



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 09:11 am BST

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](mailto: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.

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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

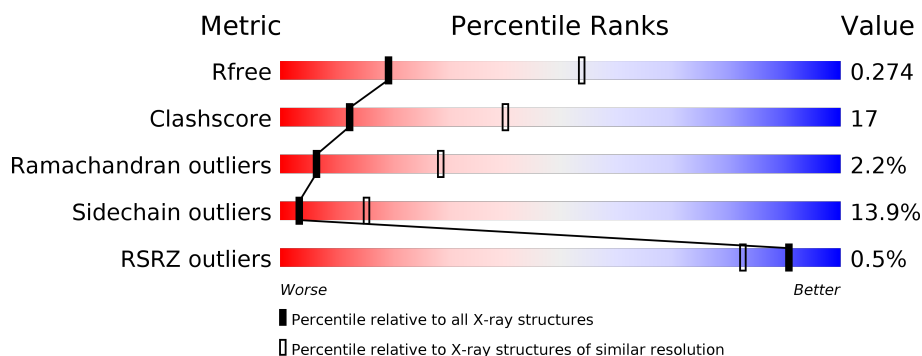
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	792	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>61%</span> <span>24%</span> <span>5% • 10%</span> </div> </div>
1	B	792	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>51%</span> <span>33%</span> <span>8% 9%</span> </div> </div>

## 2 Entry composition [i](#)

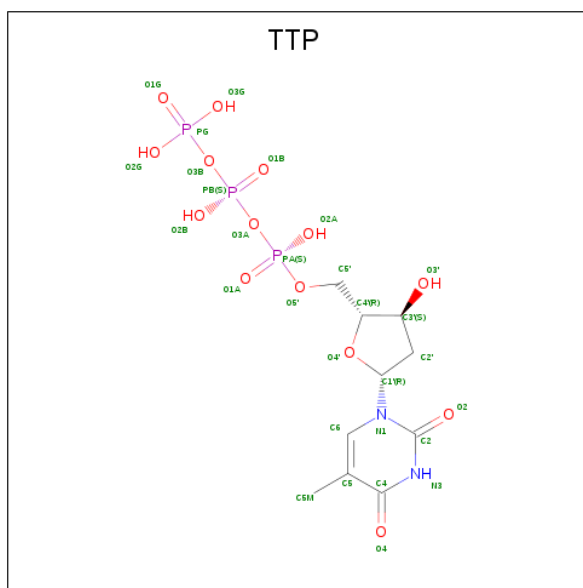
There are 6 unique types of molecules in this entry. The entry contains 11380 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
1	A	715	Total	C	N	O	S	6	1	0
			5568	3557	927	1051	33			
1	B	724	Total	C	N	O	S	0	0	0
			5644	3593	955	1062	34			

- 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
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>13</sub>P<sub>3</sub>).



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

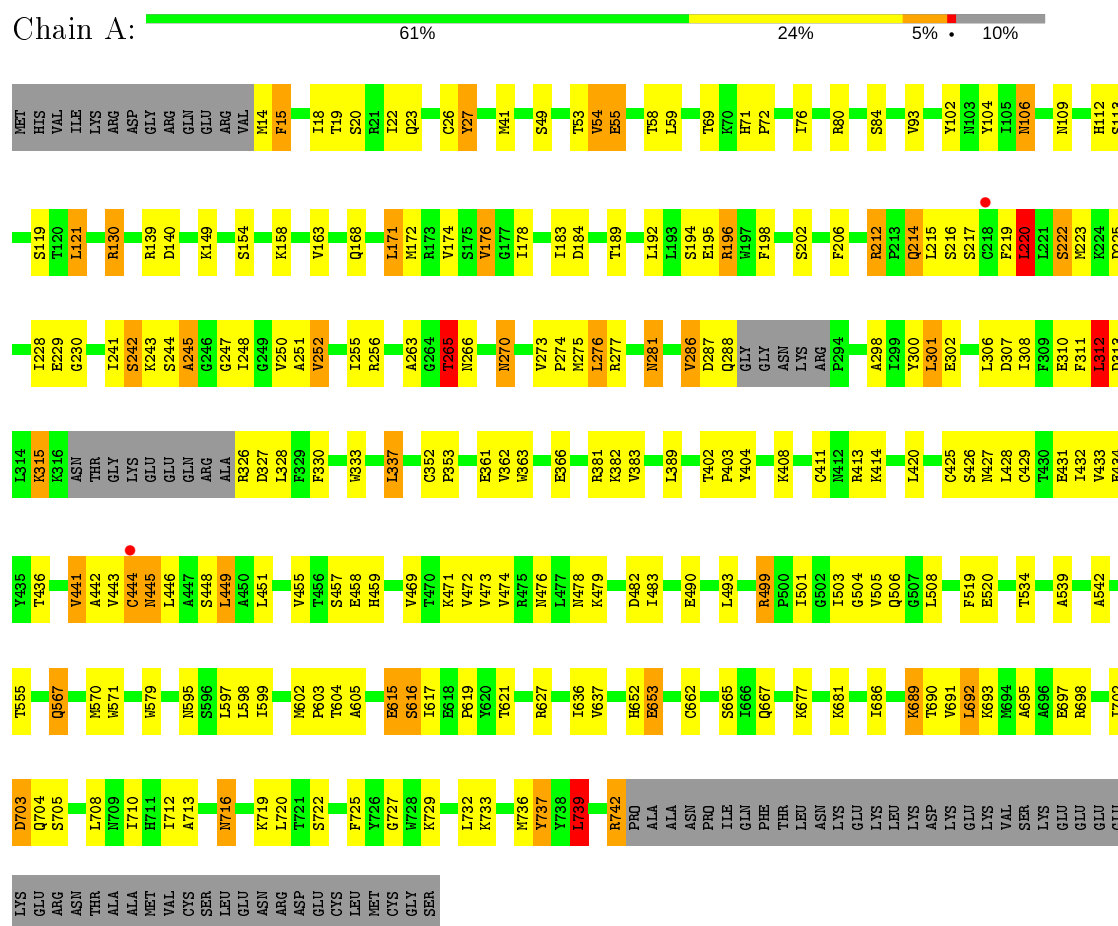
- Molecule 6 is water.

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

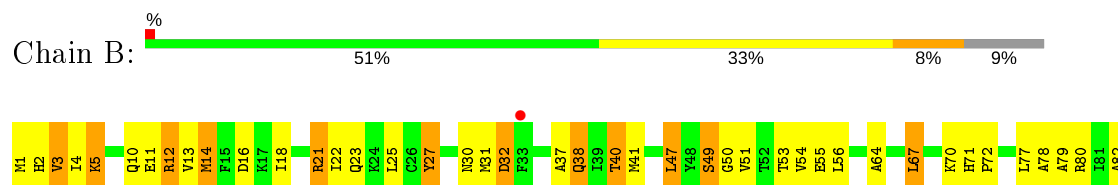
### 3 Residue-property plots

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: Ribonucleoside-diphosphate reductase large subunit



- Molecule 1: Ribonucleoside-diphosphate reductase large subunit



ASP	E685	E686	P601	I503	K315	V250	I189	V83
LYS	Q687	Q688	P602	G504	K316	A251	I189	S84
LYS	Q688	Q688	P603	Q505	THR	V252	I189	N85
VAL	K689	K689	P603	Q506	GLY	S253	K162	L86
SER	T690	T690	T607	L508	LYS	C254	R166	H87
LYS	V691	V691	T607	L508	GLY	I255	R166	K88
GLU	L692	L692	T610	F512	GLU	R256	E89	E89
GLU	L611	L611	T610	F512	GLN	A257	T90	T90
GLU	A695	A695	G612	M515	GLN	T258	H169	H169
GLU	A696	A696	G612	M515	R324	G259	M170	M170
LYS	A697	A697	G613	R516	A325	S260	L171	L171
GLU	R698	R698	G614	R517	R326	Y261	M172	M172
GLU	R698	R698	G615	P518	D327	I262	H173	H173
ARG	G699	G699	S616	P518	D327	A263	S175	S95
ASN	A700	A700	I617	E523	F330	G264	V176	D96
THR	F701	F701	E618	A524	GLU	T265	V176	L101
ALA	I702	I702	P619	Q525	GLU	N266	I187	Y102
ALA	D703	D703	Y620	Q525	GLU	N266	E188	Y102
MET	Q704	Q704	T621	M528	L337	N270	E188	P107
VAL	S705	S705	S622	K529	Q346	G271	E188	H108
CYS	Q706	Q706	G623	K529	Q346	L272	E188	N109
SER	S707	S707	G624	F532	D347	V273	E188	N109
LEU	L708	L708	G625	E533	D347	P274	E188	N109
GLU	T717	T717	T626	E533	C352	N275	E188	H112
ASN	G718	G718	ARG	Y537	P353	L276	E188	S113
ARG	K719	K719	ARG	G538	N354	R277	E188	P114
ASP	K719	K719	VAL	A539	N354	R277	E188	M115
GLU	L724	L724	LEU	L540	L359	N281	E188	V116
CYS	H724	H724	SER	E541	L359	T282	E188	A117
LEU	H724	H724	GLY	A542	V362	A283	E188	T120
MET	G727	G727	GLU	S543	V362	R284	E188	L121
CYS	Q730	Q730	G635	C544	E365	T285	E188	V124
GLY	Q730	Q730	Q635	D545	E366	V286	E188	L125
SER	Q730	Q730	L645	L546	E367	D287	E188	A126
T734	T734	T734	L645	G551	E368	G289	E188	N127
G735	G735	G735	L645	G551	Y374	GLY	E188	K128
M736	M736	M736	H651	P552	Y374	ASN	E188	D129
Y737	Y737	Y737	H652	Y553	R379	LYS	E188	R130
L739	L739	L739	E653	E554	R379	ARG	E188	L131
R740	R740	R740	E654	T555	V383	PRO	E188	N132
T741	T741	T741	R655	P560	V383	G295	E188	I135
R742	R742	R742	R656	V561	A386	A296	E188	I136
PRO	R742	R742	Q658	V561	A386	F297	E188	Y137
ALA	ALA	ALA	I659	L566	L389	A298	E188	D138
ALA	ALA	ALA	I660	Q567	L389	I299	E188	R139
ASN	ASN	ASN	A661	Y568	I393	Y300	E188	D140
PRO	PRO	PRO	G664	D569	I394	L301	E188	Y145
ILE	ILE	ILE	G664	M570	E395	E302	E188	F146
GLN	GLN	GLN	G664	M570	S396	P303	E188	G147
PHE	PHE	PHE	P673	Y573	Q397	L306	E188	F148
THR	THR	THR	D674	T574	Q397	D307	E188	K149
LEU	LEU	LEU	D675	P575	P403	I308	E188	T150
ASN	ASN	ASN	L676	T576	Y404	F309	E188	L151
LYS	LYS	LYS	R677	T576	M405	E310	E188	E152
GLU	GLU	GLU	R678	K587	L406	F311	E188	R153
LYS	LYS	LYS	L679	K587	Y407	L312	E188	S154
LEU	LEU	LEU	L683	R594	R408	D313	E188	Y155
LYS	LYS	LYS	H684	L598	S410	L314	E188	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	69.4	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 45.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TTP, SO4, 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(°)	Ideal(°)
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:N	1:A:446:LEU:HD23	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:O1B	5:B:807:ATP:H5'2	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:206:PHE:HB3	1:B:207:ASN:HD22	1.67	0.59
1:B:94:PHE:CE1	1:B:172:MET:HB3	2.37	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:C5'	5:B:807:ATP:O1B	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: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:A:76:ILE:O	1:A:80:ARG:HG3	2.06	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:N	1:B:675:ASP:OD1	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:N	1:B:129:ASP:OD2	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:287:ASP:O	1:B:289:GLY:N	2.38	0.53
1:B:248:ILE:HD12	1:B:297:PHE:HE2	1.73	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:CD1	1:B:625:TYR:C	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:N	1:A:310:GLU:CD	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:HD12	1:B:171:LEU:HA	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:432:ILE:CG2	1:A:434:GLU:HG3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:SER:OG	4:A:812:SO4:O4	2.29	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:273:VAL:HG21	1:B:310:GLU:HB3	1.97	0.47
1:B:27:TYR:HE1	1:B:80:ARG:NH1	2.13	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: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:49:SER:O	1:B:51:VAL:N	2.49	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:B:79:ALA:O	1:B:83:VAL:HG23	2.16	0.45
1:A:667:GLN:O	1:A:677:LYS:HE2	2.17	0.45
1:B:21:ARG:O	1:B:21:ARG:HD2	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:N	1:A:602:MET:SD	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:CA	1:A:742:ARG:NE	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:N	1:B:523:GLU:OE2	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:263:ALA:HB3	2:A:806:TTP:O1G	2.20	0.42
1:A:256:ARG:HA	1:A:353:PRO:HD2	2.01	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:23:GLN:HE22	1:B:31:MET:HE2	1.85	0.42
1:B:3:VAL:HG22	1:B:13:VAL:HG22	2.01	0.42
1:B:551:GLY:O	1:B:594:ARG:NH1	2.50	0.42
1:A:106:ASN:HD21	1:A:109:ASN:H	1.67	0.42
1:A:20:SER:O	1:A:23:GLN:HB3	2.19	0.42
1:A:265:THR:HG21	1:B:288:GLN:HG2	2.01	0.42
1:A:54:VAL:HG13	1:A:55:GLU:HG3	2.00	0.42
1:A:414:LYS:HD2	1:A:571:TRP:NE1	2.35	0.42
1:B:483:ILE:HA	1:B:483:ILE:HD12	1.92	0.42
1:B:611:LEU:HB2	1:B:613:ASN:HD22	1.85	0.42
1:B:256:ARG:HD2	2:B:805:TTP:H4'	1.91	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:HA	1:B:645:LEU:HD23	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:ND2	1:B:445:ASN:N	2.68	0.41
1:B:626:THR:HG22	1:B:635:GLN:HA	2.01	0.41
1:A:446:LEU:N	1:A:446:LEU:CD2	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:300:TYR:HE2	1:B:406:LEU:CD1	2.30	0.41
1:B:38:GLN:HA	1:B:38:GLN:NE2	2.35	0.41
5:B:807:ATP:PB	5:B:807:ATP:H5'2	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:520:GLU:HG2	6:A:914:HOH:O	2.21	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:A:270:ASN:N	1:A:270:ASN:ND2	2.67	0.41
1:A:603:PRO:O	1:A:604:THR:C	2.59	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:HG2	1:B:365:GLU:H	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:HA	1:B:337:LEU:HD23	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:B:93:VAL:HG23	1:B:132:ASN:OD1	2.22	0.40
1:A:243:LYS:NZ	2:B:805:TTP:O1B	2.52	0.40
1:A:448:SER:HA	1:A:504:GLY:O	2.22	0.40
1:B:477:LEU:HA	1:B:477:LEU:HD23	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 ⓘ

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

Some 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 ⓘ

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 ⓘ

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	A	812	-	4,4,4	0.14	0	6,6,6	0.47	0
4	SO4	B	813	-	4,4,4	0.17	0	6,6,6	0.57	0
4	SO4	B	811	-	4,4,4	0.18	0	6,6,6	0.53	0
4	SO4	A	808	-	4,4,4	0.18	0	6,6,6	0.40	0
4	SO4	B	810	-	4,4,4	0.21	0	6,6,6	0.34	0
2	TTP	B	805	3	23,30,30	1.10	2 (8%)	29,47,47	1.85	4 (13%)
4	SO4	A	809	-	4,4,4	0.13	0	6,6,6	0.28	0
5	ATP	B	807	3	26,33,33	1.30	2 (7%)	31,52,52	1.79	8 (25%)
2	TTP	A	806	3	23,30,30	1.06	2 (8%)	29,47,47	1.81	4 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ATP	B	807	3	-	4/18/38/38	0/3/3/3
2	TTP	A	806	3	-	11/19/34/34	0/2/2/2
2	TTP	B	805	3	-	2/19/34/34	0/2/2/2

All (6) 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	3.82	1.49	1.41
2	B	805	TTP	C4-C5	3.71	1.49	1.41
5	B	807	ATP	C5-C4	2.60	1.47	1.40
2	A	806	TTP	C2-N3	-2.10	1.34	1.38
2	B	805	TTP	C2-N3	-2.01	1.34	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	805	TTP	C4-N3-C2	7.20	121.22	115.14
2	A	806	TTP	C4-N3-C2	6.13	120.32	115.14
5	B	807	ATP	PA-O3A-PB	-4.42	117.67	132.83
2	A	806	TTP	C5-C6-N1	-4.11	117.76	122.19
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
2	B	805	TTP	C5-C6-N1	-3.19	118.76	122.19
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
5	B	807	ATP	O3G-PG-O2G	2.57	117.47	107.64
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
5	B	807	ATP	C5-C6-N6	2.08	123.52	120.35
5	B	807	ATP	O4'-C4'-C3'	-2.01	101.13	105.11

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	805	TTP	O4'-C1'-N1-C6
5	B	807	ATP	C5'-O5'-PA-O1A
5	B	807	ATP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	B	807	ATP	C5'-O5'-PA-O3A
2	A	806	TTP	C5'-O5'-PA-O1A
2	A	806	TTP	C5'-O5'-PA-O2A
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

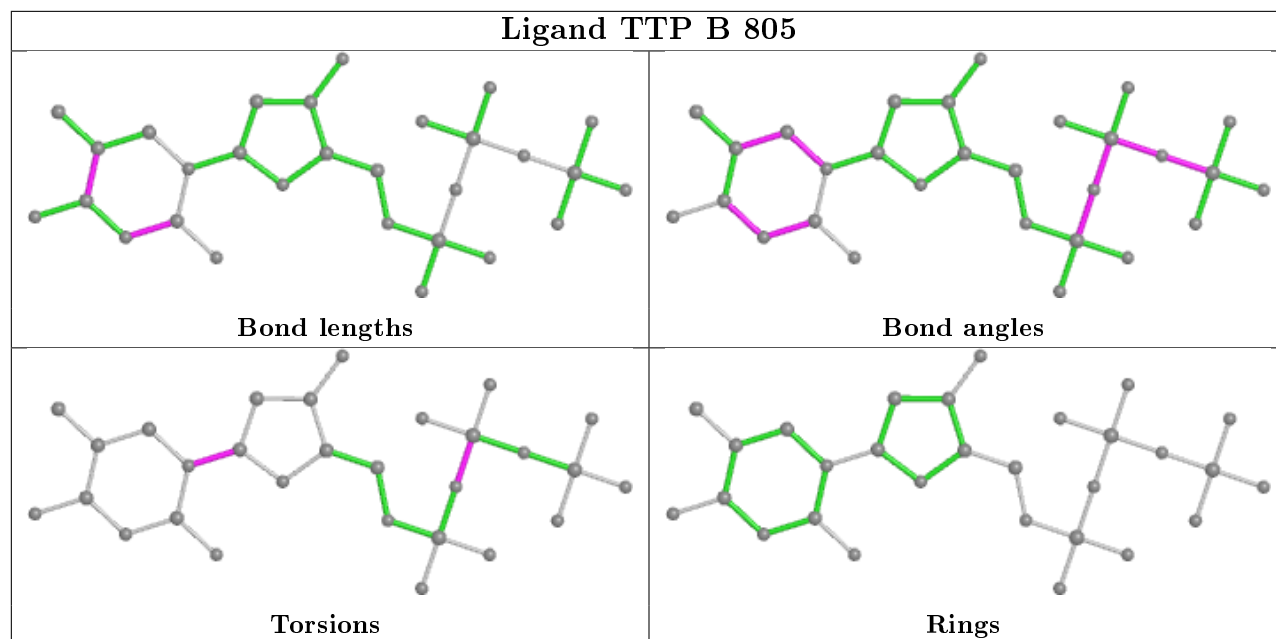
There are no ring outliers.

6 monomers are involved in 11 short contacts:

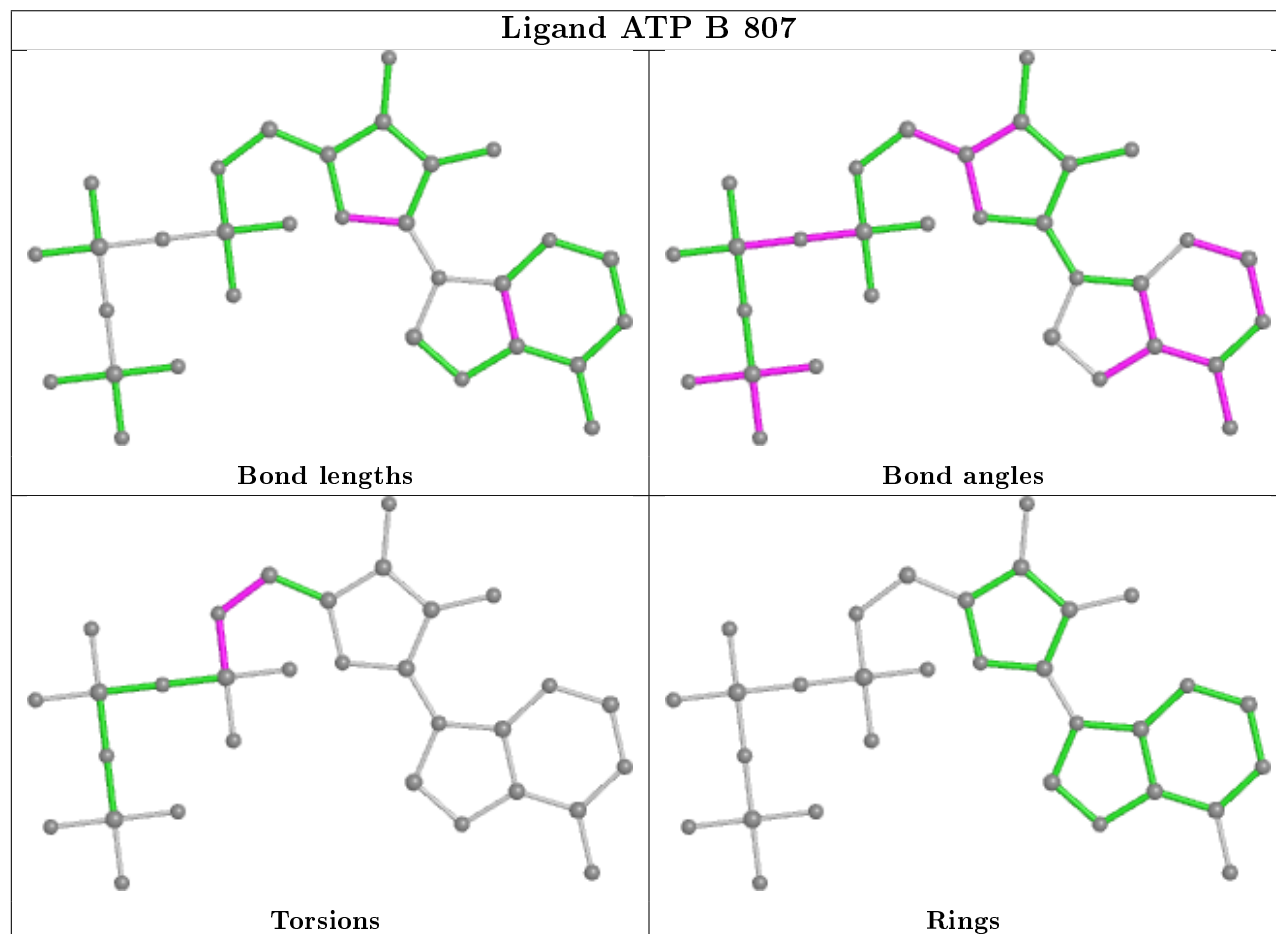
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	812	SO4	1	0
4	B	810	SO4	1	0
2	B	805	TTP	4	0
4	A	809	SO4	1	0
5	B	807	ATP	3	0
2	A	806	TTP	1	0

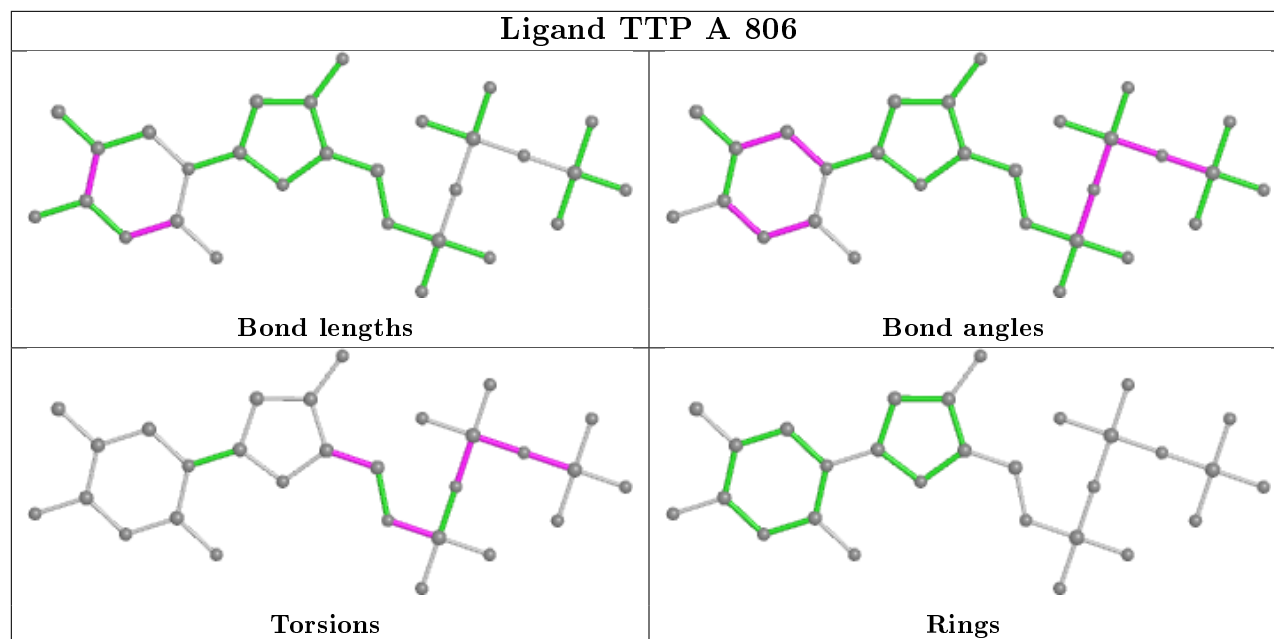
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 TTP B 805



## 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, 95<sup>th</sup> 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 <sup>2</sup> )	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 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, 95<sup>th</sup> 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.

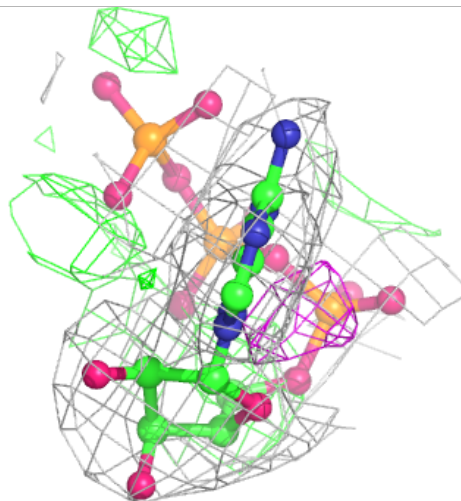
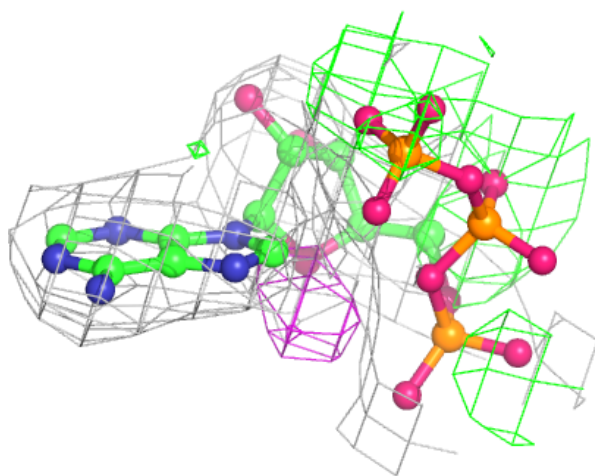
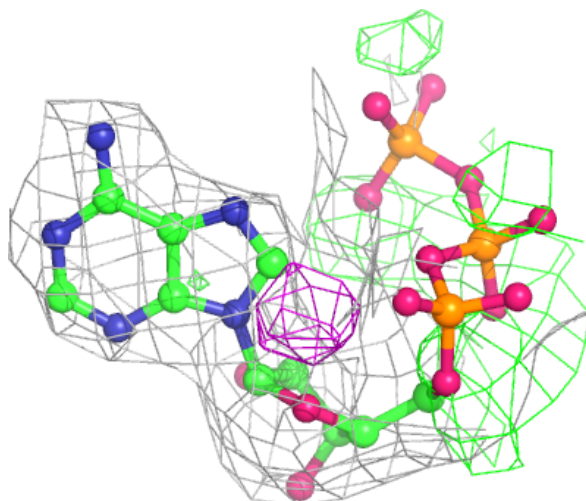
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	A	809	5/5	0.89	0.13	127,127,127,127	0
5	ATP	B	807	31/31	0.91	0.15	65,69,76,76	0
3	MG	B	804	1/1	0.92	0.12	47,47,47,47	0
4	SO4	B	813	5/5	0.93	0.27	70,70,72,72	0
4	SO4	B	811	5/5	0.94	0.13	99,100,100,100	0
3	MG	B	803	1/1	0.94	0.19	42,42,42,42	0
4	SO4	A	808	5/5	0.94	0.16	86,87,87,87	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
2	TTP	B	805	29/29	0.97	0.13	72,75,83,85	0
4	SO4	B	810	5/5	0.97	0.13	79,79,80,81	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.



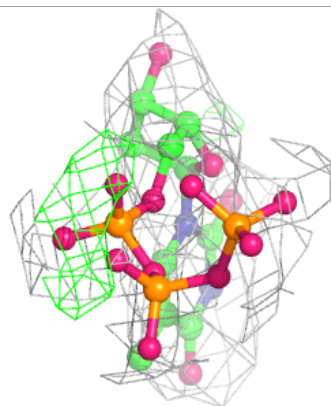
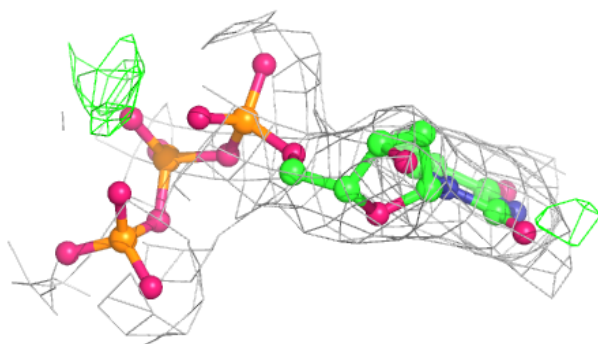
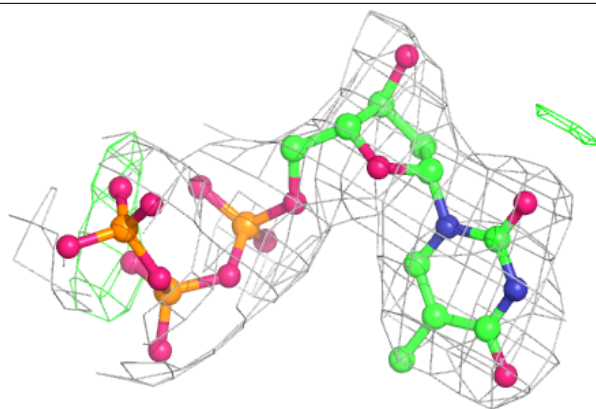
**Electron density around ATP B 807:**

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

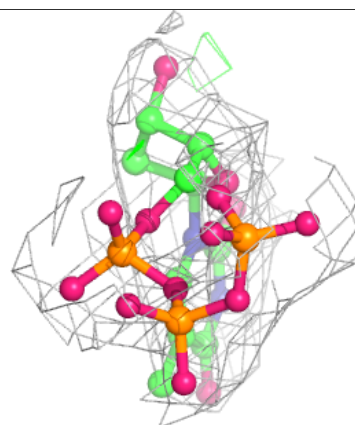
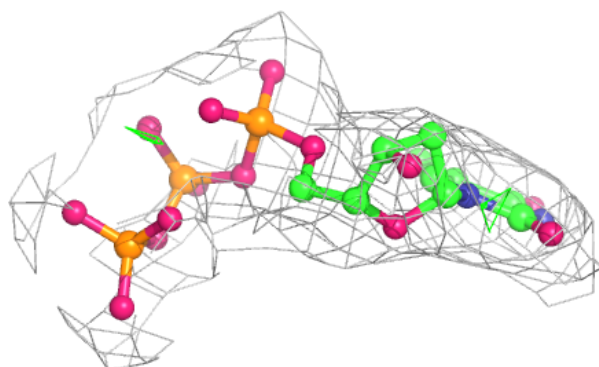
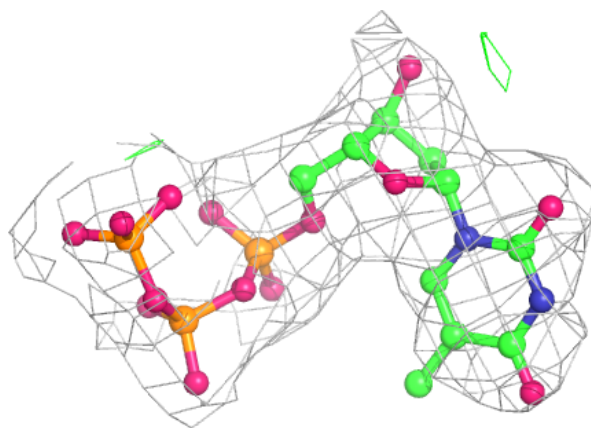


**Electron density around TTP A 806:**

$2mF_o-DF_c$  (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.