



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2023 – 06:54 PM EDT

PDB ID : 4X3V  
Title : Crystal structure of human ribonucleotide reductase 1 bound to inhibitor  
Authors : Dealwis, C.G.; Ahmad, M.F.; Alam, I.  
Deposited on : 2014-12-01  
Resolution : 3.70 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35.1  
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

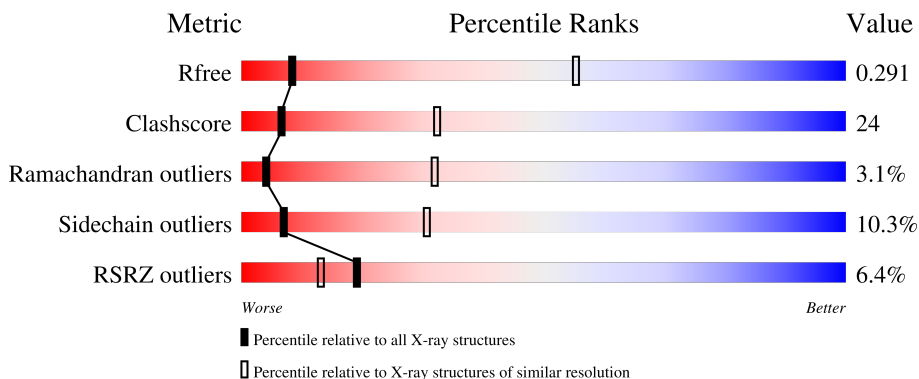
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.70 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	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)

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  $\geq 3$ , 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	
1	B	792	

## 2 Entry composition [i](#)

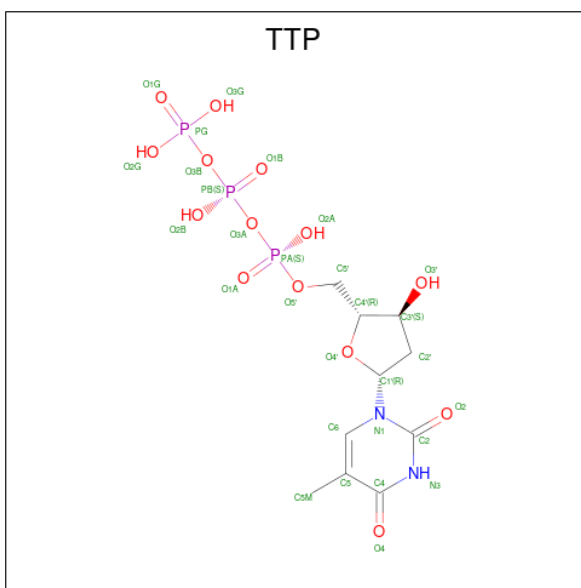
There are 3 unique types of molecules in this entry. The entry contains 11384 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

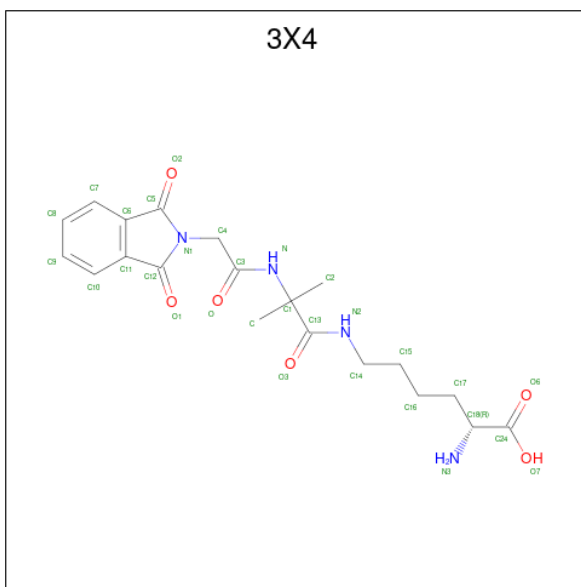
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	714	Total	C	N	O	S	7	0	0
			5545	3542	924	1047	32			
1	B	738	Total	C	N	O	S	0	0	0
			5751	3669	968	1080	34			

- 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
			Total	C	N	O	P		
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		

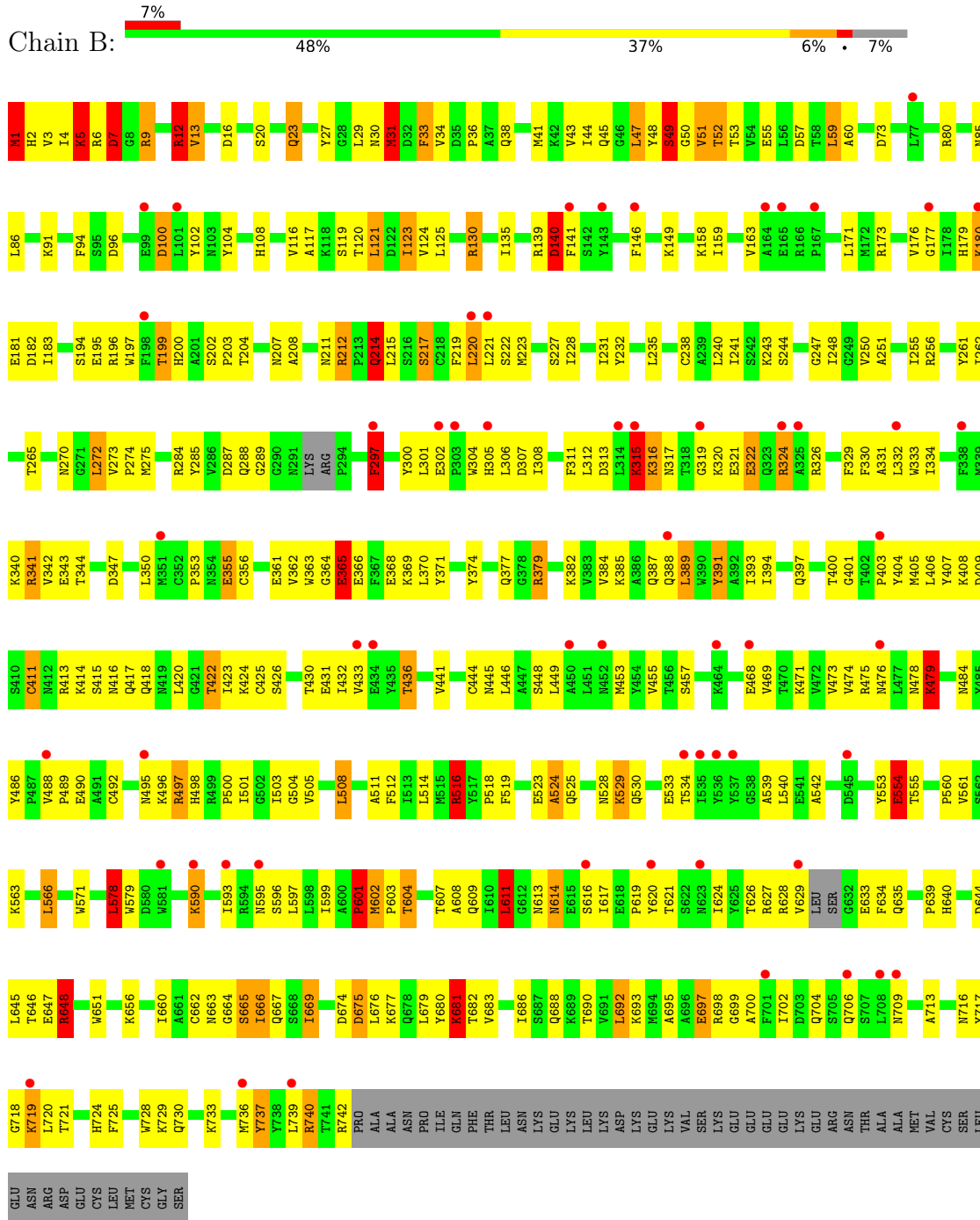
- Molecule 3 is N 6 -{N-[(1,3-dioxo-1,3-dihydro-2H-isoindol-2-yl)acetyl]-2-methyl-D-alanyl}-D-lysine (three-letter code: 3X4) (formula:  $C_{20}H_{26}N_4O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	30	20	4	6	0	0



● Molecule 1: Ribonucleoside-diphosphate reductase large subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.88Å 110.50Å 216.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.36 – 3.70 108.36 – 3.55	Depositor EDS
% Data completeness (in resolution range)	95.8 (108.36-3.70) 85.5 (108.36-3.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.58Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.232 , 0.289 0.236 , 0.291	Depositor DCC
$R_{free}$ test set	1987 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	110.3	Xtrriage
Anisotropy	0.294	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 64.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11384	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	121.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: 3X4, TTP

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	0.46	1/5666 (0.0%)	0.84	20/7709 (0.3%)
1	B	0.45	1/5877 (0.0%)	0.89	29/7989 (0.4%)
All	All	0.46	2/11543 (0.0%)	0.87	49/15698 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	8
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	GLU	CD-OE1	7.08	1.33	1.25
1	B	692	LEU	C-O	5.05	1.32	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	526	LEU	CA-CB-CG	15.65	151.29	115.30
1	B	590	LYS	CA-CB-CG	9.49	134.28	113.40
1	B	578	LEU	CA-CB-CG	9.40	136.91	115.30
1	A	656	LYS	CD-CE-NZ	8.93	132.24	111.70
1	B	648	ARG	CG-CD-NE	-7.65	95.74	111.80
1	B	140	ASP	CB-CG-OD2	7.44	125.00	118.30
1	B	1	MET	CB-CG-SD	-7.03	91.32	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	740	ARG	NE-CZ-NH2	-6.57	117.01	120.30
1	B	648	ARG	CB-CG-CD	6.44	128.34	111.60
1	B	31	MET	CB-CG-SD	6.33	131.40	112.40
1	B	675	ASP	CB-CG-OD1	6.30	123.97	118.30
1	B	590	LYS	N-CA-CB	6.29	121.93	110.60
1	B	590	LYS	CB-CG-CD	6.24	127.81	111.60
1	A	158	LYS	CD-CE-NZ	-6.04	97.80	111.70
1	A	413	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	B	648	ARG	CB-CA-C	5.94	122.28	110.40
1	A	650	LEU	CB-CG-CD2	-5.92	100.94	111.00
1	B	648	ARG	CA-CB-CG	5.89	126.36	113.40
1	B	611	LEU	CA-CB-CG	5.80	128.64	115.30
1	B	681	LYS	CD-CE-NZ	5.73	124.88	111.70
1	A	341	ARG	CG-CD-NE	5.71	123.78	111.80
1	A	689	LYS	CB-CG-CD	-5.70	96.78	111.60
1	B	315	LYS	N-CA-C	5.68	126.33	111.00
1	A	21	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	23	GLN	CA-CB-CG	5.62	125.77	113.40
1	B	578	LEU	CB-CG-CD2	5.61	120.53	111.00
1	B	365	GLU	OE1-CD-OE2	-5.60	116.58	123.30
1	B	5	LYS	CD-CE-NZ	5.51	124.36	111.70
1	B	326	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	A	23	GLN	N-CA-CB	5.50	120.49	110.60
1	A	587	LYS	CD-CE-NZ	5.49	124.32	111.70
1	B	479	LYS	CB-CG-CD	-5.41	97.53	111.60
1	A	223	MET	CA-CB-CG	5.30	122.31	113.30
1	B	12	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	223	MET	CB-CG-SD	5.26	128.18	112.40
1	B	212	ARG	CG-CD-NE	-5.25	100.78	111.80
1	A	465	LYS	CD-CE-NZ	-5.24	99.65	111.70
1	B	341	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	379	ARG	CB-CG-CD	5.20	125.11	111.60
1	A	413	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	A	224	LYS	CD-CE-NZ	-5.19	99.76	111.70
1	A	310	GLU	CA-CB-CG	5.18	124.81	113.40
1	A	341	ARG	CB-CG-CD	5.15	124.98	111.60
1	B	578	LEU	N-CA-C	-5.14	97.11	111.00
1	B	297	PHE	CB-CG-CD1	5.10	124.37	120.80
1	B	516	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	B	214	GLN	N-CA-C	-5.00	97.49	111.00
1	B	554	GLU	CB-CA-C	-5.00	100.40	110.40

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	287	ASP	Peptide
1	A	403	PRO	Peptide
1	A	546	LEU	Peptide
1	A	571	TRP	Peptide
1	A	655	MET	Peptide
1	A	91	LYS	Peptide
1	B	1	MET	Peptide
1	B	30	ASN	Peptide
1	B	315	LYS	Peptide
1	B	322	GLU	Peptide
1	B	524	ALA	Peptide
1	B	601	PRO	Peptide
1	B	614	ASN	Peptide
1	B	648	ARG	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5545	0	5342	250	0
1	B	5751	0	5586	281	0
2	A	29	0	13	5	0
2	B	29	0	13	4	0
3	A	30	0	25	3	0
All	All	11384	0	10979	527	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 24.

All (527) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:ARG:HG3	1:B:554:GLU:HG2	1.30	1.14
1:A:667:GLN:HE21	1:A:677:LYS:HB2	1.26	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:H2	1:B:12:ARG:HE	1.10	0.95
1:B:624:ILE:HD11	1:B:635:GLN:HE21	1.32	0.95
1:B:363:TRP:HD1	1:B:422:THR:HG23	1.31	0.93
1:A:52:THR:H	1:A:55:GLU:HG3	1.37	0.89
1:A:523:GLU:HA	1:A:526:LEU:HD23	1.53	0.89
1:A:270:ASN:H	2:A:801:TTP:HM53	1.37	0.87
1:A:404:TYR:HD1	1:A:404:TYR:H	1.18	0.86
1:B:365:GLU:HA	1:B:368:GLU:HG2	1.56	0.85
1:B:1:MET:N	1:B:12:ARG:HE	1.75	0.85
1:B:270:ASN:HB3	1:B:274:PRO:HG2	1.59	0.83
1:A:337:LEU:HG	1:A:368:GLU:HG2	1.58	0.83
1:B:455:VAL:HG11	1:B:514:LEU:HD22	1.58	0.83
1:B:361:GLU:HG2	1:B:424:LYS:HE2	1.60	0.83
1:A:302:GLU:HG2	1:A:333:TRP:HB3	1.59	0.82
1:B:611:LEU:HD12	1:B:613:ASN:ND2	1.94	0.81
1:B:227:SER:HA	2:B:801:TTP:H5'1	1.65	0.79
1:B:315:LYS:HD2	1:B:330:PHE:CD2	2.17	0.79
1:A:57:ASP:OD2	1:A:85:ASN:ND2	2.15	0.79
1:A:52:THR:N	1:A:55:GLU:HG3	1.99	0.77
1:A:336:ASP:HA	1:A:728:TRP:HE1	1.50	0.77
1:A:667:GLN:HE21	1:A:677:LYS:CB	1.97	0.76
1:B:418:GLN:HE21	1:B:560:PRO:HG3	1.50	0.76
1:A:256:ARG:NH2	1:A:261:TYR:O	2.19	0.76
1:B:1:MET:HG2	1:B:2:HIS:HB2	1.68	0.75
1:A:340:LYS:O	1:A:344:THR:OG1	2.05	0.75
1:B:256:ARG:NH2	2:B:801:TTP:O3B	2.20	0.75
1:B:616:SER:OG	1:B:617:ILE:N	2.19	0.75
1:A:397:GLN:HB3	1:A:739:LEU:HD12	1.69	0.75
1:A:395:GLU:HG3	1:A:717:TYR:HE1	1.52	0.75
1:B:215:LEU:N	1:B:484:ASN:OD1	2.20	0.75
1:B:363:TRP:CD1	1:B:422:THR:HG23	2.20	0.74
1:B:501:ILE:HG12	1:B:595:ASN:HD22	1.52	0.74
1:A:118:LYS:O	1:A:122:ASP:HB2	1.86	0.74
1:B:315:LYS:HD2	1:B:330:PHE:HD2	1.51	0.74
1:B:667:GLN:HA	1:B:677:LYS:HD3	1.70	0.74
1:B:44:ILE:HA	1:B:47:LEU:HD12	1.69	0.73
1:B:1:MET:HA	1:B:12:ARG:HH11	1.53	0.73
1:B:730:GLN:O	1:B:730:GLN:HG2	1.87	0.73
1:B:406:LEU:HD11	1:B:430:THR:HB	1.71	0.73
1:A:270:ASN:N	2:A:801:TTP:HM53	2.04	0.72
1:A:171:LEU:HD23	1:A:193:LEU:HB3	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:GLN:HG3	1:B:244:SER:HB3	1.71	0.72
1:B:709:ASN:OD1	1:B:740:ARG:NH2	2.16	0.72
1:A:662:CYS:HB3	1:A:665:SER:HB3	1.72	0.71
1:A:310:GLU:N	1:A:310:GLU:OE1	2.24	0.71
1:A:312:LEU:HD22	1:A:393:ILE:HA	1.72	0.71
1:B:1:MET:HB3	1:B:13:VAL:HG23	1.72	0.71
1:A:337:LEU:HB3	1:A:341:ARG:HD3	1.73	0.71
1:A:546:LEU:HD12	1:A:594:ARG:HB2	1.71	0.71
1:A:624:ILE:HD13	1:A:660:ILE:HG12	1.73	0.70
1:B:604:THR:HB	1:B:607:THR:HG23	1.71	0.70
1:A:446:LEU:HB3	1:A:602:MET:CE	2.22	0.70
1:B:256:ARG:NH1	1:B:261:TYR:O	2.26	0.69
1:A:348:TRP:HB2	1:A:386:ALA:HB2	1.74	0.69
1:B:140:ASP:OD1	1:B:140:ASP:N	2.22	0.69
1:A:516:ARG:NH2	1:A:644:ASP:OD2	2.26	0.69
1:B:80:ARG:HD3	1:B:141:PHE:HB3	1.75	0.68
1:A:537:TYR:CE2	1:A:579:TRP:HB3	2.29	0.68
1:A:23:GLN:HB3	1:A:26:CYS:HB2	1.75	0.68
1:A:504:GLY:HA3	1:A:602:MET:SD	2.34	0.68
1:B:725:PHE:O	1:B:729:LYS:HB2	1.93	0.67
1:A:499:ARG:HE	1:A:594:ARG:HD2	1.58	0.67
1:B:341:ARG:HD3	1:B:347:ASP:O	1.95	0.67
1:B:418:GLN:NE2	1:B:560:PRO:HG3	2.10	0.67
1:A:446:LEU:HB3	1:A:602:MET:HE1	1.77	0.67
1:B:603:PRO:HA	1:B:616:SER:HB2	1.76	0.67
1:A:516:ARG:NH1	1:A:679:LEU:HD13	2.09	0.66
1:A:261:TYR:HA	1:A:268:ASN:HD22	1.60	0.66
1:B:530:GLN:HB3	1:B:578:LEU:HD21	1.77	0.66
1:A:284:ARG:NH1	1:B:322:GLU:O	2.28	0.66
1:A:465:LYS:HA	1:A:468:GLU:HB2	1.78	0.66
1:A:481:ILE:HG23	1:A:495:ASN:ND2	2.11	0.66
1:B:498:HIS:HB2	1:B:500:PRO:HD3	1.76	0.66
1:B:43:VAL:HG22	1:B:59:LEU:HD22	1.76	0.66
1:A:667:GLN:NE2	1:A:677:LYS:HB2	2.06	0.66
1:B:300:TYR:HE2	1:B:406:LEU:HD13	1.61	0.66
1:A:179:HIS:HB3	1:A:182:ASP:HB3	1.77	0.65
1:B:401:GLY:HA2	1:B:739:LEU:HB2	1.78	0.65
1:B:423:ILE:HD13	1:B:433:VAL:HG12	1.78	0.65
1:A:471:LYS:HA	1:A:542:ALA:HB2	1.78	0.65
1:B:397:GLN:HB3	1:B:739:LEU:HD12	1.79	0.65
1:B:52:THR:HG23	1:B:55:GLU:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:GLY:HA3	1:B:602:MET:HG2	1.78	0.64
1:B:647:GLU:O	1:B:648:ARG:HB3	1.97	0.64
1:A:537:TYR:CD1	1:A:584:LEU:HD22	2.33	0.64
1:A:69:THR:HG21	1:A:656:LYS:NZ	2.12	0.64
1:B:256:ARG:HH12	1:B:262:ILE:HA	1.61	0.64
1:A:650:LEU:HG	1:A:650:LEU:O	1.98	0.64
1:A:337:LEU:CG	1:A:368:GLU:HG2	2.28	0.64
1:B:614:ASN:HD21	1:B:620:TYR:HA	1.63	0.63
1:A:556:TYR:HE2	1:A:561:VAL:HG23	1.64	0.63
1:B:7:ASP:HB3	1:B:9:ARG:H	1.64	0.63
1:B:52:THR:HG23	1:B:55:GLU:CB	2.29	0.63
1:B:355:GLU:O	1:B:379:ARG:HD2	1.99	0.63
1:A:423:ILE:HD13	1:A:433:VAL:HG12	1.81	0.63
1:B:48:TYR:O	1:B:50:GLY:N	2.31	0.63
1:B:297:PHE:HD1	1:B:297:PHE:N	1.97	0.63
1:A:449:LEU:H	1:A:505:VAL:HA	1.62	0.62
1:A:256:ARG:NH1	2:A:801:TTP:O1B	2.32	0.62
1:B:31:MET:HA	1:B:34:VAL:HB	1.80	0.62
1:B:272:LEU:HD11	1:B:305:HIS:CE1	2.33	0.62
1:A:170:MET:HG2	1:A:173:ARG:HH21	1.63	0.62
1:B:676:LEU:HD22	1:B:680:TYR:HE1	1.64	0.62
1:B:1:MET:H2	1:B:12:ARG:NE	1.91	0.61
1:B:179:HIS:HB3	1:B:182:ASP:HB3	1.81	0.61
1:B:207:ASN:N	1:B:207:ASN:OD1	2.33	0.61
1:B:341:ARG:HH12	1:B:371:TYR:HE2	1.49	0.61
1:A:486:TYR:OH	1:A:495:ASN:ND2	2.27	0.61
1:B:604:THR:OG1	1:B:608:ALA:HB2	2.00	0.61
1:A:445:ASN:HD21	1:A:481:ILE:HG12	1.66	0.61
1:B:475:ARG:O	1:B:479:LYS:HG3	2.01	0.61
1:A:375:GLU:HA	1:A:375:GLU:OE1	2.00	0.60
1:A:452:ASN:ND2	1:A:613:ASN:OD1	2.28	0.60
1:B:1:MET:HB3	1:B:13:VAL:CG2	2.31	0.60
1:B:690:THR:O	1:B:693:LYS:HB3	2.02	0.60
1:B:341:ARG:NH1	1:B:371:TYR:HE2	2.00	0.60
3:A:802:3X4:C3	3:A:802:3X4:H23	2.15	0.60
1:B:365:GLU:CD	1:B:413:ARG:HH22	2.05	0.60
1:A:192:LEU:HA	1:A:197:TRP:HD1	1.67	0.59
1:A:402:THR:HG22	1:A:404:TYR:CE1	2.37	0.59
1:B:57:ASP:HA	1:B:60:ALA:HB3	1.84	0.59
1:B:468:GLU:HA	1:B:471:LYS:HB2	1.84	0.59
1:A:340:LYS:HA	1:A:343:GLU:OE2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLN:HG2	1:A:488:VAL:HG11	1.84	0.59
1:B:251:ALA:HB2	1:B:425:CYS:HB3	1.84	0.59
1:A:32:ASP:OD1	1:A:32:ASP:N	2.35	0.59
1:B:331:ALA:HB2	1:B:404:TYR:HD2	1.67	0.59
1:B:611:LEU:HD12	1:B:613:ASN:HD22	1.67	0.59
1:B:297:PHE:N	1:B:297:PHE:CD1	2.69	0.59
1:A:374:TYR:HD2	1:A:379:ARG:HD2	1.67	0.58
1:B:621:THR:HA	1:B:683:VAL:HG12	1.85	0.58
1:A:285:TYR:O	1:B:270:ASN:ND2	2.35	0.58
1:A:275:MET:HG3	1:B:285:TYR:CZ	2.38	0.58
1:A:341:ARG:HH12	1:A:346:GLN:HE21	1.52	0.58
1:B:302:GLU:HG2	1:B:333:TRP:HB3	1.86	0.58
1:B:405:MET:HG3	1:B:724:HIS:CE1	2.37	0.58
1:B:528:ASN:HD21	1:B:698:ARG:HH21	1.52	0.58
2:A:801:TTP:HM52	1:B:285:TYR:CE2	2.38	0.58
1:B:709:ASN:HD21	1:B:737:TYR:HD2	1.50	0.58
1:A:300:TYR:HE2	1:A:406:LEU:HD13	1.69	0.58
1:B:149:LYS:HD2	1:B:629:VAL:HG21	1.85	0.58
1:A:404:TYR:CD1	1:A:404:TYR:N	2.70	0.57
1:B:287:ASP:HB2	1:B:289:GLY:H	1.69	0.57
1:B:377:GLN:OE1	1:B:379:ARG:NH2	2.25	0.57
1:B:501:ILE:HG12	1:B:595:ASN:ND2	2.19	0.57
1:A:23:GLN:C	1:A:25:LEU:H	2.07	0.57
1:B:57:ASP:OD2	1:B:85:ASN:ND2	2.37	0.57
1:A:690:THR:HA	1:A:693:LYS:HB2	1.86	0.57
1:B:29:LEU:HD22	1:B:73:ASP:HB3	1.86	0.57
1:B:139:ARG:NH1	1:B:194:SER:OG	2.38	0.57
1:B:350:LEU:HB2	1:B:382:LYS:HB2	1.86	0.57
1:A:410:SER:O	1:A:414:LYS:HG3	2.04	0.57
1:B:397:GLN:HG3	1:B:403:PRO:HD2	1.86	0.57
1:B:524:ALA:O	1:B:528:ASN:N	2.35	0.57
1:B:203:PRO:HG2	1:B:217:SER:HA	1.87	0.57
1:B:614:ASN:ND2	1:B:620:TYR:HA	2.20	0.57
1:A:497:ARG:HA	1:A:554:GLU:HG2	1.87	0.57
1:A:626:THR:HG22	1:A:635:GLN:HA	1.86	0.57
1:B:688:GLN:O	1:B:692:LEU:HD12	2.04	0.57
1:A:603:PRO:HA	1:A:616:SER:HB2	1.86	0.57
1:A:655:MET:SD	1:A:669:ILE:HD12	2.45	0.57
1:B:33:PHE:CE2	1:B:646:THR:HB	2.40	0.56
1:A:69:THR:HG21	1:A:656:LYS:HZ2	1.70	0.56
1:A:222:SER:HA	1:A:251:ALA:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:LEU:HD12	1:B:613:ASN:HD21	1.70	0.56
1:A:139:ARG:NH1	1:A:194:SER:OG	2.39	0.56
1:A:404:TYR:HD1	1:A:404:TYR:N	1.98	0.56
1:B:227:SER:O	1:B:231:ILE:N	2.37	0.56
1:B:256:ARG:HH22	2:B:801:TTP:PG	2.29	0.56
1:B:662:CYS:HB3	1:B:665:SER:HB3	1.88	0.56
1:B:1:MET:CA	1:B:12:ARG:HH11	2.20	0.55
1:B:49:SER:OG	1:B:49:SER:O	2.23	0.55
1:B:391:TYR:HD2	1:B:717:TYR:CD1	2.24	0.55
1:B:312:LEU:HD21	1:B:393:ILE:HA	1.89	0.55
1:B:214:GLN:HE21	1:B:244:SER:HB2	1.72	0.55
1:A:397:GLN:HB3	1:A:739:LEU:CD1	2.36	0.54
1:A:687:SER:OG	1:A:689:LYS:HD2	2.07	0.54
1:B:495:ASN:OD1	1:B:495:ASN:O	2.25	0.54
1:B:699:GLY:HA2	1:B:702:ILE:HD12	1.89	0.54
1:A:404:TYR:CE2	1:A:737:TYR:HE1	2.24	0.54
1:A:537:TYR:CE1	1:A:584:LEU:HD13	2.42	0.54
1:A:339:MET:HB2	1:A:728:TRP:CZ2	2.42	0.54
1:B:528:ASN:HD21	1:B:698:ARG:NH2	2.05	0.54
1:A:389:LEU:HD23	1:A:393:ILE:HD11	1.90	0.54
1:A:739:LEU:C	1:A:740:ARG:HG2	2.27	0.54
1:A:214:GLN:NE2	1:A:487:PRO:HD3	2.23	0.54
1:A:372:ALA:HA	1:A:375:GLU:HB2	1.90	0.54
1:B:304:TRP:HH2	1:B:353:PRO:HB3	1.72	0.54
1:B:709:ASN:N	1:B:709:ASN:HD22	2.05	0.54
1:A:285:TYR:CZ	1:B:275:MET:HG3	2.43	0.54
1:A:535:ILE:HG22	1:A:599:ILE:HD12	1.90	0.53
1:A:537:TYR:HB2	1:A:581:TRP:CH2	2.42	0.53
1:B:23:GLN:OE1	1:B:36:PRO:HG2	2.07	0.53
1:B:342:VAL:HG13	1:B:387:GLN:HG2	1.90	0.53
1:B:171:LEU:HD23	1:B:194:SER:HA	1.91	0.53
1:A:334:ILE:O	1:A:408:LYS:N	2.41	0.53
1:B:308:ILE:HG13	1:B:389:LEU:HD21	1.90	0.53
1:B:223:MET:HG2	1:B:255:ILE:HD11	1.91	0.53
1:B:301:LEU:HD11	1:B:305:HIS:HB3	1.91	0.53
1:A:495:ASN:OD1	1:A:500:PRO:HD2	2.08	0.53
1:B:384:VAL:HB	1:B:388:GLN:OE1	2.09	0.53
1:A:130:ARG:HE	1:A:187:ILE:CD1	2.22	0.52
1:A:333:TRP:NE1	1:A:408:LYS:HG3	2.24	0.52
1:A:434:GLU:HG2	1:A:597:LEU:HD12	1.91	0.52
1:A:59:LEU:HA	1:A:62:GLU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:CYS:HA	1:A:29:LEU:HD12	1.90	0.52
1:A:301:LEU:HD11	1:A:305:HIS:HB3	1.91	0.52
1:A:602:MET:HB2	1:A:604:THR:HG23	1.90	0.52
1:B:240:LEU:O	1:B:243:LYS:HB3	2.09	0.52
1:B:667:GLN:HE22	1:B:681:LYS:HA	1.75	0.52
1:A:405:MET:O	1:A:735:GLY:N	2.43	0.52
1:A:18:ILE:O	1:A:22:ILE:HG12	2.10	0.52
1:A:339:MET:HG3	1:A:728:TRP:CD1	2.45	0.52
1:A:616:SER:OG	1:A:617:ILE:N	2.43	0.52
1:B:474:VAL:HG21	1:B:539:ALA:HA	1.90	0.52
1:A:599:ILE:HB	1:A:702:ILE:HA	1.91	0.52
1:B:347:ASP:HA	1:B:385:LYS:HA	1.91	0.52
1:B:518:PRO:HA	1:B:679:LEU:HA	1.91	0.52
1:B:199:THR:HG22	1:B:448:SER:HB2	1.92	0.52
1:A:695:ALA:HB1	1:A:708:LEU:HD11	1.91	0.51
1:A:67:LEU:C	1:A:69:THR:H	2.12	0.51
1:A:537:TYR:HE2	1:A:579:TRP:HB3	1.72	0.51
1:B:709:ASN:ND2	1:B:737:TYR:HD2	2.09	0.51
1:B:57:ASP:HB2	1:B:85:ASN:HD22	1.76	0.51
1:B:214:GLN:HE21	1:B:244:SER:CB	2.23	0.51
1:B:709:ASN:ND2	1:B:737:TYR:HB3	2.25	0.51
1:A:720:LEU:HD21	1:A:739:LEU:HD11	1.92	0.51
1:A:130:ARG:HE	1:A:187:ILE:HD12	1.76	0.51
1:A:499:ARG:HG3	1:A:553:TYR:HB2	1.91	0.51
1:A:407:TYR:CD1	1:A:728:TRP:HB2	2.46	0.51
1:A:407:TYR:CE1	1:A:728:TRP:HB2	2.45	0.51
1:B:146:PHE:HE1	1:B:634:PHE:HB2	1.76	0.51
1:B:96:ASP:O	1:B:100:ASP:HB2	2.11	0.50
1:B:492:CYS:O	1:B:496:LYS:HB2	2.11	0.50
1:A:498:HIS:HB2	1:A:500:PRO:HD3	1.94	0.50
1:B:238:CYS:HB2	1:B:248:ILE:HD13	1.93	0.50
1:B:449:LEU:HB2	1:B:505:VAL:HG12	1.93	0.50
1:B:571:TRP:CD1	1:B:700:ALA:HA	2.47	0.50
1:A:167:PRO:O	1:A:171:LEU:HD12	2.11	0.50
1:B:718:GLY:HA2	1:B:721:THR:HB	1.92	0.50
1:A:649:GLY:O	1:A:651:TRP:N	2.40	0.50
1:A:650:LEU:HD12	1:A:671:GLU:HB2	1.94	0.50
1:B:341:ARG:HA	1:B:344:THR:OG1	2.11	0.50
1:A:446:LEU:HB3	1:A:602:MET:HE3	1.94	0.50
1:B:200:HIS:HB3	1:B:204:THR:HB	1.93	0.50
1:B:315:LYS:HE3	1:B:329:PHE:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:THR:HG23	1:B:441:VAL:HA	1.94	0.50
1:A:277:ARG:HH11	1:B:284:ARG:HH12	1.60	0.50
1:A:395:GLU:HG3	1:A:717:TYR:CE1	2.40	0.50
1:B:44:ILE:HG12	1:B:47:LEU:HD12	1.94	0.50
1:B:221:LEU:HB2	1:B:250:VAL:HG22	1.94	0.50
1:A:341:ARG:O	1:A:386:ALA:HB3	2.12	0.49
1:B:634:PHE:CD1	1:B:634:PHE:N	2.80	0.49
1:A:52:THR:H	1:A:55:GLU:CG	2.16	0.49
1:A:173:ARG:NH1	1:A:208:ALA:O	2.45	0.49
1:A:241:ILE:HB	1:A:248:ILE:HD11	1.93	0.49
1:A:526:LEU:O	1:A:529:LYS:HB2	2.12	0.49
1:A:629:VAL:HB	1:A:634:PHE:HE1	1.77	0.49
1:A:276:LEU:HD21	1:A:299:ILE:HG21	1.94	0.49
1:A:499:ARG:HE	1:A:594:ARG:CD	2.24	0.49
1:B:3:VAL:HG12	1:B:51:VAL:O	2.13	0.49
1:B:4:ILE:HG13	1:B:9:ARG:O	2.12	0.49
1:B:497:ARG:CG	1:B:554:GLU:HG2	2.21	0.49
1:B:681:LYS:HD3	1:B:686:ILE:HG12	1.95	0.49
1:A:349:SER:HB3	1:A:380:VAL:HG21	1.94	0.49
1:B:179:HIS:NE2	1:B:476:ASN:OD1	2.46	0.49
1:B:400:THR:OG1	1:B:401:GLY:N	2.45	0.49
1:A:288:GLN:HG3	1:B:265:THR:HG22	1.94	0.49
1:B:91:LYS:HE2	1:B:96:ASP:OD2	2.13	0.49
1:A:544:CYS:HA	1:A:592:GLY:O	2.11	0.49
1:B:363:TRP:CE3	1:B:364:GLY:HA3	2.48	0.49
1:B:416:ASN:H	1:B:597:LEU:HD21	1.77	0.49
1:B:121:LEU:HD22	1:B:125:LEU:CD1	2.42	0.49
1:A:420:LEU:HD13	1:A:498:HIS:CD2	2.48	0.49
1:A:93:VAL:HG13	1:A:96:ASP:HB2	1.95	0.49
1:B:5:LYS:HB3	1:B:6:ARG:H	1.24	0.49
1:B:273:VAL:HB	1:B:274:PRO:HD3	1.95	0.49
1:B:1:MET:N	1:B:12:ARG:NE	2.52	0.48
1:B:29:LEU:HD21	1:B:80:ARG:HH21	1.78	0.48
1:A:333:TRP:CD1	1:A:408:LYS:HG3	2.48	0.48
1:A:530:GLN:HG2	1:A:578:LEU:HD22	1.94	0.48
3:A:802:3X4:O1	3:A:802:3X4:N	2.46	0.48
1:B:130:ARG:HH21	1:B:183:ILE:HG22	1.78	0.48
1:B:332:LEU:HG	1:B:403:PRO:HB2	1.95	0.48
1:B:626:THR:HG22	1:B:635:GLN:HA	1.93	0.48
1:B:690:THR:HA	1:B:693:LYS:HB3	1.96	0.48
1:A:201:ALA:HB2	1:A:446:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:GLY:O	1:B:666:ILE:N	2.47	0.48
1:A:247:GLY:HA3	1:A:428:LEU:CD2	2.43	0.48
1:A:705:SER:OG	1:A:706:GLN:N	2.40	0.48
1:B:415:SER:O	1:B:418:GLN:HG3	2.13	0.48
1:B:431:GLU:HG2	1:B:432:ILE:HG12	1.95	0.48
1:B:540:LEU:HD11	1:B:566:LEU:HD21	1.96	0.48
1:A:79:ALA:HB2	1:A:145:TYR:N	2.28	0.48
1:A:107:PRO:HG3	1:A:160:ASN:HD21	1.78	0.48
1:A:338:PHE:O	1:A:342:VAL:HG23	2.13	0.48
1:B:669:ILE:H	1:B:669:ILE:HG13	1.49	0.48
1:B:414:LYS:HB2	1:B:733:LYS:HE2	1.96	0.48
1:B:530:GLN:HA	1:B:533:GLU:HB2	1.94	0.48
1:B:656:LYS:O	1:B:660:ILE:HG13	2.13	0.48
1:A:102:TYR:OH	1:A:118:LYS:HD2	2.13	0.48
1:B:645:LEU:HB3	1:B:651:TRP:HB2	1.96	0.48
1:B:695:ALA:O	1:B:699:GLY:N	2.45	0.48
1:A:397:GLN:HG3	1:A:403:PRO:HD2	1.96	0.48
1:B:486:TYR:OH	1:B:495:ASN:ND2	2.47	0.48
1:A:427:ASN:OD1	1:A:430:THR:N	2.48	0.47
1:A:516:ARG:HH11	1:A:679:LEU:HD13	1.76	0.47
1:A:561:VAL:HG21	1:A:593:ILE:HD11	1.94	0.47
1:A:39:ILE:O	1:A:43:VAL:HG23	2.14	0.47
1:A:204:THR:HA	1:A:215:LEU:HD22	1.96	0.47
1:B:624:ILE:HD13	1:B:660:ILE:HG12	1.96	0.47
1:A:274:PRO:HB2	1:B:285:TYR:HD2	1.79	0.47
1:B:602:MET:O	1:B:602:MET:HG3	2.14	0.47
1:A:33:PHE:CD1	1:A:33:PHE:N	2.82	0.47
1:A:97:VAL:HG21	1:A:169:HIS:ND1	2.30	0.47
1:B:41:MET:O	1:B:45:GLN:HB2	2.13	0.47
1:B:356:CYS:HB3	1:B:374:TYR:CE1	2.50	0.47
1:B:471:LYS:HG2	1:B:475:ARG:HH21	1.80	0.47
1:A:117:ALA:O	1:A:121:LEU:N	2.36	0.47
1:A:225:ASP:HB2	1:A:230:GLY:HA3	1.97	0.47
1:A:478:ASN:HD21	1:A:499:ARG:NH2	2.13	0.47
1:B:124:VAL:HG22	1:B:176:VAL:HG11	1.95	0.47
1:A:223:MET:SD	1:A:231:ILE:HA	2.55	0.47
1:A:480:ILE:O	1:A:484:ASN:HB2	2.15	0.47
1:A:650:LEU:HD11	1:A:672:ILE:HA	1.97	0.47
1:B:222:SER:OG	1:B:436:THR:HB	2.14	0.47
1:B:468:GLU:O	1:B:468:GLU:HG2	2.14	0.47
1:B:202:SER:HB2	1:B:203:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:GLY:HA3	1:B:324:ARG:HH11	1.79	0.47
1:A:221:LEU:HD22	1:A:234:THR:HG23	1.97	0.47
1:B:200:HIS:HE1	1:B:476:ASN:HB3	1.79	0.47
1:A:207:ASN:HB3	1:A:210:THR:OG1	2.14	0.47
1:A:356:CYS:HB3	1:A:374:TYR:CD1	2.49	0.47
1:A:499:ARG:HB2	1:A:594:ARG:O	2.15	0.47
1:B:196:ARG:O	1:B:453:MET:HG3	2.15	0.47
1:B:320:LYS:H	1:B:324:ARG:HD2	1.80	0.47
1:A:66:THR:HA	1:A:634:PHE:HD2	1.80	0.46
1:A:687:SER:O	1:A:690:THR:OG1	2.31	0.46
1:B:52:THR:HG23	1:B:55:GLU:HB2	1.97	0.46
1:B:208:ALA:HA	1:B:215:LEU:HD21	1.97	0.46
1:B:300:TYR:CE2	1:B:406:LEU:HD13	2.47	0.46
1:B:391:TYR:HD2	1:B:717:TYR:HD1	1.61	0.46
1:B:497:ARG:O	1:B:553:TYR:HB2	2.15	0.46
1:B:256:ARG:NH1	1:B:262:ILE:HA	2.28	0.46
1:B:602:MET:HA	1:B:603:PRO:HD3	1.81	0.46
1:B:200:HIS:HD1	1:B:204:THR:HG21	1.81	0.46
1:B:220:LEU:HD21	1:B:432:ILE:HG22	1.96	0.46
1:B:308:ILE:HG21	1:B:389:LEU:HD11	1.97	0.46
1:B:5:LYS:HZ3	1:B:9:ARG:NE	2.13	0.46
1:A:14:MET:SD	1:A:15:PHE:N	2.89	0.46
1:A:469:VAL:O	1:A:473:VAL:HG23	2.16	0.46
1:B:1:MET:N	1:B:12:ARG:HH11	2.14	0.46
1:B:102:TYR:CB	1:B:121:LEU:HD12	2.46	0.46
1:B:364:GLY:H	1:B:409:ASP:CG	2.19	0.46
1:B:340:LYS:O	1:B:344:THR:HG23	2.16	0.46
1:B:529:LYS:CE	1:B:697:GLU:HG2	2.45	0.46
1:A:224:LYS:HE3	1:A:237:GLN:NE2	2.31	0.46
1:A:604:THR:HB	1:A:607:THR:HG22	1.97	0.46
1:B:173:ARG:O	1:B:177:GLY:N	2.43	0.46
1:B:420:LEU:HD22	1:B:498:HIS:NE2	2.31	0.46
1:B:471:LYS:HA	1:B:542:ALA:HB2	1.98	0.46
1:B:553:TYR:O	1:B:555:THR:N	2.49	0.46
1:A:94:PHE:HA	1:A:169:HIS:CD2	2.51	0.45
1:A:304:TRP:HH2	1:A:353:PRO:HB3	1.80	0.45
1:A:553:TYR:CZ	1:A:556:TYR:HA	2.50	0.45
1:B:86:LEU:HD11	1:B:163:VAL:HG21	1.97	0.45
1:A:513:ILE:HA	1:A:679:LEU:HD21	1.99	0.45
1:B:313:ASP:HA	1:B:316:LYS:HE3	1.99	0.45
1:B:445:ASN:ND2	1:B:500:PRO:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:GLN:HA	1:A:677:LYS:HD2	1.99	0.45
1:B:311:PHE:CE1	1:B:330:PHE:HD1	2.35	0.45
1:B:516:ARG:NH2	1:B:644:ASP:OD2	2.44	0.45
1:A:306:LEU:CD2	1:A:381:ARG:HH21	2.29	0.45
1:A:341:ARG:NH1	1:A:346:GLN:HE21	2.14	0.45
1:B:57:ASP:CB	1:B:85:ASN:HD22	2.29	0.45
1:A:652:HIS:O	1:A:656:LYS:HB2	2.16	0.45
1:B:94:PHE:HB2	1:B:135:ILE:HD12	1.98	0.45
1:A:545:ASP:O	1:A:549:GLU:HG3	2.17	0.45
1:B:5:LYS:HZ3	1:B:9:ARG:HE	1.64	0.45
1:A:78:ALA:HA	1:A:81:ILE:HD12	1.99	0.45
1:A:94:PHE:HB2	1:A:135:ILE:HD12	1.99	0.45
1:A:280:ASN:HA	1:A:328:LEU:HG	1.99	0.45
1:A:400:THR:OG1	1:A:401:GLY:N	2.49	0.45
1:A:470:THR:O	1:A:474:VAL:HG23	2.17	0.45
1:B:508:LEU:HD12	1:B:508:LEU:O	2.17	0.45
1:B:519:PHE:CD2	1:B:619:PRO:HB3	2.52	0.45
1:B:709:ASN:N	1:B:709:ASN:ND2	2.65	0.45
1:A:247:GLY:HA3	1:A:428:LEU:HD22	1.99	0.44
1:B:599:ILE:HG22	1:B:601:PRO:HD3	1.98	0.44
1:A:37:ALA:O	1:A:41:MET:HB2	2.17	0.44
1:B:232:TYR:HA	1:B:235:LEU:HB3	2.00	0.44
1:A:203:PRO:HG2	1:A:217:SER:HB3	1.98	0.44
1:A:341:ARG:HB3	1:A:346:GLN:CG	2.47	0.44
1:B:609:GLN:CB	1:B:627:ARG:NH1	2.81	0.44
1:A:195:GLU:HB3	1:A:197:TRP:CD1	2.52	0.44
1:B:104:TYR:CE1	1:B:159:ILE:HG23	2.53	0.44
1:B:334:ILE:O	1:B:408:LYS:N	2.51	0.44
1:B:690:THR:C	1:B:693:LYS:HB3	2.38	0.44
1:A:500:PRO:HB3	1:A:596:SER:OG	2.18	0.44
1:A:705:SER:OG	1:A:734:THR:OG1	2.31	0.44
1:B:448:SER:O	1:B:449:LEU:HD23	2.18	0.44
1:A:684:TRP:CZ3	1:A:711:HIS:HB3	2.53	0.44
1:B:446:LEU:HB3	1:B:602:MET:SD	2.58	0.44
1:A:576:THR:HG22	1:A:578:LEU:H	1.82	0.43
1:A:645:LEU:HB3	1:A:651:TRP:HB2	2.00	0.43
1:B:38:GLN:HA	1:B:41:MET:SD	2.58	0.43
1:B:241:ILE:HB	1:B:248:ILE:HD11	1.98	0.43
1:B:315:LYS:HD2	1:B:330:PHE:CE2	2.52	0.43
1:B:514:LEU:HD23	1:B:514:LEU:O	2.17	0.43
1:B:634:PHE:N	1:B:634:PHE:HD1	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ILE:HD12	1:A:139:ARG:CZ	2.48	0.43
1:A:638:ASN:HB3	1:A:641:LEU:HB3	2.00	0.43
1:B:1:MET:HG2	1:B:2:HIS:CB	2.44	0.43
1:B:713:ALA:HB2	1:B:742:ARG:HH22	1.83	0.43
1:A:351:MET:HB3	1:A:356:CYS:SG	2.58	0.43
1:B:665:SER:C	1:B:667:GLN:H	2.22	0.43
1:A:431:GLU:OE2	1:A:603:PRO:HD3	2.18	0.43
1:B:441:VAL:HG22	1:B:490:GLU:HB2	1.99	0.43
1:B:508:LEU:HA	1:B:511:ALA:HB3	2.01	0.43
1:A:91:LYS:NZ	1:A:100:ASP:OD1	2.41	0.43
1:A:92:LYS:HA	1:A:166:ARG:CZ	2.49	0.43
1:A:392:ALA:HA	1:A:395:GLU:OE1	2.18	0.43
1:B:120:THR:O	1:B:124:VAL:HG23	2.19	0.43
1:B:599:ILE:HB	1:B:702:ILE:HA	2.01	0.43
1:B:377:GLN:CD	1:B:379:ARG:HH21	2.15	0.43
1:A:326:ARG:HG3	1:A:326:ARG:HH11	1.82	0.43
1:A:362:VAL:HG13	1:A:367:PHE:HD2	1.83	0.43
1:A:394:ILE:HG23	1:A:720:LEU:HD13	2.00	0.43
1:A:645:LEU:HD13	1:A:651:TRP:CE3	2.53	0.43
1:B:534:THR:HA	1:B:579:TRP:HE1	1.84	0.43
1:B:716:ASN:HB3	1:B:719:LYS:HB3	2.00	0.43
1:A:25:LEU:HD22	1:A:80:ARG:HB3	2.01	0.43
1:A:29:LEU:CD1	1:A:77:LEU:HB2	2.49	0.43
1:A:226:ASP:OD1	1:A:256:ARG:HG2	2.19	0.43
1:A:227:SER:O	1:A:231:ILE:N	2.49	0.43
1:B:561:VAL:HG21	1:B:593:ILE:HD11	2.01	0.43
1:A:306:LEU:HD22	1:A:381:ARG:HE	1.84	0.43
1:A:519:PHE:CZ	1:A:619:PRO:HG3	2.54	0.43
1:A:655:MET:O	1:A:659:ILE:HG13	2.19	0.43
1:B:432:ILE:HG13	1:B:444:CYS:SG	2.59	0.43
1:A:33:PHE:CD2	1:A:646:THR:HB	2.54	0.43
1:B:716:ASN:HB3	1:B:719:LYS:CB	2.49	0.43
1:A:29:LEU:O	1:A:31:MET:N	2.52	0.42
1:A:449:LEU:HB2	1:A:505:VAL:HG12	1.99	0.42
1:B:219:PHE:N	1:B:247:GLY:O	2.50	0.42
1:A:401:GLY:HA2	1:A:739:LEU:HB2	2.01	0.42
1:A:18:ILE:O	1:A:21:ARG:HB2	2.20	0.42
1:A:23:GLN:C	1:A:25:LEU:N	2.73	0.42
1:A:390:TRP:NE1	1:A:394:ILE:HD11	2.34	0.42
1:A:18:ILE:HB	1:A:40:THR:HG23	2.02	0.42
1:A:120:THR:O	1:A:124:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:ARG:CD	1:B:347:ASP:O	2.66	0.42
1:B:635:GLN:HE22	1:B:660:ILE:HD11	1.84	0.42
1:A:253:SER:OG	1:A:302:GLU:HG3	2.20	0.42
1:B:300:TYR:CE2	1:B:426:SER:HB3	2.54	0.42
1:A:204:THR:HG23	1:A:215:LEU:HD22	2.02	0.42
1:A:300:TYR:CZ	1:A:426:SER:HB3	2.55	0.42
1:A:405:MET:HB2	1:A:736:MET:N	2.35	0.42
1:B:306:LEU:HA	1:B:350:LEU:HB3	2.02	0.42
1:B:313:ASP:HB3	1:B:324:ARG:NH2	2.34	0.42
1:A:429:CYS:HB2	1:A:431:GLU:OE2	2.20	0.42
1:A:439:ASP:HB3	1:A:490:GLU:HG3	2.01	0.42
1:A:669:ILE:HA	1:A:670:PRO:HD3	1.54	0.42
1:B:512:PHE:CZ	1:B:524:ALA:HB1	2.54	0.42
1:A:261:TYR:HA	1:A:268:ASN:ND2	2.33	0.42
1:A:402:THR:HG22	1:A:404:TYR:HE1	1.82	0.42
1:A:456:THR:C	1:A:458:GLU:H	2.23	0.42
1:B:123:ILE:HG21	1:B:181:GLU:HA	2.01	0.42
1:B:417:GLN:NE2	1:B:596:SER:OG	2.51	0.42
1:A:642:LEU:HA	1:A:645:LEU:HB2	2.01	0.42
1:B:20:SER:HA	1:B:23:GLN:HB2	2.00	0.42
1:B:117:ALA:HB2	1:B:211:ASN:N	2.34	0.42
1:B:362:VAL:HG11	1:B:370:LEU:CD2	2.50	0.42
1:A:79:ALA:O	1:A:83:VAL:HG23	2.19	0.41
1:B:512:PHE:HD2	1:B:519:PHE:CD2	2.37	0.41
1:A:227:SER:HA	2:A:801:TTP:O3'	2.19	0.41
1:B:5:LYS:HA	1:B:53:THR:HG23	2.01	0.41
1:B:228:ILE:HG12	2:B:801:TTP:H5'2	2.03	0.41
1:A:220:LEU:CD1	1:A:434:GLU:HB2	2.50	0.41
1:B:221:LEU:O	1:B:250:VAL:HA	2.20	0.41
1:B:300:TYR:CZ	1:B:426:SER:HB3	2.56	0.41
1:A:69:THR:HG21	1:A:656:LYS:HZ3	1.83	0.41
1:A:472:VAL:HG12	1:A:476:ASN:OD1	2.20	0.41
1:B:272:LEU:HD12	1:B:307:ASP:HB2	2.03	0.41
1:B:597:LEU:HD13	1:B:704:GLN:HG2	2.02	0.41
1:A:33:PHE:N	1:A:33:PHE:HD1	2.18	0.41
1:A:532:PHE:CE2	1:A:698:ARG:HD3	2.56	0.41
1:B:628:ARG:CB	1:B:633:GLU:HG2	2.51	0.41
1:A:652:HIS:H	1:A:655:MET:HB3	1.86	0.41
1:B:195:GLU:HG3	1:B:197:TRP:CD1	2.55	0.41
1:B:407:TYR:CZ	1:B:728:TRP:HB2	2.55	0.41
1:A:304:TRP:CH2	1:A:353:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:SER:OG	1:A:427:ASN:N	2.54	0.41
1:A:308:ILE:O	1:A:312:LEU:HD12	2.21	0.41
1:A:466:LEU:O	1:A:470:THR:OG1	2.20	0.41
1:A:477:LEU:O	1:A:481:ILE:HG13	2.20	0.41
1:B:104:TYR:HE1	1:B:159:ILE:HG23	1.86	0.41
1:B:469:VAL:O	1:B:473:VAL:HG23	2.21	0.41
1:B:512:PHE:CE2	1:B:524:ALA:HB1	2.56	0.41
1:B:553:TYR:O	1:B:554:GLU:C	2.59	0.41
1:B:621:THR:O	1:B:682:THR:HB	2.20	0.41
1:B:698:ARG:HG3	1:B:706:GLN:HE22	1.86	0.41
1:B:3:VAL:CG2	1:B:13:VAL:HG13	2.51	0.41
1:B:407:TYR:O	1:B:411:CYS:N	2.54	0.41
1:B:662:CYS:O	1:B:663:ASN:HB2	2.19	0.41
1:A:121:LEU:HD23	1:A:121:LEU:O	2.21	0.40
1:B:474:VAL:HG22	1:B:503:ILE:HD11	2.02	0.40
1:A:304:TRP:CH2	1:A:359:LEU:HB3	2.56	0.40
1:A:391:TYR:CD2	1:A:394:ILE:HD12	2.56	0.40
1:A:710:ILE:CG1	1:A:736:MET:HG3	2.51	0.40
1:A:220:LEU:HD13	1:A:434:GLU:HB2	2.03	0.40
1:A:337:LEU:O	1:A:341:ARG:HG3	2.21	0.40
1:A:584:LEU:C	1:A:586:GLU:H	2.25	0.40
3:A:802:3X4:C12	3:A:802:3X4:H27	2.33	0.40
1:B:736:MET:SD	1:B:739:LEU:HG	2.61	0.40
1:A:683:VAL:HA	1:A:686:ILE:HB	2.02	0.40
1:B:204:THR:O	1:B:208:ALA:HB2	2.20	0.40
1:B:394:ILE:HG23	1:B:720:LEU:HD13	2.02	0.40
1:B:667:GLN:N	1:B:667:GLN:OE1	2.54	0.40
1:A:298:ALA:CB	1:A:428:LEU:HA	2.52	0.40
1:A:405:MET:HG3	1:A:724:HIS:CE1	2.55	0.40
1:A:553:TYR:HE1	1:A:555:THR:HG23	1.86	0.40
1:A:702:ILE:HD12	1:A:706:GLN:NE2	2.37	0.40
1:B:385:LYS:O	1:B:388:GLN:HB2	2.21	0.40
1:B:488:VAL:HA	1:B:489:PRO:HD3	1.90	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	708/792 (89%)	607 (86%)	82 (12%)	19 (3%)	5	33
1	B	732/792 (92%)	619 (85%)	88 (12%)	25 (3%)	3	30
All	All	1440/1584 (91%)	1226 (85%)	170 (12%)	44 (3%)	4	32

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	CYS
1	A	219	PHE
1	A	263	ALA
1	A	615	GLU
1	A	656	LYS
1	B	7	ASP
1	B	12	ARG
1	B	52	THR
1	B	525	GLN
1	B	554	GLU
1	B	602	MET
1	B	640	HIS
1	B	648	ARG
1	A	30	ASN
1	A	51	VAL
1	A	530	GLN
1	A	572	ASN
1	A	650	LEU
1	B	5	LYS
1	B	23	GLN
1	B	49	SER
1	B	180	LYS
1	B	288	GLN
1	B	317	ASN
1	B	639	PRO

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Mol	Chain	Res	Type
1	A	382	LYS
1	A	404	TYR
1	A	590	LYS
1	B	116	VAL
1	B	529	LYS
1	B	665	SER
1	A	116	VAL
1	A	529	LYS
1	B	51	VAL
1	B	321	GLU
1	B	737	TYR
1	A	62	GLU
1	A	224	LYS
1	A	715	PRO
1	B	316	LYS
1	A	605	ALA
1	B	217	SER
1	B	666	ILE
1	B	601	PRO

### 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	581/693 (84%)	518 (89%)	63 (11%)	<b>6</b> 29
1	B	607/693 (88%)	548 (90%)	59 (10%)	8 <b>33</b>
All	All	1188/1386 (86%)	1066 (90%)	122 (10%)	<b>7</b> <b>31</b>

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	32	ASP
1	A	55	GLU
1	A	59	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	62	GLU
1	A	69	THR
1	A	84	SER
1	A	91	LYS
1	A	93	VAL
1	A	122	ASP
1	A	129	ASP
1	A	130	ARG
1	A	158	LYS
1	A	192	LEU
1	A	214	GLN
1	A	220	LEU
1	A	221	LEU
1	A	225	ASP
1	A	229	GLU
1	A	243	LYS
1	A	270	ASN
1	A	287	ASP
1	A	288	GLN
1	A	310	GLU
1	A	341	ARG
1	A	343	GLU
1	A	344	THR
1	A	375	GLU
1	A	380	VAL
1	A	381	ARG
1	A	382	LYS
1	A	389	LEU
1	A	404	TYR
1	A	413	ARG
1	A	414	LYS
1	A	428	LEU
1	A	455	VAL
1	A	465	LYS
1	A	475	ARG
1	A	499	ARG
1	A	508	LEU
1	A	516	ARG
1	A	523	GLU
1	A	526	LEU
1	A	527	LEU
1	A	537	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	546	LEU
1	A	565	ILE
1	A	572	ASN
1	A	591	TYR
1	A	594	ARG
1	A	602	MET
1	A	606	SER
1	A	607	THR
1	A	650	LEU
1	A	669	ILE
1	A	671	GLU
1	A	677	LYS
1	A	681	LYS
1	A	685	GLU
1	A	728	TRP
1	A	739	LEU
1	A	740	ARG
1	B	7	ASP
1	B	9	ARG
1	B	13	VAL
1	B	16	ASP
1	B	27	TYR
1	B	31	MET
1	B	33	PHE
1	B	47	LEU
1	B	49	SER
1	B	59	LEU
1	B	100	ASP
1	B	108	HIS
1	B	119	SER
1	B	121	LEU
1	B	123	ILE
1	B	130	ARG
1	B	140	ASP
1	B	158	LYS
1	B	180	LYS
1	B	199	THR
1	B	212	ARG
1	B	214	GLN
1	B	220	LEU
1	B	272	LEU
1	B	297	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	324	ARG
1	B	343	GLU
1	B	355	GLU
1	B	365	GLU
1	B	366	GLU
1	B	369	LYS
1	B	379	ARG
1	B	389	LEU
1	B	391	TYR
1	B	411	CYS
1	B	422	THR
1	B	436	THR
1	B	457	SER
1	B	478	ASN
1	B	479	LYS
1	B	497	ARG
1	B	508	LEU
1	B	516	ARG
1	B	523	GLU
1	B	554	GLU
1	B	563	LYS
1	B	566	LEU
1	B	578	LEU
1	B	590	LYS
1	B	604	THR
1	B	611	LEU
1	B	648	ARG
1	B	669	ILE
1	B	674	ASP
1	B	675	ASP
1	B	681	LYS
1	B	697	GLU
1	B	719	LYS
1	B	740	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	266	ASN
1	A	268	ASN
1	A	346	GLN
1	A	530	GLN

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Mol	Chain	Res	Type
1	A	572	ASN
1	A	667	GLN
1	B	2	HIS
1	B	85	ASN
1	B	200	HIS
1	B	214	GLN
1	B	323	GLN
1	B	418	GLN
1	B	445	ASN
1	B	459	HIS
1	B	476	ASN
1	B	495	ASN
1	B	595	ASN
1	B	635	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TTP	A	801	-	26,30,30	1.34	6 (23%)	39,47,47	2.09	12 (30%)
2	TTP	B	801	-	26,30,30	1.21	4 (15%)	39,47,47	2.06	8 (20%)
3	3X4	A	802	-	30,31,31	2.33	7 (23%)	43,44,44	2.16	11 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TTP	A	801	-	-	6/22/34/34	0/2/2/2
2	TTP	B	801	-	-	7/22/34/34	0/2/2/2
3	3X4	A	802	-	-	10/27/43/43	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	3X4	O2-C5	6.61	1.35	1.22
3	A	802	3X4	O1-C12	6.56	1.35	1.22
3	A	802	3X4	C11-C12	-5.57	1.39	1.48
3	A	802	3X4	C6-C5	-3.50	1.43	1.48
2	A	801	TTP	C4-N3	-3.03	1.33	1.38
2	A	801	TTP	C2-N1	2.93	1.43	1.38
3	A	802	3X4	O6-C24	2.93	1.31	1.22
3	A	802	3X4	C4-C3	2.83	1.56	1.52
2	B	801	TTP	C4-N3	-2.67	1.33	1.38
2	A	801	TTP	C6-N1	-2.62	1.33	1.38
3	A	802	3X4	O7-C24	-2.50	1.22	1.30
2	A	801	TTP	C6-C5	2.40	1.38	1.34
2	B	801	TTP	C6-C5	2.38	1.38	1.34
2	B	801	TTP	C6-N1	-2.27	1.34	1.38
2	B	801	TTP	C2-N1	2.23	1.42	1.38
2	A	801	TTP	C4-C5	2.23	1.48	1.44
2	A	801	TTP	C2-N3	-2.07	1.34	1.38

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802	3X4	C12-N1-C5	-6.62	106.63	112.03
3	A	802	3X4	C4-N1-C12	6.15	128.79	123.71
2	A	801	TTP	N3-C2-N1	5.42	122.08	114.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	TTP	C4-N3-C2	-5.17	120.66	127.35
2	B	801	TTP	C4-N3-C2	-5.13	120.71	127.35
2	B	801	TTP	C5-C4-N3	4.83	119.44	115.31
2	B	801	TTP	O4-C4-C5	-4.81	119.33	124.90
3	A	802	3X4	O1-C12-N1	-4.76	120.18	124.81
2	B	801	TTP	N3-C2-N1	4.53	120.90	114.89
3	A	802	3X4	C11-C12-N1	4.47	109.06	105.88
3	A	802	3X4	C6-C5-N1	4.07	108.77	105.88
2	B	801	TTP	PB-O3A-PA	-4.07	118.88	132.83
2	A	801	TTP	C5-C6-N1	-3.86	119.37	123.34
3	A	802	3X4	O2-C5-N1	-3.77	121.15	124.81
2	A	801	TTP	PB-O3B-PG	-3.51	120.78	132.83
2	A	801	TTP	C5-C4-N3	3.49	118.29	115.31
2	B	801	TTP	C5-C6-N1	-3.45	119.79	123.34
2	A	801	TTP	O4-C4-C5	-3.31	121.07	124.90
2	B	801	TTP	PB-O3B-PG	-3.09	122.23	132.83
2	A	801	TTP	C1'-N1-C2	2.97	123.48	117.64
2	A	801	TTP	O2-C2-N3	-2.92	116.06	121.50
3	A	802	3X4	O7-C24-C18	2.73	122.67	113.38
2	A	801	TTP	C5M-C5-C6	-2.60	119.37	122.85
3	A	802	3X4	O6-C24-C18	-2.53	113.21	122.14
2	A	801	TTP	PB-O3A-PA	-2.50	124.26	132.83
3	A	802	3X4	C10-C11-C6	-2.30	118.48	121.07
2	A	801	TTP	C1'-N1-C6	-2.30	116.80	120.77
2	A	801	TTP	C6-C5-C4	2.21	119.88	118.03
2	B	801	TTP	C1'-N1-C2	2.15	121.88	117.64
3	A	802	3X4	C4-C3-N	2.07	118.58	114.85
3	A	802	3X4	O-C3-C4	-2.06	117.47	121.08

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	TTP	C5'-O5'-PA-O2A
2	B	801	TTP	C5'-O5'-PA-O3A
2	B	801	TTP	O4'-C4'-C5'-O5'
2	B	801	TTP	C3'-C4'-C5'-O5'
3	A	802	3X4	C3-C4-N1-C5
3	A	802	3X4	C3-C4-N1-C12
2	A	801	TTP	O4'-C1'-N1-C2
2	B	801	TTP	C4'-C5'-O5'-PA
2	A	801	TTP	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
3	A	802	3X4	N2-C14-C15-C16
3	A	802	3X4	N3-C18-C24-O7
3	A	802	3X4	C-C1-C13-N2
3	A	802	3X4	N3-C18-C24-O6
3	A	802	3X4	C2-C1-C13-N2
2	B	801	TTP	C5'-O5'-PA-O1A
3	A	802	3X4	C16-C17-C18-N3
2	A	801	TTP	PG-O3B-PB-O3A
3	A	802	3X4	C-C1-C13-O3
3	A	802	3X4	C2-C1-C13-O3
2	A	801	TTP	PA-O3A-PB-O2B
2	B	801	TTP	PG-O3B-PB-O1B
2	A	801	TTP	O4'-C4'-C5'-O5'
2	A	801	TTP	PG-O3B-PB-O1B

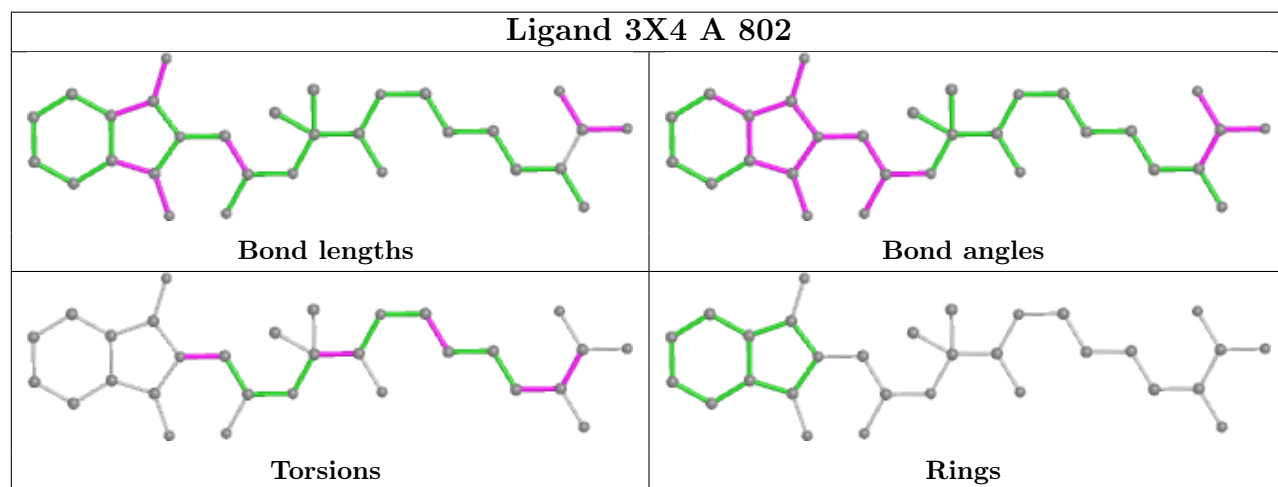
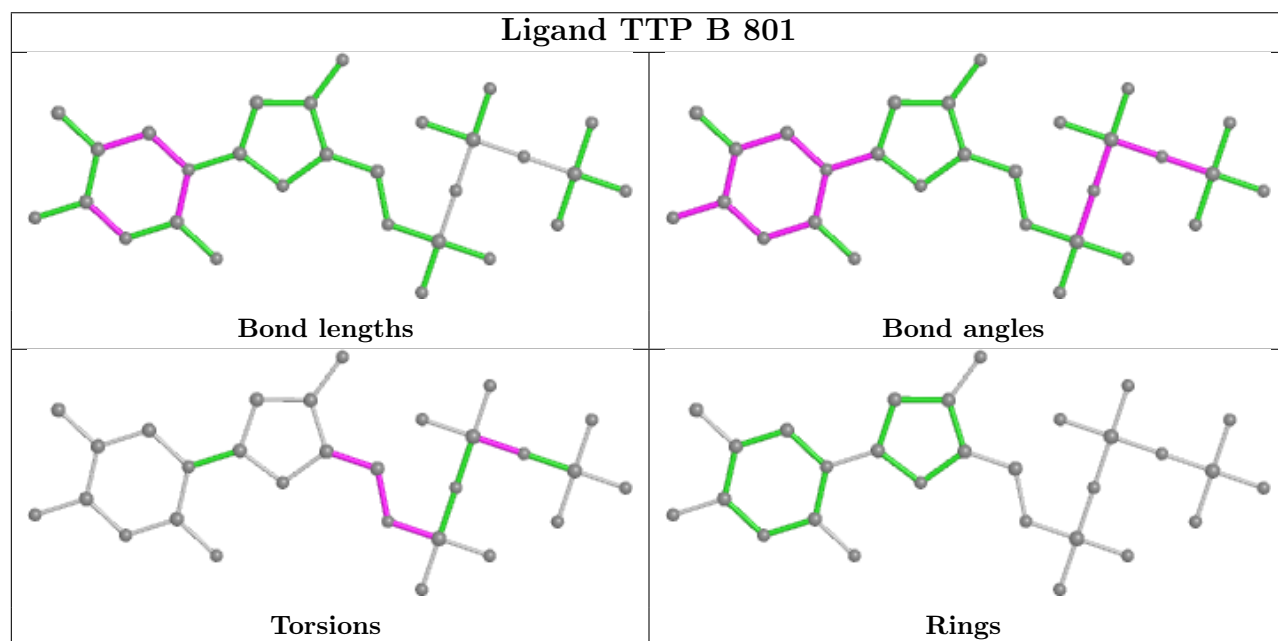
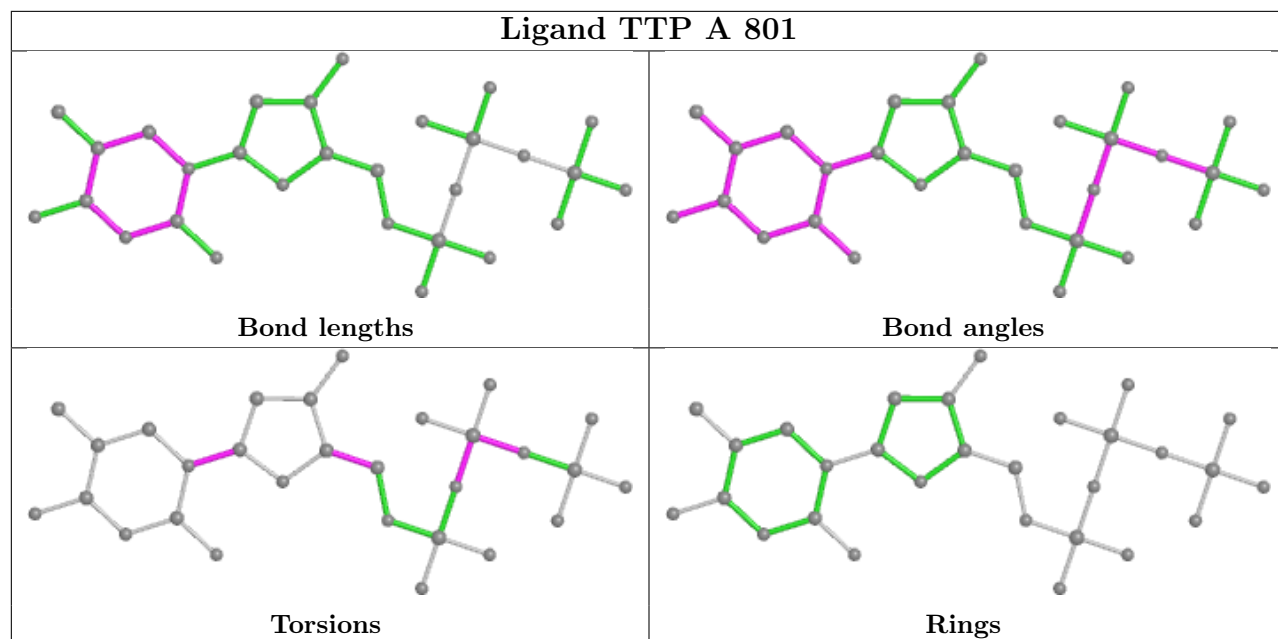
There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	TTP	5	0
2	B	801	TTP	4	0
3	A	802	3X4	3	0

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	714/792 (90%)	0.47	36 (5%) 28 21	87, 115, 140, 165	2 (0%)
1	B	738/792 (93%)	0.53	57 (7%) 13 10	90, 125, 154, 173	0
All	All	1452/1584 (91%)	0.50	93 (6%) 19 13	87, 119, 148, 173	2 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	GLU	5.4
1	A	666	ILE	4.2
1	B	198	PHE	4.1
1	A	433	VAL	3.9
1	B	434	GLU	3.6
1	B	739	LEU	3.5
1	A	23	GLN	3.5
1	B	701	PHE	3.3
1	A	711	HIS	3.2
1	B	325	ALA	3.1
1	A	330	PHE	3.1
1	B	220	LEU	3.0
1	B	616	SER	3.0
1	A	461	TYR	3.0
1	A	697	GLU	3.0
1	B	708	LEU	2.9
1	B	351	MET	2.9
1	B	141	PHE	2.9
1	A	32	ASP	2.9
1	B	146	PHE	2.9
1	B	581	TRP	2.8
1	B	164	ALA	2.8
1	A	200	HIS	2.8
1	B	468	GLU	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	450	ALA	2.8
1	A	237	GLN	2.8
1	A	620	TYR	2.8
1	B	535	ILE	2.7
1	A	331	ALA	2.7
1	A	19	THR	2.6
1	B	143	TYR	2.6
1	A	248	ILE	2.6
1	B	167	PRO	2.6
1	A	332	LEU	2.6
1	B	709	ASN	2.5
1	A	20	SER	2.5
1	B	593	ILE	2.4
1	B	537	TYR	2.4
1	A	297	PHE	2.4
1	A	650	LEU	2.4
1	B	314	LEU	2.4
1	A	146	PHE	2.4
1	B	706	GLN	2.4
1	B	177	GLY	2.4
1	B	221	LEU	2.4
1	B	476	ASN	2.3
1	A	163	VAL	2.3
1	A	33	PHE	2.3
1	A	720	LEU	2.3
1	B	302	GLU	2.3
1	B	319	GLY	2.3
1	B	338	PHE	2.3
1	B	620	TYR	2.3
1	B	495	ASN	2.3
1	A	348	TRP	2.3
1	B	623	ASN	2.2
1	B	595	ASN	2.2
1	A	616	SER	2.2
1	B	433	VAL	2.2
1	A	445	ASN	2.2
1	B	534	THR	2.2
1	B	629	VAL	2.2
1	A	389	LEU	2.2
1	B	536	TYR	2.2
1	B	388	GLN	2.2
1	B	303	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	332	LEU	2.2
1	B	305	HIS	2.2
1	B	464	LYS	2.2
1	B	590	LYS	2.2
1	B	736	MET	2.1
1	B	101	LEU	2.1
1	A	446	LEU	2.1
1	A	349	SER	2.1
1	B	719	LYS	2.1
1	B	324	ARG	2.1
1	B	297	PHE	2.1
1	B	77	LEU	2.1
1	A	214	GLN	2.1
1	A	425	CYS	2.1
1	B	452	ASN	2.1
1	B	488	VAL	2.1
1	B	403	PRO	2.1
1	B	545	ASP	2.1
1	A	739	LEU	2.1
1	B	99	GLU	2.0
1	A	388	GLN	2.0
1	A	450	ALA	2.0
1	A	224	LYS	2.0
1	B	315	LYS	2.0
1	B	180	LYS	2.0
1	A	624	ILE	2.0
1	A	676	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

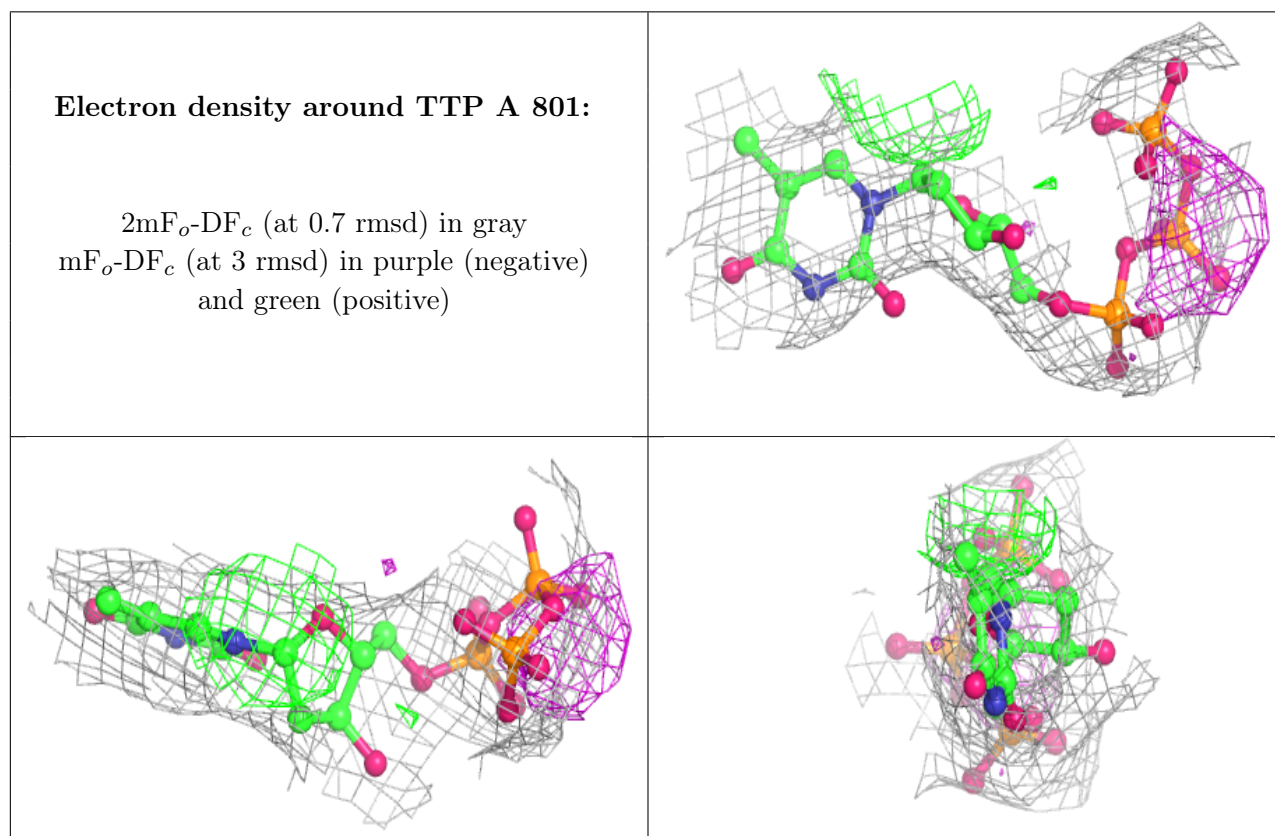
## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<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.

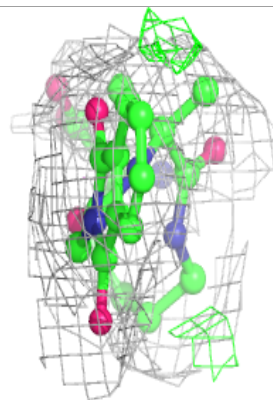
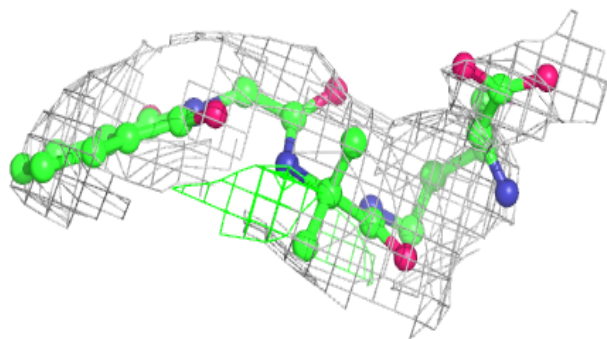
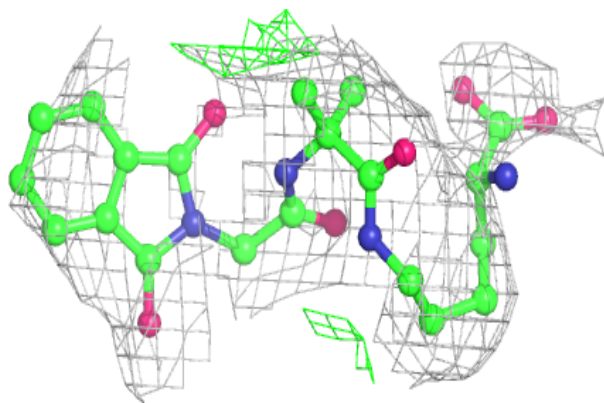
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	TTP	A	801	29/29	0.78	0.27	101,127,159,165	0
3	3X4	A	802	30/30	0.78	0.24	103,119,126,129	0
2	TTP	B	801	29/29	0.90	0.21	93,111,129,132	0

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.

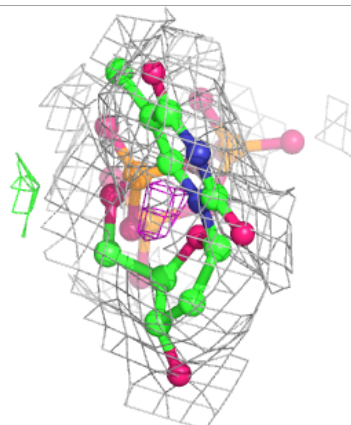
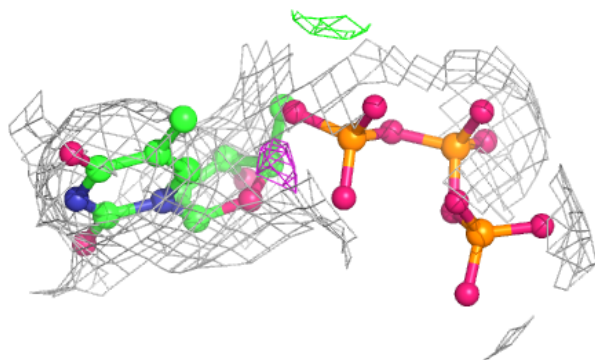
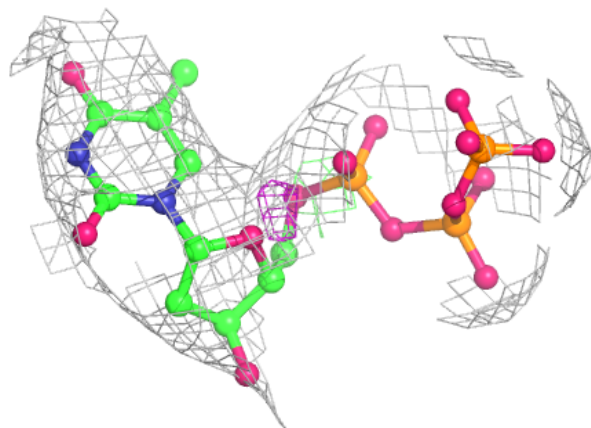


**Electron density around 3X4 A 802:**

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

**Electron density around TTP B 801:**

$2mF_o-DF_c$  (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.