



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:42 PM UTC

PDB ID : 1Q13 / pdb_00001q13
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

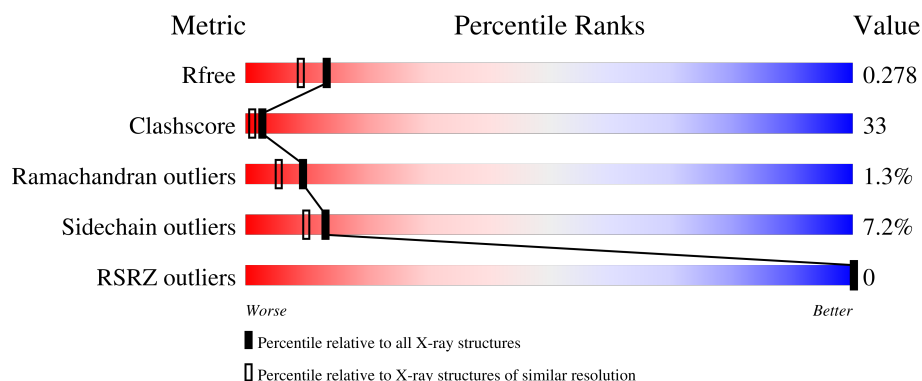
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 53% 38% 7% .
1	B	323	 51% 38% 7% ..

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
1	A	322	Total	C	N	O	S	0	0	0
			2579	1662	435	472	10			
1	B	317	Total	C	N	O	S	0	0	0
			2532	1632	428	462	10			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



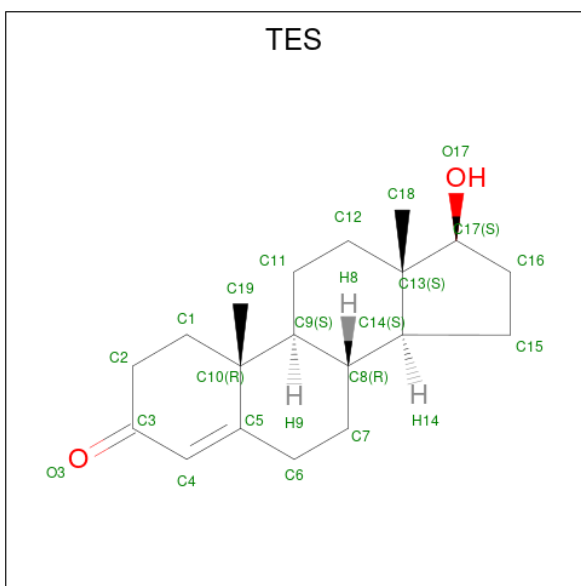
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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

- Molecule 4 is TESTOSTERONE (CCD ID: TES) (formula: $C_{19}H_{28}O_2$).



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

- Molecule 5 is water.

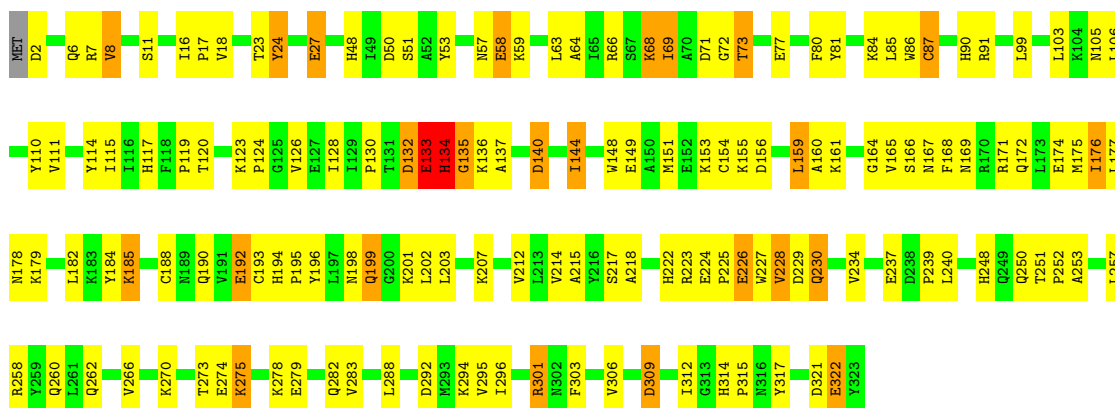
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	201	Total 201	O 201	0	0
5	B	191	Total 191	O 191	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

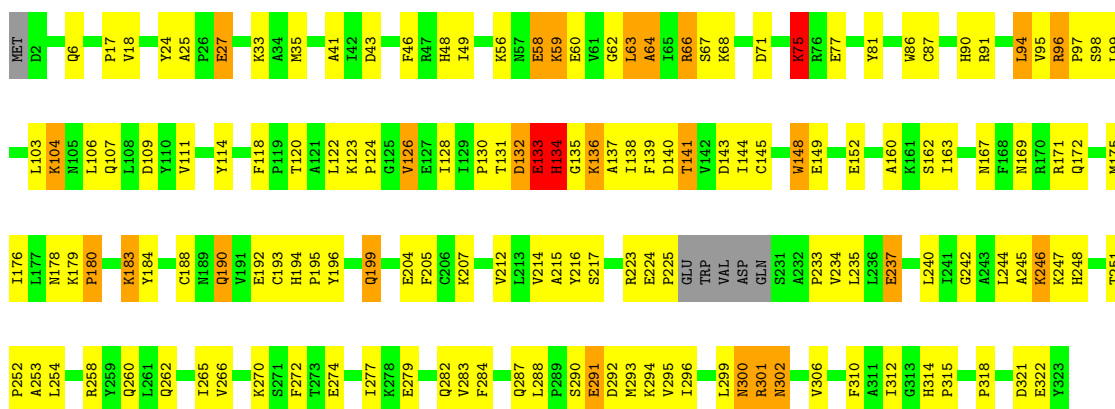
• Molecule 1: Prostaglandin-E2 9-reductase

Chain A: 



• Molecule 1: Prostaglandin-E2 9-reductase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.21Å 84.05Å 66.25Å 90.00° 91.17° 90.00°	Depositor
Resolution (Å)	20.00 – 2.08 20.00 – 2.08	Depositor EDS
% Data completeness (in resolution range)	93.5 (20.00-2.08) 90.2 (20.00-2.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.45 (at 2.09Å)	Xtriage
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 ²)	19.5	Xtriage
Anisotropy	0.693	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.177 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5625	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TES, NAP, 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	1.40	18/2642 (0.7%)	1.32	7/3575 (0.2%)
1	B	1.26	14/2592 (0.5%)	1.29	11/3504 (0.3%)
All	All	1.33	32/5234 (0.6%)	1.30	18/7079 (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 (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	TYR	C-N	9.35	1.44	1.32
1	B	59	LYS	CD-CE	9.22	1.80	1.52
1	A	253	ALA	CA-CB	8.47	1.66	1.53
1	A	322	GLU	CD-OE2	8.03	1.40	1.25
1	B	253	ALA	CA-CB	7.97	1.66	1.53
1	A	71	ASP	CA-CB	7.42	1.63	1.53
1	B	300	ASN	N-CA	6.94	1.55	1.46
1	A	192	GLU	CD-OE2	6.58	1.37	1.25
1	B	59	LYS	CE-NZ	6.18	1.67	1.49
1	A	71	ASP	C-N	6.09	1.42	1.33
1	A	24	TYR	C-O	6.07	1.31	1.24
1	A	68	LYS	CA-C	6.01	1.61	1.52
1	A	24	TYR	CG-CD2	5.88	1.51	1.39
1	B	180	PRO	N-CD	5.88	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	64	ALA	C-N	5.86	1.41	1.33
1	A	24	TYR	CE1-CZ	5.84	1.52	1.38
1	A	239	PRO	C-N	5.70	1.41	1.34
1	B	293	MET	SD-CE	-5.62	1.65	1.79
1	A	71	ASP	CA-C	5.50	1.60	1.52
1	A	23	THR	N-CA	5.41	1.52	1.46
1	B	95	VAL	CA-C	5.41	1.59	1.52
1	B	49	ILE	CA-CB	5.28	1.60	1.54
1	A	58	GLU	CD-OE2	5.27	1.35	1.25
1	B	64	ALA	CA-CB	5.25	1.61	1.53
1	B	148	TRP	C-O	5.20	1.30	1.24
1	A	50	ASP	CA-CB	5.19	1.60	1.53
1	A	85	LEU	CG-CD1	5.18	1.69	1.52
1	B	162	SER	N-CA	5.18	1.52	1.45
1	B	58	GLU	CA-C	5.18	1.59	1.52
1	B	118	PHE	N-CA	5.15	1.50	1.45
1	A	64	ALA	C-O	5.13	1.30	1.24
1	A	64	ALA	C-N	5.09	1.40	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	HIS	N-CA-C	10.09	123.47	108.14
1	B	306	VAL	N-CA-C	7.09	117.65	106.88
1	B	109	ASP	N-CA-C	6.65	120.61	112.23
1	B	190	GLN	CA-C-N	-6.31	114.25	122.51
1	B	190	GLN	C-N-CA	-6.31	114.25	122.51
1	A	69	ILE	N-CA-C	-6.25	105.64	111.45
1	B	126	VAL	CB-CA-C	-6.20	101.13	111.29
1	A	73	THR	OG1-CB-CG2	-6.04	97.22	109.30
1	A	134	HIS	CA-C-O	6.03	127.73	121.28
1	A	159	LEU	N-CA-C	5.71	117.51	111.28
1	B	66	ARG	N-CA-C	-5.69	105.60	112.54
1	A	140	ASP	N-CA-C	-5.68	100.53	109.50
1	B	253	ALA	N-CA-C	-5.50	105.36	111.36
1	B	75	LYS	N-CA-C	-5.44	101.71	110.14
1	B	283	VAL	N-CA-C	-5.38	105.92	112.76
1	A	53	TYR	N-CA-C	-5.13	105.69	111.28
1	B	64	ALA	CA-C-N	-5.06	112.45	120.55
1	B	64	ALA	C-N-CA	-5.06	112.45	120.55

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

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	181	8
1	B	2532	0	2549	166	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	346	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 33.

All (346) 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:CE	1:B:59:LYS:NZ	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:227:TRP:HA	1:A:230:GLN:HG3	1.30	1.11
1:A:275:LYS:H	1:A:275:LYS:CE	1.63	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LYS:N	1:A:275:LYS:CE	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
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:OE2	1:B:133:GLU:HA	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:133:GLU:O	1:B:134:HIS:C	2.15	0.89
1:B:262:GLN:HE22	1:B:288:LEU:H	1.15	0.88
1:B:287:GLN:CD	5:B:556:HOH:O	2.16	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:A:224:GLU:O	1:A:228:VAL:CG1	2.25	0.84
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:CE	1:B:59:LYS:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:230:GLN:CD	5:A:654:HOH:O	2.07	0.73
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:A:225:PRO:C	1:A:226:GLU:OE1	2.32	0.73
1:B:149:GLU:CG	1:B:179:LYS:HZ1	2.01	0.73
1:B:291:GLU:H	1:B:291:GLU:CD	1.97	0.73
1:A:174:GLU:O	1:A:178:ASN:HB2	1.89	0.73
1:B:94:LEU:HB3	5:B:501:HOH:O	1.87	0.73
1:B:123:LYS:HE2	1:B:140:ASP:OD1	1.89	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:6:GLN:HE21	1:A:18:VAL:HG21	1.55	0.70
1:A:270:LYS:O	3:A:401:NAP:H8A	1.91	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:A:132:ASP:C	1:A:134:HIS:N	2.50	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:NH1	1:B:171:ARG:HG2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:B:171:ARG:HH11	1.59	0.66
1:B:43:ASP:CG	5:B:467:HOH:O	2.38	0.66
1:A:59:LYS:HE3	1:A:105:ASN:ND2	2.09	0.66
1:A:260:GLN:HA	1:A:260:GLN:OE1	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
1:A:192:GLU:OE2	1:A:194:HIS:HE1	1.79	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:247:LYS:NZ	5:B:562:HOH:O	2.30	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:131:THR:HG22	1:B:136:LYS:C	2.24	0.62
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: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:A:273:THR:O	1:A:274:GLU:C	2.45	0.58
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:A:227:TRP:C	1:A:230:GLN:HG3	2.29	0.58
1:B:199:GLN:HE21	1:B:199:GLN:HA	1.69	0.58
1:A:81:TYR:CE2	1:A:106:LEU:HD11	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ASN:OD1	1:B:172:GLN:HG3	2.04	0.57
1:B:59:LYS:HD2	5:B:415:HOH:O	2.04	0.57
1:B:131:THR:HG22	1:B:136:LYS: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:B:132:ASP:C	1:B:134:HIS:N	2.63	0.56
1:A:188:CYS:HA	1:A:212:VAL:O	2.05	0.56
1:A:226:GLU:C	1:A:230:GLN:CG	2.78	0.55
1:B:242:GLY:O	1:B:246:LYS:HD2	2.07	0.55
1:A:270:LYS:HD3	1:A:270:LYS:C	2.32	0.55
1:A:234:VAL:CB	1:A:237:GLU:OE2	2.55	0.55
1:B:133:GLU:OE2	1:B:133:GLU:CA	2.47	0.54
1:B:133:GLU:O	1:B:135:GLY:N	2.39	0.54
1:B:237:GLU:OE2	5:B:542:HOH:O	2.18	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: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:A:303:PHE:C	1:A:303:PHE:CD2	2.87	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:A:164:GLY:C	1:A:165:VAL:HG13	2.34	0.52
1:B:192:GLU:OE2	1:B:194:HIS:HE1	1.92	0.52
1:B:237:GLU:CD	5:B:542:HOH:O	2.53	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:B:270:LYS:C	1:B:270:LYS:HD3	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:130:PRO:C	1:B:131:THR:HG23	2.36	0.51
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:B:171:ARG:HH11	1:B:171:ARG:CG	2.24	0.50
1:A:126:VAL:HG13	1:B:302:ASN:CG	2.32	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
1:A:126:VAL:CG1	1:A:126:VAL:O	2.58	0.50
1:A:174:GLU:OE2	1:A:174:GLU:HA	2.12	0.50
1:A:51:SER:O	1:A:84:LYS:NZ	2.43	0.50
1:B:86:TRP:CG	1:B:87:CYS:H	2.29	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: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:A:224:GLU:C	1:A:228:VAL:HG13	2.37	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:A:72:GLY:O	1:A:73:THR:C	2.54	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:225:PRO:O	1:A:226:GLU:C	2.55	0.48
1:A:309:ASP:O	1:A:312:ILE:HG12	2.12	0.48
1:B:301:ARG:HE	1:B:301:ARG:HB3	1.32	0.48
1:B:68:LYS:HD2	1:B:68:LYS:HA	1.58	0.48
1:B:149:GLU:HA	1:B:152:GLU:OE1	2.13	0.48
1:B:149:GLU:CD	1:B:179:LYS:HZ1	2.22	0.48
1:A:190:GLN:OE1	3:A:401:NAP:H2N	2.14	0.47
1:A:175:MET:HE3	1:A:175:MET:HB2	1.73	0.47
1:A:110:TYR:CD1	1:A:161:LYS:HG2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:63:LEU:HD12	1:A:66:ARG:NH2	2.29	0.47
1:A:201:LYS:O	1:A:202:LEU:C	2.56	0.47
1:A:250:GLN:NE2	5:A:756:HOH:O	2.47	0.47
1:B:75:LYS:HE3	1:B:75:LYS:HB2	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:O	1:A:306:VAL:HG12	2.13	0.47
1:B:244:LEU:O	1:B:245:ALA:C	2.58	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:57:ASN:C	1:A:57:ASN:OD1	2.58	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:24:TYR:CE1	4:A:501:TES:H61	2.50	0.46
1:A:194:HIS:CD2	1:A:196:TYR:HB2	2.50	0.46
1:A:196:TYR:CD1	1:A:301:ARG:HD3	2.50	0.46
1:A:91:ARG:HH21	1:A:140:ASP:CG	2.24	0.46
1:A:133:GLU:CD	1:A:133:GLU:H	2.23	0.46
1:B:214:VAL:HA	1:B:266:VAL:O	2.16	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:A:226:GLU:N	1:A:226:GLU:CD	2.73	0.45
1:B:172:GLN:HE22	1:B:318:PRO:HB3	1.82	0.45
1:A:7:ARG:HD3	1:A:17:PRO:HD3	1.99	0.45
1:A:130:PRO:HD3	5:A:647:HOH:O	2.16	0.45
1:A:226:GLU:C	1:A:230:GLN:HG3	2.40	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:35:MET:HB2	1:B:60:GLU:HB3	1.98	0.45
1:B:171:ARG:NH1	1:B:171:ARG:CG	2.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASP:C	1:A:134:HIS:H	2.26	0.44
1:B:67:SER:OG	5:B:411:HOH:O	2.15	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: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:A:134:HIS:C	1:A:136:LYS:N	2.75	0.43
1:A:224:GLU:C	1:A:228:VAL:CG1	2.89	0.43
1:B:87:CYS:HA	1:B:90:HIS:CD2	2.53	0.43
1:A:164:GLY:C	1:A:165:VAL:CG1	2.91	0.43
1:B:71:ASP:OD1	1:B:71:ASP:C	2.60	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:A:240:LEU:HD21	1:A:295:VAL:HG13	2.00	0.43
1:A:149:GLU:HG3	1:A:179:LYS:HE3	2.01	0.43
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.76	0.43
1:B:245:ALA:HB3	1:B:246:LYS:HE3	2.01	0.43
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:HD23	1:A:257:LEU:HA	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:80:PHE:CD1	1:A:80:PHE:C	2.97	0.42
1:A:193:CYS:O	1:A:218:ALA:HA	2.18	0.42
1:B:199:GLN:HE21	1:B:199:GLN:CA	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: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:203:LEU:HD11	1:A:207:LYS:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:321:ASP:O	1:B:322:GLU:C	2.62	0.42
1:A:155:LYS:HD3	1:A:184:TYR:CE2	2.55	0.42
1:A:198:ASN:O	1:A:199:GLN:HB2	2.19	0.42
1:A:234:VAL:HG11	1:A:237:GLU:CD	2.45	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: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:A:224:GLU:O	1:A:228:VAL:HG13	2.12	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:HA	1:A:250:GLN:HE21	1.85	0.41
1:B:194:HIS:CD2	1:B:196:TYR:H	2.31	0.41
1:B:204:GLU:O	1:B:205:PHE:C	2.61	0.41
1:B:270:LYS:HE2	1:B:272:PHE:CD1	2.56	0.41
1:B:282:GLN:C	1:B:284:PHE:N	2.77	0.41
1:B:43:ASP:OD1	5:B:467:HOH:O	2.22	0.41
1:A:91:ARG:HH22	1:A:123:LYS:NZ	2.18	0.41
1:A:130:PRO:CG	5:A:647:HOH:O	2.68	0.41
1:A:248:HIS:NE2	1:A:292:ASP:OD2	2.41	0.41
1:A:321:ASP:O	1:A:322:GLU:C	2.61	0.41
1:B:27:GLU:OE2	5:B:575:HOH:O	2.22	0.41
1:B:99:LEU:HB2	1:B:114:TYR:CE2	2.55	0.41
1:B:111:VAL:O	1:B:160:ALA:HA	2.21	0.41
1:B:251:THR:HB	1:B:252:PRO:HD2	2.03	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:63:LEU:HD12	1:A:63:LEU:HA	1.79	0.40
1:A:312:ILE:HD13	1:A:312:ILE:HA	1.89	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:68:LYS:HD3	1:A:68:LYS:HA	1.66	0.40
1:A:251:THR:HG21	1:A:279:GLU:OE1	2.21	0.40
5:A:793:HOH:O	1:B:312:ILE:CG2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ASN:HD22	1:B:178:ASN:HA	1.63	0.40
1:A:314:HIS:HA	1:A:315:PRO:HD2	1.93	0.40
1:B:63:LEU:O	1:B:64:ALA:C	2.64	0.40
1:B:130:PRO:O	1:B:131:THR:CG2	2.69	0.40
1:A:69:ILE:HD13	1:A:69:ILE:HG21	1.93	0.40
1:B:96:ARG:HB3	1:B:97:PRO:HD3	2.03	0.40
1:B:149:GLU:OE2	1:B:179:LYS:NZ	2.54	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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	320/323 (99%)	303 (95%)	14 (4%)	3 (1%)	14	10
1	B	313/323 (97%)	290 (93%)	18 (6%)	5 (2%)	7	4
All	All	633/646 (98%)	593 (94%)	32 (5%)	8 (1%)	9	5

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%)	263 (94%)	17 (6%)	17	14
1	B	275/281 (98%)	252 (92%)	23 (8%)	10	7
All	All	555/562 (99%)	515 (93%)	40 (7%)	13	10

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	27	GLU
1	A	77	GLU
1	A	87	CYS
1	A	128	ILE
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

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Mol	Chain	Res	Type
1	A	301	ARG
1	A	309	ASP
1	B	33	LYS
1	B	63	LEU
1	B	75	LYS
1	B	77	GLU
1	B	94	LEU
1	B	96	ARG
1	B	104	LYS
1	B	126	VAL
1	B	128	ILE
1	B	133	GLU
1	B	134	HIS
1	B	136	LYS
1	B	141	THR
1	B	144	ILE
1	B	176	ILE
1	B	183	LYS
1	B	199	GLN
1	B	237	GLU
1	B	246	LYS
1	B	290	SER
1	B	291	GLU
1	B	294	LYS
1	B	301	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) 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
1	A	222	HIS
1	A	230	GLN
1	A	249	GLN
1	A	250	GLN
1	A	262	GLN
1	A	282	GLN
1	B	6	GLN

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Mol	Chain	Res	Type
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 oligosaccharides 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	B	402	-	50,52,52	1.76	6 (12%)	71,80,80	1.98	18 (25%)
2	SO4	A	601	-	4,4,4	0.38	0	6,6,6	0.43	0
4	TES	A	501	-	24,24,24	1.11	1 (4%)	39,39,39	2.01	9 (23%)
3	NAP	A	401	-	50,52,52	1.93	13 (26%)	71,80,80	1.86	19 (26%)

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	B	402	-	-	10/35/67/67	0/5/5/5
4	TES	A	501	-	-	-	0/4/4/4
3	NAP	A	401	-	-	8/35/67/67	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NAP	O7N-C7N	8.61	1.40	1.24
3	A	401	NAP	O7N-C7N	8.50	1.40	1.24
3	B	402	NAP	P2B-O2B	4.58	1.67	1.59
3	A	401	NAP	P2B-O2B	3.98	1.66	1.59
4	A	501	TES	C7-C6	3.72	1.60	1.53
3	A	401	NAP	C2A-N1A	3.62	1.40	1.33
3	A	401	NAP	C2A-N3A	2.65	1.38	1.33
3	A	401	NAP	C4A-N3A	2.54	1.39	1.34
3	A	401	NAP	C5A-N7A	-2.45	1.34	1.39
3	A	401	NAP	C2N-N1N	2.44	1.37	1.35
3	B	402	NAP	C8A-N7A	2.39	1.36	1.31
3	A	401	NAP	O2B-C2B	-2.38	1.36	1.44
3	A	401	NAP	O2D-C2D	-2.34	1.37	1.43
3	A	401	NAP	C6A-N1A	2.33	1.42	1.35
3	A	401	NAP	C8A-N7A	2.32	1.36	1.31
3	A	401	NAP	PN-O2N	-2.31	1.44	1.55
3	B	402	NAP	C2N-N1N	2.23	1.37	1.35
3	B	402	NAP	C2A-N1A	2.20	1.37	1.33
3	B	402	NAP	C2A-N3A	2.17	1.37	1.33
3	A	401	NAP	PN-O3	2.08	1.61	1.59

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	NAP	N3A-C2A-N1A	-6.57	118.64	128.58
3	B	402	NAP	N3A-C2A-N1A	-5.95	119.57	128.58
4	A	501	TES	C1-C10-C9	5.63	116.19	108.74
3	B	402	NAP	N9A-C8A-N7A	-5.14	106.64	113.94
3	B	402	NAP	C5A-N7A-C8A	4.77	110.94	103.45
3	A	401	NAP	N9A-C8A-N7A	-4.76	107.19	113.94
4	A	501	TES	C19-C10-C9	-4.72	106.36	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	NAP	C5A-C4A-N3A	-4.56	120.44	126.72
4	A	501	TES	C16-C17-C13	-4.25	101.17	104.52
3	A	401	NAP	C3N-C7N-N7N	3.95	122.60	117.74
3	A	401	NAP	C5A-N7A-C8A	3.90	109.58	103.45
3	B	402	NAP	C4A-C5A-N7A	-3.73	106.32	110.58
3	A	401	NAP	O7N-C7N-C3N	-3.69	115.08	119.60
3	B	402	NAP	C2A-N3A-C4A	3.65	120.74	111.83
4	A	501	TES	C7-C8-C9	3.59	114.83	110.52
3	B	402	NAP	C3N-C7N-N7N	3.59	122.16	117.74
3	A	401	NAP	C2B-C1B-N9A	-3.51	107.97	113.75
3	B	402	NAP	O3B-C3B-C4B	-3.46	101.14	111.08
3	A	401	NAP	O2A-PA-O3	3.40	116.46	107.27
3	B	402	NAP	C6N-N1N-C2N	-3.26	119.10	121.88
3	B	402	NAP	N3A-C4A-N9A	3.08	132.41	127.17
3	B	402	NAP	C4A-N9A-C8A	3.02	108.91	105.74
3	B	402	NAP	O7N-C7N-C3N	-2.95	115.99	119.60
3	A	401	NAP	C2A-N1A-C6A	2.92	123.52	118.73
3	B	402	NAP	C4D-O4D-C1D	2.90	112.58	109.92
4	A	501	TES	C6-C5-C4	-2.71	116.53	120.86
3	A	401	NAP	C4A-N9A-C8A	2.66	108.53	105.74
3	B	402	NAP	C5N-C4N-C3N	-2.65	117.76	120.36
3	A	401	NAP	O3X-P2B-O2X	2.64	117.71	107.80
4	A	501	TES	C11-C12-C13	-2.62	108.32	112.74
3	A	401	NAP	C2A-N3A-C4A	2.59	118.16	111.83
4	A	501	TES	C12-C13-C17	2.56	119.13	115.23
3	B	402	NAP	C5B-C4B-C3B	-2.49	106.23	115.21
3	A	401	NAP	O2D-C2D-C3D	-2.45	103.96	111.82
3	B	402	NAP	C2N-C3N-C4N	2.40	121.06	118.26
3	A	401	NAP	O4B-C1B-N9A	2.36	112.63	108.09
3	A	401	NAP	C5A-C4A-N3A	-2.33	123.51	126.72
3	A	401	NAP	O4D-C4D-C5D	2.26	116.58	109.33
3	B	402	NAP	C2B-C3B-C4B	2.26	106.85	101.99
3	A	401	NAP	C2N-C3N-C4N	2.22	120.83	118.26
3	A	401	NAP	C4D-O4D-C1D	2.20	111.94	109.92
4	A	501	TES	C11-C9-C8	-2.19	108.73	111.78
3	A	401	NAP	O5D-PN-O1N	-2.05	100.80	108.94
3	A	401	NAP	N3A-C4A-N9A	2.04	130.63	127.17
3	B	402	NAP	O3X-P2B-O2X	2.02	115.38	107.80
4	A	501	TES	C6-C5-C10	2.00	120.29	116.76

There are no chirality outliers.

All (18) torsion outliers are listed below:

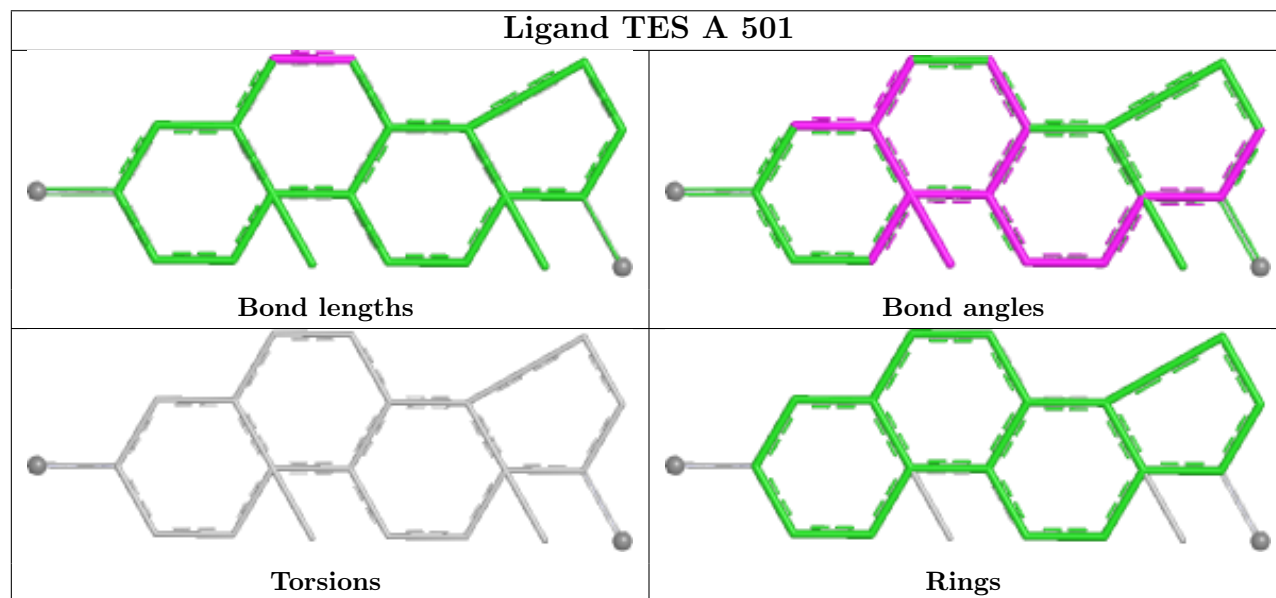
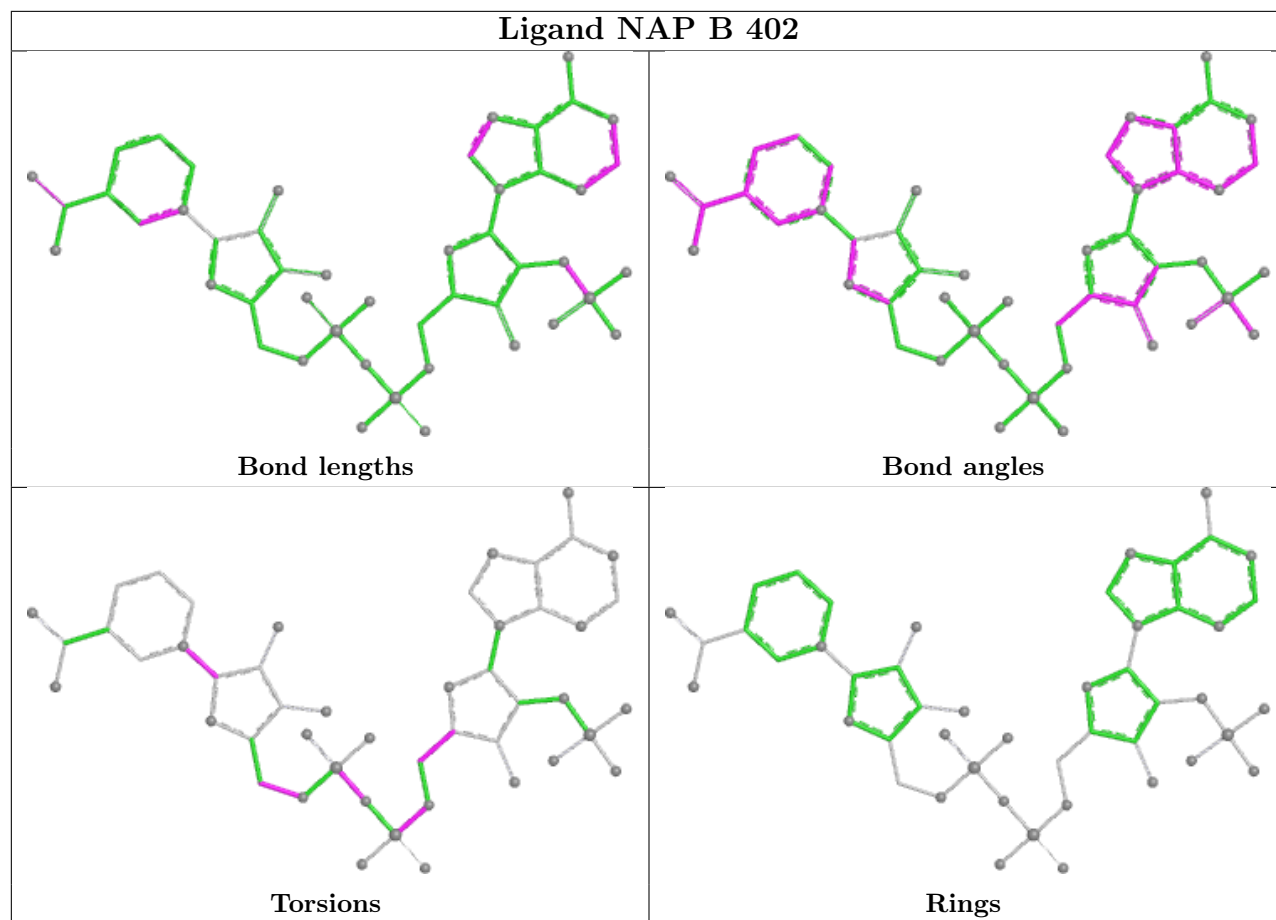
Mol	Chain	Res	Type	Atoms
3	A	401	NAP	C5B-O5B-PA-O1A
3	A	401	NAP	C5B-O5B-PA-O2A
3	B	402	NAP	C5B-O5B-PA-O2A
3	B	402	NAP	C5B-O5B-PA-O3
3	A	401	NAP	C3B-C4B-C5B-O5B
3	B	402	NAP	C3B-C4B-C5B-O5B
3	A	401	NAP	PA-O3-PN-O5D
3	B	402	NAP	PA-O3-PN-O5D
3	A	401	NAP	O4B-C4B-C5B-O5B
3	B	402	NAP	C4D-C5D-O5D-PN
3	B	402	NAP	O4B-C4B-C5B-O5B
3	A	401	NAP	C5B-O5B-PA-O3
3	B	402	NAP	C5B-O5B-PA-O1A
3	A	401	NAP	C4D-C5D-O5D-PN
3	B	402	NAP	O4D-C1D-N1N-C2N
3	B	402	NAP	O4D-C1D-N1N-C6N
3	B	402	NAP	PA-O3-PN-O2N
3	A	401	NAP	C2B-O2B-P2B-O2X

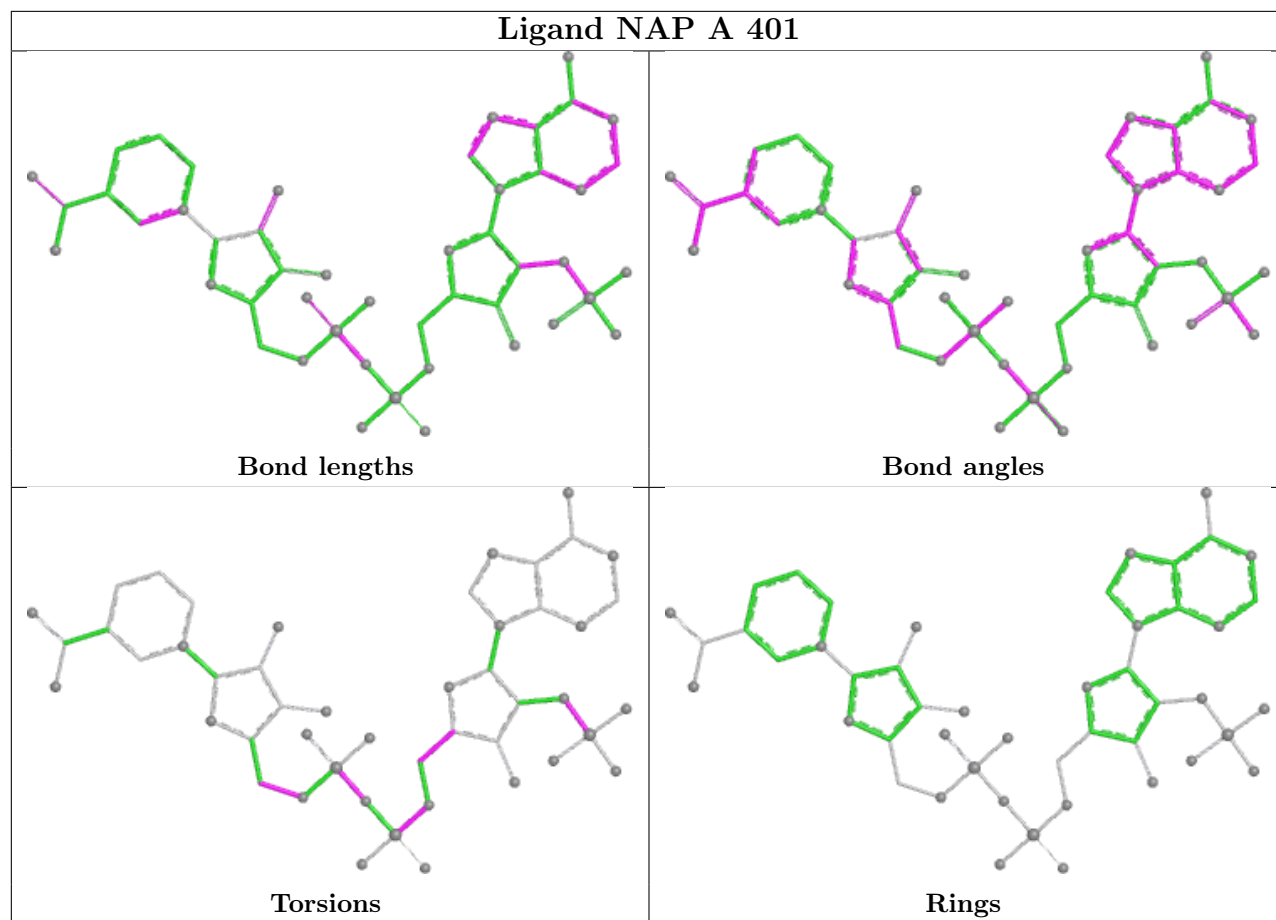
There are no ring outliers.

3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	NAP	4	0
4	A	501	TES	7	0
3	A	401	NAP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	322/323 (99%)	-0.63	0 100 100	8, 14, 27, 38	0
1	B	317/323 (98%)	-0.66	0 100 100	5, 13, 24, 37	0
All	All	639/646 (98%)	-0.64	0 100 100	5, 13, 26, 38	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

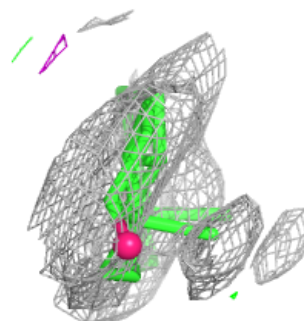
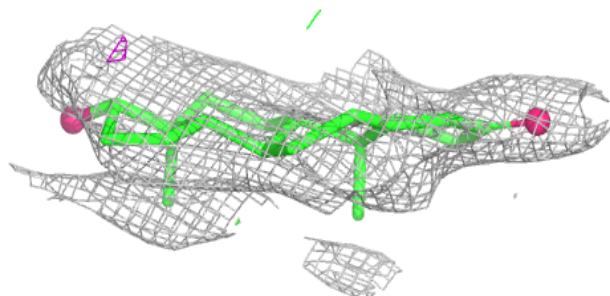
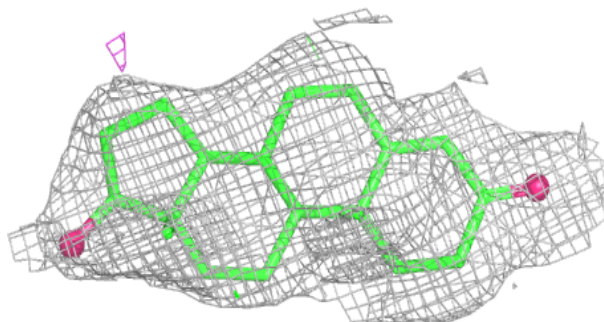
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	601	5/5	0.96	0.10	60,62,65,66	0
4	TES	A	501	21/21	0.97	0.08	43,49,51,52	0
3	NAP	B	402	48/48	0.99	0.05	4,12,14,18	0
3	NAP	A	401	48/48	0.99	0.04	3,12,15,17	0

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.

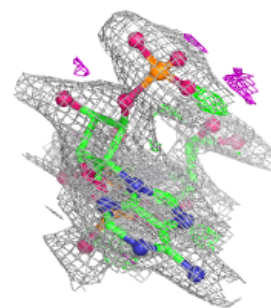
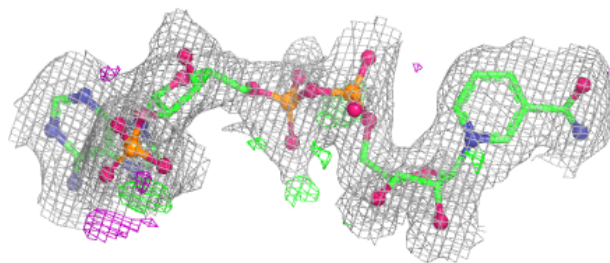
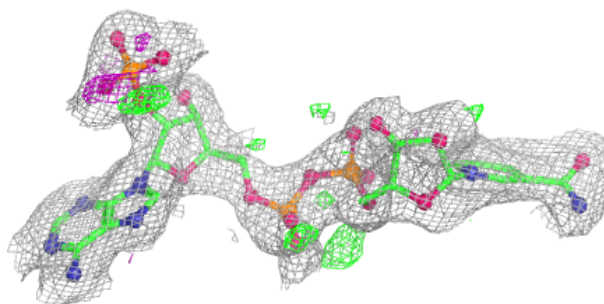
Electron density around TES A 501:

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



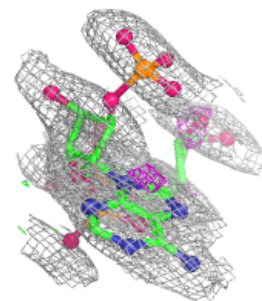
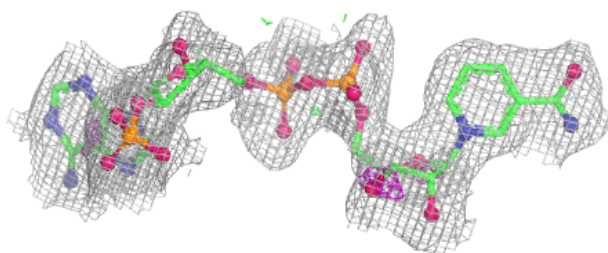
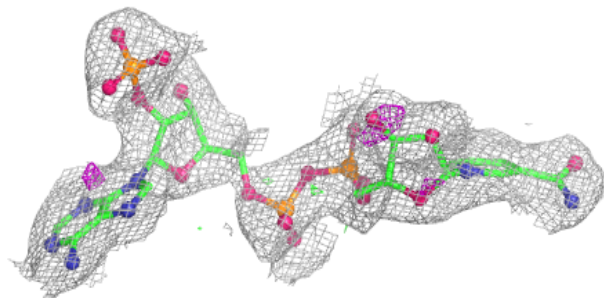
Electron density around NAP B 402:

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



Electron density around NAP A 401:

$2mF_o-DF_c$ (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.