



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 02:00 pm BST

PDB ID : 1Q13  
Title : Crystal structure of rabbit 20alpha hydroxysteroid dehydrogenase in ternary complex with NADP and testosterone  
Authors : Couture, J.-F.; Cantin, L.; Legrand, P.; Luu-The, V.; Labrie, F.; Breton, R.  
Deposited on : 2003-07-18  
Resolution : 2.08 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

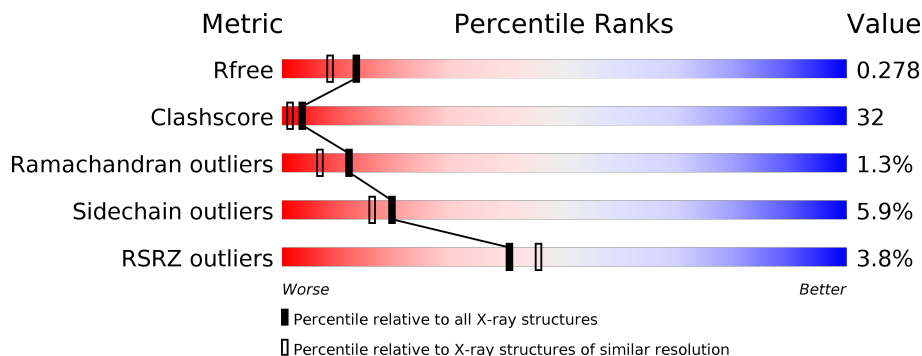
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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	323	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 55%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 36%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">4%      55%      36%      8%      •</p>
1	B	323	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 54%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 37%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="margin-top: 5px;">4%      54%      37%      6%      ••</p>

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5625 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 Prostaglandin-E2 9-reductase.

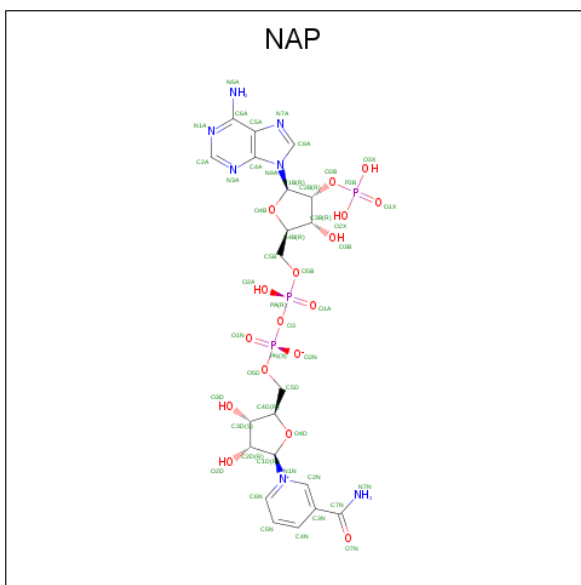
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	322	Total 2579	C 1662	N 435	O 472	S 10	0	0	0
1	B	317	Total 2532	C 1632	N 428	O 462	S 10	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



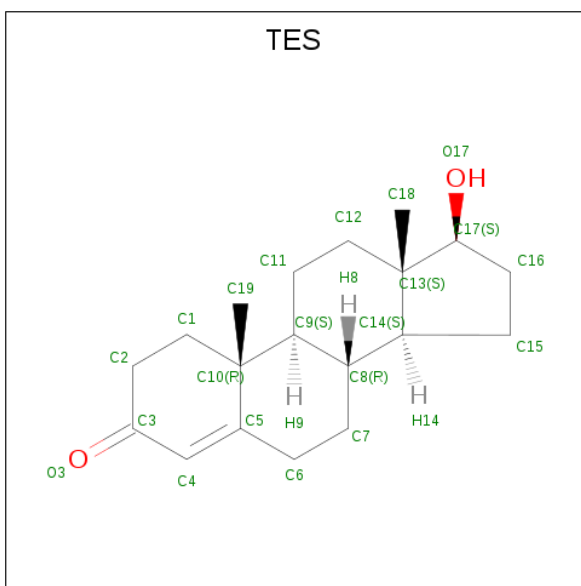
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
3	A	1	48	21	7	17	3	0	0
3	B	1	48	21	7	17	3	0	0

- Molecule 4 is TESTOSTERONE (three-letter code: TES) (formula:  $C_{19}H_{28}O_2$ ).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	C			O
4	A	1	21	19	2	0	0

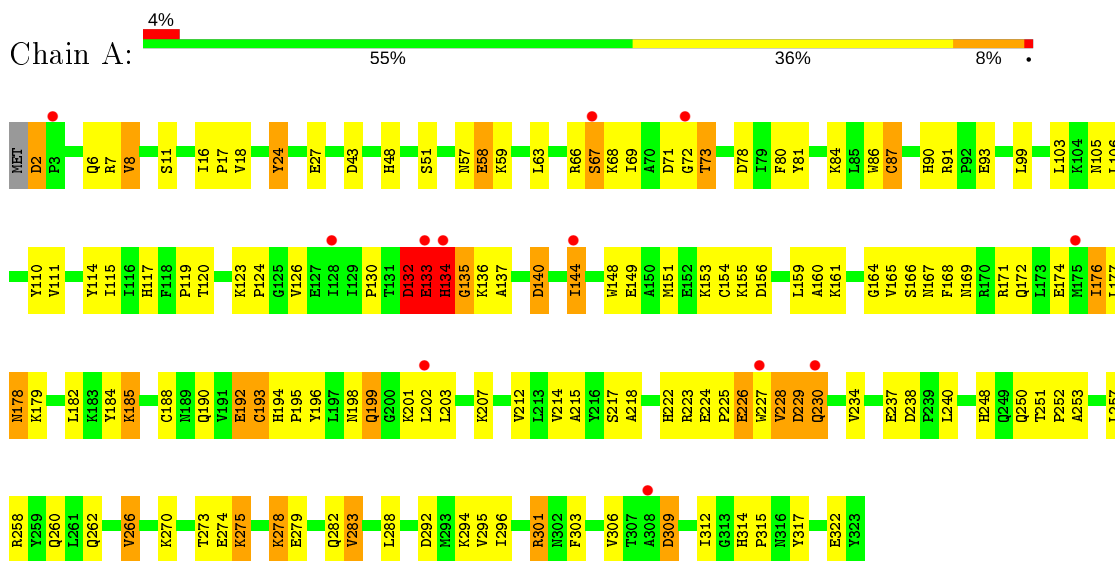
- Molecule 5 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	201	Total 201	O 201	0	0
5	B	191	Total 191	O 191	0	0

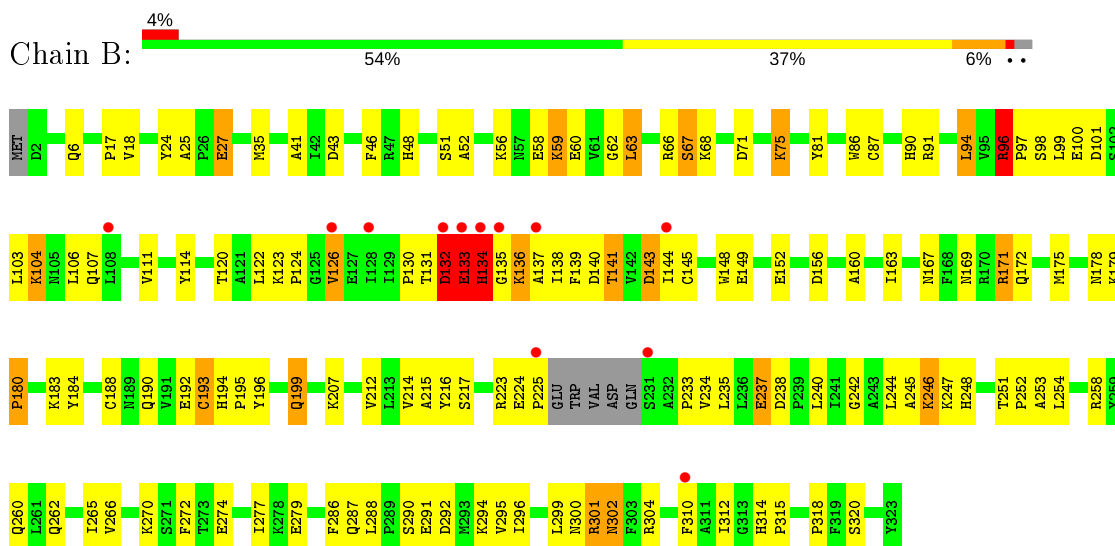
### 3 Residue-property plots i

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: Prostaglandin-E2 9-reductase



- Molecule 1: Prostaglandin-E2 9-reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	57.21Å 84.05Å 66.25Å 90.00° 91.17° 90.00°	Depositor
Resolution (Å)	20.00 – 2.08 19.72 – 2.08	Depositor EDS
% Data completeness (in resolution range)	93.5 (20.00-2.08) 90.2 (19.72-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.09Å)	Xtrriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.226 , 0.280 0.226 , 0.278	Depositor DCC
$R_{free}$ test set	1754 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.5	Xtrriage
Anisotropy	0.693	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	0.177 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5625	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.10% 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: NAP, TES, 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	1.22	15/2642 (0.6%)	1.06	9/3575 (0.3%)
1	B	1.08	9/2592 (0.3%)	1.02	10/3504 (0.3%)
All	All	1.16	24/5234 (0.5%)	1.04	19/7079 (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	2
1	B	0	1
All	All	0	3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	GLU	CD-OE2	13.60	1.40	1.25
1	B	59	LYS	CD-CE	11.55	1.80	1.51
1	A	192	GLU	CD-OE2	11.10	1.37	1.25
1	A	24	TYR	CE1-CZ	10.56	1.52	1.38
1	A	24	TYR	CG-CD2	9.66	1.51	1.39
1	A	58	GLU	CD-OE2	8.84	1.35	1.25
1	B	67	SER	CB-OG	7.59	1.52	1.42
1	B	59	LYS	CE-NZ	7.54	1.67	1.49
1	B	320	SER	CB-OG	7.45	1.51	1.42
1	B	193	CYS	CB-SG	7.24	1.94	1.82
1	A	322	GLU	CD-OE1	6.79	1.33	1.25
1	A	67	SER	CB-OG	6.78	1.51	1.42
1	A	253	ALA	CA-CB	6.70	1.66	1.52
1	A	283	VAL	CB-CG2	6.54	1.66	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	ALA	CA-CB	6.43	1.66	1.52
1	B	180	PRO	N-CD	5.81	1.55	1.47
1	A	266	VAL	CB-CG1	-5.77	1.40	1.52
1	A	93	GLU	CD-OE1	5.76	1.31	1.25
1	A	178	ASN	CB-CG	5.51	1.63	1.51
1	A	193	CYS	CB-SG	5.23	1.91	1.82
1	A	71	ASP	C-N	5.19	1.42	1.33
1	B	286	PHE	CE1-CZ	5.15	1.47	1.37
1	B	100	GLU	CG-CD	5.04	1.59	1.51
1	A	278	LYS	CE-NZ	5.03	1.61	1.49

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	ASP	CB-CG-OD2	7.11	124.70	118.30
1	B	71	ASP	CB-CG-OD2	7.10	124.69	118.30
1	A	134	HIS	CA-C-N	-6.77	102.67	116.20
1	B	238	ASP	CB-CG-OD2	6.66	124.30	118.30
1	A	78	ASP	CB-CG-OD2	6.53	124.17	118.30
1	B	156	ASP	CB-CG-OD2	6.49	124.14	118.30
1	A	238	ASP	CB-CG-OD2	6.43	124.08	118.30
1	A	140	ASP	CB-CG-OD2	6.15	123.84	118.30
1	B	96	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	A	43	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	132	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	101	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	73	THR	OG1-CB-CG2	-5.56	97.22	110.00
1	B	126	VAL	CB-CA-C	-5.41	101.13	111.40
1	A	132	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	143	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	171	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	A	2	ASP	CB-CG-OD2	5.06	122.85	118.30
1	B	171	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	133	GLU	Peptide
1	A	134	HIS	Mainchain
1	B	224	GLU	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	2579	0	2587	172	8
1	B	2532	0	2549	160	2
2	A	5	0	0	0	0
3	A	48	0	25	3	0
3	B	48	0	25	4	0
4	A	21	0	28	7	0
5	A	201	0	0	22	1
5	B	191	0	0	30	3
All	All	5625	0	5214	332	10

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 32.

All (332) 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:59:LYS:CD	1:B:59:LYS:CE	1.80	1.56
1:B:59:LYS:NZ	1:B:59:LYS:CE	1.67	1.53
1:A:275:LYS:HE3	1:A:275:LYS:N	1.20	1.41
1:B:223:ARG:HD3	5:B:586:HOH:O	1.30	1.24
1:A:230:GLN:NE2	5:A:654:HOH:O	1.57	1.24
1:A:172:GLN:OE1	5:A:689:HOH:O	1.55	1.22
1:A:226:GLU:O	1:A:230:GLN:HG2	1.48	1.14
1:A:126:VAL:HG13	1:B:302:ASN:OD1	1.48	1.13
1:A:274:GLU:HB3	1:A:275:LYS:HE2	1.18	1.12
1:A:275:LYS:CE	1:A:275:LYS:H	1.63	1.11
1:A:227:TRP:HA	1:A:230:GLN:HG3	1.30	1.11
1:A:275:LYS:CE	1:A:275:LYS:N	2.16	1.09
1:A:63:LEU:HD22	5:A:793:HOH:O	1.54	1.05
1:B:133:GLU:HB3	1:B:136:LYS:HB2	1.07	1.04
3:A:401:NAP:O2N	5:A:602:HOH:O	1.77	1.03
1:B:133:GLU:CB	1:B:136:LYS:HB2	1.88	1.02
1:A:226:GLU:O	1:A:230:GLN:CG	2.08	1.01
1:B:291:GLU:OE2	1:B:291:GLU:N	1.92	1.00
1:A:2:ASP:N	5:A:744:HOH:O	1.94	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ASN:H	1:B:172:GLN:HE21	1.02	0.99
1:B:107:GLN:HG2	5:B:554:HOH:O	1.63	0.98
1:A:224:GLU:O	1:A:228:VAL:HG11	1.64	0.96
1:A:227:TRP:CA	1:A:230:GLN:HG3	1.95	0.96
1:A:134:HIS:CG	1:A:135:GLY:H	1.84	0.95
1:B:131:THR:HG22	1:B:137:ALA:HA	1.49	0.95
1:B:133:GLU:HA	1:B:133:GLU:OE2	1.65	0.93
1:A:225:PRO:HB2	1:A:226:GLU:OE1	1.68	0.93
1:B:18:VAL:HG11	5:B:570:HOH:O	1.70	0.92
1:A:262:GLN:HE22	1:A:288:LEU:H	1.10	0.91
1:A:278:LYS:NZ	5:A:742:HOH:O	2.04	0.89
1:B:258:ARG:HE	1:B:262:GLN:HE21	1.11	0.89
1:A:134:HIS:O	1:A:136:LYS:N	2.04	0.89
1:B:169:ASN:H	1:B:172:GLN:NE2	1.69	0.89
1:B:262:GLN:HE22	1:B:288:LEU:H	1.15	0.88
1:B:133:GLU:HB3	1:B:136:LYS:CB	2.01	0.88
1:A:274:GLU:HB3	1:A:275:LYS:CE	2.03	0.88
1:A:225:PRO:CB	1:A:226:GLU:OE1	2.21	0.87
1:A:275:LYS:HE3	1:A:275:LYS:CA	2.03	0.86
1:A:134:HIS:CG	1:A:135:GLY:N	2.43	0.85
1:A:258:ARG:HE	1:A:262:GLN:HE21	1.22	0.85
1:B:123:LYS:HG3	1:B:138:ILE:HG22	1.59	0.84
1:B:132:ASP:O	1:B:134:HIS:N	2.11	0.84
1:B:133:GLU:O	1:B:134:HIS:C	2.15	0.84
1:A:224:GLU:O	1:A:228:VAL:CG1	2.25	0.84
1:B:287:GLN:CD	5:B:556:HOH:O	2.16	0.83
1:A:24:TYR:CZ	4:A:501:TES:C6	2.62	0.83
1:B:149:GLU:HG3	1:B:179:LYS:HZ3	1.43	0.83
1:A:223:ARG:O	1:A:229:ASP:HB2	1.78	0.82
1:A:226:GLU:OE1	1:A:226:GLU:N	2.13	0.82
1:B:59:LYS:CG	1:B:59:LYS:CE	2.58	0.81
1:B:149:GLU:HG3	1:B:179:LYS:NZ	1.95	0.81
1:A:24:TYR:CZ	4:A:501:TES:H62	2.16	0.81
1:A:126:VAL:CG1	1:B:302:ASN:OD1	2.30	0.78
1:A:169:ASN:H	1:A:172:GLN:HE21	1.30	0.78
1:A:225:PRO:O	1:A:227:TRP:N	2.18	0.77
1:A:8:VAL:HG22	1:A:18:VAL:HG12	1.65	0.77
1:A:149:GLU:OE1	1:A:179:LYS:NZ	2.18	0.76
1:A:103:LEU:HD21	1:A:111:VAL:HG13	1.67	0.76
1:A:274:GLU:CB	1:A:275:LYS:HE2	2.09	0.76
1:B:94:LEU:HD12	5:B:539:HOH:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLU:CG	1:B:179:LYS:NZ	2.49	0.75
1:A:136:LYS:HG2	1:A:137:ALA:O	1.87	0.74
1:B:240:LEU:HD21	1:B:295:VAL:CG1	2.18	0.73
1:A:156:ASP:OD1	1:A:184:TYR:OH	2.07	0.73
1:B:149:GLU:CG	1:B:179:LYS:HZ1	2.01	0.73
1:A:174:GLU:O	1:A:178:ASN:HB2	1.89	0.73
1:B:123:LYS:HE2	1:B:140:ASP:OD1	1.89	0.73
1:B:94:LEU:HB3	5:B:501:HOH:O	1.87	0.73
1:A:171:ARG:HD3	5:A:786:HOH:O	1.88	0.72
1:B:131:THR:HG22	1:B:137:ALA:CA	2.19	0.72
1:A:225:PRO:CA	1:A:226:GLU:OE1	2.38	0.72
1:B:270:LYS:O	3:B:402:NAP:H8A	1.90	0.71
1:B:240:LEU:HD21	1:B:295:VAL:HG12	1.70	0.71
1:A:279:GLU:HA	1:A:282:GLN:HE21	1.55	0.71
1:B:6:GLN:NE2	5:B:570:HOH:O	2.23	0.71
1:A:169:ASN:H	1:A:172:GLN:NE2	1.89	0.71
1:A:270:LYS:O	3:A:401:NAP:H8A	1.91	0.70
1:A:6:GLN:HE21	1:A:18:VAL:HG21	1.55	0.70
1:B:98:SER:HA	5:B:510:HOH:O	1.91	0.70
1:B:63:LEU:HD12	1:B:66:ARG:NH2	2.07	0.70
1:A:227:TRP:HA	1:A:230:GLN:CG	2.16	0.70
1:B:141:THR:HG23	5:B:504:HOH:O	1.92	0.69
1:B:247:LYS:CE	5:B:562:HOH:O	2.40	0.69
1:A:149:GLU:CG	1:A:179:LYS:HE3	2.22	0.69
1:B:171:ARG:HG2	1:B:171:ARG:NH1	2.05	0.69
1:A:24:TYR:CE2	4:A:501:TES:H62	2.28	0.69
1:B:123:LYS:HE3	1:B:139:PHE:O	1.93	0.69
1:A:225:PRO:C	1:A:226:GLU:OE1	2.32	0.68
1:A:226:GLU:O	1:A:230:GLN:HG3	1.92	0.68
1:A:222:HIS:CE1	5:A:602:HOH:O	2.46	0.67
1:A:230:GLN:CD	5:A:654:HOH:O	2.07	0.67
1:B:223:ARG:CD	5:B:586:HOH:O	2.08	0.67
1:A:194:HIS:HD2	1:A:196:TYR:H	1.43	0.67
1:A:234:VAL:HB	1:A:237:GLU:OE2	1.95	0.66
1:A:148:TRP:CG	1:A:176:ILE:HD13	2.31	0.66
1:B:171:ARG:HH11	1:B:171:ARG:HG2	1.59	0.66
1:A:59:LYS:HE3	1:A:105:ASN:ND2	2.09	0.66
1:A:260:GLN:OE1	1:A:260:GLN:HA	1.96	0.65
1:B:169:ASN:N	1:B:172:GLN:HE21	1.85	0.65
1:A:27:GLU:O	5:A:784:HOH:O	2.13	0.65
1:B:195:PRO:HD2	1:B:235:LEU:HD11	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:GLU:OE2	1:A:194:HIS:HE1	1.79	0.65
1:A:132:ASP:C	1:A:134:HIS:N	2.50	0.65
1:B:194:HIS:HD2	1:B:196:TYR:H	1.46	0.64
1:A:133:GLU:O	1:A:134:HIS:HB2	1.97	0.64
1:A:24:TYR:CZ	4:A:501:TES:H61	2.32	0.64
1:A:99:LEU:HB2	1:A:114:TYR:CE2	2.33	0.63
1:B:314:HIS:ND1	1:B:315:PRO:HD2	2.13	0.63
1:A:149:GLU:HG2	1:A:179:LYS:HE3	1.81	0.63
1:B:258:ARG:HE	1:B:262:GLN:NE2	1.92	0.63
1:B:91:ARG:HG3	5:B:539:HOH:O	1.98	0.62
1:B:123:LYS:HG3	1:B:138:ILE:CG2	2.29	0.62
1:A:222:HIS:HE1	5:A:602:HOH:O	1.80	0.61
1:B:43:ASP:CG	5:B:467:HOH:O	2.38	0.61
1:A:81:TYR:OH	1:A:106:LEU:HD21	2.01	0.61
1:B:265:ILE:O	5:B:564:HOH:O	2.16	0.61
1:B:6:GLN:HE21	1:B:18:VAL:HG21	1.66	0.61
1:B:143:ASP:OD2	1:B:145:CYS:HB2	2.01	0.60
1:A:240:LEU:HD21	1:A:295:VAL:CG1	2.31	0.60
1:B:194:HIS:HD2	1:B:196:TYR:N	2.00	0.60
1:B:247:LYS:HE2	5:B:562:HOH:O	2.02	0.59
1:B:24:TYR:CG	1:B:25:ALA:N	2.70	0.59
1:A:275:LYS:HE3	1:A:275:LYS:H	0.76	0.59
1:B:260:GLN:OE1	1:B:260:GLN:HA	2.03	0.59
1:A:81:TYR:HE2	1:A:106:LEU:HD11	1.68	0.59
1:B:58:GLU:HG3	5:B:526:HOH:O	2.02	0.58
1:A:81:TYR:CZ	1:A:106:LEU:HD21	2.38	0.58
1:B:131:THR:HG22	1:B:136:LYS:C	2.24	0.58
1:B:199:GLN:HA	1:B:199:GLN:HE21	1.69	0.58
1:A:81:TYR:CE2	1:A:106:LEU:HD11	2.38	0.57
1:B:169:ASN:OD1	1:B:172:GLN:HG3	2.04	0.57
1:B:131:THR:HG22	1:B:136:LYS:O	2.04	0.57
1:B:59:LYS:HD2	5:B:415:HOH:O	2.04	0.57
1:A:117:HIS:O	1:A:166:SER:HB3	2.04	0.57
1:B:145:CYS:HB3	1:B:179:LYS:HD2	1.86	0.57
1:A:58:GLU:HG2	1:A:81:TYR:OH	2.03	0.57
1:B:56:LYS:HA	5:B:434:HOH:O	2.05	0.57
1:A:87:CYS:HB3	1:A:120:THR:O	2.04	0.56
1:A:132:ASP:OD2	1:A:134:HIS:O	2.22	0.56
1:A:188:CYS:HA	1:A:212:VAL:O	2.05	0.56
1:B:291:GLU:H	1:B:291:GLU:CD	1.97	0.56
1:B:242:GLY:O	1:B:246:LYS:HD2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:CB	1:A:237:GLU:OE2	2.55	0.55
1:B:133:GLU:O	1:B:135:GLY:N	2.39	0.54
1:B:133:GLU:OE2	1:B:133:GLU:CA	2.47	0.54
1:B:237:GLU:OE2	5:B:542:HOH:O	2.18	0.54
1:A:273:THR:O	1:A:274:GLU:C	2.45	0.54
1:B:183:LYS:HG2	1:B:184:TYR:CD2	2.43	0.54
1:B:86:TRP:CG	1:B:87:CYS:N	2.76	0.53
1:A:11:SER:HB3	5:A:799:HOH:O	2.07	0.53
1:B:274:GLU:HA	1:B:277:ILE:HD12	1.88	0.53
1:A:148:TRP:CD2	1:A:176:ILE:HD13	2.43	0.53
1:A:227:TRP:C	1:A:230:GLN:HG3	2.29	0.53
1:B:195:PRO:O	1:B:300:ASN:N	2.40	0.53
1:A:149:GLU:OE1	1:A:179:LYS:CE	2.57	0.53
1:A:312:ILE:HD13	1:A:317:TYR:CE1	2.44	0.53
1:B:234:VAL:HB	1:B:237:GLU:HG3	1.91	0.52
1:B:207:LYS:HG2	5:B:544:HOH:O	2.09	0.52
1:B:120:THR:HB	1:B:314:HIS:CD2	2.44	0.52
1:B:132:ASP:C	1:B:134:HIS:N	2.63	0.52
1:B:192:GLU:OE2	1:B:194:HIS:HE1	1.92	0.52
1:B:254:LEU:HD21	1:B:279:GLU:O	2.10	0.52
1:A:124:PRO:HG3	5:A:650:HOH:O	2.09	0.52
1:B:122:LEU:HD11	1:B:310:PHE:CE2	2.45	0.52
1:A:8:VAL:HG23	1:A:16:ILE:HG23	1.91	0.51
1:B:62:GLY:O	1:B:66:ARG:HG3	2.10	0.51
1:A:155:LYS:HD3	1:A:184:TYR:CD2	2.46	0.51
1:B:104:LYS:NZ	5:B:512:HOH:O	1.83	0.51
1:B:247:LYS:NZ	5:B:562:HOH:O	2.30	0.51
1:B:122:LEU:HD11	1:B:310:PHE:HE2	1.75	0.51
1:B:190:GLN:OE1	3:B:402:NAP:H2N	2.10	0.51
1:B:148:TRP:CZ2	1:B:163:ILE:HD12	2.46	0.51
1:A:226:GLU:C	1:A:230:GLN:CG	2.78	0.50
1:A:81:TYR:CE2	1:A:106:LEU:CD1	2.94	0.50
1:A:312:ILE:CD1	1:A:317:TYR:CZ	2.94	0.50
1:A:270:LYS:HD3	1:A:270:LYS:C	2.32	0.50
1:B:171:ARG:HH11	1:B:171:ARG:CG	2.24	0.50
1:A:169:ASN:OD1	1:A:172:GLN:HG3	2.10	0.50
1:A:240:LEU:HD21	1:A:295:VAL:HG12	1.93	0.50
1:B:130:PRO:O	1:B:137:ALA:HA	2.11	0.50
1:B:262:GLN:HE22	1:B:288:LEU:N	1.97	0.50
1:A:225:PRO:HD3	4:A:501:TES:H162	1.93	0.50
1:B:131:THR:CG2	1:B:137:ALA:HA	2.33	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:VAL:O	1:A:126:VAL:CG1	2.58	0.50
1:A:174:GLU:OE2	1:A:174:GLU:HA	2.12	0.50
1:A:151:MET:O	1:A:154:CYS:HB2	2.12	0.50
1:B:195:PRO:HD2	1:B:235:LEU:CD1	2.42	0.49
1:A:165:VAL:HB	1:A:168:PHE:CE1	2.47	0.49
1:A:51:SER:O	1:A:84:LYS:NZ	2.43	0.49
1:A:87:CYS:HA	1:A:90:HIS:CD2	2.47	0.49
1:B:63:LEU:CD1	1:B:66:ARG:NH2	2.76	0.49
1:B:87:CYS:HB3	1:B:120:THR:O	2.13	0.49
1:B:193:CYS:HB3	1:B:215:ALA:HB1	1.93	0.49
1:B:258:ARG:NE	1:B:262:GLN:HE21	1.94	0.49
1:A:91:ARG:HH22	1:A:123:LYS:HZ2	1.59	0.48
1:B:188:CYS:HA	1:B:212:VAL:O	2.13	0.48
1:B:172:GLN:O	1:B:175:MET:HB2	2.13	0.48
1:A:155:LYS:HE2	5:A:636:HOH:O	2.13	0.48
1:A:309:ASP:O	1:A:312:ILE:HG12	2.12	0.48
1:B:301:ARG:HB3	1:B:301:ARG:HE	1.32	0.48
1:B:68:LYS:HA	1:B:68:LYS:HD2	1.58	0.48
1:B:149:GLU:HA	1:B:152:GLU:OE1	2.13	0.48
1:B:270:LYS:C	1:B:270:LYS:HD3	2.34	0.48
1:A:303:PHE:CD2	1:A:303:PHE:C	2.87	0.47
1:A:190:GLN:OE1	3:A:401:NAP:H2N	2.14	0.47
1:A:110:TYR:CD1	1:A:161:LYS:HG2	2.49	0.47
1:A:164:GLY:C	1:A:165:VAL:HG13	2.34	0.47
1:B:237:GLU:CD	5:B:542:HOH:O	2.53	0.47
1:A:130:PRO:O	1:A:137:ALA:HA	2.15	0.47
5:A:793:HOH:O	1:B:312:ILE:HG22	2.14	0.47
1:A:250:GLN:NE2	5:A:756:HOH:O	2.47	0.47
1:A:63:LEU:HD12	1:A:66:ARG:NH2	2.29	0.47
1:B:75:LYS:HB2	1:B:75:LYS:HE3	1.61	0.47
1:A:182:LEU:HD21	1:A:185:LYS:HG2	1.97	0.47
1:A:194:HIS:HD2	1:A:196:TYR:N	2.11	0.47
1:A:306:VAL:HG12	1:A:306:VAL:O	2.13	0.47
1:A:132:ASP:O	1:A:134:HIS:N	2.47	0.46
1:A:119:PRO:HB2	1:A:144:ILE:HD11	1.97	0.46
1:A:250:GLN:NE2	1:A:250:GLN:HA	2.29	0.46
1:A:301:ARG:HD2	5:A:700:HOH:O	2.15	0.46
1:A:194:HIS:CD2	1:A:196:TYR:HB2	2.50	0.46
1:A:24:TYR:CE1	4:A:501:TES:H61	2.50	0.46
1:A:196:TYR:CD1	1:A:301:ARG:HD3	2.50	0.46
1:B:214:VAL:HA	1:B:266:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PRO:C	1:B:131:THR:HG23	2.36	0.46
1:B:225:PRO:HD2	5:B:514:HOH:O	2.15	0.46
1:B:193:CYS:HB3	1:B:215:ALA:CB	2.46	0.45
1:B:179:LYS:HA	1:B:180:PRO:HD2	1.78	0.45
1:A:63:LEU:CD1	1:A:66:ARG:NH2	2.79	0.45
1:B:81:TYR:CZ	1:B:106:LEU:HD21	2.51	0.45
3:B:402:NAP:O2N	3:B:402:NAP:H3D	2.16	0.45
1:A:48:HIS:HA	1:A:80:PHE:O	2.17	0.45
1:B:172:GLN:HE22	1:B:318:PRO:HB3	1.82	0.45
1:A:130:PRO:HD3	5:A:647:HOH:O	2.16	0.45
1:A:7:ARG:HD3	1:A:17:PRO:HD3	1.99	0.45
1:B:123:LYS:HG2	1:B:139:PHE:O	2.16	0.45
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.78	0.45
1:B:171:ARG:CG	1:B:171:ARG:NH1	2.74	0.45
1:B:35:MET:HB2	1:B:60:GLU:HB3	1.98	0.45
1:B:167:ASN:ND2	5:B:409:HOH:O	2.50	0.45
1:B:217:SER:HA	3:B:402:NAP:O1A	2.17	0.45
1:A:224:GLU:C	1:A:228:VAL:HG13	2.37	0.44
1:A:8:VAL:HG23	1:A:16:ILE:CG2	2.48	0.44
1:A:86:TRP:CG	1:A:87:CYS:N	2.85	0.44
1:B:67:SER:OG	5:B:411:HOH:O	2.15	0.44
1:A:224:GLU:O	1:A:228:VAL:HG13	2.12	0.44
1:B:43:ASP:OD1	1:B:68:LYS:CE	2.66	0.44
1:A:166:SER:O	1:A:167:ASN:HB2	2.17	0.44
1:B:17:PRO:HB2	1:B:48:HIS:HB2	1.99	0.44
1:A:11:SER:CB	5:A:799:HOH:O	2.66	0.44
1:A:72:GLY:O	1:A:73:THR:C	2.54	0.44
1:B:66:ARG:NE	1:B:107:GLN:HB2	2.33	0.44
1:A:111:VAL:O	1:A:160:ALA:HA	2.17	0.43
1:B:131:THR:HG22	1:B:137:ALA:N	2.32	0.43
1:B:87:CYS:HA	1:B:90:HIS:CD2	2.53	0.43
1:A:225:PRO:O	1:A:226:GLU:C	2.55	0.43
1:B:130:PRO:O	1:B:131:THR:HG23	2.17	0.43
1:B:247:LYS:HD3	1:B:248:HIS:NE2	2.33	0.43
1:B:296:ILE:O	1:B:299:LEU:HB2	2.18	0.43
1:B:51:SER:OG	1:B:52:ALA:N	2.49	0.43
1:A:240:LEU:HD21	1:A:295:VAL:HG13	2.00	0.43
1:A:159:LEU:HA	1:A:159:LEU:HD23	1.76	0.43
1:A:149:GLU:HG3	1:A:179:LYS:HE3	2.01	0.43
1:B:149:GLU:CD	1:B:179:LYS:HZ1	2.22	0.43
1:B:245:ALA:HB3	1:B:246:LYS:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LYS:HE2	1:A:140:ASP:OD1	2.19	0.43
1:A:228:VAL:HG22	1:A:229:ASP:N	2.34	0.43
1:B:94:LEU:CD1	5:B:539:HOH:O	2.55	0.43
1:A:193:CYS:HB3	1:A:215:ALA:HB1	2.01	0.43
1:B:103:LEU:HD21	1:B:111:VAL:HG13	2.01	0.43
1:A:257:LEU:HA	1:A:257:LEU:HD23	1.86	0.42
1:A:292:ASP:O	1:A:296:ILE:HG13	2.19	0.42
1:B:169:ASN:HD21	1:B:171:ARG:NH2	2.17	0.42
1:B:192:GLU:N	1:B:216:TYR:CE2	2.87	0.42
1:B:91:ARG:HB2	1:B:94:LEU:HG	2.01	0.42
1:A:193:CYS:O	1:A:218:ALA:HA	2.18	0.42
1:B:199:GLN:CA	1:B:199:GLN:HE21	2.31	0.42
1:B:314:HIS:ND1	1:B:315:PRO:CD	2.82	0.42
1:A:192:GLU:HG3	1:A:217:SER:HB2	2.02	0.42
1:A:201:LYS:O	1:A:202:LEU:C	2.56	0.42
1:A:258:ARG:HB2	1:A:283:VAL:HG23	2.00	0.42
1:B:194:HIS:HB2	1:B:195:PRO:CD	2.48	0.42
1:B:251:THR:HG21	1:B:279:GLU:OE2	2.19	0.42
1:A:130:PRO:HG3	5:A:647:HOH:O	2.19	0.42
1:A:198:ASN:O	1:A:199:GLN:HB2	2.19	0.42
1:A:203:LEU:HD11	1:A:207:LYS:HE3	2.00	0.42
1:B:133:GLU:CB	1:B:136:LYS:CB	2.78	0.42
1:B:223:ARG:NE	5:B:586:HOH:O	2.43	0.42
1:B:244:LEU:O	1:B:245:ALA:C	2.58	0.42
1:A:155:LYS:HD3	1:A:184:TYR:CE2	2.55	0.42
1:A:57:ASN:OD1	1:A:57:ASN:C	2.58	0.42
1:A:190:GLN:HA	1:A:214:VAL:O	2.20	0.41
1:A:194:HIS:HB2	1:A:195:PRO:CD	2.49	0.41
1:A:262:GLN:HE22	1:A:288:LEU:N	1.94	0.41
1:B:81:TYR:OH	1:B:106:LEU:HD21	2.19	0.41
1:A:248:HIS:O	1:A:250:GLN:HG2	2.21	0.41
1:B:131:THR:CB	1:B:136:LYS:O	2.68	0.41
1:A:133:GLU:CD	1:A:133:GLU:H	2.23	0.41
1:A:91:ARG:HH21	1:A:140:ASP:CG	2.24	0.41
1:B:223:ARG:NH1	1:B:233:PRO:O	2.54	0.41
1:A:193:CYS:HB3	1:A:215:ALA:CB	2.50	0.41
1:B:123:LYS:HA	1:B:124:PRO:HD3	1.82	0.41
1:A:115:ILE:HD13	1:A:115:ILE:HG21	1.89	0.41
1:A:250:GLN:HE21	1:A:250:GLN:HA	1.85	0.41
1:B:194:HIS:CD2	1:B:196:TYR:H	2.31	0.41
1:B:270:LYS:HE2	1:B:272:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:ASP:OD1	5:B:467:HOH:O	2.22	0.41
1:A:130:PRO:CG	5:A:647:HOH:O	2.68	0.41
1:A:91:ARG:HH22	1:A:123:LYS:NZ	2.18	0.41
1:B:111:VAL:O	1:B:160:ALA:HA	2.21	0.41
1:B:27:GLU:OE2	5:B:575:HOH:O	2.22	0.41
1:A:248:HIS:NE2	1:A:292:ASP:OD2	2.41	0.41
1:B:251:THR:HB	1:B:252:PRO:HD2	2.03	0.41
1:B:99:LEU:HB2	1:B:114:TYR:CE2	2.55	0.41
1:A:214:VAL:HA	1:A:266:VAL:O	2.21	0.41
1:B:292:ASP:O	1:B:296:ILE:HG13	2.21	0.41
1:A:312:ILE:HD13	1:A:312:ILE:HA	1.89	0.40
1:A:63:LEU:HD12	1:A:63:LEU:HA	1.79	0.40
1:B:41:ALA:HA	1:B:277:ILE:HG21	2.03	0.40
1:B:41:ALA:O	1:B:46:PHE:HB2	2.21	0.40
1:A:24:TYR:OH	4:A:501:TES:H71	2.21	0.40
1:A:251:THR:HG21	1:A:279:GLU:OE1	2.21	0.40
1:A:68:LYS:HD3	1:A:68:LYS:HA	1.66	0.40
1:B:178:ASN:HD22	1:B:178:ASN:HA	1.63	0.40
5:A:793:HOH:O	1:B:312:ILE:CG2	2.69	0.40
1:A:226:GLU:CD	1:A:226:GLU:N	2.73	0.40
1:A:314:HIS:HA	1:A:315:PRO:HD2	1.93	0.40
1:B:130:PRO:O	1:B:131:THR:CG2	2.69	0.40
1:A:226:GLU:C	1:A:230:GLN:HG3	2.40	0.40
1:A:69:ILE:HD13	1:A:69:ILE:HG21	1.93	0.40
1:B:149:GLU:OE2	1:B:179:LYS:NZ	2.54	0.40
1:B:96:ARG:HB3	1:B:97:PRO:HD3	2.03	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ARG:NH1	1:A:237:GLU:OE1[2_656]	1.56	0.64
1:A:91:ARG:NH1	1:A:237:GLU:CD[2_656]	1.73	0.47
1:A:153:LYS:NZ	1:A:230:GLN:OE1[2_656]	1.90	0.30
1:B:237:GLU:CG	5:B:584:HOH:O[2_655]	1.93	0.27
1:A:230:GLN:OE1	5:A:694:HOH:O[2_646]	2.08	0.12
1:A:91:ARG:CZ	1:A:237:GLU:OE1[2_656]	2.09	0.11
1:B:237:GLU:CD	5:B:584:HOH:O[2_655]	2.11	0.09
1:A:153:LYS:CD	1:A:230:GLN:OE1[2_656]	2.13	0.07
1:A:153:LYS:NZ	1:A:230:GLN:CD[2_656]	2.15	0.05
1:A:275:LYS:CG	5:B:592:HOH:O[2_645]	2.19	0.01

## 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	320/323 (99%)	303 (95%)	14 (4%)	3 (1%)	17	12
1	B	313/323 (97%)	290 (93%)	18 (6%)	5 (2%)	9	4
All	All	633/646 (98%)	593 (94%)	32 (5%)	8 (1%)	12	7

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	GLY
1	A	226	GLU
1	B	133	GLU
1	B	134	HIS
1	A	133	GLU
1	B	27	GLU
1	B	132	ASP
1	B	302	ASN

### 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	280/281 (100%)	265 (95%)	15 (5%)	22	19
1	B	275/281 (98%)	257 (94%)	18 (6%)	17	13
All	All	555/562 (99%)	522 (94%)	33 (6%)	19	16

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	67	SER
1	A	87	CYS
1	A	132	ASP
1	A	144	ILE
1	A	176	ILE
1	A	185	LYS
1	A	199	GLN
1	A	228	VAL
1	A	230	GLN
1	A	252	PRO
1	A	275	LYS
1	A	294	LYS
1	A	301	ARG
1	A	309	ASP
1	B	63	LEU
1	B	75	LYS
1	B	94	LEU
1	B	96	ARG
1	B	104	LYS
1	B	126	VAL
1	B	133	GLU
1	B	134	HIS
1	B	136	LYS
1	B	141	THR
1	B	144	ILE
1	B	199	GLN
1	B	237	GLU
1	B	246	LYS
1	B	290	SER
1	B	294	LYS
1	B	301	ARG
1	B	304	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	6	GLN
1	A	105	ASN
1	A	167	ASN
1	A	172	GLN
1	A	194	HIS
1	A	199	GLN

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Mol	Chain	Res	Type
1	A	222	HIS
1	A	230	GLN
1	A	250	GLN
1	A	262	GLN
1	A	282	GLN
1	B	6	GLN
1	B	105	ASN
1	B	134	HIS
1	B	167	ASN
1	B	172	GLN
1	B	178	ASN
1	B	194	HIS
1	B	199	GLN
1	B	262	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

4 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
3	NAP	A	401	-	45,52,52	1.90	9 (20%)	56,80,80	1.64	9 (16%)
2	SO4	A	601	-	4,4,4	0.28	0	6,6,6	0.49	0
4	TES	A	501	-	24,24,24	1.08	1 (4%)	39,39,39	1.95	8 (20%)
3	NAP	B	402	-	45,52,52	1.84	6 (13%)	56,80,80	1.63	12 (21%)

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	NAP	A	401	-	-	8/31/67/67	0/5/5/5
4	TES	A	501	-	-	-	0/4/4/4
3	NAP	B	402	-	-	8/31/67/67	0/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAP	O7N-C7N	8.36	1.40	1.24
3	A	401	NAP	O7N-C7N	8.25	1.40	1.24
3	B	402	NAP	P2B-O2B	4.37	1.67	1.59
3	A	401	NAP	C2A-N3A	4.07	1.38	1.32
3	A	401	NAP	P2B-O2B	3.81	1.66	1.59
4	A	501	TES	C7-C6	3.56	1.60	1.52
3	B	402	NAP	C2A-N3A	3.53	1.37	1.32
3	A	401	NAP	C2A-N1A	3.47	1.40	1.33
3	A	401	NAP	C4A-N3A	2.55	1.39	1.35
3	A	401	NAP	O2D-C2D	-2.47	1.37	1.43
3	B	402	NAP	O4B-C1B	2.34	1.44	1.41
3	A	401	NAP	PN-O2N	-2.28	1.44	1.55
3	A	401	NAP	O2B-C2B	-2.23	1.36	1.44
3	A	401	NAP	C2N-N1N	2.22	1.37	1.35
3	B	402	NAP	C2A-N1A	2.12	1.37	1.33
3	B	402	NAP	C2N-N1N	2.03	1.37	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAP	N3A-C2A-N1A	-6.43	118.64	128.68
3	B	402	NAP	N3A-C2A-N1A	-5.83	119.57	128.68
4	A	501	TES	C1-C10-C9	5.34	116.19	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	501	TES	C19-C10-C9	-4.47	106.36	111.68
4	A	501	TES	C16-C17-C13	-4.23	101.17	104.53
3	A	401	NAP	C3N-C7N-N7N	4.04	122.60	117.75
3	A	401	NAP	O7N-C7N-C3N	-3.80	115.08	119.63
3	B	402	NAP	C3N-C7N-N7N	3.67	122.16	117.75
4	A	501	TES	C7-C8-C9	3.49	114.83	110.49
3	B	402	NAP	O3B-C3B-C4B	-3.43	101.14	111.05
3	B	402	NAP	C6N-N1N-C2N	-3.15	119.10	121.97
3	B	402	NAP	O7N-C7N-C3N	-3.04	115.99	119.63
3	B	402	NAP	C4A-C5A-N7A	-2.96	106.32	109.40
3	A	401	NAP	C2A-N1A-C6A	2.79	123.52	118.75
4	A	501	TES	C12-C13-C17	2.72	119.13	115.24
3	A	401	NAP	O3X-P2B-O2X	2.64	117.71	107.64
4	A	501	TES	C11-C12-C13	-2.60	108.32	112.78
4	A	501	TES	C6-C5-C4	-2.60	116.53	120.87
3	B	402	NAP	C2N-C3N-C4N	2.47	121.06	118.26
3	A	401	NAP	O2D-C2D-C3D	-2.43	103.96	111.82
3	B	402	NAP	C5B-C4B-C3B	-2.39	106.23	115.18
3	B	402	NAP	O2D-C2D-C1D	-2.33	102.24	110.85
3	A	401	NAP	C2N-C3N-C4N	2.27	120.83	118.26
3	B	402	NAP	C2B-C3B-C4B	2.24	106.85	101.99
3	A	401	NAP	O4D-C4D-C5D	2.19	116.58	109.37
3	B	402	NAP	C5N-C4N-C3N	-2.18	117.76	120.34
3	A	401	NAP	O5D-PN-O1N	-2.12	100.80	109.07
4	A	501	TES	C11-C9-C8	-2.10	108.73	111.75
3	B	402	NAP	O3X-P2B-O2X	2.03	115.38	107.64

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	NAP	C5B-O5B-PA-O1A
3	A	401	NAP	C5B-O5B-PA-O2A
3	A	401	NAP	C5B-O5B-PA-O3
3	B	402	NAP	C5B-O5B-PA-O3
3	A	401	NAP	C3B-C4B-C5B-O5B
3	B	402	NAP	C3B-C4B-C5B-O5B
3	A	401	NAP	C4D-C5D-O5D-PN
3	B	402	NAP	C4D-C5D-O5D-PN
3	A	401	NAP	PA-O3-PN-O5D
3	B	402	NAP	PA-O3-PN-O5D
3	A	401	NAP	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
3	B	402	NAP	C5B-O5B-PA-O1A
3	B	402	NAP	C5B-O5B-PA-O2A
3	B	402	NAP	O4B-C4B-C5B-O5B
3	A	401	NAP	C2B-O2B-P2B-O2X
3	B	402	NAP	PA-O3-PN-O2N

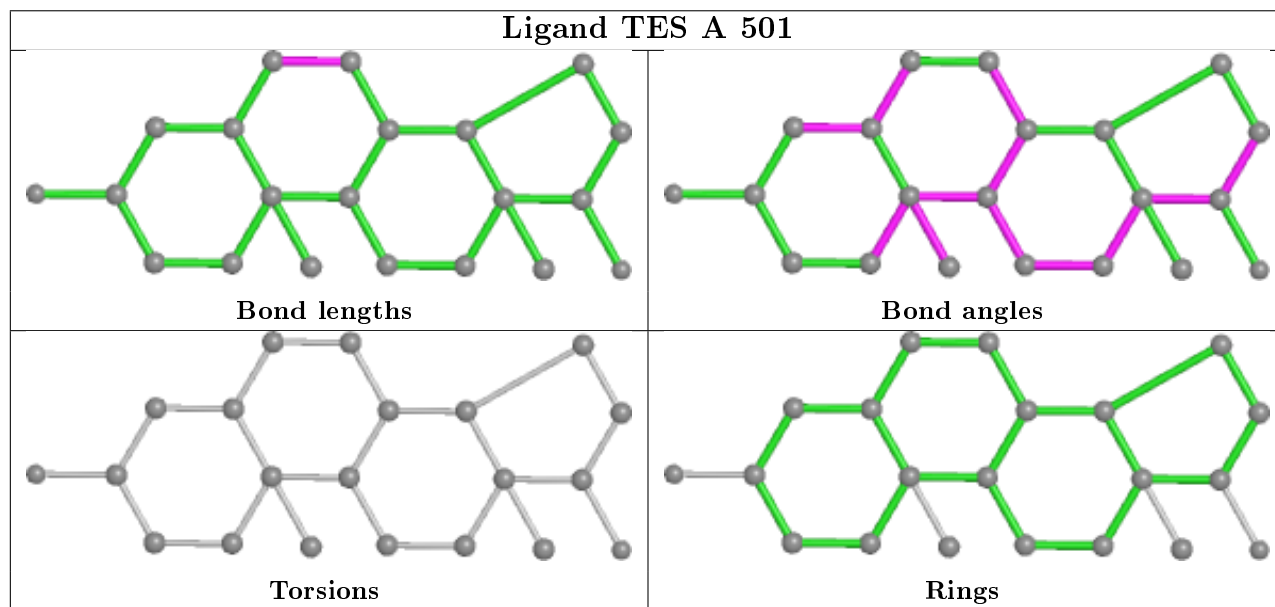
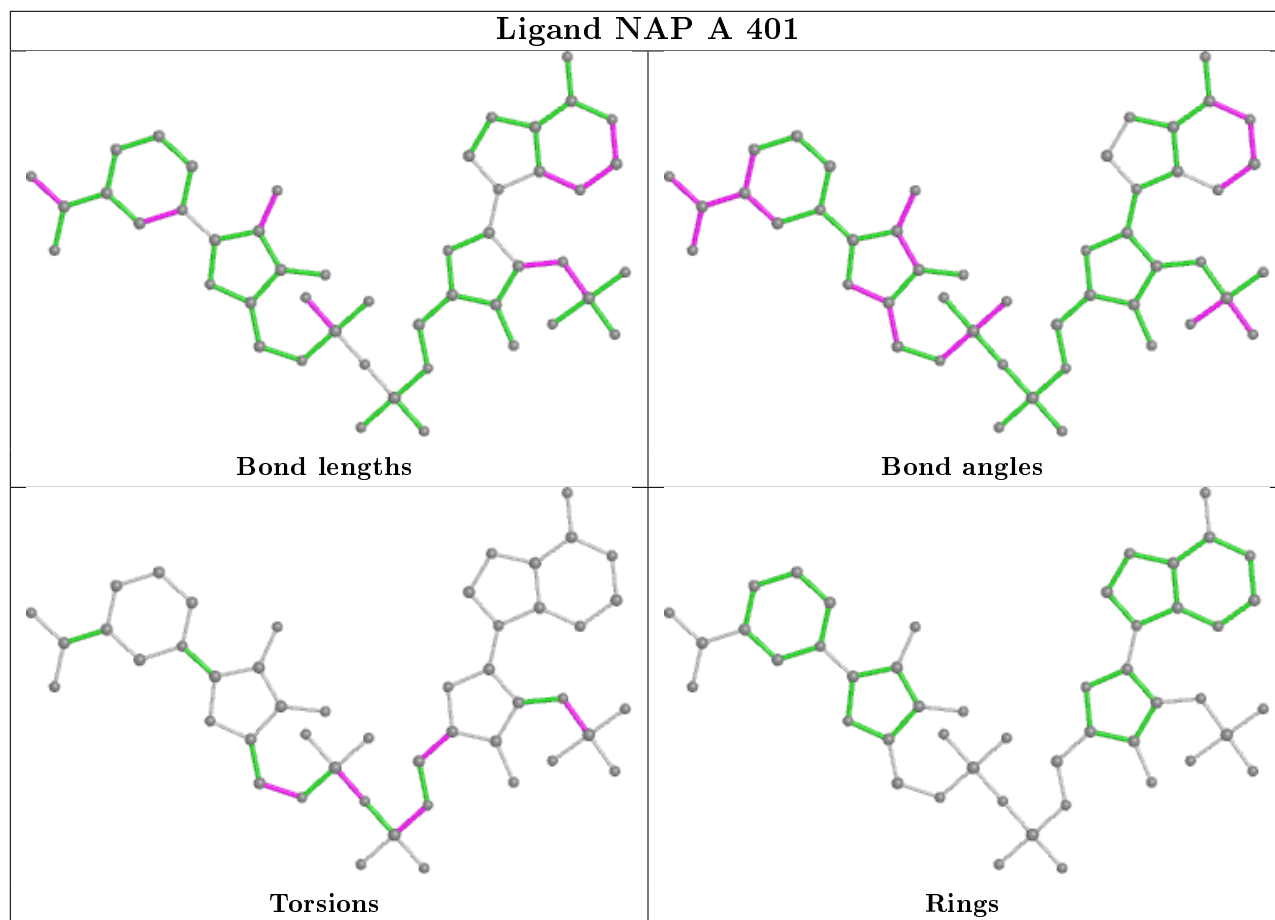
There are no ring outliers.

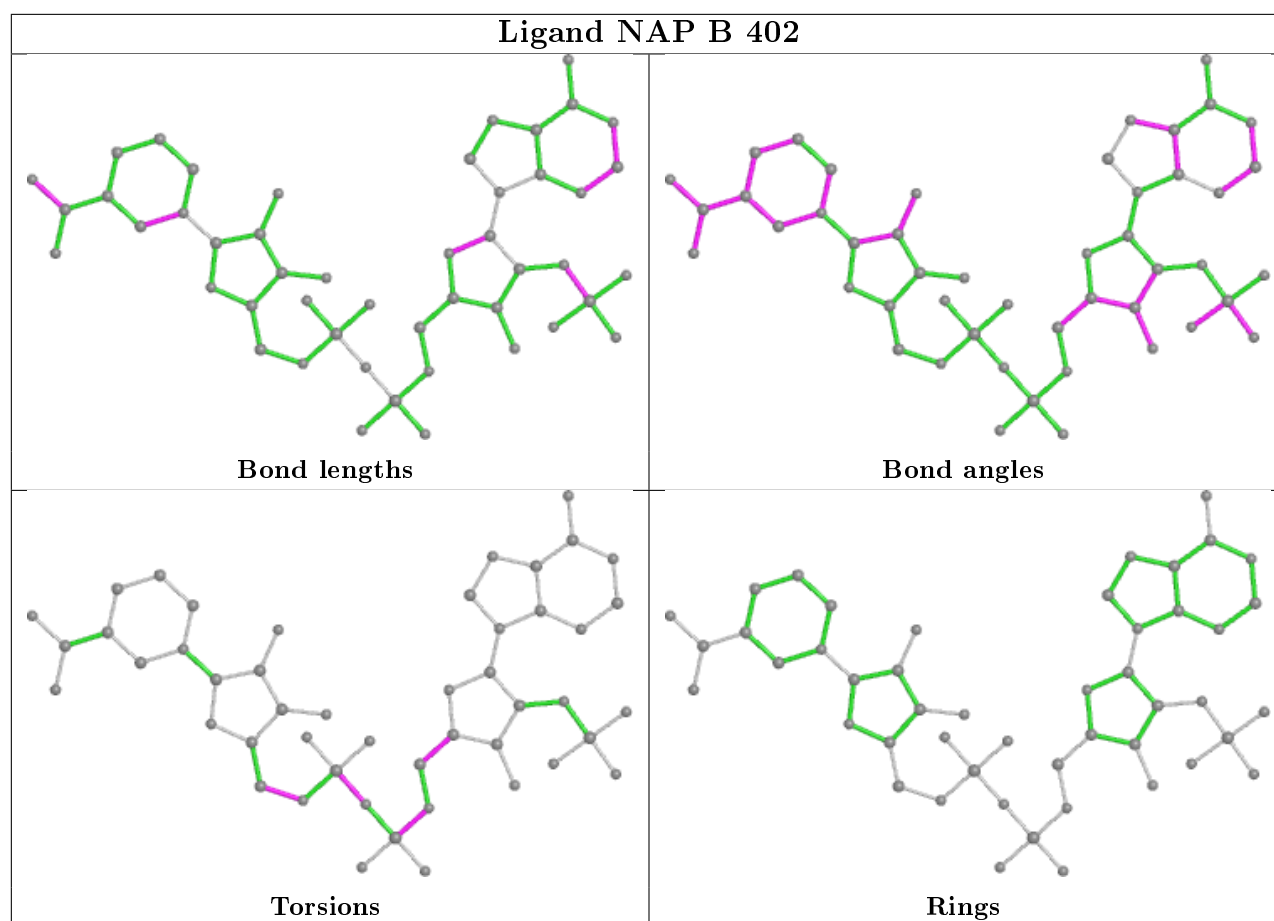
3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAP	3	0
4	A	501	TES	7	0
3	B	402	NAP	4	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	322/323 (99%)	0.39	12 (3%) 41 46	8, 14, 27, 38	0
1	B	317/323 (98%)	0.38	12 (3%) 40 45	5, 13, 24, 37	0
All	All	639/646 (98%)	0.38	24 (3%) 40 45	5, 13, 26, 38	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	135	GLY	7.5
1	A	134	HIS	7.5
1	B	134	HIS	4.5
1	A	133	GLU	4.2
1	B	132	ASP	4.0
1	A	308	ALA	3.8
1	B	225	PRO	3.8
1	B	128	ILE	3.6
1	A	175	MET	3.0
1	B	231	SER	2.8
1	B	126	VAL	2.7
1	B	133	GLU	2.6
1	A	227	TRP	2.4
1	A	3	PRO	2.3
1	A	230	GLN	2.3
1	B	137	ALA	2.2
1	B	108	LEU	2.2
1	A	67	SER	2.2
1	A	202	LEU	2.2
1	B	310	PHE	2.1
1	A	128	ILE	2.0
1	A	144	ILE	2.0
1	B	144	ILE	2.0
1	A	72	GLY	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](#)

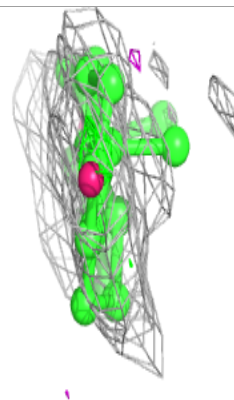
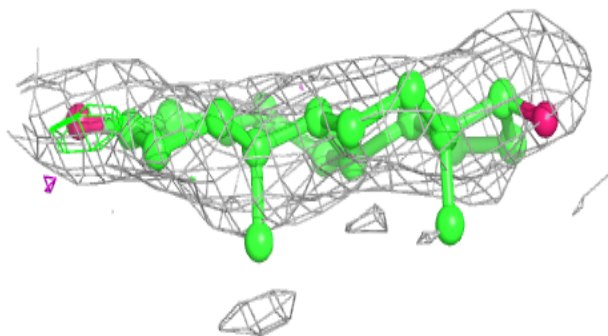
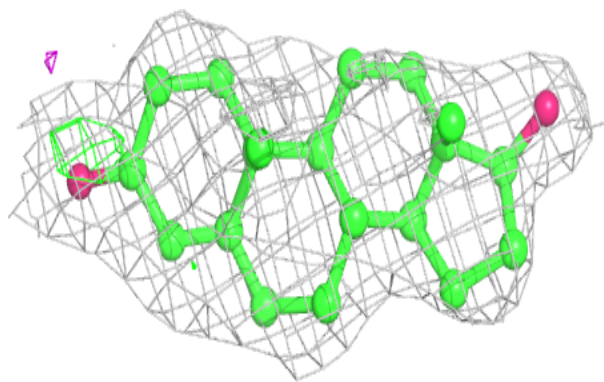
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	TES	A	501	21/21	0.86	0.23	43,49,51,52	0
2	SO4	A	601	5/5	0.89	0.16	60,62,65,66	0
3	NAP	B	402	48/48	0.94	0.13	4,12,14,18	0
3	NAP	A	401	48/48	0.96	0.12	3,12,15,17	0

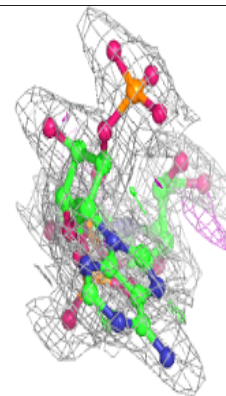
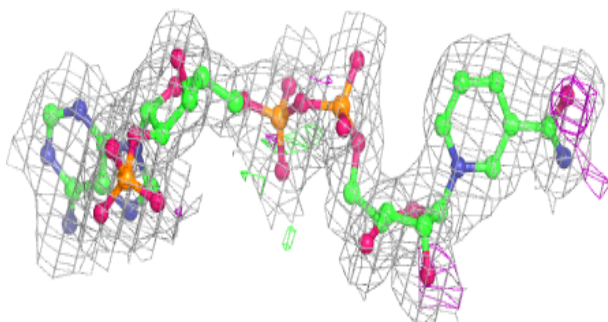
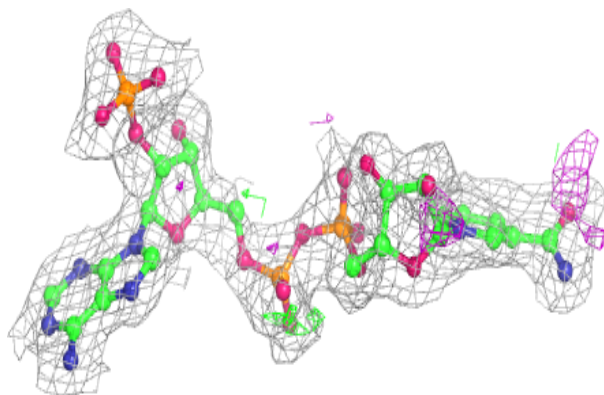
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

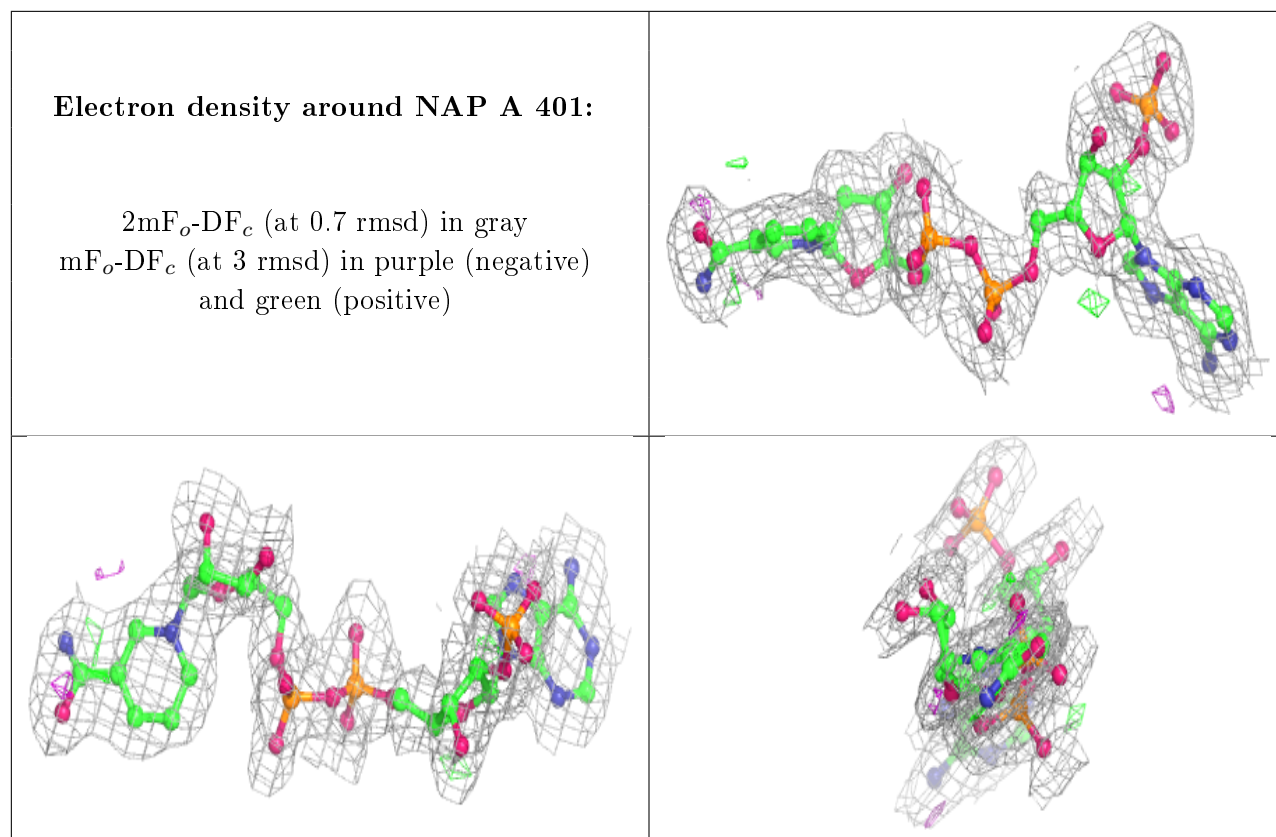
**Electron density around TES A 501:**

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

**Electron density around NAP B 402:**

$2mF_o-DF_c$  (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.