Full wwPDB X-ray Structure Validation Report (i)

Apr 30, 2024 – 10:48 pm BST

PDB ID	:	2YDX
Title	:	Crystal structure of human S-adenosylmethionine synthetase 2, beta subunit
Authors	:	Muniz, J.R.C.; Shafqat, N.; Pike, A.C.W.; Yue, W.W.; Vollmar, M.; Papagriogriou, V.; Roos, A.; Gileadi, O.; von Delft, F.; Kavanagh, K.L.; Arrowsmith, C.H.; Edwards, A.M.; Weigelt, J.; Bountra, C.; Oppermann, U.
Deposited on	:	2011-03-25
Resolution	:	2.80 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 (i) 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 (i)) were used in the production of this report:

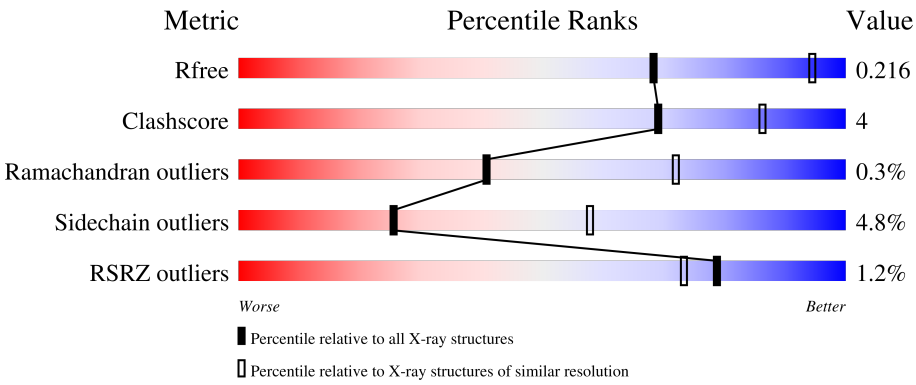
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	315	87% 10% • •
1	B	315	85% 12% • •
1	C	315	% 89% 9% • •
1	D	315	3% 90% 8% • •

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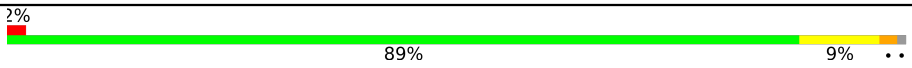
Mol	Chain	Length	Quality of chain
1	E	315	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	STL	A	501	-	X	-	-
2	STL	A	502	-	X	-	-
2	STL	B	501	-	X	-	-
2	STL	B	502	-	X	-	-
2	STL	C	501	-	X	-	-
2	STL	C	502	-	X	-	-
2	STL	D	501	-	X	-	-
2	STL	D	502	-	X	-	-
2	STL	E	501	-	X	-	-
2	STL	E	502	-	X	-	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 13178 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 METHIONINE ADENOSYLTRANSFERASE 2 SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	312	2452	1553	441	447	11	0	2	0
1	B	312	2440	1543	444	442	11	0	1	0
1	C	312	2440	1542	441	446	11	0	1	0
1	D	312	2409	1522	435	441	11	0	1	0
1	E	312	2408	1522	433	442	11	0	1	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP Q9NZL9
A	335	ALA	-	expression tag	UNP Q9NZL9
A	336	GLU	-	expression tag	UNP Q9NZL9
A	337	ASN	-	expression tag	UNP Q9NZL9
A	338	LEU	-	expression tag	UNP Q9NZL9
A	339	TYR	-	expression tag	UNP Q9NZL9
A	340	PHE	-	expression tag	UNP Q9NZL9
A	341	GLN	-	expression tag	UNP Q9NZL9
B	27	MET	-	expression tag	UNP Q9NZL9
B	335	ALA	-	expression tag	UNP Q9NZL9
B	336	GLU	-	expression tag	UNP Q9NZL9
B	337	ASN	-	expression tag	UNP Q9NZL9
B	338	LEU	-	expression tag	UNP Q9NZL9
B	339	TYR	-	expression tag	UNP Q9NZL9
B	340	PHE	-	expression tag	UNP Q9NZL9
B	341	GLN	-	expression tag	UNP Q9NZL9
C	27	MET	-	expression tag	UNP Q9NZL9
C	335	ALA	-	expression tag	UNP Q9NZL9

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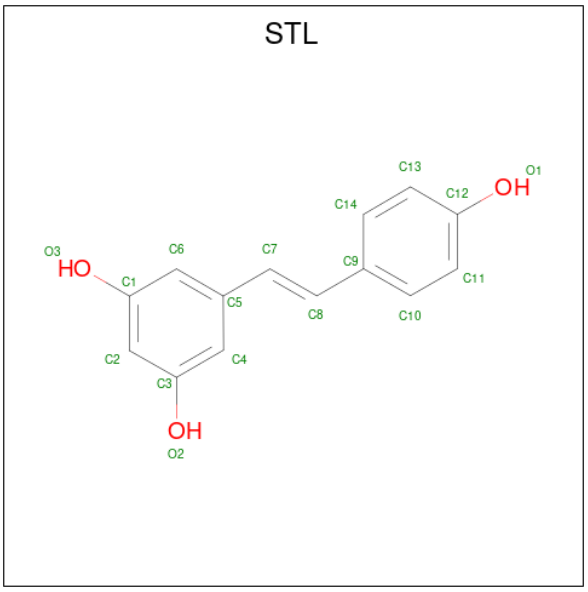
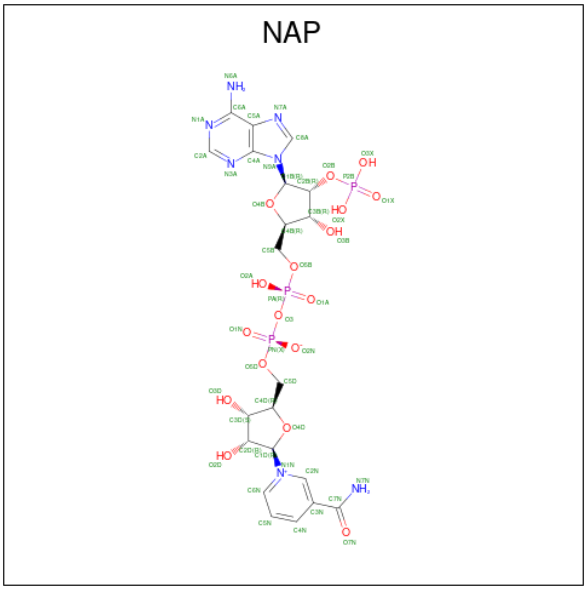
Chain	Residue	Modelled	Actual	Comment	Reference
C	336	GLU	-	expression tag	UNP Q9NZL9
C	337	ASN	-	expression tag	UNP Q9NZL9
C	338	LEU	-	expression tag	UNP Q9NZL9
C	339	TYR	-	expression tag	UNP Q9NZL9
C	340	PHE	-	expression tag	UNP Q9NZL9
C	341	GLN	-	expression tag	UNP Q9NZL9
D	27	MET	-	expression tag	UNP Q9NZL9
D	335	ALA	-	expression tag	UNP Q9NZL9
D	336	GLU	-	expression tag	UNP Q9NZL9
D	337	ASN	-	expression tag	UNP Q9NZL9
D	338	LEU	-	expression tag	UNP Q9NZL9
D	339	TYR	-	expression tag	UNP Q9NZL9
D	340	PHE	-	expression tag	UNP Q9NZL9
D	341	GLN	-	expression tag	UNP Q9NZL9
E	27	MET	-	expression tag	UNP Q9NZL9
E	335	ALA	-	expression tag	UNP Q9NZL9
E	336	GLU	-	expression tag	UNP Q9NZL9
E	337	ASN	-	expression tag	UNP Q9NZL9
E	338	LEU	-	expression tag	UNP Q9NZL9
E	339	TYR	-	expression tag	UNP Q9NZL9
E	340	PHE	-	expression tag	UNP Q9NZL9
E	341	GLN	-	expression tag	UNP Q9NZL9

- Molecule 2 is RESVERATROL (three-letter code: STL) (formula: $C_{14}H_{12}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
2	A	1	17	14	3		0	0
			Total	C	O			
2	A	1	17	14	3		0	0
			Total	C	O			
2	B	1	17	14	3		0	0
			Total	C	O			
2	B	1	17	14	3		0	0
			Total	C	O			
2	C	1	17	14	3		0	0
			Total	C	O			
2	C	1	17	14	3		0	0
			Total	C	O			
2	D	1	17	14	3		0	0
			Total	C	O			
2	D	1	17	14	3		0	0
			Total	C	O			
2	E	1	17	14	3		0	0
			Total	C	O			
2	E	1	17	14	3		0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

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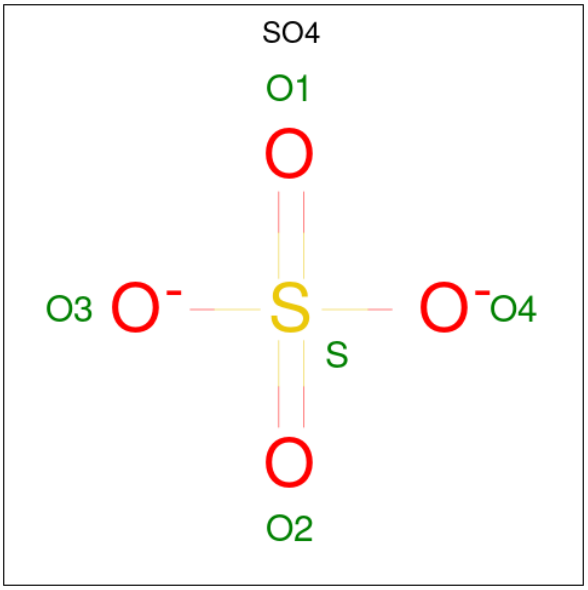
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	C	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
3	D	1	48	21	7	17	3	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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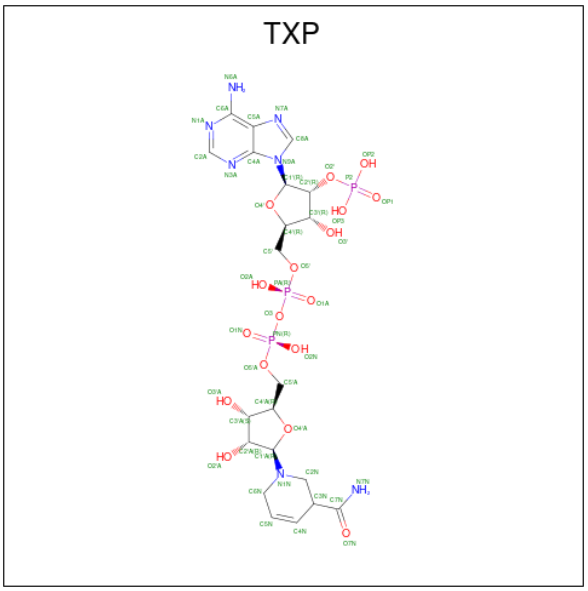
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	B	1	5	4	1	0	0
			Total	O	S		
4	C	1	5	4	1	0	0
			Total	O	S		
4	C	1	5	4	1	0	0
			Total	O	S		
4	C	1	5	4	1	0	0
			Total	O	S		
4	D	1	5	4	1	0	0
			Total	O	S		
4	D	1	5	4	1	0	0
			Total	O	S		
4	D	1	5	4	1	0	0
			Total	O	S		
4	E	1	5	4	1	0	0
			Total	O	S		
4	E	1	5	4	1	0	0
			Total	O	S		
4	E	1	5	4	1	0	0
			Total	O	S		
4	E	1	5	4	1	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	A	1	1	1	0	0

- Molecule 6 is 1,4,5,6-TETRAHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE PHOSPHATE (three-letter code: TXP) (formula: $C_{21}H_{32}N_7O_{17}P_3$).



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

- Molecule 7 is water.

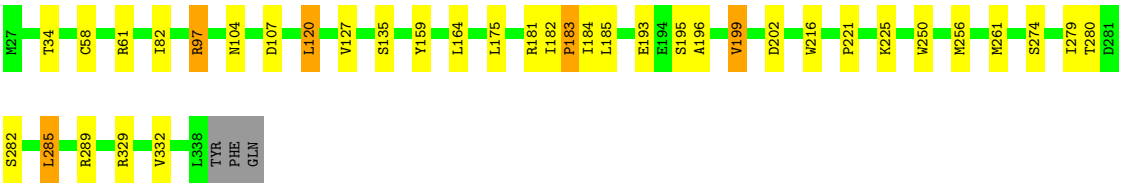
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	156	156	156	0	0
7	B	129	Total 129	O 129	0	0
7	C	103	Total 103	O 103	0	0
7	D	65	Total 65	O 65	0	0
7	E	70	Total 70	O 70	0	0

3 Residue-property plots (i)

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.

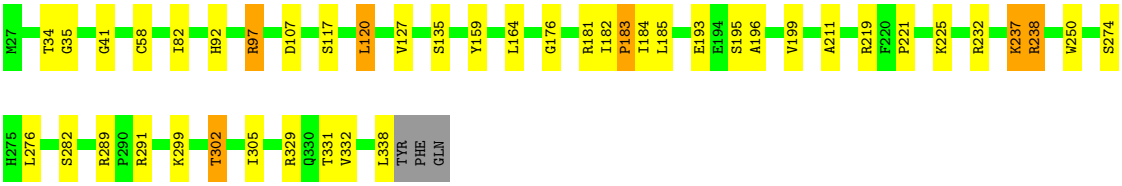
• Molecule 1: METHIONINE ADENOSYLTRANSFERASE 2 SUBUNIT BETA

Chain A:



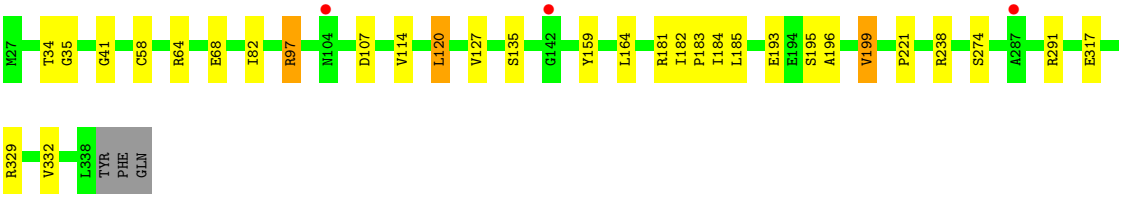
• Molecule 1: METHIONINE ADENOSYLTRANSFERASE 2 SUBUNIT BETA

Chain B:



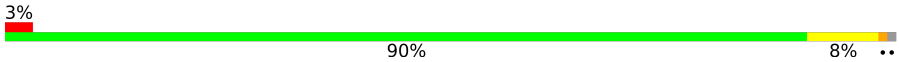
• Molecule 1: METHIONINE ADENOSYLTRANSFERASE 2 SUBUNIT BETA

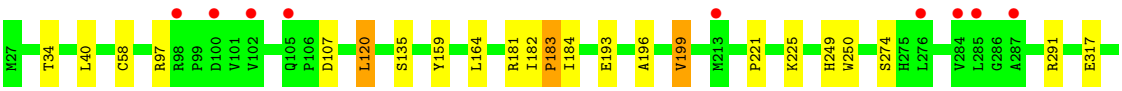
Chain C:

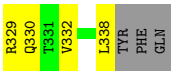


• Molecule 1: METHIONINE ADENOSYLTRANSFERASE 2 SUBUNIT BETA

Chain D:

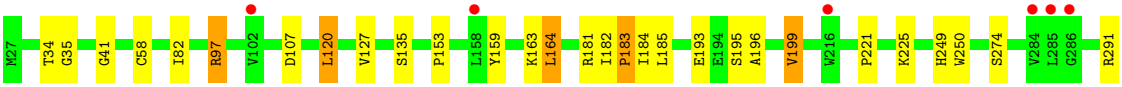


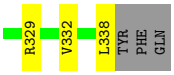




• Molecule 1: METHIONINE ADENOSYLTRANSFERASE 2 SUBUNIT BETA

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	163.39Å 163.39Å 252.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.96 – 2.80 58.96 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (58.96-2.80) 93.0 (58.96-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.168 , 0.188 0.194 , 0.216	Depositor DCC
R_{free} test set	3936 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	53.8	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13178	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, STL, CA, NAP, TXP

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	0.51	0/2511	0.66	0/3412
1	B	0.52	0/2499	0.67	0/3395
1	C	0.47	0/2499	0.64	0/3397
1	D	0.47	0/2468	0.64	0/3360
1	E	0.47	0/2467	0.64	0/3358
All	All	0.49	0/12444	0.65	0/16922

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2452	0	2381	20	0
1	B	2440	0	2366	28	0
1	C	2440	0	2362	16	0
1	D	2409	0	2290	13	0
1	E	2408	0	2284	19	0
2	A	34	0	22	1	0
2	B	34	0	22	3	0
2	C	34	0	20	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	34	0	20	1	0
2	E	34	0	21	2	0
3	A	48	0	24	1	0
3	B	48	0	24	1	0
3	C	48	0	23	1	0
3	D	48	0	23	2	0
4	A	20	0	0	0	0
4	B	25	0	0	1	0
4	C	15	0	0	0	0
4	D	15	0	0	0	0
4	E	20	0	0	0	0
5	A	1	0	0	0	0
6	E	48	0	25	1	0
7	A	156	0	0	0	0
7	B	129	0	0	2	0
7	C	103	0	0	0	0
7	D	65	0	0	0	0
7	E	70	0	0	1	0
All	All	13178	0	11907	92	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 4.

All (92) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:TRP:HE1	1:B:302:THR:HG21	1.13	1.08
1:A:216:TRP:HE1	1:B:302:THR:CG2	2.00	0.68
1:D:193:GLU:HA	1:D:199:VAL:HG13	1.77	0.66
1:E:193:GLU:HA	1:E:199:VAL:HG13	1.77	0.66
1:C:193:GLU:HA	1:C:199:VAL:HG13	1.78	0.66
1:B:331:THR:O	2:B:502:STL:H8	1.96	0.65
1:A:193:GLU:HA	1:A:199:VAL:HG13	1.79	0.65
1:A:184:ILE:HD11	1:A:196:ALA:HB3	1.81	0.62
1:A:216:TRP:NE1	1:B:302:THR:HG21	1.99	0.59
1:B:34:THR:HG21	1:B:120:LEU:HD21	1.87	0.57
1:B:211:ALA:HB3	1:B:276:LEU:HD23	1.88	0.55
1:A:202:ASP:OD1	1:C:64:ARG:NH2	2.39	0.55
1:E:182:ILE:O	6:E:1339:TXP:H5N	2.05	0.55
1:C:135:SER:HB3	1:C:181:ARG:HG2	1.88	0.55
1:E:329:ARG:HG2	2:E:502:STL:H2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:SER:HB3	1:A:181:ARG:HG2	1.89	0.55
1:B:58:CYS:HB3	7:B:2032:HOH:O	2.07	0.55
1:C:182:ILE:HD12	1:C:185:LEU:HD21	1.90	0.54
1:E:135:SER:HB3	1:E:181:ARG:HG2	1.89	0.54
1:C:82:ILE:HG22	1:C:127:VAL:HG21	1.88	0.54
1:B:195:SER:O	1:B:199:VAL:HG23	2.08	0.54
1:B:135:SER:HB3	1:B:181:ARG:HG2	1.89	0.53
1:A:182:ILE:HD12	1:A:185:LEU:HD21	1.91	0.53
1:E:34:THR:HA	1:E:58:CYS:HB2	1.91	0.53
1:E:182:ILE:HD12	1:E:185:LEU:HD21	1.91	0.53
1:B:182:ILE:HD12	1:B:185:LEU:HD21	1.91	0.52
1:E:58:CYS:HB3	7:E:2022:HOH:O	2.08	0.52
1:A:34:THR:HA	1:A:58:CYS:HB2	1.92	0.52
1:B:184:ILE:HD11	1:B:196:ALA:HB3	1.91	0.52
1:A:82:ILE:HG22	1:A:127:VAL:HG21	1.92	0.52
1:B:196:ALA:N	2:B:501:STL:H11	2.25	0.52
1:B:34:THR:HA	1:B:58:CYS:HB2	1.91	0.52
1:C:184:ILE:HD11	1:C:196:ALA:HB3	1.93	0.51
1:E:82:ILE:HG22	1:E:127:VAL:HG21	1.92	0.51
1:D:181:ARG:HB2	1:D:249:HIS:CD2	2.45	0.51
1:D:182:ILE:O	3:D:1339:NAP:H5N	2.11	0.50
1:E:184:ILE:HD11	1:E:196:ALA:HB3	1.94	0.50
1:D:34:THR:HA	1:D:58:CYS:HB2	1.94	0.50
1:D:135:SER:HB3	1:D:181:ARG:HG2	1.94	0.49
1:A:282:SER:HB3	1:A:285:LEU:HD23	1.95	0.49
1:D:329:ARG:HG2	2:D:502:STL:H2	1.95	0.49
1:C:182:ILE:O	3:C:1339:NAP:H5N	2.13	0.48
1:D:184:ILE:HD11	1:D:196:ALA:HB3	1.96	0.48
1:B:184:ILE:HG23	1:B:221:PRO:HA	1.95	0.47
1:C:97:ARG:HA	1:C:159:TYR:CE1	2.49	0.47
1:E:184:ILE:HG23	1:E:221:PRO:HA	1.96	0.47
1:A:97:ARG:HA	1:A:159:TYR:CE1	2.50	0.47
1:B:176:GLY:O	1:B:238:ARG:NH2	2.47	0.47
1:A:195:SER:O	1:A:199:VAL:HG22	2.15	0.47
1:C:34:THR:HG21	1:C:120:LEU:HD21	1.97	0.46
1:D:97:ARG:HA	1:D:159:TYR:CE1	2.50	0.46
1:B:82:ILE:HG22	1:B:127:VAL:HG21	1.97	0.46
1:B:237:LYS:HD3	1:B:305:ILE:HD11	1.97	0.46
1:B:329:ARG:HG2	2:B:502:STL:H2	1.98	0.46
1:B:182:ILE:O	3:B:1339:NAP:H5N	2.16	0.45
1:B:97:ARG:HA	1:B:159:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:THR:HG21	1:D:120:LEU:HD21	1.97	0.45
1:D:184:ILE:HG23	1:D:221:PRO:HA	1.98	0.45
1:A:184:ILE:HG23	1:A:221:PRO:HA	1.99	0.45
1:A:34:THR:HG21	1:A:120:LEU:HD21	1.99	0.45
1:C:184:ILE:HG23	1:C:221:PRO:HA	1.98	0.45
1:E:34:THR:HG21	1:E:120:LEU:HD21	1.98	0.45
1:E:97:ARG:HA	1:E:159:TYR:CE1	2.51	0.45
1:B:183:PRO:HD3	1:B:250:TRP:O	2.17	0.44
1:E:97:ARG:O	2:E:501:STL:H14	2.17	0.44
1:E:153:PRO:HB2	1:E:164:LEU:HD11	1.99	0.44
1:D:183:PRO:HD3	1:D:250:TRP:O	2.19	0.43
1:A:182:ILE:O	3:A:1339:NAP:H5N	2.17	0.42
1:B:238:ARG:HD2	7:B:2087:HOH:O	2.18	0.42
1:C:159:TYR:OH	2:C:502:STL:O2	2.23	0.42
1:E:35:GLY:O	1:E:41:GLY:HA3	2.18	0.42
1:E:181:ARG:HD2	1:E:249:HIS:NE2	2.34	0.42
1:E:183:PRO:HD3	1:E:250:TRP:O	2.20	0.42
1:C:195:SER:O	1:C:199:VAL:HG22	2.19	0.42
1:E:329:ARG:HB3	1:E:332:VAL:HB	2.02	0.42
1:C:329:ARG:HG2	2:C:501:STL:H2	2.01	0.42
1:A:329:ARG:HB3	1:A:332:VAL:HB	2.02	0.42
1:C:35:GLY:O	1:C:41:GLY:HA3	2.20	0.42
1:B:35:GLY:O	1:B:41:GLY:HA3	2.20	0.42
1:B:34:THR:OG1	1:B:92:HIS:HA	2.20	0.41
1:B:193:GLU:HA	1:B:199:VAL:HG22	2.02	0.41
1:A:256:MET:HB3	1:A:261:MET:HG3	2.03	0.41
1:B:219:ARG:NH2	4:B:1342:SO4:S	2.92	0.41
1:B:329:ARG:HB3	1:B:332:VAL:HB	2.02	0.41
1:B:299:LYS:O	1:B:302:THR:HG22	2.21	0.41
1:C:58:CYS:HB3	1:C:68:GLU:HB2	2.03	0.41
1:D:329:ARG:HB3	1:D:332:VAL:HB	2.02	0.41
1:E:195:SER:O	1:E:199:VAL:HG22	2.20	0.41
1:A:183:PRO:HD3	1:A:250:TRP:O	2.20	0.41
1:A:196:ALA:N	2:A:502:STL:H11	2.36	0.40
1:C:329:ARG:HB3	1:C:332:VAL:HB	2.02	0.40
1:D:40:LEU:HB3	3:D:1339:NAP:H52N	2.04	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	312/315 (99%)	301 (96%)	10 (3%)	1 (0%)	41	72
1	B	311/315 (99%)	298 (96%)	12 (4%)	1 (0%)	41	72
1	C	311/315 (99%)	301 (97%)	9 (3%)	1 (0%)	41	72
1	D	311/315 (99%)	302 (97%)	8 (3%)	1 (0%)	41	72
1	E	311/315 (99%)	299 (96%)	11 (4%)	1 (0%)	41	72
All	All	1556/1575 (99%)	1501 (96%)	50 (3%)	5 (0%)	41	72

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	183	PRO
1	B	183	PRO
1	C	183	PRO
1	D	183	PRO
1	E	183	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	255/267 (96%)	241 (94%)	14 (6%)	21	52
1	B	252/267 (94%)	237 (94%)	15 (6%)	19	48
1	C	254/267 (95%)	244 (96%)	10 (4%)	32	66
1	D	244/267 (91%)	234 (96%)	10 (4%)	30	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	243/267 (91%)	233 (96%)	10 (4%)	30	64
All	All	1248/1335 (94%)	1189 (95%)	59 (5%)	25	59

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ARG
1	A	97	ARG
1	A	104	ASN
1	A	107	ASP
1	A	120	LEU
1	A	164	LEU
1	A	175	LEU
1	A	199	VAL
1	A	225	LYS
1	A	274	SER
1	A	279	ILE
1	A	280	THR
1	A	285	LEU
1	A	289	ARG
1	B	97	ARG
1	B	107	ASP
1	B	117	SER
1	B	120	LEU
1	B	164	LEU
1	B	225	LYS
1	B	232	ARG
1	B	237	LYS
1	B	238	ARG
1	B	274	SER
1	B	282	SER
1	B	289	ARG
1	B	291	ARG
1	B	302	THR
1	B	338	LEU
1	C	97	ARG
1	C	107	ASP
1	C	114	VAL
1	C	120	LEU
1	C	164	LEU
1	C	199	VAL
1	C	238	ARG

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Mol	Chain	Res	Type
1	C	274	SER
1	C	291	ARG
1	C	317	GLU
1	D	107	ASP
1	D	120	LEU
1	D	164	LEU
1	D	199	VAL
1	D	225	LYS
1	D	274	SER
1	D	291	ARG
1	D	317	GLU
1	D	330	GLN
1	D	338	LEU
1	E	97	ARG
1	E	107	ASP
1	E	120	LEU
1	E	163	LYS
1	E	164	LEU
1	E	199	VAL
1	E	225	LYS
1	E	274	SER
1	E	291	ARG
1	E	338	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 35 ligands modelled in this entry, 1 is monoatomic - leaving 34 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	B	1342	-	4,4,4	0.46	0	6,6,6	0.39	0
4	SO4	B	1340	-	4,4,4	0.12	0	6,6,6	0.32	0
4	SO4	C	1341	-	4,4,4	0.32	0	6,6,6	0.37	0
4	SO4	E	1342	-	4,4,4	0.37	0	6,6,6	0.19	0
2	STL	A	502	-	18,18,18	3.92	11 (61%)	24,24,24	2.05	8 (33%)
4	SO4	A	1340	-	4,4,4	0.67	0	6,6,6	0.43	0
4	SO4	E	1341	-	4,4,4	0.19	0	6,6,6	0.19	0
2	STL	B	502	-	18,18,18	4.70	12 (66%)	24,24,24	2.01	10 (41%)
4	SO4	C	1340	-	4,4,4	0.27	0	6,6,6	0.13	0
2	STL	D	502	-	18,18,18	4.61	12 (66%)	24,24,24	1.53	5 (20%)
4	SO4	B	1341	-	4,4,4	0.40	0	6,6,6	0.35	0
6	TXP	E	1339	-	45,52,52	2.57	20 (44%)	55,80,80	2.19	20 (36%)
4	SO4	D	1342	-	4,4,4	0.44	0	6,6,6	0.21	0
2	STL	B	501	-	18,18,18	5.42	11 (61%)	24,24,24	1.98	8 (33%)
2	STL	A	501	-	18,18,18	4.60	11 (61%)	24,24,24	1.42	5 (20%)
2	STL	D	501	-	18,18,18	5.25	14 (77%)	24,24,24	1.84	7 (29%)
4	SO4	C	1342	-	4,4,4	0.29	0	6,6,6	0.17	0
4	SO4	E	1340	-	4,4,4	0.81	0	6,6,6	0.69	0
4	SO4	D	1341	-	4,4,4	0.31	0	6,6,6	0.15	0
2	STL	C	502	-	18,18,18	4.47	14 (77%)	24,24,24	1.66	4 (16%)
2	STL	E	502	-	18,18,18	4.53	12 (66%)	24,24,24	1.44	5 (20%)
2	STL	E	501	-	18,18,18	5.00	13 (72%)	24,24,24	1.92	7 (29%)
4	SO4	A	1343	-	4,4,4	0.22	0	6,6,6	0.26	0
3	NAP	B	1339	-	45,52,52	3.22	25 (55%)	56,80,80	2.60	13 (23%)
4	SO4	B	1343	-	4,4,4	0.41	0	6,6,6	0.16	0
4	SO4	A	1342	-	4,4,4	0.20	0	6,6,6	0.23	0
4	SO4	B	1344	-	4,4,4	0.43	0	6,6,6	0.32	0
3	NAP	A	1339	-	45,52,52	2.78	24 (53%)	56,80,80	2.35	16 (28%)
3	NAP	D	1339	-	45,52,52	2.92	26 (57%)	56,80,80	2.51	17 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	E	1343	-	4,4,4	0.20	0	6,6,6	0.07	0
4	SO4	D	1340	-	4,4,4	0.17	0	6,6,6	0.19	0
4	SO4	A	1341	-	4,4,4	0.48	0	6,6,6	0.22	0
3	NAP	C	1339	-	45,52,52	2.80	22 (48%)	56,80,80	2.04	15 (26%)
2	STL	C	501	-	18,18,18	4.40	12 (66%)	24,24,24	1.91	9 (37%)

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	STL	C	502	-	-	4/5/5/5	0/2/2/2
3	NAP	A	1339	-	-	17/31/67/67	0/5/5/5
3	NAP	D	1339	-	-	13/31/67/67	0/5/5/5
2	STL	B	501	-	-	2/5/5/5	0/2/2/2
2	STL	A	501	-	-	4/5/5/5	0/2/2/2
2	STL	E	502	-	-	4/5/5/5	0/2/2/2
2	STL	A	502	-	-	2/5/5/5	0/2/2/2
2	STL	D	501	-	-	2/5/5/5	0/2/2/2
3	NAP	C	1339	-	-	8/31/67/67	0/5/5/5
2	STL	E	501	-	-	2/5/5/5	0/2/2/2
2	STL	D	502	-	-	4/5/5/5	0/2/2/2
2	STL	B	502	-	-	2/5/5/5	0/2/2/2
3	NAP	B	1339	-	-	11/31/67/67	0/5/5/5
2	STL	C	501	-	-	4/5/5/5	0/2/2/2
6	TXP	E	1339	-	-	10/31/77/77	0/5/5/5

All (239) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	STL	C14-C13	9.31	1.55	1.38
2	B	501	STL	C6-C5	9.22	1.55	1.39
2	C	501	STL	C2-C1	9.00	1.52	1.39
2	E	501	STL	C14-C13	8.89	1.54	1.38
3	B	1339	NAP	C4N-C3N	8.86	1.54	1.39
2	E	502	STL	C2-C1	8.57	1.51	1.39
2	D	502	STL	C2-C1	8.40	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	STL	C14-C13	8.33	1.53	1.38
2	B	501	STL	C6-C1	8.28	1.51	1.39
2	B	502	STL	C2-C1	8.12	1.51	1.39
2	B	501	STL	C2-C1	8.10	1.51	1.39
2	D	501	STL	C6-C1	8.09	1.51	1.39
2	D	502	STL	O3-C1	8.09	1.55	1.37
2	A	501	STL	C14-C13	8.08	1.53	1.38
2	B	501	STL	C14-C13	7.88	1.53	1.38
2	E	502	STL	C14-C13	7.84	1.53	1.38
2	E	501	STL	C6-C1	7.77	1.50	1.39
3	B	1339	NAP	C7N-N7N	7.75	1.47	1.33
2	B	502	STL	C14-C13	7.73	1.52	1.38
2	A	501	STL	C2-C1	7.69	1.50	1.39
3	B	1339	NAP	C2D-C1D	-7.65	1.42	1.53
2	D	501	STL	C6-C5	7.57	1.52	1.39
2	D	501	STL	C2-C3	7.55	1.50	1.39
2	E	501	STL	O3-C1	7.45	1.54	1.37
2	B	501	STL	O3-C1	7.44	1.54	1.37
2	C	502	STL	C2-C3	7.28	1.49	1.39
2	B	501	STL	C2-C3	7.19	1.49	1.39
2	B	502	STL	C2-C3	7.15	1.49	1.39
2	D	501	STL	C14-C9	7.14	1.53	1.39
2	C	502	STL	C14-C13	7.06	1.51	1.38
2	A	501	STL	O3-C1	6.93	1.53	1.37
2	D	502	STL	C14-C13	6.92	1.51	1.38
6	E	1339	TXP	C4N-C5N	6.84	1.49	1.32
2	E	501	STL	C6-C5	6.81	1.51	1.39
2	E	502	STL	C6-C1	6.74	1.49	1.39
2	C	502	STL	C6-C5	6.69	1.51	1.39
2	E	501	STL	C14-C9	6.59	1.52	1.39
2	C	501	STL	O3-C1	6.58	1.52	1.37
3	A	1339	NAP	C2D-C1D	-6.54	1.43	1.53
2	D	501	STL	C2-C1	6.52	1.48	1.39
2	C	502	STL	C11-C12	6.50	1.51	1.38
2	E	501	STL	C2-C1	6.48	1.48	1.39
2	A	501	STL	C6-C5	6.36	1.50	1.39
2	A	501	STL	C6-C1	6.34	1.48	1.39
2	C	501	STL	C6-C5	6.33	1.50	1.39
2	C	501	STL	C2-C3	6.31	1.48	1.39
2	E	501	STL	C2-C3	6.30	1.48	1.39
2	D	502	STL	C6-C1	6.28	1.48	1.39
2	D	501	STL	O3-C1	6.27	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	STL	C14-C9	6.26	1.51	1.39
2	D	502	STL	C2-C3	6.23	1.48	1.39
3	B	1339	NAP	C6N-C5N	6.23	1.52	1.38
2	E	502	STL	O3-C1	6.18	1.51	1.37
3	A	1339	NAP	C4N-C3N	6.13	1.49	1.39
2	B	502	STL	C6-C1	6.09	1.48	1.39
2	C	501	STL	C14-C13	6.05	1.49	1.38
2	B	501	STL	C4-C5	6.00	1.49	1.39
2	B	502	STL	O3-C1	5.99	1.51	1.37
2	E	502	STL	C6-C5	5.98	1.49	1.39
2	C	502	STL	C6-C1	5.97	1.48	1.39
3	C	1339	NAP	C7N-N7N	5.86	1.44	1.33
2	E	502	STL	C2-C3	5.81	1.47	1.39
3	A	1339	NAP	C7N-N7N	5.78	1.44	1.33
3	D	1339	NAP	C2D-C1D	-5.75	1.45	1.53
2	A	502	STL	C6-C5	5.73	1.49	1.39
2	B	502	STL	C4-C5	5.71	1.49	1.39
2	B	501	STL	C13-C12	5.70	1.49	1.38
2	A	501	STL	C2-C3	5.61	1.47	1.39
3	D	1339	NAP	C2N-C3N	5.48	1.47	1.39
3	B	1339	NAP	C2N-C3N	5.46	1.47	1.39
2	C	501	STL	C6-C1	5.42	1.47	1.39
3	D	1339	NAP	O4D-C1D	5.38	1.48	1.41
2	C	502	STL	C14-C9	5.36	1.49	1.39
3	D	1339	NAP	C6N-C5N	5.36	1.50	1.38
3	D	1339	NAP	C7N-N7N	5.33	1.43	1.33
2	D	502	STL	C11-C12	5.30	1.49	1.38
2	B	502	STL	C11-C12	5.24	1.48	1.38
2	A	502	STL	C14-C9	5.22	1.49	1.39
2	A	502	STL	C6-C1	5.21	1.46	1.39
2	B	502	STL	C6-C5	5.19	1.48	1.39
2	D	502	STL	C4-C5	5.17	1.48	1.39
2	D	501	STL	C13-C12	5.08	1.48	1.38
3	D	1339	NAP	C5N-C4N	5.05	1.49	1.38
2	A	501	STL	C4-C5	5.02	1.48	1.39
3	C	1339	NAP	C6N-C5N	5.01	1.49	1.38
3	C	1339	NAP	C2N-N1N	5.00	1.41	1.35
2	A	501	STL	C11-C12	4.98	1.48	1.38
3	C	1339	NAP	C2D-C1D	-4.96	1.46	1.53
2	B	502	STL	C14-C9	4.88	1.48	1.39
2	E	501	STL	C11-C12	4.87	1.48	1.38
2	E	501	STL	C13-C12	4.83	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1339	TXP	C7N-N7N	4.82	1.45	1.32
2	D	501	STL	C11-C12	4.81	1.48	1.38
2	A	502	STL	C13-C12	4.80	1.48	1.38
2	C	502	STL	O3-C1	4.77	1.48	1.37
2	D	502	STL	C6-C5	4.77	1.47	1.39
3	C	1339	NAP	C5N-C4N	4.75	1.48	1.38
2	A	502	STL	C4-C5	4.72	1.47	1.39
3	C	1339	NAP	O4D-C1D	4.61	1.47	1.41
3	B	1339	NAP	O4D-C4D	-4.61	1.34	1.45
2	E	502	STL	C11-C12	4.59	1.47	1.38
2	A	502	STL	O3-C1	4.58	1.47	1.37
2	E	502	STL	C4-C5	4.54	1.47	1.39
3	D	1339	NAP	C4N-C3N	4.54	1.47	1.39
2	C	502	STL	C4-C5	4.53	1.47	1.39
6	E	1339	TXP	C2N-C3N	-4.49	1.48	1.52
2	C	502	STL	C2-C1	4.49	1.45	1.39
2	C	501	STL	C14-C9	4.44	1.48	1.39
2	C	501	STL	C4-C5	4.40	1.47	1.39
3	C	1339	NAP	C4N-C3N	4.35	1.46	1.39
3	A	1339	NAP	O7N-C7N	-4.32	1.15	1.24
2	A	502	STL	C11-C12	4.31	1.47	1.38
3	B	1339	NAP	C5N-C4N	4.25	1.47	1.38
3	A	1339	NAP	O4D-C4D	-4.23	1.35	1.45
3	B	1339	NAP	C3D-C4D	-4.21	1.42	1.53
2	A	501	STL	C14-C9	4.18	1.47	1.39
3	C	1339	NAP	O4D-C4D	-4.09	1.35	1.45
2	B	501	STL	C11-C12	4.07	1.46	1.38
6	E	1339	TXP	C3'-C2'	-4.06	1.43	1.52
6	E	1339	TXP	C2'A-C3'A	-4.04	1.42	1.53
2	A	501	STL	C13-C12	4.00	1.46	1.38
2	C	501	STL	C11-C12	3.99	1.46	1.38
2	D	501	STL	C4-C5	3.95	1.46	1.39
6	E	1339	TXP	O3'-C3'	-3.95	1.33	1.43
2	D	502	STL	C14-C9	3.88	1.47	1.39
2	E	502	STL	C14-C9	3.87	1.47	1.39
2	A	502	STL	C2-C3	3.87	1.44	1.39
3	D	1339	NAP	C2N-N1N	3.86	1.39	1.35
3	C	1339	NAP	C2N-C3N	3.82	1.44	1.39
3	A	1339	NAP	C2N-C3N	3.77	1.44	1.39
2	E	501	STL	C4-C5	3.77	1.46	1.39
3	D	1339	NAP	O2D-C2D	-3.76	1.34	1.43
6	E	1339	TXP	O2'A-C2'A	-3.76	1.34	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	STL	C13-C12	3.72	1.46	1.38
3	D	1339	NAP	C3B-C2B	-3.71	1.44	1.52
3	A	1339	NAP	C3B-C2B	-3.70	1.44	1.52
3	A	1339	NAP	C2D-C3D	-3.66	1.43	1.53
3	C	1339	NAP	C8A-N7A	-3.54	1.28	1.34
3	C	1339	NAP	C3B-C4B	-3.54	1.44	1.53
3	A	1339	NAP	O4D-C1D	3.52	1.46	1.41
3	B	1339	NAP	O4D-C1D	3.46	1.45	1.41
2	D	502	STL	C13-C12	3.43	1.45	1.38
6	E	1339	TXP	C2N-N1N	-3.38	1.42	1.47
3	A	1339	NAP	C5N-C4N	3.36	1.46	1.38
3	A	1339	NAP	C6N-C5N	3.35	1.46	1.38
3	D	1339	NAP	O4D-C4D	-3.35	1.37	1.45
3	B	1339	NAP	O5B-C5B	-3.33	1.31	1.44
3	A	1339	NAP	PN-O2N	-3.33	1.39	1.55
3	D	1339	NAP	O3B-C3B	-3.31	1.35	1.43
3	C	1339	NAP	O3B-C3B	-3.30	1.35	1.43
3	B	1339	NAP	P2B-O2X	-3.26	1.42	1.54
3	D	1339	NAP	C3B-C4B	-3.22	1.44	1.53
3	D	1339	NAP	C2D-C3D	-3.19	1.44	1.53
2	E	502	STL	C13-C12	3.17	1.45	1.38
6	E	1339	TXP	O4'-C1'	-3.16	1.36	1.41
2	C	502	STL	C13-C12	3.15	1.44	1.38
6	E	1339	TXP	O4'A-C4'A	-3.10	1.38	1.45
2	D	501	STL	C9-C8	3.08	1.56	1.47
3	A	1339	NAP	P2B-O2X	-3.05	1.43	1.54
3	C	1339	NAP	P2B-O2X	-2.98	1.43	1.54
6	E	1339	TXP	O4'-C4'	-2.98	1.38	1.45
3	B	1339	NAP	C3B-C4B	-2.97	1.45	1.53
6	E	1339	TXP	C3'-C4'	-2.95	1.45	1.53
2	B	501	STL	O2-C3	-2.91	1.30	1.37
3	D	1339	NAP	C5B-C4B	-2.83	1.42	1.51
3	A	1339	NAP	PN-O1N	-2.82	1.40	1.50
3	B	1339	NAP	O3B-C3B	-2.80	1.36	1.43
6	E	1339	TXP	P2-OP2	-2.77	1.44	1.54
3	A	1339	NAP	O3B-C3B	-2.76	1.36	1.43
2	A	502	STL	C2-C1	2.76	1.43	1.39
2	C	502	STL	C4-C3	2.76	1.43	1.39
6	E	1339	TXP	P2-OP3	-2.76	1.44	1.54
2	C	501	STL	C13-C12	2.75	1.44	1.38
3	C	1339	NAP	C2D-C3D	-2.74	1.45	1.53
2	D	501	STL	C10-C9	2.73	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1339	NAP	O2D-C2D	-2.72	1.36	1.43
2	C	502	STL	C11-C10	2.72	1.43	1.38
6	E	1339	TXP	C2'A-C1'A	-2.69	1.44	1.53
3	C	1339	NAP	O7N-C7N	-2.68	1.19	1.24
3	D	1339	NAP	C6A-N6A	2.67	1.43	1.34
3	D	1339	NAP	O5B-C5B	-2.65	1.34	1.44
3	B	1339	NAP	PN-O2N	-2.62	1.43	1.55
2	C	502	STL	C10-C9	2.62	1.44	1.39
3	C	1339	NAP	C6A-N6A	2.62	1.43	1.34
3	A	1339	NAP	O4B-C1B	-2.60	1.37	1.41
3	C	1339	NAP	C6N-N1N	2.60	1.41	1.35
3	D	1339	NAP	PA-O5B	-2.59	1.48	1.59
2	E	502	STL	O2-C3	-2.59	1.31	1.37
3	C	1339	NAP	C3B-C2B	-2.58	1.47	1.52
3	B	1339	NAP	C2D-C3D	-2.58	1.46	1.53
3	A	1339	NAP	C3B-C4B	-2.58	1.46	1.53
2	B	502	STL	C4-C3	2.57	1.43	1.39
3	C	1339	NAP	C5B-C4B	-2.54	1.43	1.51
3	A	1339	NAP	PA-O5B	-2.54	1.49	1.59
3	B	1339	NAP	O4B-C4B	-2.53	1.39	1.45
2	B	502	STL	C9-C8	2.53	1.54	1.47
6	E	1339	TXP	C6N-N1N	-2.53	1.41	1.47
6	E	1339	TXP	PN-O2N	-2.51	1.43	1.55
3	C	1339	NAP	PN-O1N	-2.49	1.42	1.50
2	D	502	STL	O2-C3	-2.48	1.31	1.37
3	D	1339	NAP	PN-O2N	-2.46	1.43	1.55
3	B	1339	NAP	C5B-C4B	-2.46	1.43	1.51
3	D	1339	NAP	PN-O1N	-2.45	1.42	1.50
3	A	1339	NAP	C2A-N1A	2.44	1.38	1.33
2	A	501	STL	C4-C3	2.43	1.42	1.39
2	A	502	STL	C4-C3	2.43	1.42	1.39
3	B	1339	NAP	C2N-N1N	2.41	1.37	1.35
3	D	1339	NAP	O7N-C7N	-2.40	1.19	1.24
3	D	1339	NAP	O4B-C4B	-2.39	1.39	1.45
2	E	501	STL	O2-C3	-2.37	1.31	1.37
3	A	1339	NAP	C2N-N1N	2.36	1.37	1.35
3	A	1339	NAP	C6N-N1N	2.35	1.41	1.35
3	B	1339	NAP	O3D-C3D	-2.34	1.37	1.43
2	C	501	STL	C5-C7	-2.29	1.40	1.47
3	C	1339	NAP	C2A-N3A	2.28	1.35	1.32
3	B	1339	NAP	C5A-N7A	-2.28	1.31	1.39
6	E	1339	TXP	P2-OP1	-2.26	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	STL	C11-C10	2.25	1.42	1.38
3	D	1339	NAP	P2B-O2X	-2.24	1.46	1.54
3	A	1339	NAP	O2D-C2D	-2.23	1.37	1.43
6	E	1339	TXP	O3'A-C3'A	-2.23	1.37	1.43
3	B	1339	NAP	O4B-C1B	-2.23	1.38	1.41
2	C	501	STL	C4-C3	2.22	1.42	1.39
3	B	1339	NAP	C6N-N1N	2.21	1.40	1.35
6	E	1339	TXP	P2-O2'	-2.20	1.55	1.59
3	B	1339	NAP	C4A-N3A	-2.20	1.32	1.35
3	B	1339	NAP	C3B-C2B	-2.20	1.48	1.52
2	C	502	STL	O2-C3	-2.19	1.31	1.37
3	D	1339	NAP	C3D-C4D	-2.16	1.47	1.53
3	B	1339	NAP	C3N-C7N	2.15	1.53	1.50
3	D	1339	NAP	O4B-C1B	-2.13	1.38	1.41
2	D	501	STL	C4-C3	2.13	1.42	1.39
3	D	1339	NAP	P2B-O3X	-2.13	1.46	1.54
3	A	1339	NAP	O5B-C5B	-2.10	1.36	1.44
3	A	1339	NAP	P2B-O1X	-2.10	1.43	1.50
2	E	502	STL	C4-C3	2.07	1.42	1.39
2	E	501	STL	C9-C8	2.05	1.53	1.47
2	D	502	STL	C4-C3	2.05	1.42	1.39
2	E	501	STL	C10-C9	2.00	1.43	1.39

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1339	NAP	C2N-N1N-C1D	9.83	141.03	119.14
3	D	1339	NAP	C2N-N1N-C1D	9.43	140.15	119.14
3	B	1339	NAP	C2N-N1N-C1D	8.27	137.56	119.14
3	C	1339	NAP	C2N-N1N-C1D	8.07	137.11	119.14
3	B	1339	NAP	C5N-C4N-C3N	-7.59	111.37	120.34
3	B	1339	NAP	O4D-C1D-C2D	-7.34	96.20	106.93
3	D	1339	NAP	C5N-C4N-C3N	-6.63	112.50	120.34
3	A	1339	NAP	C3N-C7N-N7N	6.14	125.12	117.75
3	D	1339	NAP	C6N-N1N-C2N	-5.80	116.69	121.97
6	E	1339	TXP	C4N-C3N-C7N	5.61	125.62	110.08
3	B	1339	NAP	O5D-C5D-C4D	5.25	127.07	108.99
3	B	1339	NAP	O4B-C1B-C2B	-5.21	97.56	106.59
2	C	502	STL	C5-C4-C3	-5.09	115.74	120.28
6	E	1339	TXP	C3N-C4N-C5N	-5.02	114.65	123.09
3	A	1339	NAP	C5N-C4N-C3N	-4.69	114.79	120.34
3	D	1339	NAP	N3A-C2A-N1A	-4.60	121.48	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1339	TXP	O4'A-C1'A-C2'A	-4.59	96.63	106.64
2	A	502	STL	C5-C4-C3	-4.59	116.19	120.28
3	D	1339	NAP	C4A-C5A-N7A	-4.57	104.63	109.40
3	B	1339	NAP	N3A-C2A-N1A	-4.51	121.63	128.68
3	D	1339	NAP	C3D-C2D-C1D	4.51	107.76	100.98
3	D	1339	NAP	O4D-C1D-C2D	-4.45	100.43	106.93
3	B	1339	NAP	C3D-C2D-C1D	4.31	107.47	100.98
6	E	1339	TXP	C6N-N1N-C1'A	-4.26	100.34	112.83
3	C	1339	NAP	N3A-C2A-N1A	-4.22	122.08	128.68
6	E	1339	TXP	N3A-C2A-N1A	-4.14	122.21	128.68
2	E	501	STL	C4-C3-C2	4.13	126.13	120.43
3	A	1339	NAP	O7N-C7N-C3N	-4.13	114.69	119.63
3	B	1339	NAP	C6N-N1N-C2N	-4.08	118.26	121.97
3	D	1339	NAP	O5D-C5D-C4D	4.05	122.93	108.99
2	B	501	STL	O1-C12-C11	-4.04	108.52	120.02
2	D	501	STL	C11-C10-C9	3.79	126.19	121.25
2	B	501	STL	O1-C12-C13	3.78	130.80	120.02
3	C	1339	NAP	O4D-C1D-C2D	-3.78	101.40	106.93
2	D	501	STL	C4-C3-C2	3.62	125.42	120.43
3	C	1339	NAP	C3N-C2N-N1N	3.61	123.95	120.43
2	C	502	STL	C4-C3-C2	3.60	125.40	120.43
6	E	1339	TXP	C4A-C5A-N7A	-3.58	105.67	109.40
3	C	1339	NAP	C5N-C4N-C3N	-3.57	116.11	120.34
6	E	1339	TXP	O4'A-C1'A-N1N	-3.57	104.33	109.47
3	A	1339	NAP	C1B-N9A-C4A	-3.57	120.38	126.64
2	C	501	STL	C5-C4-C3	-3.50	117.16	120.28
2	A	502	STL	C4-C3-C2	3.49	125.25	120.43
2	E	501	STL	C14-C13-C12	-3.48	116.06	119.88
2	B	502	STL	C11-C10-C9	3.44	125.73	121.25
2	E	501	STL	O1-C12-C11	-3.44	110.22	120.02
2	A	502	STL	O1-C12-C13	3.42	129.78	120.02
3	D	1339	NAP	C2N-C3N-C4N	-3.42	114.38	118.26
2	E	501	STL	C11-C10-C9	3.42	125.70	121.25
2	B	501	STL	C14-C13-C12	-3.41	116.14	119.88
2	C	501	STL	C6-C5-C4	3.39	123.72	119.12
2	D	501	STL	O1-C12-C11	-3.39	110.36	120.02
2	B	502	STL	C3-C2-C1	-3.37	115.17	119.20
3	C	1339	NAP	C3N-C7N-N7N	3.36	121.79	117.75
2	E	502	STL	C11-C10-C9	3.34	125.60	121.25
3	C	1339	NAP	C4A-C5A-N7A	-3.34	105.92	109.40
2	B	502	STL	C4-C3-C2	3.33	125.04	120.43
3	A	1339	NAP	N3A-C2A-N1A	-3.31	123.50	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	STL	O1-C12-C11	-3.28	110.68	120.02
3	C	1339	NAP	O5D-C5D-C4D	3.27	120.25	108.99
2	A	501	STL	C11-C10-C9	3.27	125.51	121.25
6	E	1339	TXP	C3N-C7N-N7N	3.25	120.35	116.85
2	B	501	STL	C4-C3-C2	3.23	124.89	120.43
2	D	501	STL	O1-C12-C13	3.20	129.15	120.02
3	A	1339	NAP	C2N-C3N-C4N	3.19	121.87	118.26
2	E	501	STL	C5-C4-C3	-3.18	117.45	120.28
2	A	502	STL	C5-C6-C1	-3.18	117.45	120.28
6	E	1339	TXP	C3'A-C2'A-C1'A	3.17	107.46	101.43
6	E	1339	TXP	C2'-C3'-C4'	3.16	108.87	101.99
6	E	1339	TXP	C2N-C3N-C4N	3.15	113.12	108.63
3	A	1339	NAP	O2B-C2B-C1B	3.11	121.31	110.10
3	B	1339	NAP	C3N-C7N-N7N	3.10	121.47	117.75
2	A	502	STL	O1-C12-C11	-3.08	111.23	120.02
2	B	502	STL	C14-C13-C12	-2.99	116.60	119.88
2	E	502	STL	C4-C3-C2	2.96	124.52	120.43
6	E	1339	TXP	C5N-C6N-N1N	2.95	118.05	111.03
3	A	1339	NAP	C6N-N1N-C2N	-2.95	119.29	121.97
2	D	502	STL	C11-C10-C9	2.93	125.06	121.25
2	C	501	STL	C5-C6-C1	-2.91	117.69	120.28
2	E	501	STL	O1-C12-C13	2.88	128.25	120.02
2	B	501	STL	O2-C3-C4	-2.87	112.37	119.84
2	B	502	STL	O1-C12-C13	2.85	128.16	120.02
3	C	1339	NAP	O5B-C5B-C4B	2.82	118.71	108.99
2	D	501	STL	C5-C4-C3	-2.82	117.77	120.28
2	C	501	STL	C11-C10-C9	2.81	124.91	121.25
3	A	1339	NAP	O5D-C5D-C4D	2.81	118.65	108.99
3	D	1339	NAP	C2N-C3N-C7N	-2.80	111.33	119.46
6	E	1339	TXP	C3'-C2'-C1'	-2.78	97.66	102.89
3	A	1339	NAP	O4D-C1D-C2D	-2.78	102.86	106.93
6	E	1339	TXP	O5'-C5'-C4'	2.78	118.55	108.99
2	B	501	STL	C11-C10-C9	2.77	124.86	121.25
3	B	1339	NAP	C2N-C3N-C7N	-2.77	111.43	119.46
2	B	501	STL	C5-C4-C3	-2.75	117.83	120.28
3	B	1339	NAP	O3B-C3B-C2B	-2.74	103.38	111.17
2	B	502	STL	O1-C12-C11	-2.73	112.24	120.02
2	B	502	STL	C5-C4-C3	-2.71	117.87	120.28
3	B	1339	NAP	O2B-C2B-C3B	2.70	121.46	111.68
2	E	502	STL	O1-C12-C13	2.66	127.62	120.02
2	A	501	STL	C5-C4-C3	-2.65	117.92	120.28
2	D	502	STL	C5-C4-C3	-2.65	117.92	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1339	TXP	O7N-C7N-N7N	-2.60	118.47	123.00
6	E	1339	TXP	O5'A-C5'A-C4'A	2.60	117.93	108.99
3	B	1339	NAP	C4A-C5A-N7A	-2.57	106.72	109.40
3	D	1339	NAP	O4B-C1B-C2B	-2.56	102.15	106.59
2	C	501	STL	C14-C13-C12	-2.55	117.08	119.88
2	D	502	STL	C4-C3-C2	2.55	123.95	120.43
2	A	501	STL	O1-C12-C13	2.46	127.03	120.02
6	E	1339	TXP	O2'A-C2'A-C1'A	2.45	118.20	110.02
3	A	1339	NAP	O4B-C1B-C2B	-2.44	102.36	106.59
3	C	1339	NAP	C2B-C3B-C4B	2.43	107.28	101.99
2	A	502	STL	C13-C14-C9	-2.42	118.09	121.25
2	C	501	STL	O1-C12-C13	2.38	126.79	120.02
3	A	1339	NAP	C3D-C2D-C1D	2.37	104.55	100.98
3	A	1339	NAP	O5B-C5B-C4B	2.33	117.00	108.99
2	D	501	STL	C14-C13-C12	-2.32	117.33	119.88
3	D	1339	NAP	C2B-C3B-C4B	2.32	107.04	101.99
2	B	502	STL	C5-C6-C1	-2.32	118.22	120.28
2	B	501	STL	C6-C1-C2	-2.32	117.23	120.43
3	D	1339	NAP	C6N-C5N-C4N	2.31	122.79	119.44
3	D	1339	NAP	O7N-C7N-N7N	-2.30	119.31	122.58
3	C	1339	NAP	O7N-C7N-N7N	-2.30	119.31	122.58
2	E	502	STL	O1-C12-C11	-2.30	113.47	120.02
3	C	1339	NAP	O2B-C2B-C3B	2.28	119.96	111.68
3	A	1339	NAP	O2B-P2B-O1X	-2.28	100.59	109.39
2	A	501	STL	C4-C3-C2	2.28	123.58	120.43
2	B	502	STL	O2-C3-C4	-2.27	113.95	119.84
3	D	1339	NAP	O2X-P2B-O2B	2.26	116.13	105.99
3	C	1339	NAP	C2N-C3N-C7N	-2.20	113.07	119.46
2	A	501	STL	O1-C12-C11	-2.18	113.81	120.02
2	C	501	STL	C4-C3-C2	2.18	123.44	120.43
2	C	501	STL	C10-C11-C12	-2.17	117.49	119.88
2	D	502	STL	O1-C12-C11	-2.15	113.89	120.02
3	C	1339	NAP	O4B-C1B-C2B	-2.15	102.86	106.59
2	D	501	STL	O2-C3-C4	-2.14	114.27	119.84
2	C	502	STL	C6-C5-C4	2.14	122.02	119.12
2	A	502	STL	C14-C13-C12	-2.12	117.55	119.88
2	C	502	STL	C14-C13-C12	-2.11	117.56	119.88
2	B	502	STL	O3-C1-C6	-2.11	114.35	119.84
6	E	1339	TXP	PN-O5'A-C5'A	2.10	133.98	121.68
3	D	1339	NAP	C5N-C6N-N1N	-2.09	117.40	120.40
2	E	501	STL	O2-C3-C4	-2.08	114.43	119.84
2	A	502	STL	C9-C8-C7	-2.06	117.73	125.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	1339	TXP	OP2-P2-O2'	2.05	115.19	105.99
3	D	1339	NAP	O4B-C4B-C5B	-2.05	102.62	109.37
3	C	1339	NAP	C4N-C3N-C7N	2.03	126.48	121.04
3	A	1339	NAP	C2N-C3N-C7N	-2.02	113.59	119.46
2	E	502	STL	C3-C2-C1	-2.01	116.79	119.20
6	E	1339	TXP	C1'-N9A-C4A	-2.01	123.12	126.64
2	D	502	STL	O3-C1-C2	2.01	125.05	119.84

There are no chirality outliers.

All (89) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1339	NAP	C5B-O5B-PA-O1A
3	A	1339	NAP	C5B-O5B-PA-O2A
3	A	1339	NAP	O4B-C4B-C5B-O5B
3	A	1339	NAP	C2B-O2B-P2B-O1X
3	A	1339	NAP	C2B-O2B-P2B-O2X
3	A	1339	NAP	C5D-O5D-PN-O3
3	A	1339	NAP	C5D-O5D-PN-O2N
3	A	1339	NAP	O4D-C1D-N1N-C2N
3	A	1339	NAP	O4D-C1D-N1N-C6N
3	A	1339	NAP	C2D-C1D-N1N-C2N
3	A	1339	NAP	C2D-C1D-N1N-C6N
3	B	1339	NAP	C2B-O2B-P2B-O1X
3	B	1339	NAP	O4D-C1D-N1N-C2N
3	B	1339	NAP	C2D-C1D-N1N-C2N
3	B	1339	NAP	C2D-C1D-N1N-C6N
3	C	1339	NAP	C5B-O5B-PA-O1A
3	C	1339	NAP	C2B-O2B-P2B-O1X
3	C	1339	NAP	O4D-C1D-N1N-C2N
3	D	1339	NAP	C5D-O5D-PN-O3
3	D	1339	NAP	O4D-C1D-N1N-C2N
3	D	1339	NAP	O4D-C1D-N1N-C6N
3	D	1339	NAP	C2D-C1D-N1N-C2N
3	D	1339	NAP	C2D-C1D-N1N-C6N
6	E	1339	TXP	C5'A-O5'A-PN-O3
6	E	1339	TXP	C2'A-C1'A-N1N-C2N
6	E	1339	TXP	O4'A-C1'A-N1N-C6N
6	E	1339	TXP	C2N-C3N-C7N-O7N
6	E	1339	TXP	C2N-C3N-C7N-N7N
2	C	502	STL	C7-C8-C9-C14
2	E	502	STL	C6-C5-C7-C8

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Mol	Chain	Res	Type	Atoms
2	C	501	STL	C6-C5-C7-C8
2	D	501	STL	C7-C8-C9-C14
2	A	502	STL	C7-C8-C9-C14
2	A	501	STL	C6-C5-C7-C8
2	D	502	STL	C6-C5-C7-C8
3	D	1339	NAP	O4D-C4D-C5D-O5D
2	C	501	STL	C7-C8-C9-C14
2	E	502	STL	C7-C8-C9-C14
2	A	501	STL	C4-C5-C7-C8
2	A	502	STL	C7-C8-C9-C10
2	C	501	STL	C7-C8-C9-C10
2	D	502	STL	C4-C5-C7-C8
2	C	501	STL	C4-C5-C7-C8
2	C	502	STL	C7-C8-C9-C10
2	D	501	STL	C7-C8-C9-C10
2	E	502	STL	C4-C5-C7-C8
2	E	502	STL	C7-C8-C9-C10
3	A	1339	NAP	C3B-C4B-C5B-O5B
2	A	501	STL	C7-C8-C9-C14
2	A	501	STL	C7-C8-C9-C10
2	B	501	STL	C7-C8-C9-C14
2	B	502	STL	C6-C5-C7-C8
2	B	501	STL	C7-C8-C9-C10
2	B	502	STL	C4-C5-C7-C8
2	D	502	STL	C7-C8-C9-C14
6	E	1339	TXP	C4N-C3N-C7N-N7N
2	D	502	STL	C7-C8-C9-C10
3	A	1339	NAP	O4D-C4D-C5D-O5D
3	B	1339	NAP	O4D-C4D-C5D-O5D
6	E	1339	TXP	O4'A-C4'A-C5'A-O5'A
3	A	1339	NAP	C3D-C4D-C5D-O5D
3	B	1339	NAP	C3D-C4D-C5D-O5D
6	E	1339	TXP	C3'A-C4'A-C5'A-O5'A
3	D	1339	NAP	C3D-C4D-C5D-O5D
3	D	1339	NAP	C2B-O2B-P2B-O1X
2	C	502	STL	C6-C5-C7-C8
3	C	1339	NAP	C5B-O5B-PA-O3
3	C	1339	NAP	C5D-O5D-PN-O3
3	D	1339	NAP	C2B-O2B-P2B-O2X
3	D	1339	NAP	PA-O3-PN-O1N
3	A	1339	NAP	C5D-O5D-PN-O1N
3	C	1339	NAP	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	C	1339	NAP	C5D-O5D-PN-O1N
2	E	501	STL	C7-C8-C9-C10
2	C	502	STL	C4-C5-C7-C8
3	B	1339	NAP	PA-O3-PN-O2N
3	D	1339	NAP	PA-O3-PN-O2N
3	B	1339	NAP	C4D-C5D-O5D-PN
3	D	1339	NAP	O4B-C4B-C5B-O5B
2	E	501	STL	C7-C8-C9-C14
3	A	1339	NAP	C5B-O5B-PA-O3
3	B	1339	NAP	C2B-O2B-P2B-O3X
3	D	1339	NAP	C5B-O5B-PA-O3
3	C	1339	NAP	O4B-C4B-C5B-O5B
3	A	1339	NAP	PA-O3-PN-O2N
3	B	1339	NAP	PA-O3-PN-O1N
6	E	1339	TXP	C5'A-O5'A-PN-O2N
3	B	1339	NAP	O4B-C4B-C5B-O5B
6	E	1339	TXP	O4'-C4'-C5'-O5'

There are no ring outliers.

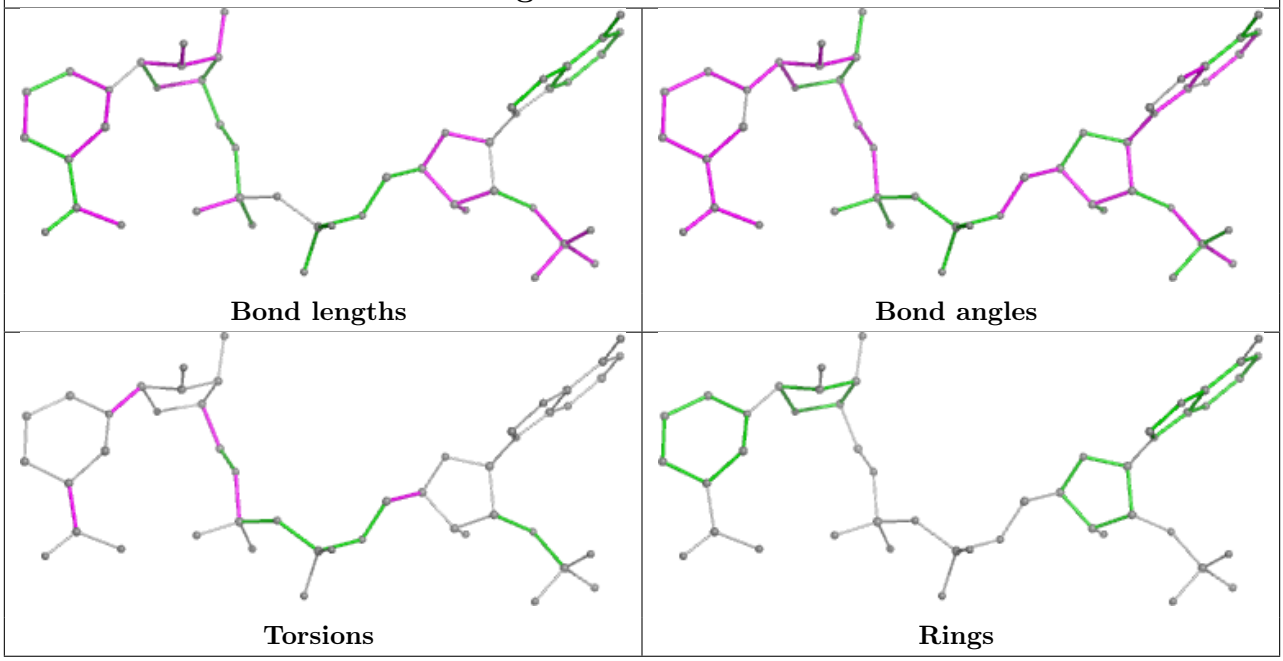
14 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1342	SO4	1	0
2	A	502	STL	1	0
2	B	502	STL	2	0
2	D	502	STL	1	0
6	E	1339	TXP	1	0
2	B	501	STL	1	0
2	C	502	STL	1	0
2	E	502	STL	1	0
2	E	501	STL	1	0
3	B	1339	NAP	1	0
3	A	1339	NAP	1	0
3	D	1339	NAP	2	0
3	C	1339	NAP	1	0
2	C	501	STL	1	0

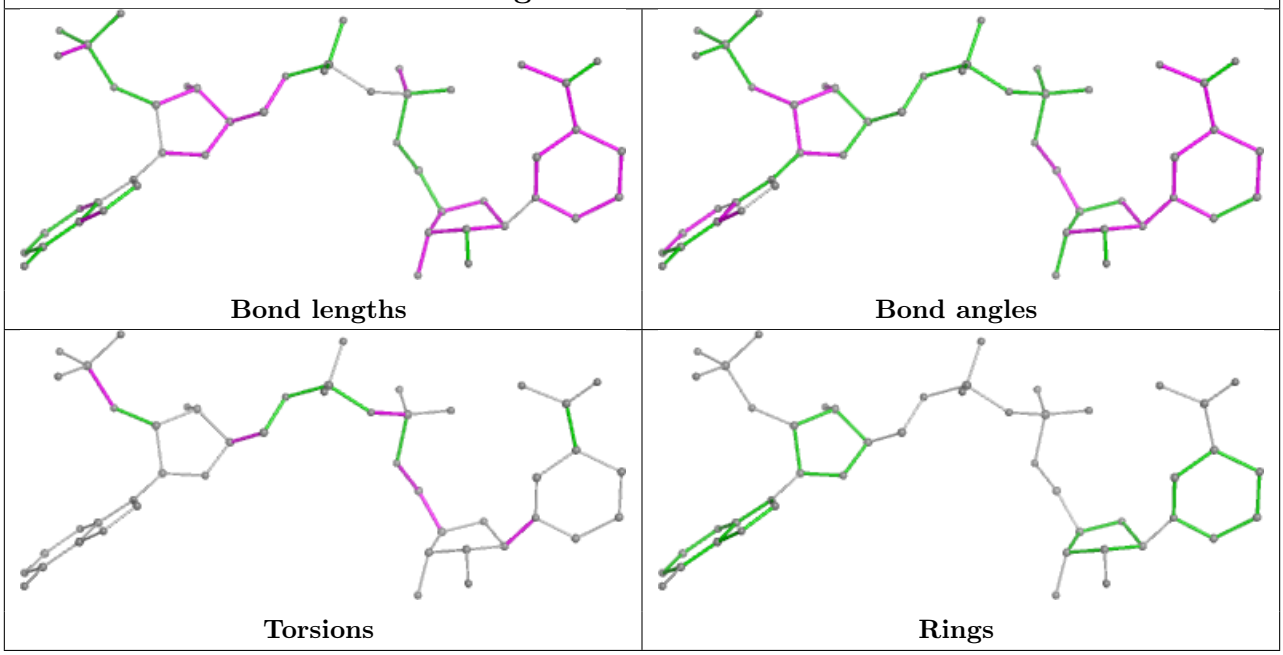
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand TXP E 1339



Ligand NAP B 1339



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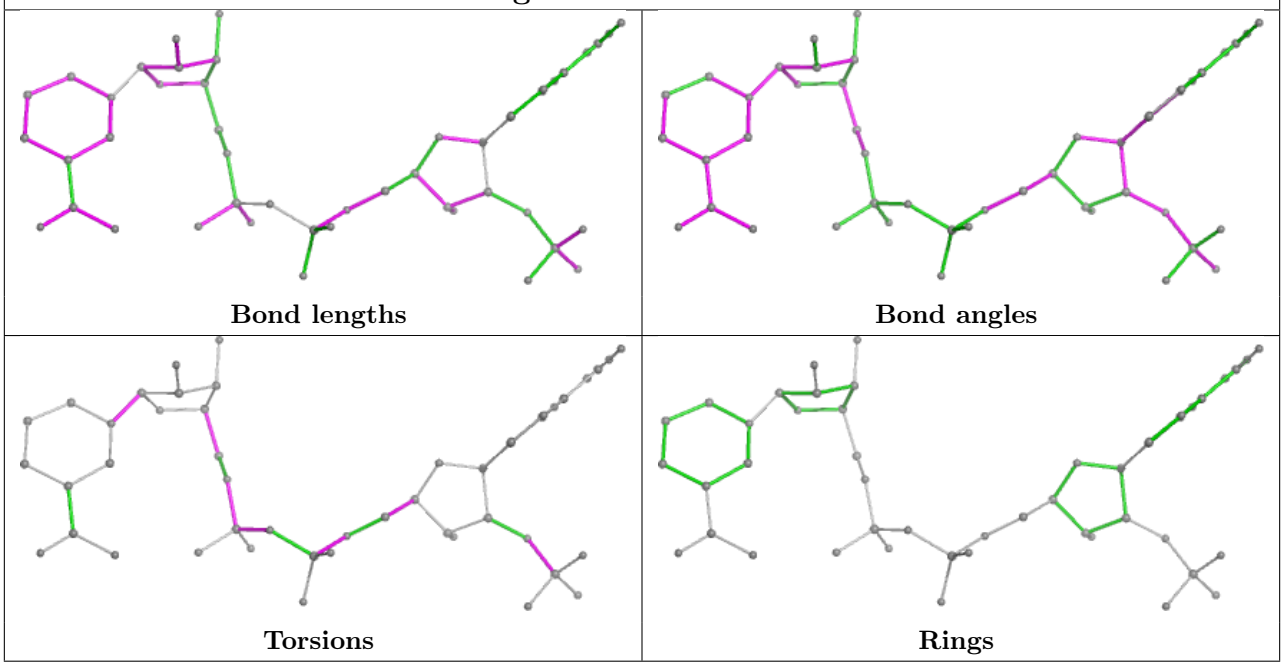
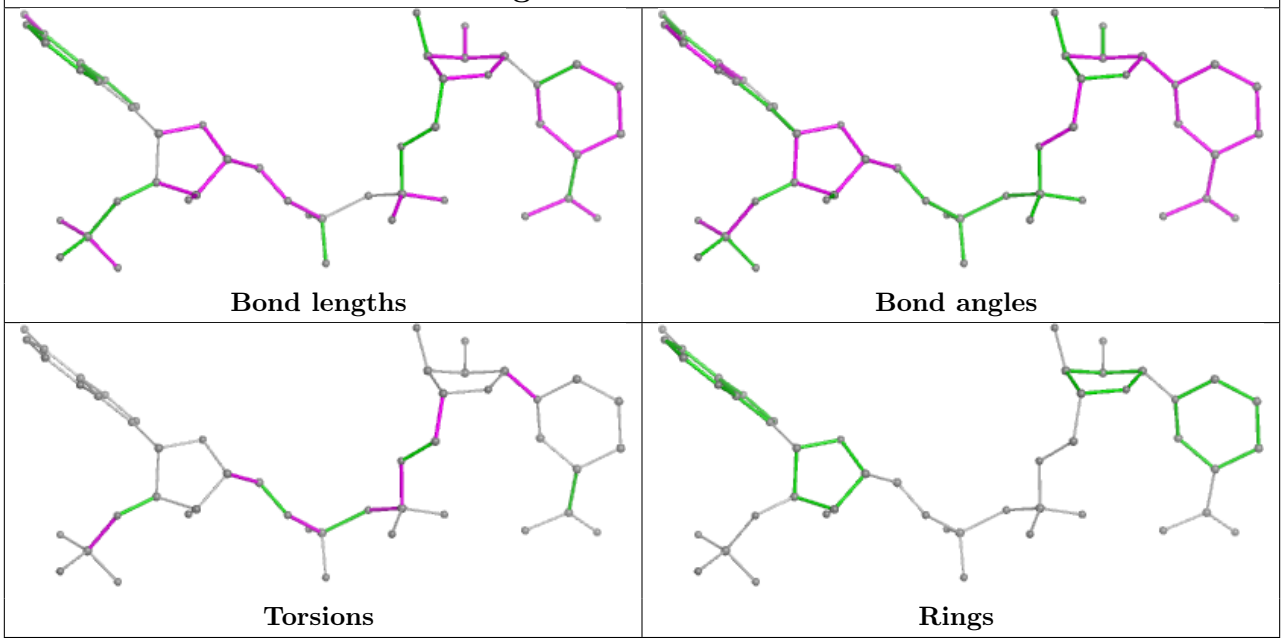


Ligand NAP D 1339



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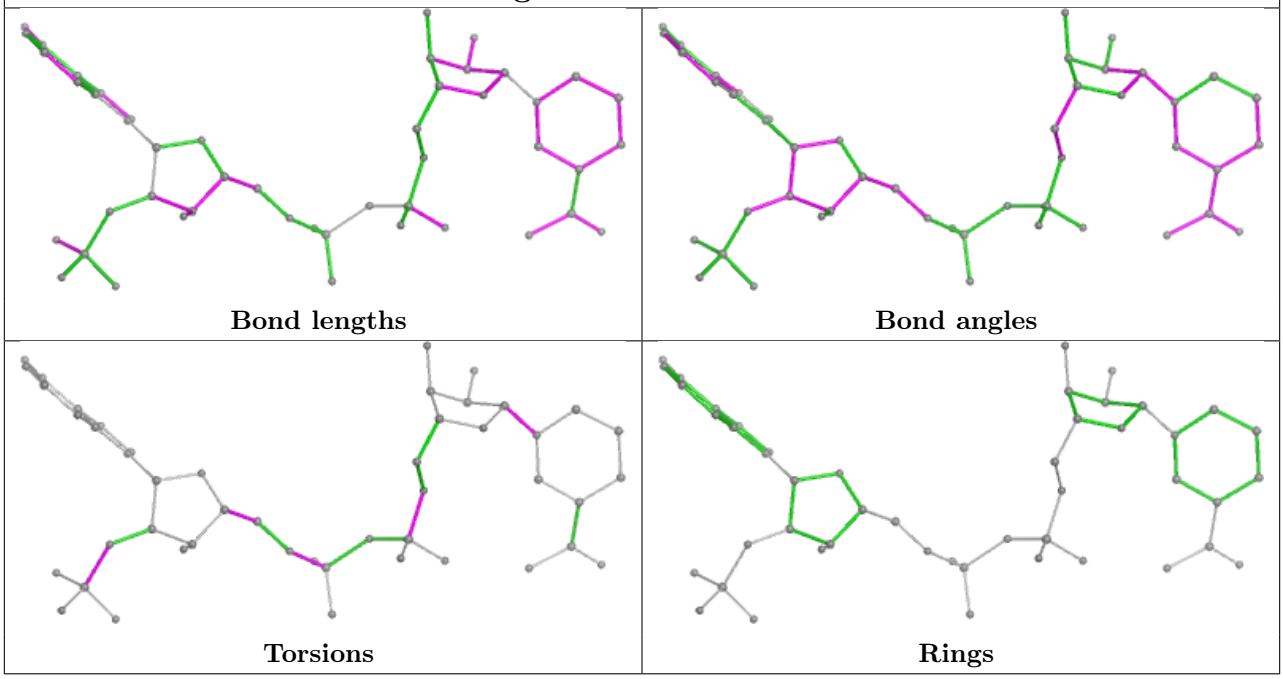

5.7 Other polymers (i)

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	312/315 (99%)	-0.41	0	100	100	30, 48, 82, 118	0
1	B	312/315 (99%)	-0.27	0	100	100	28, 55, 103, 116	0
1	C	312/315 (99%)	-0.11	3 (0%)	82	77	32, 60, 101, 118	0
1	D	312/315 (99%)	0.16	9 (2%)	51	41	43, 73, 120, 138	0
1	E	312/315 (99%)	-0.11	6 (1%)	66	59	42, 73, 119, 134	0
All	All	1560/1575 (99%)	-0.15	18 (1%)	79	73	28, 62, 106, 138	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	285	LEU	3.4
1	C	142	GLY	3.3
1	D	213	MET	2.8
1	D	285	LEU	2.7
1	D	105	GLN	2.7
1	D	100	ASP	2.7
1	E	158	LEU	2.7
1	E	216	TRP	2.5
1	E	286	GLY	2.5
1	D	102	VAL	2.4
1	D	284	VAL	2.3
1	C	104	ASN	2.3
1	E	284	VAL	2.3
1	D	98	ARG	2.3
1	D	276	LEU	2.3
1	E	102	VAL	2.1
1	D	287	ALA	2.1
1	C	287	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no 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, 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
4	SO4	E	1343	5/5	0.59	0.25	171,176,177,177	0
2	STL	E	501	17/17	0.86	0.38	104,107,111,111	0
4	SO4	B	1343	5/5	0.89	0.35	131,135,136,138	0
2	STL	D	501	17/17	0.90	0.42	90,97,110,110	0
2	STL	C	502	17/17	0.90	0.21	83,88,96,97	0
4	SO4	B	1340	5/5	0.91	0.18	121,126,127,127	0
4	SO4	B	1342	5/5	0.91	0.22	115,119,120,122	0
4	SO4	E	1342	5/5	0.92	0.20	112,116,117,117	0
4	SO4	D	1340	5/5	0.92	0.15	111,116,116,116	0
2	STL	D	502	17/17	0.93	0.35	66,73,85,86	0
4	SO4	D	1341	5/5	0.93	0.26	140,144,145,146	0
4	SO4	D	1342	5/5	0.93	0.17	112,116,116,117	0
2	STL	B	501	17/17	0.93	0.37	59,72,85,85	0
2	STL	E	502	17/17	0.93	0.35	64,70,85,86	0
4	SO4	A	1342	5/5	0.94	0.28	102,106,108,110	0
4	SO4	E	1340	5/5	0.94	0.23	63,66,68,71	0
4	SO4	B	1341	5/5	0.94	0.18	102,105,107,108	0
4	SO4	A	1343	5/5	0.94	0.19	130,134,135,136	0
2	STL	C	501	17/17	0.95	0.22	47,49,57,60	0
4	SO4	C	1340	5/5	0.95	0.17	124,128,129,130	0
2	STL	A	501	17/17	0.96	0.30	45,51,70,72	0
4	SO4	C	1341	5/5	0.96	0.16	84,88,89,89	0
4	SO4	E	1341	5/5	0.96	0.14	112,116,118,118	0
2	STL	B	502	17/17	0.96	0.26	39,44,58,61	0
4	SO4	B	1344	5/5	0.96	0.12	79,84,84,84	0
4	SO4	A	1341	5/5	0.97	0.17	83,88,89,90	0
2	STL	A	502	17/17	0.97	0.17	39,51,64,65	0

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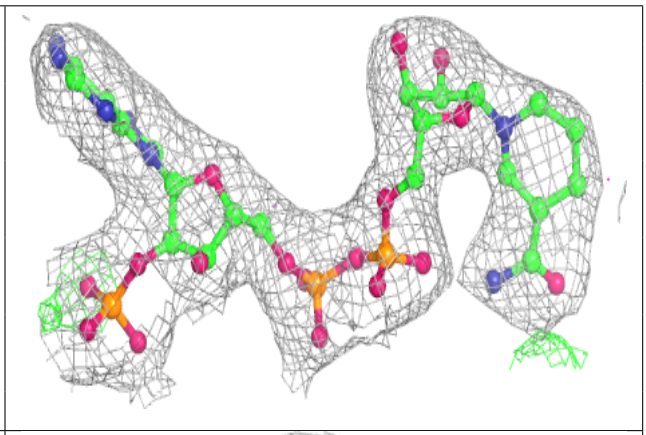
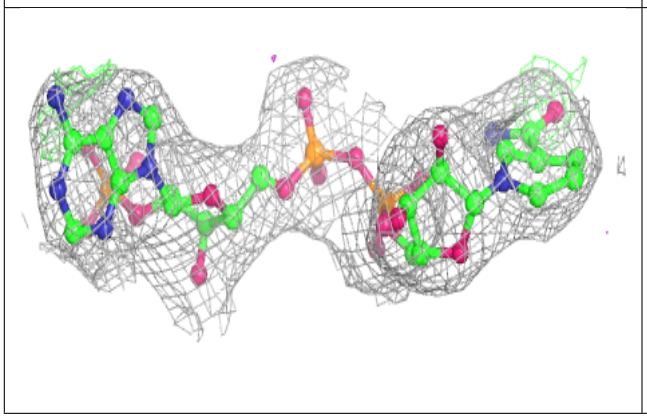
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	C	1342	5/5	0.97	0.16	95,98,101,101	0
3	NAP	D	1339	48/48	0.97	0.14	58,69,72,76	0
4	SO4	A	1340	5/5	0.97	0.19	64,68,69,70	0
3	NAP	C	1339	48/48	0.98	0.12	44,50,56,57	0
5	CA	A	1344	1/1	0.98	0.15	85,85,85,85	0
6	TXP	E	1339	48/48	0.98	0.14	51,63,77,78	0
3	NAP	B	1339	48/48	0.99	0.15	32,41,49,52	0
3	NAP	A	1339	48/48	0.99	0.14	34,45,51,52	0

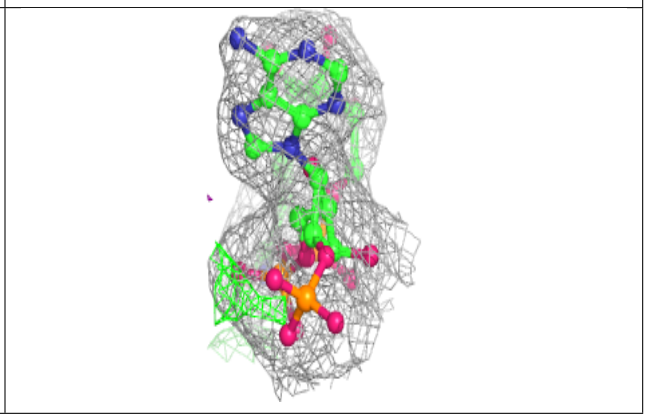
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAP D 1339:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

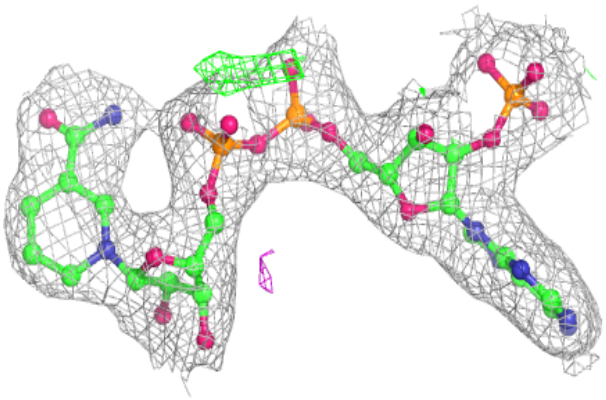


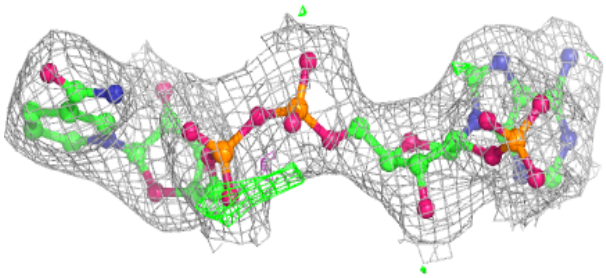


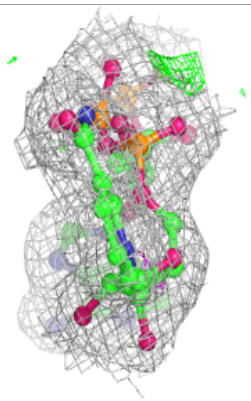


Electron density around NAP C 1339:

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

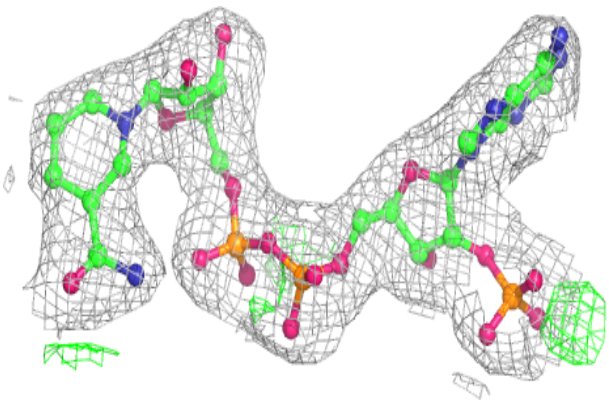


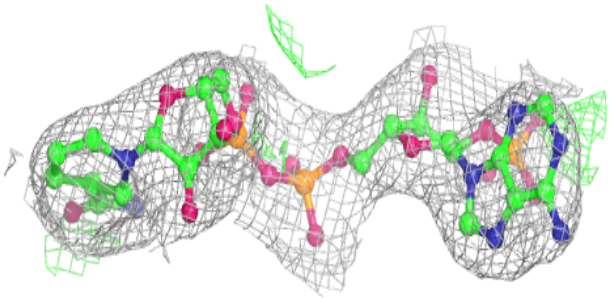


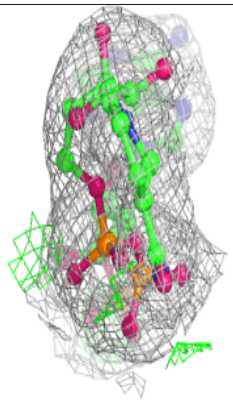


Electron density around TXP E 1339:

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

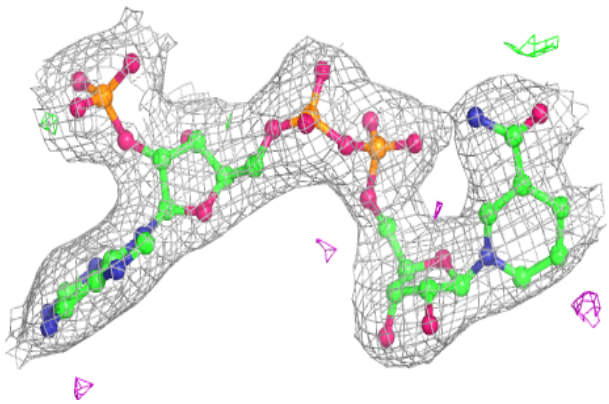


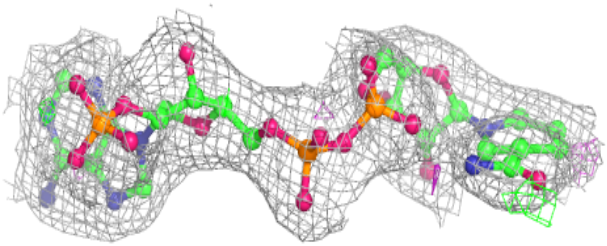


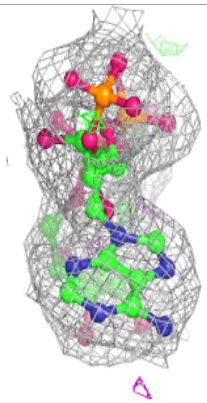


Electron density around NAP B 1339:

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

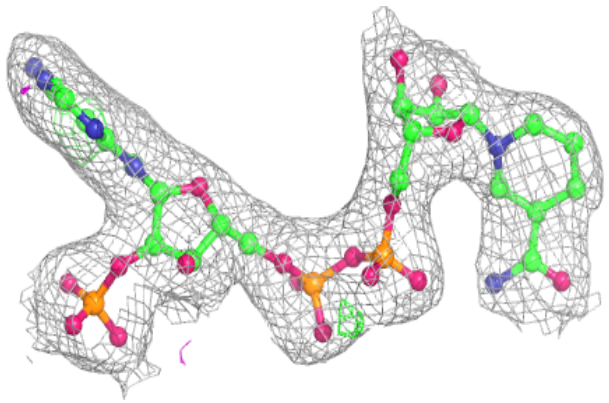


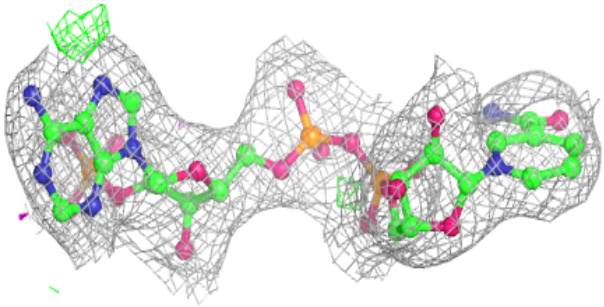


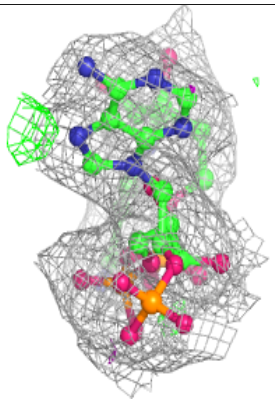


Electron density around NAP A 1339:

$2mF_o$-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.