42	0.55
1:B:443:VAL:CG2	1:B:491:ALA:HB1	2.37	0.55
1:B:166:ARG:HD2	1:B:169:HIS:CE1	2.42	0.55
1:B:651:TRP:CD1	1:B:651:TRP:C	2.80	0.55
1:B:675:ASP:OD1	1:B:675:ASP:N	2.39	0.55
1:B:625:TYR:HD1	1:B:625:TYR:C	2.11	0.55
1:A:432:ILE:HG22	1:A:434:GLU:HG3	1.89	0.54
1:B:248:ILE:CD1	1:B:297:PHE:CE2	2.90	0.54
1:B:287:ASP:C	1:B:289:GLY:H	2.10	0.54
1:A:471:LYS:HA	1:A:542:ALA:HB2	1.89	0.54
1:A:308:ILE:O	1:A:312:LEU:HD22	2.07	0.54
1:B:129:ASP:OD2	1:B:129:ASP:N	2.37	0.54
1:A:627:ARG:HG2	1:A:636:ILE:HD12	1.89	0.54
1:A:652[B]:HIS:CD2	1:A:653:GLU:N	2.76	0.54
1:A:228:ILE:O	1:A:229:GLU:C	2.45	0.54
1:B:87:HIS:NE2	1:B:140:ASP:OD1	2.30	0.54
1:B:405:MET:HG3	1:B:724:HIS:CE1	2.43	0.54
1:B:443:VAL:HG12	1:B:444:CYS:N	2.22	0.54
1:B:448:SER:HA	1:B:504:GLY:O	2.07	0.54
1:A:172:MET:O	1:A:176:VAL:HG22	2.07	0.53
1:B:256:ARG:HG3	1:B:354:ASN:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ALA:HA	1:A:698:ARG:NH1	2.23	0.53
1:B:248:ILE:HD12	1:B:297:PHE:HE2	1.73	0.53
1:B:287:ASP:O	1:B:289:GLY:N	2.38	0.53
1:B:416:ASN:HA	1:B:560:PRO:HG2	1.91	0.53
1:B:79:ALA:HB2	1:B:145:TYR:N	2.23	0.53
1:A:174:VAL:HG12	1:A:178:ILE:HD12	1.91	0.53
1:A:315:LYS:NZ	1:A:326:ARG:HA	2.23	0.53
1:B:284:ARG:CZ	1:B:324:ARG:HB3	2.38	0.53
1:B:195:GLU:C	1:B:196:ARG:HG3	2.29	0.53
1:B:102:TYR:CG	1:B:121:LEU:HD12	2.44	0.53
1:A:315:LYS:NZ	1:A:328:LEU:O	2.42	0.52
1:B:624:ILE:HG22	1:B:664:GLY:HA2	1.91	0.52
1:B:727:GLY:O	1:B:730:GLN:HB2	2.08	0.52
1:A:479:LYS:HA	6:A:910:HOH:O	2.10	0.52
1:B:326:ARG:O	1:B:327:ASP:HB2	2.08	0.52
1:A:212:ARG:O	1:A:214:GLN:N	2.37	0.52
1:B:687:SER:HB3	1:B:690:THR:OG1	2.09	0.52
1:B:696:ALA:O	1:B:699:GLY:N	2.42	0.52
1:B:64:ALA:HB3	1:B:78:ALA:HB2	1.90	0.52
1:B:362:VAL:HG23	1:B:366:GLU:OE2	2.10	0.52
1:B:420:LEU:HD22	1:B:498:HIS:CE1	2.40	0.52
1:A:27:TYR:O	1:A:80:ARG:NH2	2.42	0.51
1:B:346:GLN:CG	1:B:347:ASP:H	2.23	0.51
1:B:394:ILE:HD11	1:B:717:TYR:CE1	2.45	0.51
1:A:198:PHE:CE2	1:A:473:VAL:HG22	2.45	0.51
1:B:394:ILE:HD12	1:B:394:ILE:C	2.30	0.51
1:A:382:LYS:HG2	1:A:383:VAL:N	2.26	0.51
1:A:189:THR:CG2	1:A:476:ASN:HD21	2.23	0.51
1:B:3:VAL:HG23	1:B:11:GLU:O	2.10	0.51
1:B:601:PRO:HG2	1:B:702:ILE:HD13	1.91	0.51
1:A:139:ARG:HD3	1:A:194:SER:HB2	1.91	0.51
1:B:625:TYR:C	1:B:625:TYR:CD1	2.84	0.51
1:A:310:GLU:HA	1:A:313:ASP:HB2	1.93	0.51
1:B:602:MET:HB2	1:B:603:PRO:HD2	1.93	0.51
1:A:652[B]:HIS:CG	1:A:653:GLU:N	2.77	0.50
1:B:101:LEU:O	1:B:115:MET:HB2	2.11	0.50
1:B:212:ARG:HG2	1:B:485:TYR:CZ	2.46	0.50
1:A:195:GLU:O	1:A:196:ARG:HB2	2.11	0.50
1:A:402:THR:HB	1:A:403:PRO:HA	1.92	0.50
1:A:520:GLU:HB2	1:A:690:THR:HG21	1.92	0.50
1:B:454:TYR:HB2	1:B:461:TYR:CZ	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:LYS:O	1:B:468:GLU:HG2	2.11	0.50
1:B:1:MET:HE1	1:B:47:LEU:HD12	1.93	0.50
1:B:443:VAL:HG23	1:B:491:ALA:HB1	1.93	0.50
1:A:362:VAL:CG2	1:A:366:GLU:HB2	2.42	0.50
1:B:22:ILE:HG23	1:B:77:LEU:HD21	1.94	0.50
1:B:474:VAL:HG21	1:B:539:ALA:HA	1.93	0.50
1:A:275:MET:CE	1:A:276:LEU:CD1	2.90	0.50
1:B:532:PHE:CE2	1:B:698:ARG:HD3	2.47	0.49
1:B:734:THR:HG22	1:B:736:MET:H	1.76	0.49
1:A:310:GLU:CD	1:A:310:GLU:N	2.61	0.49
1:B:735:GLY:O	1:B:736:MET:HB2	2.11	0.49
1:B:206:PHE:HB3	1:B:207:ASN:ND2	2.27	0.49
1:B:261:TYR:CE2	1:B:266:ASN:O	2.66	0.49
1:B:420:LEU:CD2	1:B:498:HIS:HE1	2.23	0.49
1:B:446:LEU:HD13	1:B:602:MET:HG3	1.94	0.49
1:B:541:GLU:O	1:B:542:ALA:C	2.49	0.49
1:A:26:CYS:O	1:A:27:TYR:O	2.30	0.49
1:B:567:GLN:CD	1:B:703:ASP:HA	2.32	0.49
1:A:242:SER:HB3	1:A:286:VAL:HG22	1.95	0.49
1:B:374:TYR:CE2	1:B:379:ARG:NH2	2.77	0.49
1:B:498:HIS:CE1	1:B:555:THR:HG21	2.48	0.49
1:A:333:TRP:CD1	1:A:408:LYS:HD2	2.48	0.49
1:A:716:ASN:O	1:A:719:LYS:N	2.46	0.49
1:A:71:HIS:CG	1:A:72:PRO:CD	2.97	0.48
1:B:441:VAL:O	1:B:491:ALA:HA	2.14	0.48
1:B:695:ALA:CB	1:B:708:LEU:HD11	2.39	0.48
1:A:482:ASP:OD1	1:A:499:ARG:NH2	2.47	0.48
1:A:102:TYR:CG	1:A:121:LEU:HD12	2.48	0.48
1:B:220:LEU:N	1:B:220:LEU:HD23	2.29	0.48
1:B:94:PHE:HB2	1:B:135:ILE:CD1	2.44	0.48
1:A:219:PHE:HB2	1:A:247:GLY:O	2.14	0.48
1:B:171:LEU:HA	1:B:171:LEU:HD12	1.62	0.48
1:B:277:ARG:O	1:B:281:ASN:HB2	2.14	0.48
1:B:443:VAL:CG1	1:B:444:CYS:N	2.77	0.48
1:A:220:LEU:HG	1:A:442:ALA:HB3	1.95	0.48
1:A:457:SER:C	1:A:459:HIS:H	2.17	0.48
1:B:4:ILE:O	1:B:53:THR:HG23	2.14	0.48
1:A:431:GLU:HG2	1:A:432:ILE:CD1	2.44	0.47
1:A:692:LEU:CD1	1:A:710:ILE:HD11	2.44	0.47
1:B:300:TYR:CE2	1:B:406:LEU:HD13	2.46	0.47
1:A:202:SER:OG	4:A:812:SO4:O4	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ILE:CG2	1:A:434:GLU:HG3	2.44	0.47
1:B:652:HIS:CG	1:B:653:GLU:H	2.32	0.47
1:A:330:PHE:N	1:A:330:PHE:CD2	2.83	0.47
1:B:448:SER:HB2	1:B:506:GLN:HG2	1.97	0.47
1:B:544:CYS:SG	1:B:587:LYS:HG2	2.54	0.47
1:B:237:GLN:O	1:B:241:ILE:HG13	2.14	0.47
1:B:518:PRO:HB3	1:B:678:GLN:O	2.15	0.47
1:A:183:ILE:O	1:A:184:ASP:C	2.52	0.47
1:A:411:CYS:HA	1:A:733:LYS:HG2	1.95	0.47
1:B:27:TYR:HE1	1:B:80:ARG:NH1	2.13	0.47
1:B:273:VAL:HG21	1:B:310:GLU:HB3	1.97	0.47
1:A:427:ASN:HB2	6:A:903:HOH:O	2.14	0.47
1:A:443:VAL:CG1	1:A:444:CYS:N	2.52	0.47
1:B:130:ARG:NH1	1:B:187:ILE:HD13	2.29	0.47
1:B:5:LYS:HE2	1:B:11:GLU:CD	2.34	0.47
1:A:275:MET:HE1	1:A:276:LEU:CD1	2.44	0.47
1:B:257:ALA:HB1	1:B:306:LEU:HD23	1.97	0.46
1:B:137:TYR:HE2	1:B:169:HIS:NE2	2.13	0.46
1:B:610:ILE:HG22	1:B:611:LEU:HD23	1.96	0.46
1:A:202:SER:HB3	1:A:206:PHE:CE1	2.51	0.46
1:A:198:PHE:CD2	1:A:473:VAL:HG22	2.51	0.46
1:B:542:ALA:O	1:B:546:LEU:HD12	2.16	0.46
1:B:695:ALA:O	1:B:706:GLN:NE2	2.49	0.46
1:A:192:LEU:HD23	1:A:469:VAL:HG13	1.96	0.45
1:B:49:SER:O	1:B:51:VAL:N	2.49	0.45
1:B:94:PHE:HB2	1:B:135:ILE:HD13	1.98	0.45
1:B:261:TYR:HE2	1:B:266:ASN:O	1.98	0.45
1:B:79:ALA:O	1:B:83:VAL:HG23	2.16	0.45
1:B:199:THR:HG21	1:B:607:THR:HB	1.97	0.45
1:B:420:LEU:CD2	1:B:498:HIS:CE1	3.00	0.45
1:B:508:LEU:HD13	1:B:512:PHE:CE2	2.51	0.45
1:A:667:GLN:O	1:A:677:LYS:HE2	2.17	0.45
1:B:21:ARG:HD2	1:B:21:ARG:O	2.16	0.45
1:B:220:LEU:HD22	1:B:427:ASN:HB3	1.97	0.45
1:B:315:LYS:NZ	1:B:326:ARG:HB3	2.32	0.45
1:B:408:LYS:HE3	6:B:926:HOH:O	2.15	0.45
1:B:218:CYS:SG	1:B:432:ILE:HG13	2.56	0.45
1:A:158:LYS:HD3	1:A:163:VAL:HG23	1.98	0.45
1:A:681:LYS:HB2	1:A:686:ILE:HD11	1.99	0.45
1:A:71:HIS:ND1	1:A:72:PRO:CD	2.80	0.45
1:A:26:CYS:C	1:A:27:TYR:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:SER:OG	1:B:664:GLY:HA3	2.15	0.45
1:B:250:VAL:N	1:B:298:ALA:O	2.47	0.45
1:A:281:ASN:HD22	1:A:281:ASN:HA	1.52	0.44
1:B:202:SER:O	1:B:203:PRO:C	2.56	0.44
1:A:665:SER:OG	1:A:667:GLN:HG2	2.17	0.44
1:B:22:ILE:CG2	1:B:77:LEU:HD21	2.48	0.44
1:B:652:HIS:CD2	1:B:653:GLU:H	2.36	0.44
1:B:493:LEU:CD1	1:B:497:ARG:NH1	2.80	0.44
1:A:215:LEU:HD11	1:A:483:ILE:HD11	1.99	0.44
1:A:519:PHE:CE2	1:A:619:PRO:HG3	2.53	0.44
1:A:602:MET:SD	1:A:602:MET:N	2.89	0.44
1:B:207:ASN:O	1:B:210:THR:OG1	2.28	0.44
1:A:275:MET:CE	1:A:276:LEU:HD12	2.48	0.44
1:A:363:TRP:CH2	1:A:413:ARG:HA	2.53	0.44
1:B:2:HIS:ND1	1:B:10:GLN:HG2	2.33	0.44
1:B:451:LEU:CD1	1:B:508:LEU:HD23	2.48	0.44
1:B:214:GLN:HG3	1:B:244:SER:HB3	2.00	0.44
1:B:312:LEU:HD21	1:B:393:ILE:HG12	1.99	0.44
1:B:501:ILE:HG13	1:B:598:LEU:HA	1.99	0.44
1:A:742:ARG:NE	1:A:742:ARG:CA	2.71	0.43
1:B:451:LEU:HD13	1:B:508:LEU:HD23	2.00	0.43
1:B:120:THR:O	1:B:124:VAL:HG23	2.18	0.43
1:A:404:TYR:CZ	1:A:737:TYR:HE1	2.37	0.43
1:A:308:ILE:O	1:A:311:PHE:HB3	2.18	0.43
1:B:136:ILE:HB	1:B:139:ARG:HG3	2.00	0.43
1:B:708:LEU:O	1:B:737:TYR:HB3	2.18	0.43
1:A:216:SER:HB3	1:A:443:VAL:CG1	2.48	0.43
1:B:226:ASP:OD1	1:B:256:ARG:HD2	2.18	0.43
1:A:337:LEU:HD22	1:A:337:LEU:HA	1.74	0.43
1:B:346:GLN:HG3	1:B:347:ASP:N	2.33	0.43
1:B:653:GLU:O	1:B:655:MET:N	2.51	0.43
1:A:252:VAL:HG12	1:A:300:TYR:O	2.18	0.43
1:B:283:ALA:HB2	1:B:297:PHE:CD1	2.54	0.43
1:B:362:VAL:HG23	1:B:366:GLU:HB3	1.98	0.43
1:B:523:GLU:OE2	1:B:523:GLU:N	2.31	0.42
1:A:216:SER:CB	1:A:443:VAL:CG1	2.96	0.42
1:A:690:THR:O	1:A:691:VAL:C	2.57	0.42
1:A:265:THR:CG2	1:B:288:GLN:HG2	2.50	0.42
1:A:256:ARG:HA	1:A:353:PRO:HD2	2.01	0.42
1:A:263:ALA:HB3	2:A:806:TTP:O1G	2.20	0.42
1:B:256:ARG:HH21	1:B:262:ILE:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:HG22	1:B:13:VAL:HG22	2.01	0.42
1:B:23:GLN:HE22	1:B:31:MET:HE2	1.85	0.42
1:B:551:GLY:O	1:B:594:ARG:NH1	2.50	0.42
1:A:20:SER:O	1:A:23:GLN:HB3	2.19	0.42
1:A:54:VAL:HG13	1:A:55:GLU:HG3	2.00	0.42
1:A:106:ASN:HD21	1:A:109:ASN:H	1.67	0.42
1:A:265:THR:HG21	1:B:288:GLN:HG2	2.01	0.42
1:A:414:LYS:HD2	1:A:571:TRP:NE1	2.35	0.42
1:B:256:ARG:HD2	2:B:805:TTP:H4'	1.91	0.42
1:B:483:ILE:HD12	1:B:483:ILE:HA	1.92	0.42
1:B:611:LEU:HB2	1:B:613:ASN:HD22	1.85	0.42
1:A:307:ASP:C	1:A:310:GLU:OE1	2.57	0.42
1:A:627:ARG:CG	1:A:636:ILE:HD12	2.49	0.42
1:B:112:HIS:CE1	1:B:114:PRO:HG3	2.55	0.42
1:B:515:MET:O	1:B:516:ARG:HB2	2.18	0.42
1:B:83:VAL:CG1	1:B:140:ASP:HB3	2.48	0.42
1:A:241:ILE:HG22	1:A:248:ILE:HD11	2.01	0.42
1:B:414:LYS:HG2	1:B:570:MET:HB2	2.01	0.42
1:B:441:VAL:HG12	1:B:490:GLU:HB2	2.02	0.42
1:A:71:HIS:CG	1:A:72:PRO:HD2	2.55	0.41
1:B:516:ARG:HH21	1:B:679:LEU:CD1	2.33	0.41
1:B:645:LEU:HD23	1:B:645:LEU:HA	1.87	0.41
1:A:106:ASN:ND2	1:A:109:ASN:H	2.18	0.41
1:B:219:PHE:CE2	1:B:443:VAL:HG22	2.55	0.41
1:B:222:SER:HA	1:B:251:ALA:HB3	2.02	0.41
1:B:308:ILE:HG13	1:B:312:LEU:HD13	2.02	0.41
1:B:445:ASN:N	1:B:445:ASN:ND2	2.68	0.41
1:B:626:THR:HG22	1:B:635:GLN:HA	2.01	0.41
1:A:446:LEU:CD2	1:A:446:LEU:N	2.43	0.41
1:B:67:LEU:O	1:B:70:LYS:N	2.52	0.41
1:A:330:PHE:N	1:A:330:PHE:HD2	2.19	0.41
1:B:38:GLN:NE2	1:B:38:GLN:HA	2.35	0.41
1:B:300:TYR:HE2	1:B:406:LEU:CD1	2.30	0.41
5:B:807:ATP:H5'2	5:B:807:ATP:PB	2.60	0.41
1:A:451:LEU:HG	1:A:505:VAL:HB	2.02	0.41
1:A:689:LYS:HB2	4:A:809:SO4:O1	2.21	0.41
1:B:330:PHE:N	1:B:330:PHE:CD2	2.88	0.41
1:B:528:ASN:O	1:B:529:LYS:C	2.59	0.41
1:B:566:LEU:O	1:B:567:GLN:C	2.58	0.41
1:A:171:LEU:HD23	1:A:194:SER:HA	2.03	0.41
1:B:272:LEU:HD23	1:B:272:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:ND2	1:A:270:ASN:N	2.67	0.41
1:A:520:GLU:HG2	6:A:914:HOH:O	2.21	0.41
1:A:603:PRO:O	1:A:604:THR:C	2.59	0.41
1:A:692:LEU:HD13	1:A:710:ILE:HD11	2.03	0.41
1:B:12:ARG:HH21	1:B:14:MET:CE	2.34	0.41
1:B:253:SER:OG	1:B:301:LEU:HD23	2.21	0.41
1:B:705:SER:OG	1:B:706:GLN:N	2.54	0.41
1:B:128:LYS:O	1:B:132:ASN:ND2	2.49	0.41
1:B:471:LYS:HA	1:B:542:ALA:HB2	2.02	0.41
1:A:104:TYR:HD2	1:A:113:SER:HB2	1.86	0.40
1:A:192:LEU:HD22	1:A:472:VAL:HG11	2.03	0.40
1:A:448:SER:HB2	1:A:506:GLN:HG2	2.03	0.40
1:A:725:PHE:O	1:A:729:LYS:HB2	2.21	0.40
1:B:365:GLU:H	1:B:365:GLU:HG2	1.43	0.40
1:A:301:LEU:HD12	1:A:311:PHE:CG	2.56	0.40
1:B:151:LEU:HD23	1:B:155:TYR:HB2	2.03	0.40
1:B:337:LEU:HD23	1:B:337:LEU:HA	1.95	0.40
1:A:215:LEU:CD1	1:A:483:ILE:HD11	2.51	0.40
1:A:275:MET:HE2	1:A:276:LEU:CD1	2.51	0.40
1:A:695:ALA:CB	1:A:708:LEU:HD11	2.51	0.40
1:A:727:GLY:CA	1:A:732:LEU:HD12	2.51	0.40
1:B:533:GLU:HG2	1:B:701:PHE:CE1	2.55	0.40
1:A:243:LYS:NZ	2:B:805:TTP:O1B	2.52	0.40
1:B:93:VAL:HG23	1:B:132:ASN:OD1	2.22	0.40
1:A:448:SER:HA	1:A:504:GLY:O	2.22	0.40
1:B:477:LEU:HD23	1:B:477:LEU:HA	1.86	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	710/792 (90%)	636 (90%)	61 (9%)	13 (2%)	8	33
1	B	716/792 (90%)	616 (86%)	82 (12%)	18 (2%)	5	26
All	All	1426/1584 (90%)	1252 (88%)	143 (10%)	31 (2%)	6	28

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	ASP
1	B	130	ARG
1	B	288	GLN
1	B	316	LYS
1	B	327	ASP
1	B	653	GLU
1	B	654	GLU
1	A	245	ALA
1	A	444	CYS
1	A	458	GLU
1	A	605	ALA
1	A	616	SER
1	A	713	ALA
1	A	737	TYR
1	B	50	GLY
1	B	484	ASN
1	B	736	MET
1	B	128	LYS
1	B	258	THR
1	B	313	ASP
1	B	576	THR
1	B	661	ALA
1	B	737	TYR
1	A	112	HIS
1	A	196	ARG
1	B	537	TYR
1	A	49	SER
1	A	265	THR
1	B	303	PRO
1	B	245	ALA
1	A	212	ARG

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	586/693 (85%)	523 (89%)	63 (11%)	6 25
1	B	593/693 (86%)	492 (83%)	101 (17%)	2 9
All	All	1179/1386 (85%)	1015 (86%)	164 (14%)	3 15

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	PHE
1	A	19	THR
1	A	27	TYR
1	A	41	MET
1	A	53	THR
1	A	54	VAL
1	A	55	GLU
1	A	58	THR
1	A	59	LEU
1	A	69	THR
1	A	84	SER
1	A	93	VAL
1	A	106	ASN
1	A	119	SER
1	A	121	LEU
1	A	130	ARG
1	A	149	LYS
1	A	154	SER
1	A	171	LEU
1	A	176	VAL
1	A	214	GLN
1	A	217	SER
1	A	220	LEU
1	A	222	SER
1	A	242	SER
1	A	250	VAL
1	A	252	VAL

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Mol	Chain	Res	Type
1	A	265	THR
1	A	270	ASN
1	A	276	LEU
1	A	281	ASN
1	A	286	VAL
1	A	287	ASP
1	A	301	LEU
1	A	312	LEU
1	A	315	LYS
1	A	337	LEU
1	A	361	GLU
1	A	389	LEU
1	A	441	VAL
1	A	445	ASN
1	A	449	LEU
1	A	455	VAL
1	A	493	LEU
1	A	499	ARG
1	A	508	LEU
1	A	567	GLN
1	A	615	GLU
1	A	621	THR
1	A	637	VAL
1	A	653	GLU
1	A	689	LYS
1	A	692	LEU
1	A	693	LYS
1	A	697	GLU
1	A	703	ASP
1	A	705	SER
1	A	712	ILE
1	A	716	ASN
1	A	720	LEU
1	A	722	SER
1	A	739	LEU
1	A	742	ARG
1	B	3	VAL
1	B	5	LYS
1	B	12	ARG
1	B	14	MET
1	B	16	ASP
1	B	21	ARG

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Mol	Chain	Res	Type
1	B	25	LEU
1	B	27	TYR
1	B	32	ASP
1	B	38	GLN
1	B	40	THR
1	B	47	LEU
1	B	49	SER
1	B	54	VAL
1	B	55	GLU
1	B	56	LEU
1	B	67	LEU
1	B	85	ASN
1	B	92	LYS
1	B	93	VAL
1	B	109	ASN
1	B	121	LEU
1	B	125	LEU
1	B	127	ASN
1	B	129	ASP
1	B	138	ASP
1	B	149	LYS
1	B	153	ARG
1	B	154	SER
1	B	159	ILE
1	B	162	LYS
1	B	171	LEU
1	B	175	SER
1	B	188	GLU
1	B	196	ARG
1	B	214	GLN
1	B	216	SER
1	B	218	CYS
1	B	220	LEU
1	B	229	GLU
1	B	234	THR
1	B	237	GLN
1	B	241	ILE
1	B	252	VAL
1	B	256	ARG
1	B	265	THR
1	B	272	LEU
1	B	276	LEU

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Mol	Chain	Res	Type
1	B	277	ARG
1	B	286	VAL
1	B	301	LEU
1	B	313	ASP
1	B	314	LEU
1	B	324	ARG
1	B	326	ARG
1	B	337	LEU
1	B	352	CYS
1	B	359	LEU
1	B	365	GLU
1	B	366	GLU
1	B	383	VAL
1	B	389	LEU
1	B	410	SER
1	B	420	LEU
1	B	426	SER
1	B	439	ASP
1	B	441	VAL
1	B	445	ASN
1	B	457	SER
1	B	503	ILE
1	B	506	GLN
1	B	508	LEU
1	B	525	GLN
1	B	541	GLU
1	B	546	LEU
1	B	570	MET
1	B	573	VAL
1	B	575	PRO
1	B	587	LYS
1	B	602	MET
1	B	615	GLU
1	B	618	GLU
1	B	620	TYR
1	B	625	TYR
1	B	626	THR
1	B	655	MET
1	B	657	ASN
1	B	675	ASP
1	B	678	GLN
1	B	683	VAL

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Mol	Chain	Res	Type
1	B	685	GLU
1	B	690	THR
1	B	692	LEU
1	B	697	GLU
1	B	707	SER
1	B	708	LEU
1	B	719	LYS
1	B	723	MET
1	B	739	LEU
1	B	740	ARG
1	B	742	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	106	ASN
1	A	200	HIS
1	A	211	ASN
1	A	270	ASN
1	A	281	ASN
1	A	387	GLN
1	A	388	GLN
1	A	476	ASN
1	A	478	ASN
1	A	567	GLN
1	A	595	ASN
1	A	716	ASN
1	B	23	GLN
1	B	38	GLN
1	B	109	ASN
1	B	207	ASN
1	B	214	GLN
1	B	281	ASN
1	B	445	ASN
1	B	459	HIS
1	B	525	GLN
1	B	652	HIS
1	B	711	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 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
4	SO4	B	810	-	4,4,4	0.21	0	6,6,6	0.34	0
4	SO4	B	811	-	4,4,4	0.18	0	6,6,6	0.53	0
2	TTP	B	805	3	26,30,30	1.35	5 (19%)	39,47,47	1.88	9 (23%)
4	SO4	A	808	-	4,4,4	0.18	0	6,6,6	0.40	0
2	TTP	A	806	3	26,30,30	1.36	6 (23%)	39,47,47	2.08	9 (23%)
5	ATP	B	807	3	26,33,33	1.30	2 (7%)	31,52,52	1.79	8 (25%)
4	SO4	B	813	-	4,4,4	0.17	0	6,6,6	0.57	0
4	SO4	A	812	-	4,4,4	0.14	0	6,6,6	0.47	0
4	SO4	A	809	-	4,4,4	0.13	0	6,6,6	0.28	0

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
5	ATP	B	807	3	-	4/18/38/38	0/3/3/3
2	TTP	A	806	3	-	11/22/34/34	0/2/2/2
2	TTP	B	805	3	-	1/22/34/34	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	807	ATP	O4'-C1'	4.57	1.47	1.41
2	A	806	TTP	C4-C5	2.93	1.49	1.44
2	A	806	TTP	C4-N3	-2.89	1.33	1.38
2	B	805	TTP	C6-C5	2.84	1.39	1.34
2	B	805	TTP	C4-C5	2.78	1.49	1.44
5	B	807	ATP	C5-C4	2.60	1.47	1.40
2	B	805	TTP	C6-N1	-2.54	1.33	1.38
2	B	805	TTP	C4-N3	-2.50	1.34	1.38
2	A	806	TTP	C2-N1	2.49	1.42	1.38
2	A	806	TTP	C6-N1	-2.37	1.34	1.38
2	A	806	TTP	C2-N3	-2.22	1.34	1.38
2	B	805	TTP	C2-N3	-2.12	1.34	1.38
2	A	806	TTP	C6-C5	2.00	1.37	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	806	TTP	C4-N3-C2	-5.43	120.32	127.35
2	A	806	TTP	C5-C6-N1	-5.42	117.76	123.34
2	B	805	TTP	C4-N3-C2	-4.73	121.22	127.35
2	A	806	TTP	N3-C2-N1	4.65	121.06	114.89
2	B	805	TTP	C5-C6-N1	-4.45	118.76	123.34
5	B	807	ATP	PA-O3A-PB	-4.42	117.67	132.83
2	A	806	TTP	C5-C4-N3	4.25	118.94	115.31
2	B	805	TTP	C5-C4-N3	4.18	118.88	115.31
2	B	805	TTP	N3-C2-N1	4.08	120.30	114.89
2	A	806	TTP	PB-O3A-PA	-4.05	118.92	132.83
2	A	806	TTP	PB-O3B-PG	-3.62	120.41	132.83
2	B	805	TTP	PB-O3A-PA	-3.61	120.43	132.83
5	B	807	ATP	C4-C5-N7	-3.61	105.64	109.40
5	B	807	ATP	O4'-C4'-C5'	3.02	119.31	109.37
2	B	805	TTP	PB-O3B-PG	-2.99	122.57	132.83
2	B	805	TTP	O4-C4-C5	-2.78	121.67	124.90
2	A	806	TTP	C5M-C5-C6	-2.62	119.35	122.85
2	A	806	TTP	O4-C4-C5	-2.59	121.90	124.90
5	B	807	ATP	O3G-PG-O2G	2.57	117.47	107.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	807	ATP	O3G-PG-O1G	2.49	120.45	110.68
5	B	807	ATP	N3-C2-N1	-2.44	124.86	128.68
2	B	805	TTP	C5M-C5-C4	2.36	121.37	118.77
2	A	806	TTP	C6-C5-C4	2.12	119.81	118.03
5	B	807	ATP	C5-C6-N6	2.08	123.52	120.35
2	B	805	TTP	C5M-C5-C6	-2.02	120.15	122.85
5	B	807	ATP	O4'-C4'-C3'	-2.01	101.13	105.11

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	806	TTP	C5'-O5'-PA-O1A
2	A	806	TTP	C5'-O5'-PA-O2A
5	B	807	ATP	C5'-O5'-PA-O1A
5	B	807	ATP	C5'-O5'-PA-O2A
5	B	807	ATP	C5'-O5'-PA-O3A
2	A	806	TTP	O4'-C4'-C5'-O5'
2	A	806	TTP	C3'-C4'-C5'-O5'
2	A	806	TTP	PB-O3B-PG-O3G
2	B	805	TTP	PA-O3A-PB-O2B
5	B	807	ATP	C4'-C5'-O5'-PA
2	A	806	TTP	PA-O3A-PB-O2B
2	A	806	TTP	PA-O3A-PB-O1B
2	A	806	TTP	PG-O3B-PB-O1B
2	A	806	TTP	PB-O3B-PG-O2G
2	A	806	TTP	C5'-O5'-PA-O3A
2	A	806	TTP	PG-O3B-PB-O2B

There are no ring outliers.

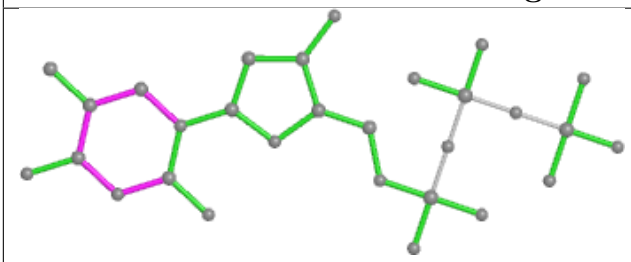
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	810	SO4	1	0
2	B	805	TTP	4	0
2	A	806	TTP	1	0
5	B	807	ATP	3	0
4	A	812	SO4	1	0
4	A	809	SO4	1	0

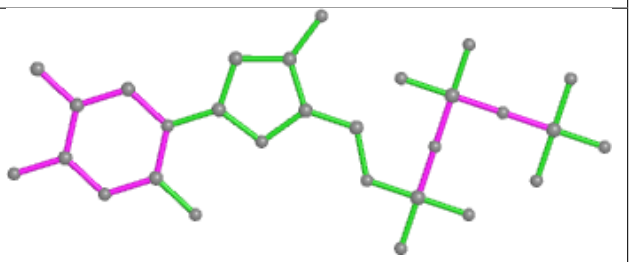
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

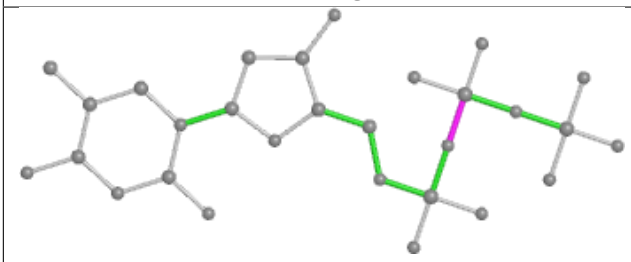
Ligand TTP B 805



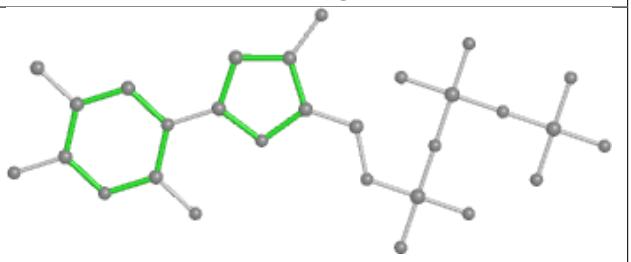
Bond lengths



Bond angles

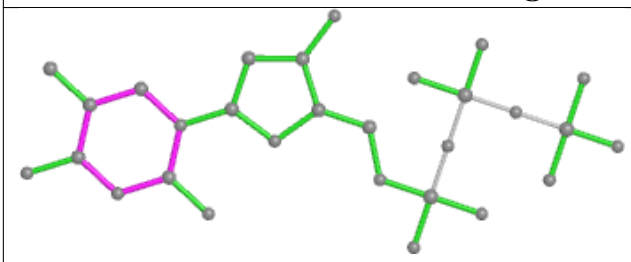


Torsions

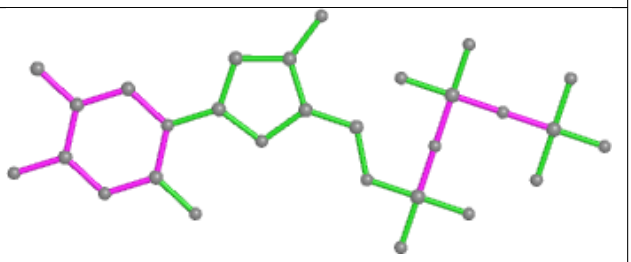


Rings

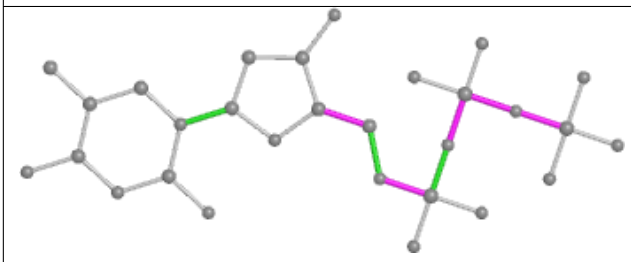
Ligand TTP A 806



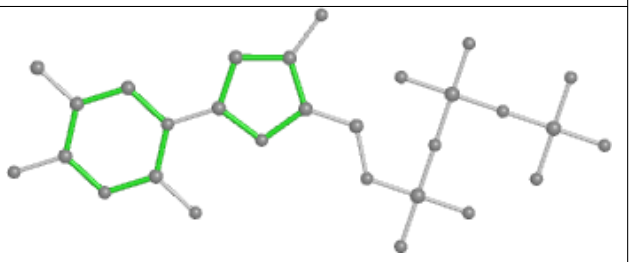
Bond lengths



Bond angles

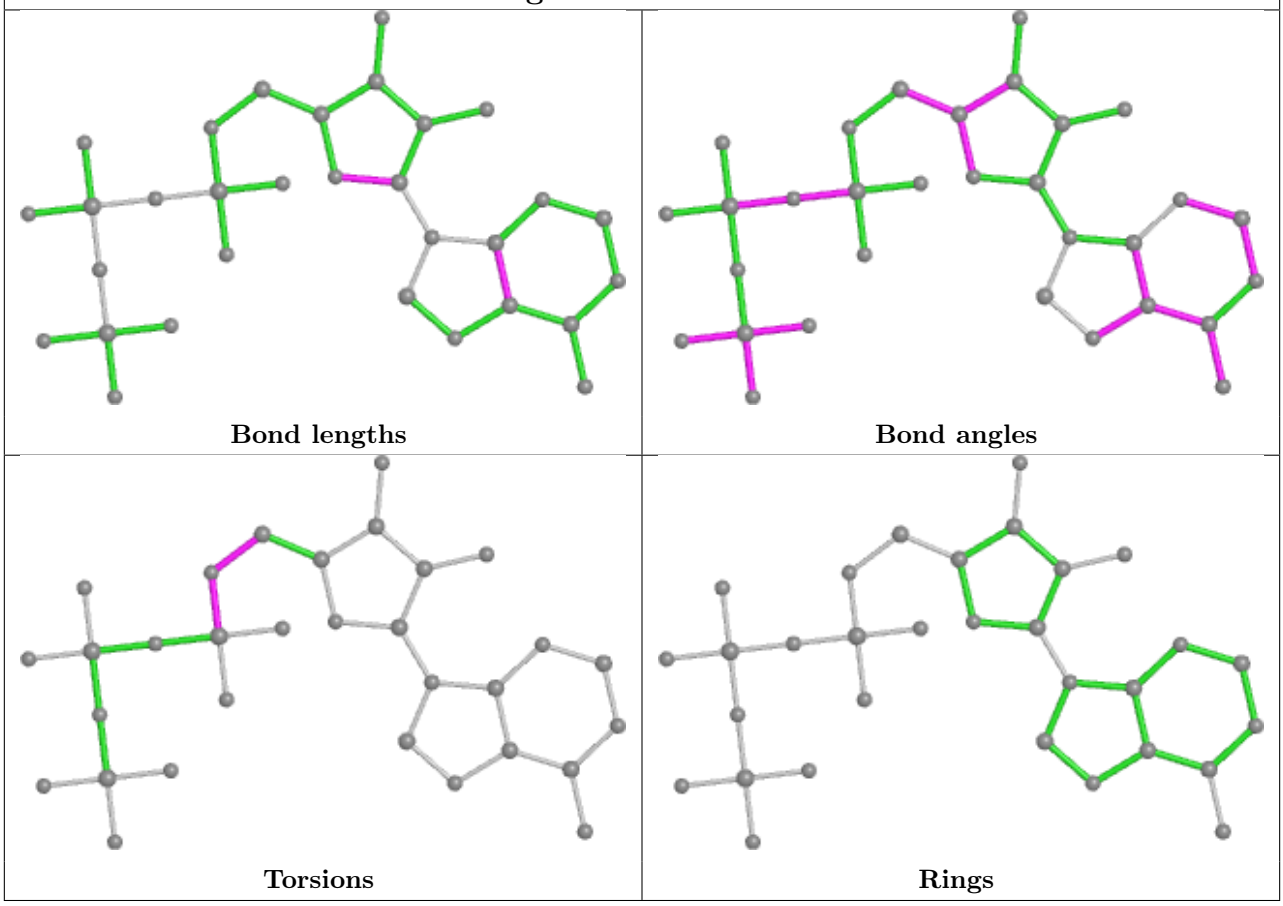


Torsions



Rings

Ligand ATP B 807



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	715/792 (90%)	-0.47	2 (0%)	94	89	46, 61, 81, 110	2 (0%)
1	B	724/792 (91%)	-0.42	5 (0%)	87	77	46, 65, 94, 126	0
All	All	1439/1584 (90%)	-0.45	7 (0%)	91	82	46, 63, 90, 126	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	6.4
1	A	218	CYS	6.1
1	B	107	PRO	2.5
1	B	676	LEU	2.2
1	B	659	ILE	2.2
1	B	33	PHE	2.1
1	B	108	HIS	2.1

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)

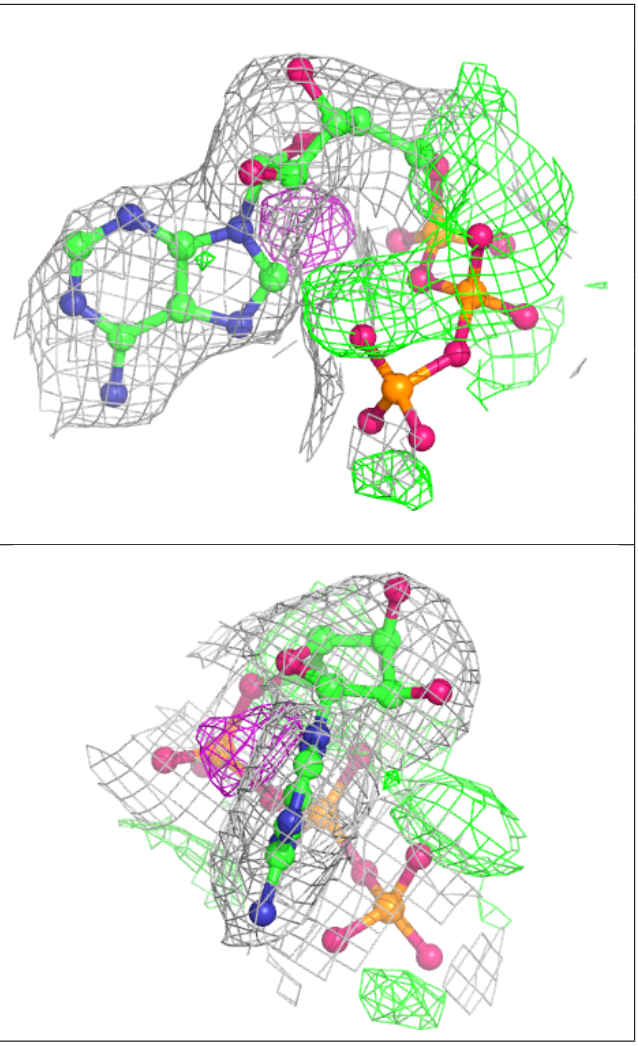
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	809	5/5	0.89	0.13	127,127,127,127	0
5	ATP	B	807	31/31	0.91	0.15	65,69,76,76	0
3	MG	B	804	1/1	0.92	0.12	47,47,47,47	0
4	SO4	B	813	5/5	0.93	0.27	70,70,72,72	0
4	SO4	B	811	5/5	0.94	0.13	99,100,100,100	0
4	SO4	A	808	5/5	0.94	0.16	86,87,87,87	0
3	MG	B	803	1/1	0.94	0.19	42,42,42,42	0
3	MG	B	802	1/1	0.95	0.10	62,62,62,62	0
4	SO4	A	812	5/5	0.96	0.21	83,83,85,86	0
2	TTP	A	806	29/29	0.96	0.14	59,63,74,75	0
4	SO4	B	810	5/5	0.97	0.13	79,79,80,81	0
2	TTP	B	805	29/29	0.97	0.13	72,75,83,85	0
3	MG	A	801	1/1	0.98	0.20	56,56,56,56	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.

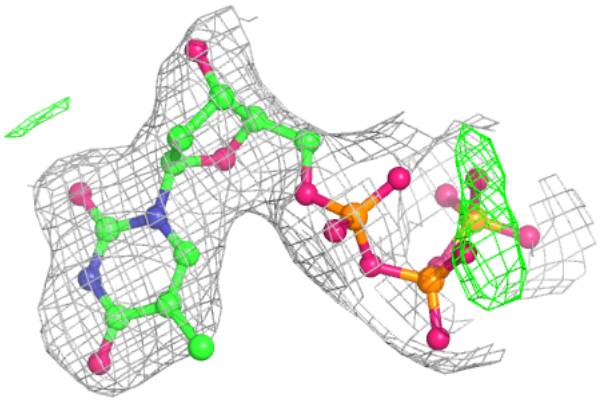
Electron density around ATP B 807:

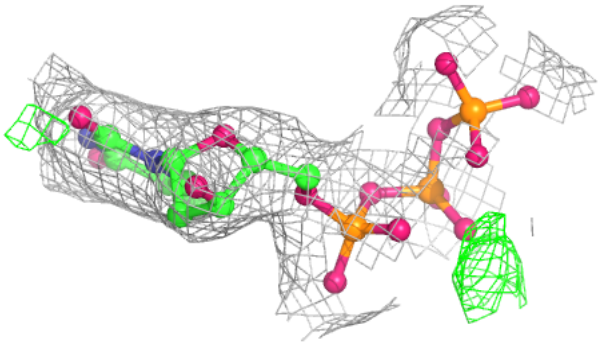
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

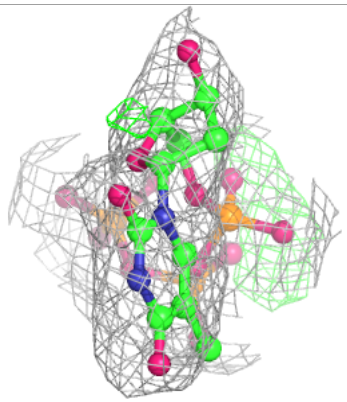


Electron density around TTP A 806:

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

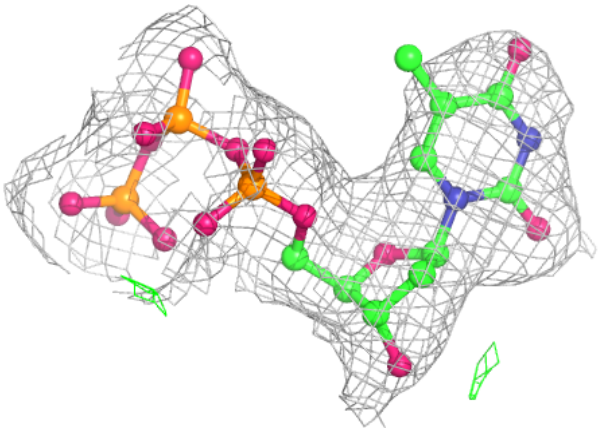


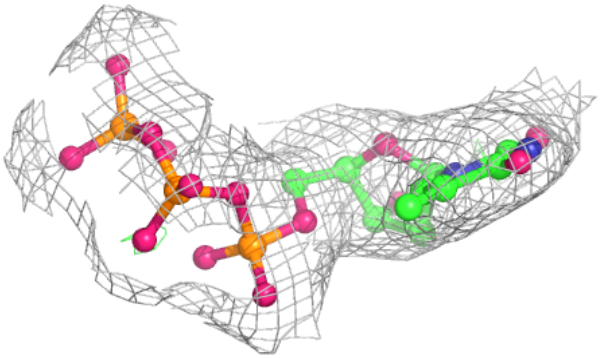


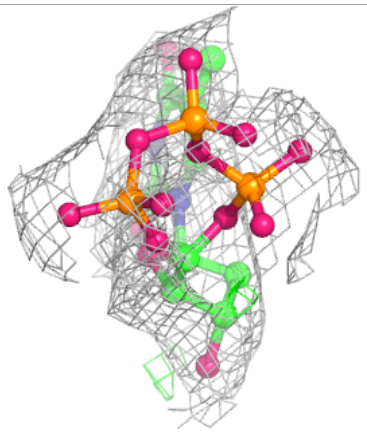


Electron density around TTP B 805:

$2mF_o$-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.