



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:49 am BST

PDB ID : 3HNF  
Title : Crystal structure of human ribonucleotide reductase 1 bound to the effectors  
TTP and dATP  
Authors : Fairman, J.W.; Wijerathna, S.R.; Xu, H.; Dealwis, C.G.  
Deposited on : 2009-05-31  
Resolution : 3.16 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

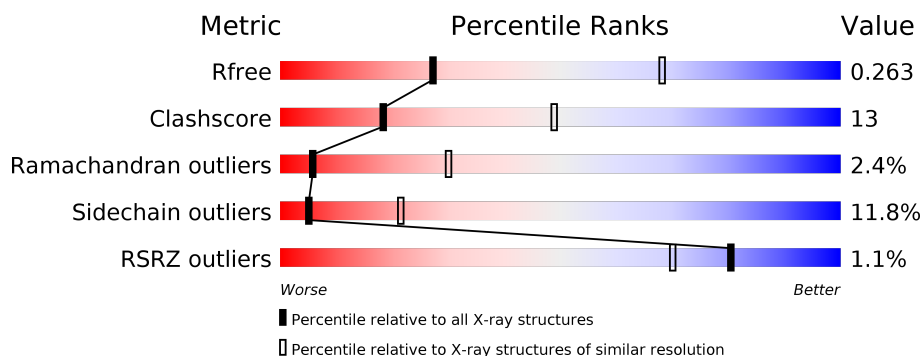
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.16 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	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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></div> <div>58%</div> <div>28%</div> <div>•</div> <div>10%</div> </div>
1	B	792	<div> <div></div> <div>61%</div> <div>27%</div> <div>5%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11549 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.

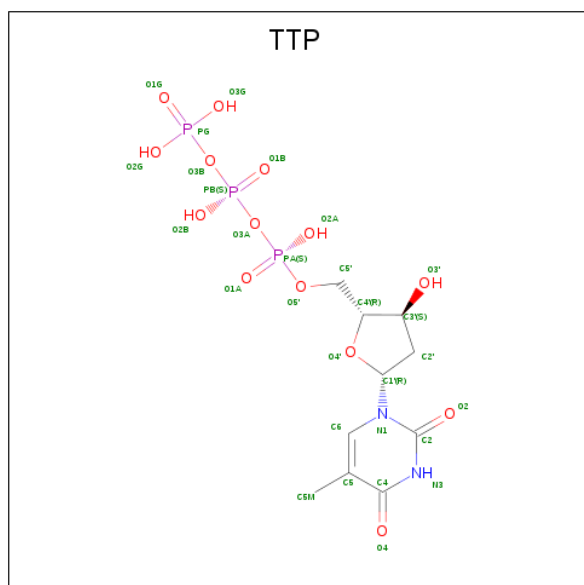
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	715	Total	C	N	O	S	6	0	0
			5596	3579	925	1059	33			
1	B	737	Total	C	N	O	S	0	0	0
			5795	3698	980	1083	34			

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

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

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>2</sub>O<sub>14</sub>P<sub>3</sub>).



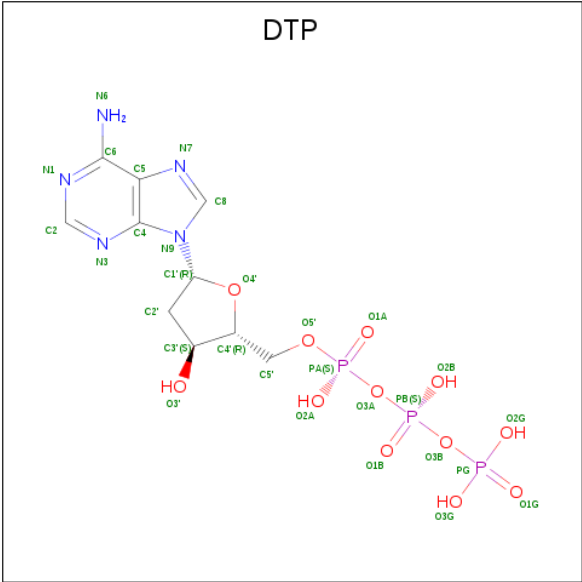
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
3	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

- 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	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>).



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

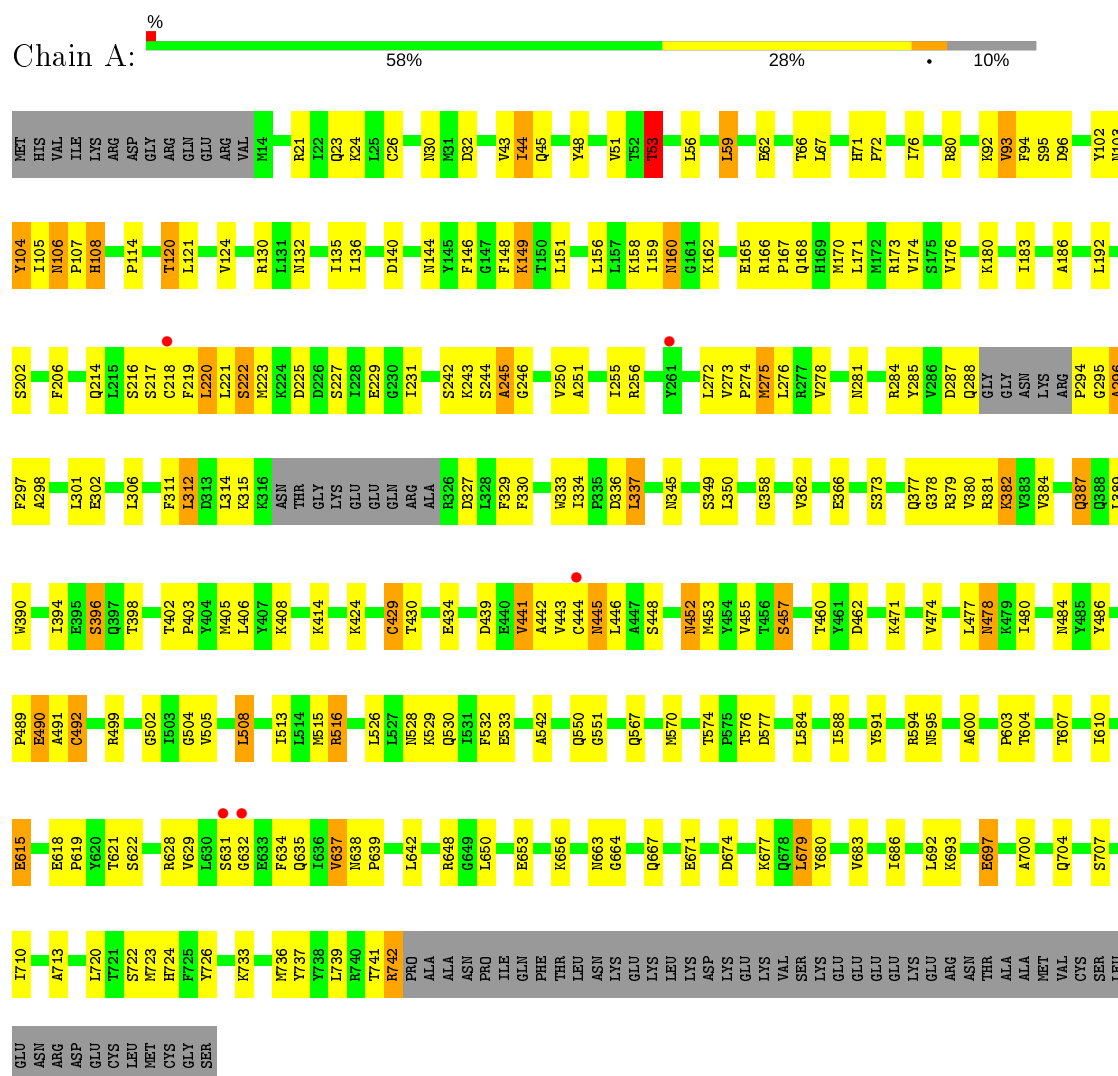
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	22	Total O	0	0
			22 22		
6	B	26	Total O	0	0
			26 26		

### 3 Residue-property plots [i](#)

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



M1	K92	S202	ASN	S373	V629	M736
K5	V93	P203	K292	Q377	LEU	LEU
R6	V97	T204	A298	L389	Q525	G632
D7	M98	L205	I299	E395	I531	Q635
G8	M106	A208	Y300	S396	T534	I636
R9	F107	R212	L301	E399	I535	V637
Q10	H108	L215	E302	E399	Y536	M638
E11	M109	R212	P303	E399	Y536	L642
D16	G110	L215	I308	L406	L540	L642
K17	K111	S216	F309	Y407	E541	K643
I18	H112	S217	E310	K408	A542	D644
T19	S113	S222	F311	Q413	A542	R648
I22	M114	M223	L312	S415	A547	M655
C26	M115	K224	D313	M416	G551	LEU
Y27	L121	D225	L314	Q417	P552	ASN
G28	Y124	D226	K315	Q418	Y553	LYS
L29	L125	S227	K316	S426	E554	GLU
N30	D129	I231	M317	C429	V561	LYS
F33	R130	T234	T318	T430	S562	LEU
D35	I136	L240	G319	E431	K563	ASP
I39	I136	K243	E321	Y441	G564	LYS
T40	R139	R243	R324	A442	I565	GLU
M41	D140	I248	A325	V443	L566	LYS
K42	G147	G249	R326	C444	D675	VAL
V43	F148	Y250	D327	M445	D676	LYS
L47	K149	A251	L328	L446	K677	GLU
Y48	T150	I255	F329	A447	Q678	GLU
S49	L151	R256	F330	S448	L679	GLU
T52	E152	S260	A331	L449	M681	LYS
T53	R153	T261	L332	M452	I588	GLU
V54	Y155	I262	W333	V455	I593	ARG
E55	L156	T265	L337	K464	R594	ASN
L56	L157	N266	F338	K471	M595	THR
D57	M160	G267	V342	I480	S596	ALA
T58	R166	L272	E343	I481	P601	ALA
L59	P167	V273	T344	M478	M602	VAL
T66	Q168	P274	N345	K479	S606	SER
T69	H169	N275	Q346	I481	T607	LEU
A79	M170	L276	G352	Y485	I610	ASN
R80	L171	R277	L359	E490	E615	ASP
V83	M172	N280	V362	E490	E615	GLU
S84	V174	N281	K363	L493	E618	CYS
H87	I187	R284	G364	S494	P619	LEU
T90	L192	Q288	E365	M495	T621	MET
K91	T199	GLY	E366	L508	S622	CYS
			F367	R516	R627	GLY
			E368		R628	SER

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.86Å 114.39Å 220.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.86 – 3.16 40.85 – 3.16	Depositor EDS
% Data completeness (in resolution range)	89.4 (40.86-3.16) 89.4 (40.85-3.16)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.185 , 0.260 0.185 , 0.263	Depositor DCC
$R_{free}$ test set	1335 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	63.0	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11549	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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, DTP, TTP, SO4

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	0.59	1/5721 (0.0%)	0.70	1/7782 (0.0%)
1	B	0.57	0/5920	0.70	2/8035 (0.0%)
All	All	0.58	1/11641 (0.0%)	0.70	3/15817 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	492	CYS	CB-SG	-5.55	1.72	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	LEU	CA-CB-CG	7.19	131.84	115.30
1	B	449	LEU	CA-CB-CG	5.76	128.55	115.30
1	A	508	LEU	CA-CB-CG	5.10	127.03	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	5596	0	5436	151	0
1	B	5795	0	5687	156	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	29	0	13	3	0
3	B	29	0	13	7	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
5	B	30	0	12	1	0
6	A	22	0	0	0	0
6	B	26	0	0	1	0
All	All	11549	0	11161	301	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (301) 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:219:PHE:C	1:A:220:LEU:HD23	1.40	1.42
1:A:443:VAL:HG12	1:A:444:CYS:N	1.67	1.10
1:A:220:LEU:N	1:A:220:LEU:HD23	1.48	1.09
1:B:416:ASN:OD1	1:B:561:VAL:CG2	2.09	1.00
1:A:219:PHE:C	1:A:220:LEU:CD2	2.30	0.99
1:B:130:ARG:HG2	1:B:130:ARG:HH11	1.30	0.97
1:B:90:THR:HG21	1:B:166:ARG:HG3	1.47	0.95
1:A:443:VAL:CG1	1:A:444:CYS:N	2.29	0.94
1:A:220:LEU:N	1:A:220:LEU:CD2	2.30	0.92
1:B:689:LYS:HG2	4:B:809:SO4:O1	1.71	0.90
1:B:223:MET:HE2	1:B:231:ILE:HA	1.55	0.88
1:A:742:ARG:HH11	1:A:742:ARG:HB2	1.39	0.87
1:B:223:MET:CE	1:B:231:ILE:HA	2.04	0.87
1:A:243:LYS:HG3	3:B:803:TTP:HM53	1.57	0.86
1:B:416:ASN:OD1	1:B:561:VAL:HG22	1.74	0.86
1:A:92:LYS:HD2	1:A:166:ARG:HH12	1.42	0.84
1:B:416:ASN:OD1	1:B:561:VAL:HG23	1.77	0.82
1:B:130:ARG:HG2	1:B:130:ARG:NH1	1.91	0.82
1:A:219:PHE:O	1:A:220:LEU:HD23	1.78	0.81
1:B:273:VAL:HB	1:B:274:PRO:HD3	1.61	0.81
1:B:212:ARG:HH11	1:B:485:TYR:HE1	1.28	0.81
1:A:219:PHE:O	1:A:220:LEU:CD2	2.30	0.78
1:A:311:PHE:CZ	1:A:330:PHE:HB3	2.19	0.77
1:B:107:PRO:HG2	1:B:160:ASN:ND2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:CYS:HA	1:B:29:LEU:HD12	1.67	0.76
1:A:471:LYS:HG2	1:A:542:ALA:HB2	1.68	0.76
1:A:106:ASN:OD1	1:A:108:HIS:HB3	1.84	0.76
1:A:53:THR:HA	1:A:56:LEU:HG	1.67	0.73
1:A:219:PHE:CD2	1:A:443:VAL:HG22	2.24	0.73
1:A:256:ARG:NH1	3:A:804:TTP:O3G	2.22	0.72
1:B:490:GLU:N	1:B:490:GLU:OE1	2.18	0.72
1:B:212:ARG:NH1	1:B:485:TYR:HE1	1.87	0.71
1:B:273:VAL:HB	1:B:274:PRO:CD	2.20	0.71
1:A:302:GLU:HG2	1:A:333:TRP:HB3	1.72	0.69
1:B:107:PRO:HG2	1:B:160:ASN:HD21	1.57	0.69
1:B:149:LYS:HE2	1:B:152:GLU:OE2	1.91	0.69
1:A:515:MET:O	1:A:516:ARG:HB2	1.93	0.69
1:A:443:VAL:CG1	1:A:444:CYS:H	2.04	0.69
1:B:30:ASN:HD21	1:B:33:PHE:HD1	1.40	0.69
1:B:314:LEU:HD23	1:B:323:GLN:O	1.94	0.68
3:A:804:TTP:HM53	1:B:243:LYS:HB2	1.73	0.68
1:A:92:LYS:HD2	1:A:166:ARG:NH1	2.06	0.68
1:B:416:ASN:CG	1:B:561:VAL:CG2	2.61	0.68
1:B:212:ARG:NH1	1:B:485:TYR:CE1	2.60	0.66
1:A:219:PHE:CE2	1:A:443:VAL:HG22	2.30	0.66
1:B:121:LEU:HD22	1:B:125:LEU:HG	1.76	0.66
1:B:52:THR:HB	1:B:54:VAL:HG13	1.79	0.65
1:B:362:VAL:HG22	1:B:366:GLU:OE1	1.97	0.64
1:B:481:ILE:HG23	1:B:495:ASN:HD22	1.61	0.64
1:A:584:LEU:O	1:A:588:ILE:HG13	1.97	0.64
1:B:222:SER:HA	1:B:251:ALA:HB3	1.80	0.64
1:A:243:LYS:NZ	3:B:803:TTP:O3A	2.31	0.63
1:B:441:VAL:HG13	1:B:490:GLU:HB2	1.81	0.63
1:B:6:ARG:HG3	1:B:53:THR:HG21	1.79	0.63
1:A:43:VAL:HG22	1:A:59:LEU:HD22	1.81	0.63
1:B:561:VAL:C	1:B:563:LYS:H	2.02	0.63
1:B:90:THR:HB	1:B:166:ARG:HE	1.62	0.63
1:B:471:LYS:HG3	1:B:542:ALA:HB2	1.81	0.62
1:B:302:GLU:HG2	1:B:333:TRP:HB3	1.80	0.62
1:B:478:ASN:HD21	1:B:594:ARG:HG2	1.64	0.62
1:B:265:THR:HG21	3:B:803:TTP:HM52	1.82	0.62
1:A:93:VAL:HG13	1:A:96:ASP:HB2	1.81	0.62
1:B:260:SER:OG	1:B:352:CYS:SG	2.46	0.61
1:B:644:ASP:N	1:B:644:ASP:OD1	2.33	0.61
1:A:704:GLN:O	1:A:733:LYS:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:GLU:O	1:B:399:GLU:HG2	2.00	0.61
1:B:644:ASP:O	1:B:648:ARG:HG3	2.01	0.60
1:A:231:ILE:HD13	1:A:275:MET:HG3	1.83	0.60
1:B:226:ASP:OD1	1:B:256:ARG:HD2	2.01	0.60
1:B:167:PRO:O	1:B:171:LEU:HD22	2.01	0.60
1:B:130:ARG:CG	1:B:130:ARG:HH11	2.08	0.59
1:B:256:ARG:HD3	3:B:803:TTP:H4'	1.85	0.59
1:B:223:MET:HE3	1:B:234:THR:HB	1.84	0.59
1:B:224:LYS:O	1:B:225:ASP:HB3	2.02	0.58
1:B:525:GLN:HB3	6:B:813:HOH:O	2.03	0.58
1:B:373:SER:O	1:B:377:GLN:HG3	2.04	0.58
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.84	0.58
1:A:243:LYS:HG3	3:B:803:TTP:C5M	2.31	0.58
1:B:552:PRO:HA	1:B:593:ILE:O	2.04	0.58
1:B:43:VAL:HG13	1:B:59:LEU:HD12	1.85	0.58
1:A:94:PHE:HB3	1:A:132:ASN:OD1	2.05	0.57
1:A:533:GLU:OE1	1:A:576:THR:HG22	2.05	0.57
1:A:120:THR:O	1:A:124:VAL:HG23	2.05	0.57
1:B:174:VAL:HG22	1:B:208:ALA:HB3	1.87	0.57
1:B:415:SER:O	1:B:418:GLN:HB2	2.04	0.56
1:B:695:ALA:O	1:B:699:GLY:N	2.38	0.56
1:B:280:ASN:O	1:B:284:ARG:HG3	2.05	0.56
1:A:710:ILE:HG12	1:A:736:MET:HG3	1.88	0.56
1:A:439:ASP:O	1:A:490:GLU:HB3	2.06	0.55
1:B:561:VAL:O	1:B:563:LYS:N	2.39	0.55
1:A:229:GLU:HG3	1:B:240:LEU:HD11	1.87	0.55
1:A:103:ASN:O	1:A:104:TYR:C	2.44	0.55
1:A:284:ARG:NH2	1:B:277:ARG:NH2	2.55	0.55
1:B:478:ASN:OD1	1:B:595:ASN:ND2	2.37	0.55
1:A:683:VAL:HA	1:A:686:ILE:HD12	1.89	0.55
1:A:362:VAL:CG1	1:A:366:GLU:HB2	2.37	0.55
1:A:380:VAL:HG12	1:A:382:LYS:H	1.72	0.54
1:A:378:GLY:O	1:A:380:VAL:N	2.40	0.54
1:B:516:ARG:NH2	1:B:644:ASP:OD2	2.40	0.54
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.73	0.54
1:B:561:VAL:C	1:B:563:LYS:N	2.61	0.54
1:A:273:VAL:HG13	1:A:314:LEU:HD11	1.90	0.54
1:A:406:LEU:HD11	1:A:430:THR:HB	1.89	0.54
1:B:531:ILE:O	1:B:534:THR:HB	2.08	0.54
1:A:607:THR:HA	1:A:610:ILE:HD12	1.88	0.54
1:A:223:MET:HG2	1:A:255:ILE:HD11	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:VAL:HA	1:B:281:ASN:ND2	2.23	0.53
1:A:30:ASN:OD1	1:A:32:ASP:HB2	2.08	0.53
1:A:281:ASN:HD22	1:B:281:ASN:HB2	1.74	0.53
1:A:529:LYS:HE2	1:A:697:GLU:HG2	1.91	0.53
1:A:382:LYS:HE3	1:A:384:VAL:HG13	1.91	0.53
1:B:115:MET:HE2	1:B:157:LEU:HD22	1.90	0.53
1:A:513:ILE:HG23	1:A:679:LEU:HD11	1.91	0.53
1:A:281:ASN:HD22	1:B:281:ASN:CB	2.22	0.53
1:A:140:ASP:OD2	1:A:168:GLN:HG2	2.09	0.53
1:A:295:GLY:O	1:A:296:ALA:HB2	2.09	0.53
1:A:146:PHE:HE1	1:A:634:PHE:HB2	1.74	0.52
1:A:102:TYR:O	1:A:114:PRO:HA	2.10	0.52
1:B:431:GLU:N	1:B:431:GLU:OE2	2.39	0.52
1:A:170:MET:SD	1:A:170:MET:C	2.88	0.52
1:A:478:ASN:OD1	1:A:499:ARG:NH1	2.43	0.52
1:B:1:MET:HG2	1:B:49:SER:HB2	1.92	0.52
1:A:170:MET:O	1:A:174:VAL:HG23	2.10	0.51
1:A:445:ASN:ND2	1:A:445:ASN:N	2.58	0.51
1:A:489:PRO:HG2	1:A:490:GLU:OE1	2.11	0.51
1:B:87:HIS:CD2	1:B:166:ARG:HD3	2.46	0.51
1:B:224:LYS:O	1:B:225:ASP:CB	2.58	0.51
1:A:462:ASP:C	1:A:462:ASP:OD2	2.49	0.51
1:B:135:ILE:HD11	1:B:172:MET:HG2	1.92	0.51
1:B:298:ALA:HA	1:B:329:PHE:O	2.11	0.51
1:A:136:ILE:HG23	4:A:808:SO4:O1	2.11	0.50
1:B:83:VAL:HG11	1:B:140:ASP:HB3	1.93	0.50
1:A:621:THR:HA	1:A:683:VAL:HG12	1.94	0.50
1:A:373:SER:O	1:A:377:GLN:HG3	2.11	0.50
1:B:313:ASP:HA	1:B:316:LYS:HD3	1.93	0.50
1:B:416:ASN:ND2	1:B:561:VAL:CG2	2.75	0.50
1:A:720:LEU:O	1:A:723:MET:HB2	2.11	0.50
1:B:551:GLY:O	1:B:594:ARG:NH1	2.45	0.50
1:A:105:ILE:O	1:A:107:PRO:HD3	2.12	0.49
1:B:256:ARG:CD	3:B:803:TTP:H4'	2.41	0.49
1:A:159:ILE:O	1:A:160:ASN:O	2.30	0.49
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.94	0.49
1:B:364:GLY:O	1:B:368:GLU:HG3	2.13	0.49
1:A:222:SER:OG	1:A:424:LYS:HD2	2.12	0.49
1:B:170:MET:HG2	1:B:173:ARG:NH2	2.27	0.49
1:A:281:ASN:ND2	1:B:281:ASN:HB2	2.27	0.49
1:A:515:MET:O	1:A:516:ARG:CB	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:LEU:HD13	1:A:381:ARG:HB3	1.94	0.49
1:B:256:ARG:HH21	1:B:262:ILE:HA	1.76	0.49
1:A:742:ARG:HB2	1:A:742:ARG:NH1	2.19	0.48
1:A:159:ILE:O	1:A:160:ASN:C	2.52	0.48
1:B:310:GLU:N	1:B:310:GLU:CD	2.67	0.48
1:B:109:ASN:O	1:B:111:LYS:N	2.46	0.48
1:B:330:PHE:N	1:B:330:PHE:CD2	2.81	0.48
1:B:98:MET:HG3	1:B:124:VAL:HG11	1.96	0.48
1:B:256:ARG:NH1	3:B:803:TTP:H5'1	2.28	0.48
1:A:93:VAL:HG22	1:A:96:ASP:H	1.78	0.48
1:A:405:MET:HG3	1:A:724:HIS:CE1	2.49	0.48
1:A:600:ALA:HB2	1:A:704:GLN:HB2	1.96	0.48
1:B:678:GLN:O	1:B:681:LYS:HG3	2.13	0.48
1:B:277:ARG:HD2	1:B:322:GLU:O	2.13	0.48
1:B:540:LEU:HB2	1:B:584:LEU:HD21	1.96	0.48
1:A:443:VAL:HG13	1:A:444:CYS:H	1.78	0.48
1:B:601:PRO:HG2	1:B:702:ILE:HD13	1.95	0.47
1:B:715:PRO:HG3	1:B:741:THR:HG21	1.95	0.47
1:A:219:PHE:O	1:A:220:LEU:HD22	2.12	0.47
1:A:244:SER:O	1:A:245:ALA:HB3	2.14	0.47
1:A:217:SER:O	1:A:217:SER:OG	2.30	0.47
1:A:156:LEU:HD21	1:A:167:PRO:HA	1.96	0.47
1:B:566:LEU:O	1:B:569:ASP:HB2	2.15	0.47
1:A:48:TYR:CE2	1:A:51:VAL:HG12	2.50	0.47
1:A:53:THR:HA	1:A:56:LEU:CG	2.41	0.47
1:A:43:VAL:HG13	1:A:59:LEU:HD13	1.97	0.47
1:B:140:ASP:OD2	1:B:168:GLN:HG2	2.14	0.47
1:A:149:LYS:HG2	1:A:629:VAL:HG13	1.97	0.47
1:B:619:PRO:HG2	1:B:683:VAL:HG23	1.96	0.47
1:A:170:MET:HG2	1:A:173:ARG:NH2	2.29	0.46
1:B:215:LEU:HD13	1:B:480:ILE:HG12	1.97	0.46
1:B:659:ILE:HG22	1:B:664:GLY:HA2	1.97	0.46
1:A:478:ASN:ND2	1:A:595:ASN:HD21	2.13	0.46
1:A:603:PRO:HD3	1:A:707:SER:OG	2.15	0.46
1:A:76:ILE:O	1:A:80:ARG:HG3	2.15	0.46
1:B:5:LYS:HE3	1:B:11:GLU:HG3	1.97	0.46
1:A:334:ILE:O	1:A:408:LYS:HB3	2.16	0.46
1:A:336:ASP:O	1:A:337:LEU:C	2.53	0.46
1:A:567:GLN:HG3	1:A:700:ALA:O	2.16	0.46
1:B:273:VAL:CB	1:B:274:PRO:CD	2.91	0.46
1:A:667:GLN:O	1:A:677:LYS:HE2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:PHE:HA	1:A:151:LEU:HD12	1.98	0.46
1:B:152:GLU:HA	1:B:156:LEU:HD12	1.97	0.45
1:A:615:GLU:CD	1:A:615:GLU:H	2.20	0.45
1:A:349:SER:HB3	1:A:380:VAL:HG11	1.98	0.45
1:B:53:THR:HG21	5:B:805:DTP:O2B	2.16	0.45
1:B:406:LEU:HD22	1:B:426:SER:HB2	1.99	0.45
1:B:667:GLN:O	1:B:677:LYS:HD3	2.17	0.45
1:A:358:GLY:O	1:A:362:VAL:HG23	2.17	0.45
1:A:679:LEU:HD12	1:A:680:TYR:CZ	2.52	0.45
1:B:519:PHE:CD2	1:B:619:PRO:HB3	2.52	0.45
1:A:484:ASN:HB3	1:A:486:TYR:CE2	2.51	0.45
1:B:445:ASN:ND2	1:B:445:ASN:H	2.15	0.45
1:A:446:LEU:HA	1:A:502:GLY:O	2.17	0.45
1:B:6:ARG:CG	1:B:53:THR:HG21	2.45	0.45
1:A:227:SER:HB2	3:A:804:TTP:O2A	2.16	0.45
1:B:226:ASP:CG	1:B:256:ARG:HD2	2.38	0.45
1:A:452:ASN:ND2	1:A:453:MET:HG2	2.32	0.44
1:A:526:LEU:O	1:A:530:GLN:HG3	2.17	0.44
1:B:308:ILE:HD11	1:B:332:LEU:HD21	1.99	0.44
1:B:553:TYR:O	1:B:554:GLU:C	2.56	0.44
1:A:434:GLU:OE1	1:A:442:ALA:HB1	2.17	0.44
1:A:216:SER:OG	1:A:443:VAL:HG11	2.16	0.44
1:B:199:THR:HG21	1:B:607:THR:HB	1.99	0.44
1:B:202:SER:N	1:B:203:PRO:HD2	2.32	0.44
1:B:16:ASP:HA	1:B:19:THR:HG23	1.99	0.44
1:B:140:ASP:OD2	1:B:167:PRO:HB2	2.17	0.44
1:B:255:ILE:HB	1:B:272:LEU:HD21	1.98	0.44
1:A:441:VAL:O	1:A:491:ALA:HA	2.18	0.44
1:B:79:ALA:O	1:B:83:VAL:HG23	2.16	0.44
1:A:135:ILE:HG23	1:A:168:GLN:HB3	1.99	0.44
1:B:563:LYS:HB2	1:B:565:ILE:HD12	2.00	0.43
1:A:287:ASP:HB2	1:A:294:PRO:HD2	2.00	0.43
1:B:320:LYS:O	1:B:324:ARG:HG2	2.18	0.43
1:B:485:TYR:CD2	1:B:485:TYR:C	2.92	0.43
1:B:674:ASP:N	1:B:674:ASP:OD1	2.49	0.43
1:B:27:TYR:O	1:B:80:ARG:NH2	2.51	0.43
1:B:280:ASN:ND2	1:B:284:ARG:HD2	2.33	0.43
1:B:147:GLY:HA2	1:B:610:ILE:HA	2.00	0.43
1:B:648:ARG:HH11	1:B:648:ARG:HG2	1.83	0.43
1:B:107:PRO:CG	1:B:160:ASN:HD21	2.28	0.43
1:B:481:ILE:HG23	1:B:495:ASN:ND2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:CYS:C	1:A:430:THR:HG23	2.39	0.43
1:A:722:SER:O	1:A:726:TYR:N	2.43	0.43
1:A:71:HIS:ND1	1:A:72:PRO:HD2	2.34	0.43
1:A:202:SER:HB3	1:A:206:PHE:CE1	2.54	0.43
1:A:223:MET:HB2	1:A:251:ALA:O	2.19	0.43
1:A:474:VAL:O	1:A:478:ASN:HB2	2.18	0.43
1:B:225:ASP:O	1:B:227:SER:N	2.49	0.43
1:B:618:GLU:OE1	1:B:711:HIS:HE1	2.00	0.43
1:A:448:SER:HA	1:A:504:GLY:O	2.19	0.43
1:A:551:GLY:O	1:A:594:ARG:NH1	2.52	0.43
1:B:205:LEU:HA	1:B:205:LEU:HD23	1.93	0.42
1:B:303:PRO:HD3	1:B:333:TRP:O	2.18	0.42
1:B:429:CYS:C	1:B:430:THR:HG23	2.40	0.42
1:B:443:VAL:HG12	1:B:444:CYS:N	2.34	0.42
1:B:448:SER:HB3	1:B:602:MET:HE1	2.00	0.42
1:A:298:ALA:HA	1:A:329:PHE:O	2.20	0.42
1:B:637:VAL:O	1:B:638:ASN:C	2.57	0.42
1:A:396:SER:HB3	1:A:403:PRO:HD2	2.01	0.42
1:A:622:SER:OG	1:A:664:GLY:HA3	2.18	0.42
1:A:144:ASN:C	1:A:144:ASN:OD1	2.58	0.42
1:A:23:GLN:O	1:A:26:CYS:HB2	2.19	0.42
1:A:628:ARG:HA	1:A:632:GLY:O	2.19	0.42
1:A:637:VAL:HG22	1:A:642:LEU:HB2	2.01	0.42
1:B:136:ILE:HG13	1:B:139:ARG:CZ	2.50	0.42
1:B:265:THR:C	1:B:267:GLY:H	2.23	0.42
1:A:306:LEU:HA	1:A:350:LEU:HB3	2.02	0.42
1:A:306:LEU:HD22	1:A:381:ARG:HG2	2.02	0.42
1:A:480:ILE:O	1:A:484:ASN:HB2	2.19	0.42
1:A:603:PRO:O	1:A:604:THR:C	2.58	0.42
1:A:650:LEU:HD22	1:A:671:GLU:HG3	2.01	0.42
1:B:588:ILE:HG23	1:B:593:ILE:HG23	2.02	0.42
1:A:273:VAL:HB	1:A:274:PRO:HD3	2.02	0.42
1:B:490:GLU:H	1:B:490:GLU:CD	2.16	0.42
1:A:21:ARG:HA	1:A:24:LYS:HG2	2.02	0.41
1:A:287:ASP:OD1	1:A:288:GLN:N	2.54	0.41
1:A:297:PHE:CD2	1:A:297:PHE:N	2.87	0.41
1:B:47:LEU:HD23	1:B:56:LEU:HD21	2.02	0.41
1:A:584:LEU:HG	1:A:588:ILE:HD11	2.03	0.41
1:B:333:TRP:CD1	1:B:408:LYS:HD2	2.55	0.41
1:A:489:PRO:O	1:A:492:CYS:HB3	2.20	0.41
1:A:146:PHE:CE1	1:A:634:PHE:HB2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PHE:HB2	1:A:135:ILE:HD12	2.01	0.41
1:A:183:ILE:O	1:A:186:ALA:HB3	2.21	0.41
1:A:394:ILE:O	1:A:398:THR:HG23	2.21	0.41
1:A:414:LYS:HA	1:A:570:MET:SD	2.61	0.41
1:B:344:THR:O	1:B:346:GLN:HG3	2.21	0.41
1:B:710:ILE:HG12	1:B:736:MET:HG3	2.02	0.41
1:A:387:GLN:O	1:A:390:TRP:HB3	2.20	0.41
1:A:477:LEU:HA	1:A:477:LEU:HD23	1.83	0.41
1:A:528:ASN:O	1:A:532:PHE:HD2	2.03	0.41
1:A:618:GLU:HA	1:A:619:PRO:HD3	1.93	0.41
1:B:416:ASN:ND2	1:B:561:VAL:HG21	2.36	0.41
1:B:536:TYR:CZ	1:B:540:LEU:HD11	2.56	0.41
1:A:441:VAL:HG22	1:A:491:ALA:HA	2.02	0.41
1:B:97:VAL:HG21	1:B:169:HIS:CE1	2.56	0.41
1:A:156:LEU:HD22	1:A:165:GLU:O	2.21	0.41
1:A:315:LYS:CB	1:A:330:PHE:HE2	2.34	0.41
1:A:638:ASN:HA	1:A:639:PRO:HD2	1.89	0.41
1:A:402:THR:HB	1:A:403:PRO:HA	2.03	0.41
1:B:248:ILE:HG22	1:B:249:GLY:N	2.35	0.41
1:B:338:PHE:O	1:B:342:VAL:HG23	2.21	0.40
1:B:547:ALA:O	1:B:551:GLY:N	2.39	0.40
1:B:18:ILE:O	1:B:22:ILE:HG12	2.21	0.40
1:B:324:ARG:HG3	1:B:326:ARG:NH2	2.35	0.40
1:B:359:LEU:HA	1:B:359:LEU:HD12	1.96	0.40
1:B:452:ASN:OD1	1:B:452:ASN:N	2.50	0.40
1:B:553:TYR:CZ	1:B:596:SER:HB3	2.55	0.40
1:A:71:HIS:CG	1:A:72:PRO:HD2	2.57	0.40
1:B:39:ILE:O	1:B:40:THR:C	2.57	0.40
1:B:90:THR:HG22	1:B:91:LYS:O	2.21	0.40
1:A:135:ILE:CG2	1:A:168:GLN:HB3	2.52	0.40
1:B:648:ARG:HE	1:B:676:LEU:HD11	1.86	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	709/792 (90%)	633 (89%)	54 (8%)	22 (3%)	4	23
1	B	731/792 (92%)	639 (87%)	79 (11%)	13 (2%)	8	37
All	All	1440/1584 (91%)	1272 (88%)	133 (9%)	35 (2%)	6	30

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	296	ALA
1	A	327	ASP
1	A	379	ARG
1	B	110	GLY
1	B	225	ASP
1	B	713	ALA
1	A	104	TYR
1	A	162	LYS
1	A	218	CYS
1	A	245	ALA
1	A	246	GLY
1	A	345	ASN
1	A	516	ARG
1	B	327	ASP
1	A	180	LYS
1	A	457	SER
1	A	653	GLU
1	A	663	ASN
1	A	713	ALA
1	B	6	ARG
1	B	226	ASP
1	B	345	ASN
1	B	516	ARG
1	B	562	SER
1	A	53	THR
1	A	737	TYR
1	B	7	ASP
1	B	601	PRO
1	A	285	TYR
1	A	312	LEU
1	B	267	GLY
1	B	493	LEU

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Mol	Chain	Res	Type
1	A	106	ASN
1	A	44	ILE

### 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	597/693 (86%)	533 (89%)	64 (11%)	6	25
1	B	617/693 (89%)	538 (87%)	79 (13%)	4	18
All	All	1214/1386 (88%)	1071 (88%)	143 (12%)	5	21

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ILE
1	A	45	GLN
1	A	53	THR
1	A	59	LEU
1	A	62	GLU
1	A	66	THR
1	A	67	LEU
1	A	93	VAL
1	A	95	SER
1	A	108	HIS
1	A	120	THR
1	A	121	LEU
1	A	130	ARG
1	A	149	LYS
1	A	158	LYS
1	A	171	LEU
1	A	176	VAL
1	A	192	LEU
1	A	214	GLN
1	A	220	LEU
1	A	221	LEU

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Mol	Chain	Res	Type
1	A	222	SER
1	A	225	ASP
1	A	242	SER
1	A	250	VAL
1	A	272	LEU
1	A	275	MET
1	A	276	LEU
1	A	301	LEU
1	A	312	LEU
1	A	337	LEU
1	A	382	LYS
1	A	387	GLN
1	A	389	LEU
1	A	396	SER
1	A	429	CYS
1	A	441	VAL
1	A	445	ASN
1	A	452	ASN
1	A	455	VAL
1	A	457	SER
1	A	460	THR
1	A	478	ASN
1	A	490	GLU
1	A	505	VAL
1	A	508	LEU
1	A	550	GLN
1	A	574	THR
1	A	577	ASP
1	A	591	TYR
1	A	615	GLU
1	A	631	SER
1	A	635	GLN
1	A	637	VAL
1	A	648	ARG
1	A	656	LYS
1	A	674	ASP
1	A	679	LEU
1	A	692	LEU
1	A	693	LYS
1	A	697	GLU
1	A	739	LEU
1	A	741	THR

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Mol	Chain	Res	Type
1	A	742	ARG
1	B	9	ARG
1	B	11	GLU
1	B	16	ASP
1	B	19	THR
1	B	30	ASN
1	B	35	ASP
1	B	41	MET
1	B	47	LEU
1	B	53	THR
1	B	54	VAL
1	B	58	THR
1	B	59	LEU
1	B	66	THR
1	B	69	THR
1	B	80	ARG
1	B	84	SER
1	B	93	VAL
1	B	106	ASN
1	B	113	SER
1	B	121	LEU
1	B	129	ASP
1	B	130	ARG
1	B	149	LYS
1	B	154	SER
1	B	171	LEU
1	B	187	ILE
1	B	192	LEU
1	B	217	SER
1	B	256	ARG
1	B	265	THR
1	B	266	ASN
1	B	273	VAL
1	B	276	LEU
1	B	281	ASN
1	B	301	LEU
1	B	310	GLU
1	B	312	LEU
1	B	313	ASP
1	B	326	ARG
1	B	327	ASP
1	B	337	LEU

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Mol	Chain	Res	Type
1	B	349	SER
1	B	359	LEU
1	B	389	LEU
1	B	396	SER
1	B	431	GLU
1	B	444	CYS
1	B	445	ASN
1	B	446	LEU
1	B	449	LEU
1	B	455	VAL
1	B	464	LYS
1	B	471	LYS
1	B	493	LEU
1	B	508	LEU
1	B	516	ARG
1	B	541	GLU
1	B	554	GLU
1	B	561	VAL
1	B	570	MET
1	B	583	VAL
1	B	602	MET
1	B	606	SER
1	B	615	GLU
1	B	621	THR
1	B	622	SER
1	B	627	ARG
1	B	642	LEU
1	B	644	ASP
1	B	655	MET
1	B	674	ASP
1	B	679	LEU
1	B	685	GLU
1	B	692	LEU
1	B	708	LEU
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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	108	HIS
1	A	281	ASN
1	A	387	GLN
1	A	418	GLN
1	A	445	ASN
1	A	478	ASN
1	A	595	ASN
1	A	652	HIS
1	B	2	HIS
1	B	106	ASN
1	B	207	ASN
1	B	268	ASN
1	B	281	ASN
1	B	346	GLN
1	B	445	ASN
1	B	459	HIS
1	B	495	ASN
1	B	663	ASN
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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	TTP	A	804	2	23,30,30	1.06	1 (4%)	29,47,47	1.59	4 (13%)
4	SO4	B	809	-	4,4,4	0.20	0	6,6,6	0.18	0
4	SO4	A	807	-	4,4,4	0.17	0	6,6,6	0.20	0
4	SO4	A	808	-	4,4,4	0.14	0	6,6,6	0.29	0
4	SO4	B	806	-	4,4,4	0.18	0	6,6,6	0.47	0
5	DTP	B	805	-	26,32,32	0.92	2 (7%)	30,50,50	1.30	3 (10%)
3	TTP	B	803	2	23,30,30	1.06	1 (4%)	29,47,47	1.72	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
3	TTP	A	804	2	-	10/19/34/34	0/2/2/2
5	DTP	B	805	-	-	3/18/34/34	0/3/3/3
3	TTP	B	803	2	-	4/19/34/34	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	803	TTP	C4-C5	4.10	1.50	1.41
3	A	804	TTP	C4-C5	3.93	1.49	1.41
5	B	805	DTP	C5-C4	2.51	1.47	1.40
5	B	805	DTP	C2-N3	2.07	1.35	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	804	TTP	C4-N3-C2	5.76	120.01	115.14
3	B	803	TTP	C4-N3-C2	4.71	119.12	115.14
3	B	803	TTP	PB-O3A-PA	-4.60	117.03	132.83
5	B	805	DTP	N3-C2-N1	-3.71	122.87	128.68
3	B	803	TTP	PB-O3B-PG	-3.57	120.57	132.83
3	B	803	TTP	C5-C6-N1	-3.46	118.47	122.19
3	A	804	TTP	C5-C6-N1	-3.44	118.49	122.19
5	B	805	DTP	C4-C5-N7	-2.59	106.70	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	804	TTP	PB-O3B-PG	-2.52	124.19	132.83
3	A	804	TTP	PB-O3A-PA	-2.23	125.18	132.83
5	B	805	DTP	PB-O3B-PG	-2.10	125.63	132.83

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	804	TTP	C5'-O5'-PA-O1A
3	A	804	TTP	O4'-C1'-N1-C6
3	B	803	TTP	C5'-O5'-PA-O1A
3	B	803	TTP	O4'-C4'-C5'-O5'
3	B	803	TTP	C3'-C4'-C5'-O5'
3	A	804	TTP	O4'-C4'-C5'-O5'
3	A	804	TTP	C3'-C4'-C5'-O5'
5	B	805	DTP	PB-O3B-PG-O1G
3	A	804	TTP	C5'-O5'-PA-O3A
3	A	804	TTP	PB-O3A-PA-O2A
3	A	804	TTP	PA-O3A-PB-O2B
3	A	804	TTP	PG-O3B-PB-O1B
5	B	805	DTP	PG-O3B-PB-O1B
3	B	803	TTP	PB-O3B-PG-O3G
3	A	804	TTP	PB-O3A-PA-O1A
3	A	804	TTP	PG-O3B-PB-O2B
5	B	805	DTP	PG-O3B-PB-O2B

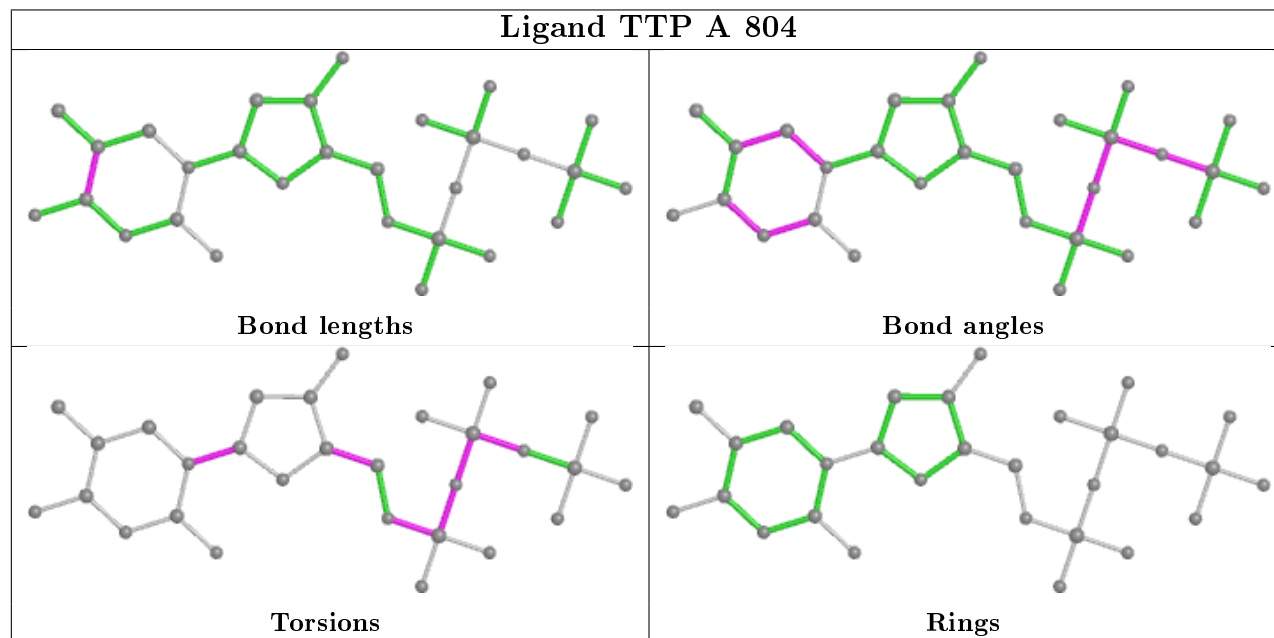
There are no ring outliers.

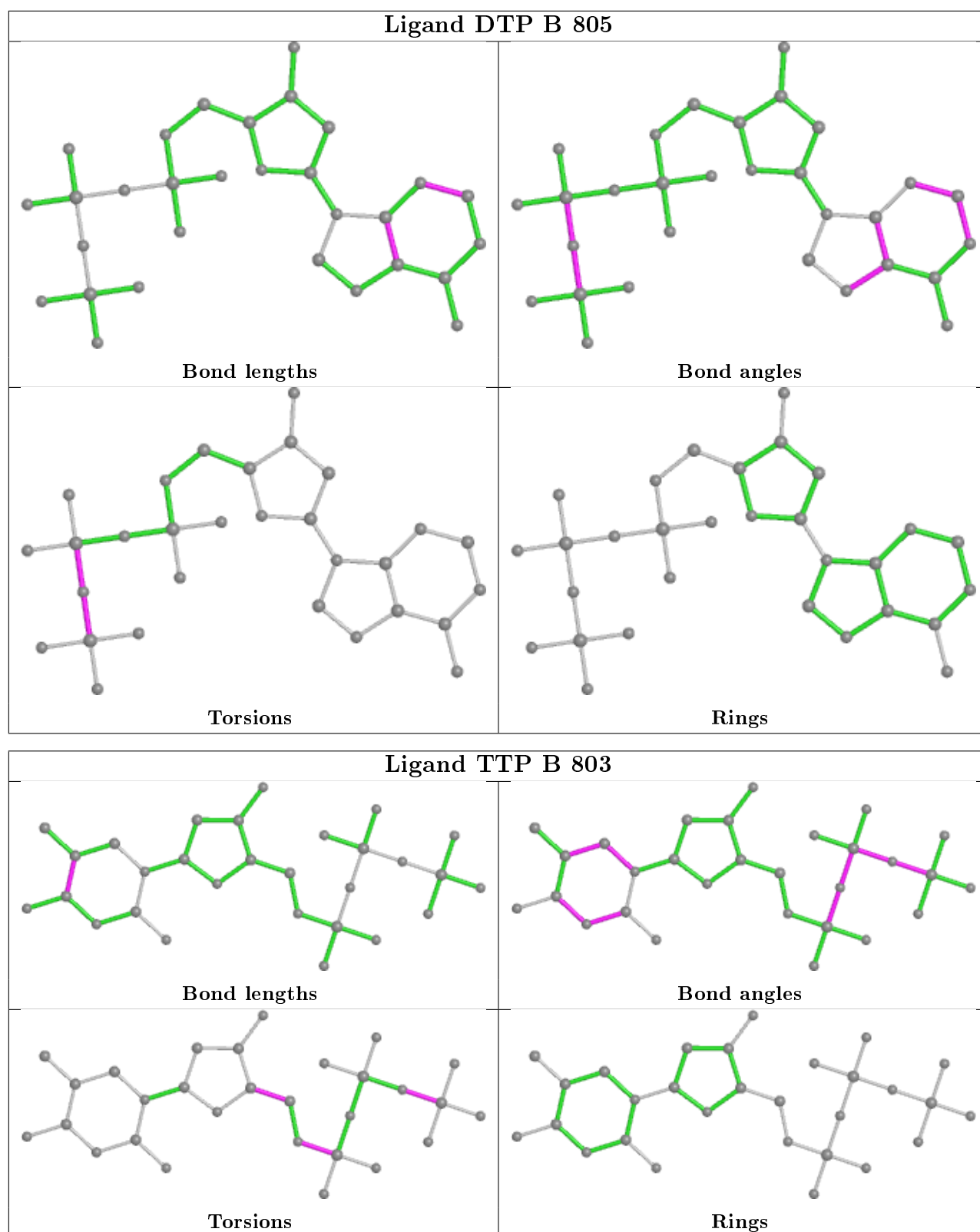
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	804	TTP	3	0
4	B	809	SO4	1	0
4	A	808	SO4	1	0
5	B	805	DTP	1	0
3	B	803	TTP	7	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.





## 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 [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%)	-0.36	5 (0%) 87 81	45, 63, 85, 123	2 (0%)
1	B	737/792 (93%)	-0.27	11 (1%) 73 61	38, 58, 94, 110	0
All	All	1452/1584 (91%)	-0.31	16 (1%) 80 70	38, 61, 91, 123	2 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	444	CYS	5.3
1	A	218	CYS	4.7
1	A	632	GLY	3.2
1	B	49	SER	2.9
1	B	323	GLN	2.6
1	B	675	ASP	2.6
1	B	318	THR	2.5
1	B	635	GLN	2.4
1	B	319	GLY	2.4
1	B	48	TYR	2.2
1	A	261	TYR	2.2
1	B	660	ILE	2.2
1	A	631	SER	2.1
1	B	324	ARG	2.1
1	B	672	ILE	2.1
1	B	160	ASN	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

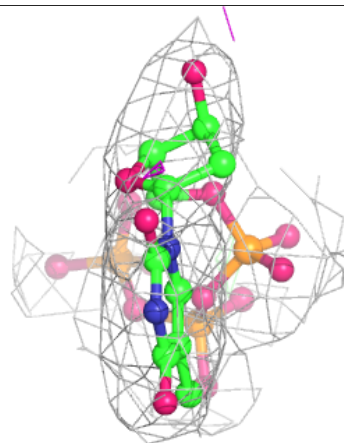
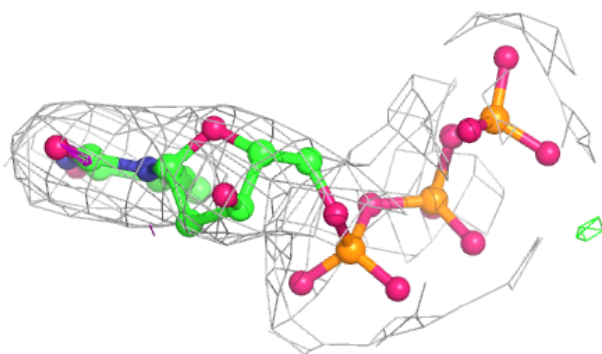
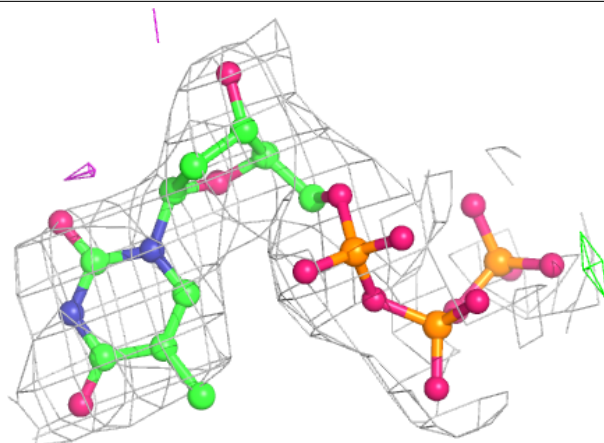
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	B	806	5/5	0.91	0.52	101,102,102,102	0
4	SO4	A	808	5/5	0.93	0.19	76,76,77,78	0
2	MG	B	802	1/1	0.94	0.18	48,48,48,48	0
3	TTP	A	804	29/29	0.95	0.14	58,60,66,67	0
5	DTP	B	805	30/30	0.96	0.17	83,84,88,89	0
2	MG	A	801	1/1	0.96	0.17	46,46,46,46	0
4	SO4	B	809	5/5	0.97	0.10	74,75,75,75	0
3	TTP	B	803	29/29	0.97	0.12	54,57,66,67	0
4	SO4	A	807	5/5	0.97	0.20	91,91,91,91	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.

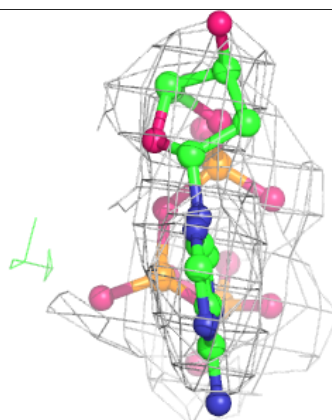
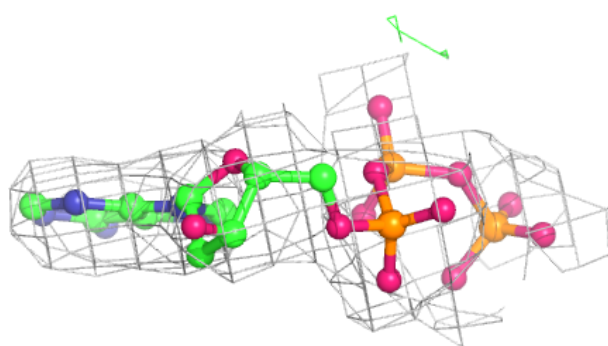
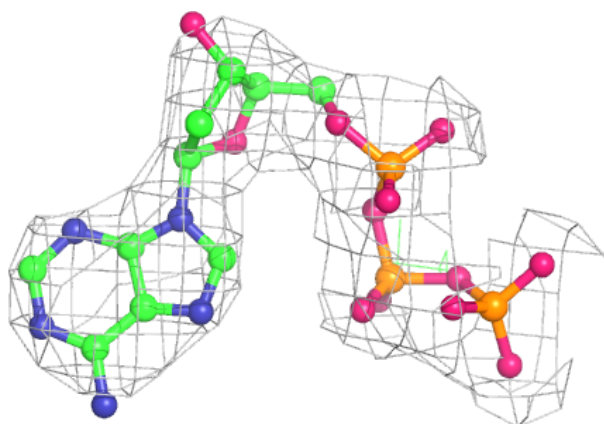
**Electron density around TTP A 804:**

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

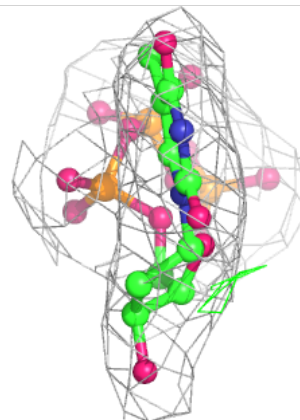
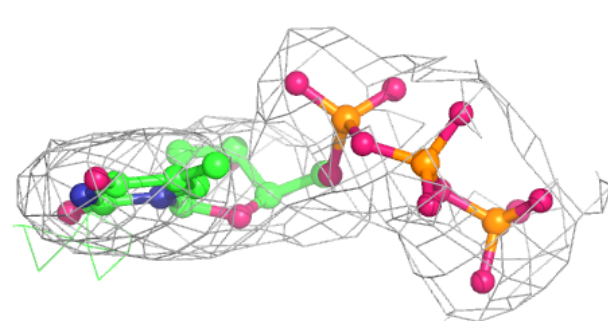
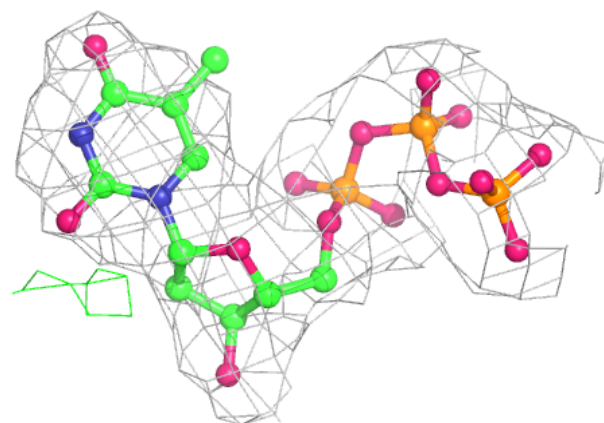


**Electron density around DTP B 805:**

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

**Electron density around TTP B 803:**

$2mF_o-DF_c$  (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.