



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 12:42 AM EST

PDB ID : 3OQ1  
Title : Crystal Structure of 11beta-Hydroxysteroid Dehydrogenase-1 (11b-HSD1) in Complex with Diarylsulfone Inhibitor  
Authors : Wang, Z.; Sudom, A.; Walker, N.P.  
Deposited on : 2010-09-02  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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

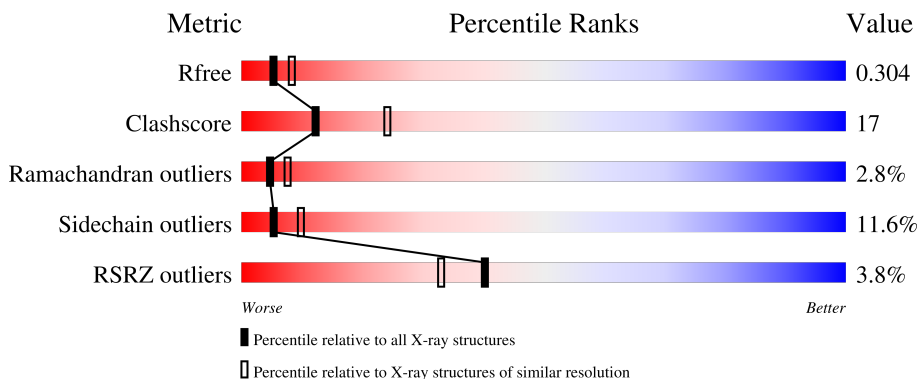
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	286	
1	B	286	
1	C	286	
1	D	286	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8469 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 Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	261	2001	1277	339	370	15	0	0	0
1	B	267	2057	1311	348	382	16	0	1	0
1	C	269	2072	1321	351	384	16	0	0	0
1	D	261	2008	1282	341	370	15	0	1	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP P28845
A	8	LYS	-	expression tag	UNP P28845
A	9	HIS	-	expression tag	UNP P28845
A	10	GLN	-	expression tag	UNP P28845
A	11	HIS	-	expression tag	UNP P28845
A	12	GLN	-	expression tag	UNP P28845
A	13	HIS	-	expression tag	UNP P28845
A	14	GLN	-	expression tag	UNP P28845
A	15	HIS	-	expression tag	UNP P28845
A	16	GLN	-	expression tag	UNP P28845
A	17	HIS	-	expression tag	UNP P28845
A	18	GLN	-	expression tag	UNP P28845
A	19	HIS	-	expression tag	UNP P28845
A	20	GLN	-	expression tag	UNP P28845
A	21	GLN	-	expression tag	UNP P28845
A	22	PRO	-	expression tag	UNP P28845
A	23	LEU	-	expression tag	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
B	7	MET	-	expression tag	UNP P28845
B	8	LYS	-	expression tag	UNP P28845
B	9	HIS	-	expression tag	UNP P28845

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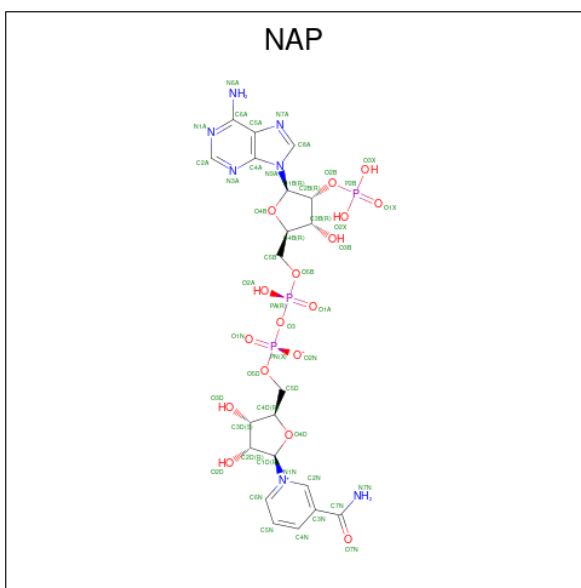
Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	expression tag	UNP P28845
B	11	HIS	-	expression tag	UNP P28845
B	12	GLN	-	expression tag	UNP P28845
B	13	HIS	-	expression tag	UNP P28845
B	14	GLN	-	expression tag	UNP P28845
B	15	HIS	-	expression tag	UNP P28845
B	16	GLN	-	expression tag	UNP P28845
B	17	HIS	-	expression tag	UNP P28845
B	18	GLN	-	expression tag	UNP P28845
B	19	HIS	-	expression tag	UNP P28845
B	20	GLN	-	expression tag	UNP P28845
B	21	GLN	-	expression tag	UNP P28845
B	22	PRO	-	expression tag	UNP P28845
B	23	LEU	-	expression tag	UNP P28845
B	272	SER	CYS	engineered mutation	UNP P28845
C	7	MET	-	expression tag	UNP P28845
C	8	LYS	-	expression tag	UNP P28845
C	9	HIS	-	expression tag	UNP P28845
C	10	GLN	-	expression tag	UNP P28845
C	11	HIS	-	expression tag	UNP P28845
C	12	GLN	-	expression tag	UNP P28845
C	13	HIS	-	expression tag	UNP P28845
C	14	GLN	-	expression tag	UNP P28845
C	15	HIS	-	expression tag	UNP P28845
C	16	GLN	-	expression tag	UNP P28845
C	17	HIS	-	expression tag	UNP P28845
C	18	GLN	-	expression tag	UNP P28845
C	19	HIS	-	expression tag	UNP P28845
C	20	GLN	-	expression tag	UNP P28845
C	21	GLN	-	expression tag	UNP P28845
C	22	PRO	-	expression tag	UNP P28845
C	23	LEU	-	expression tag	UNP P28845
C	272	SER	CYS	engineered mutation	UNP P28845
D	7	MET	-	expression tag	UNP P28845
D	8	LYS	-	expression tag	UNP P28845
D	9	HIS	-	expression tag	UNP P28845
D	10	GLN	-	expression tag	UNP P28845
D	11	HIS	-	expression tag	UNP P28845
D	12	GLN	-	expression tag	UNP P28845
D	13	HIS	-	expression tag	UNP P28845
D	14	GLN	-	expression tag	UNP P28845
D	15	HIS	-	expression tag	UNP P28845

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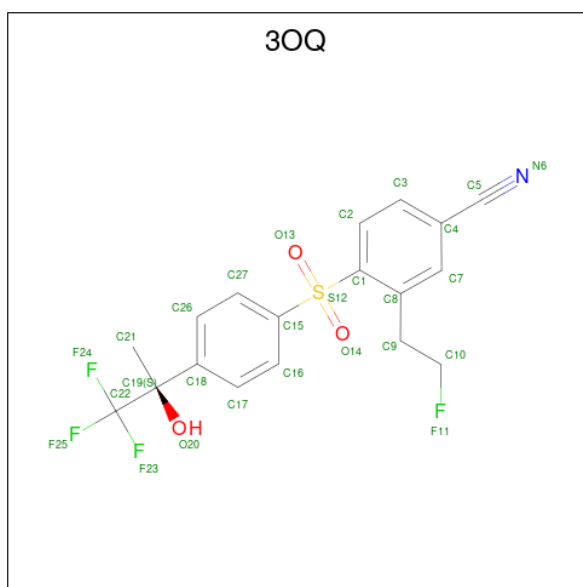
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	expression tag	UNP P28845
D	17	HIS	-	expression tag	UNP P28845
D	18	GLN	-	expression tag	UNP P28845
D	19	HIS	-	expression tag	UNP P28845
D	20	GLN	-	expression tag	UNP P28845
D	21	GLN	-	expression tag	UNP P28845
D	22	PRO	-	expression tag	UNP P28845
D	23	LEU	-	expression tag	UNP P28845
D	272	SER	CYS	engineered mutation	UNP P28845

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



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

- Molecule 3 is 3-(2-fluoroethyl)-4-({4-[(2S)-1,1,1-trifluoro-2-hydroxypropan-2-yl]phenyl}sulfonyl)benzotrile (three-letter code: 3OQ) (formula: C<sub>18</sub>H<sub>15</sub>F<sub>4</sub>NO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
3	A	1	Total	C	F	N	O	S	0	0
			27	18	4	1	3	1		
3	B	1	Total	C	F	N	O	S	0	0
			27	18	4	1	3	1		
3	C	1	Total	C	F	N	O	S	0	0
			27	18	4	1	3	1		
3	D	1	Total	C	F	N	O	S	0	0
			27	18	4	1	3	1		

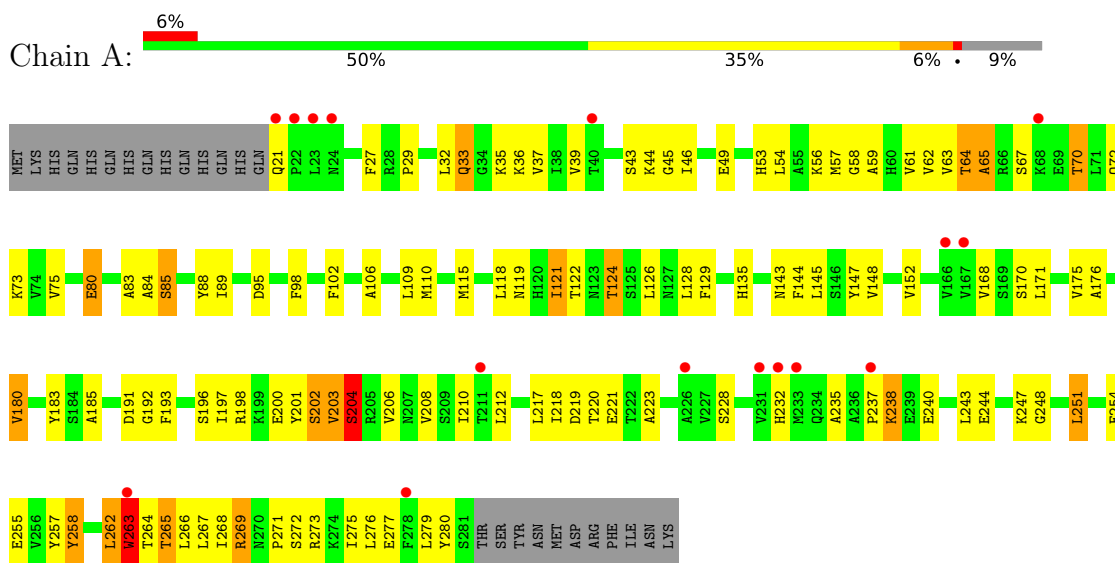
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	10	Total	O	0	0
			10	10		
4	C	10	Total	O	0	0
			10	10		
4	D	9	Total	O	0	0
			9	9		

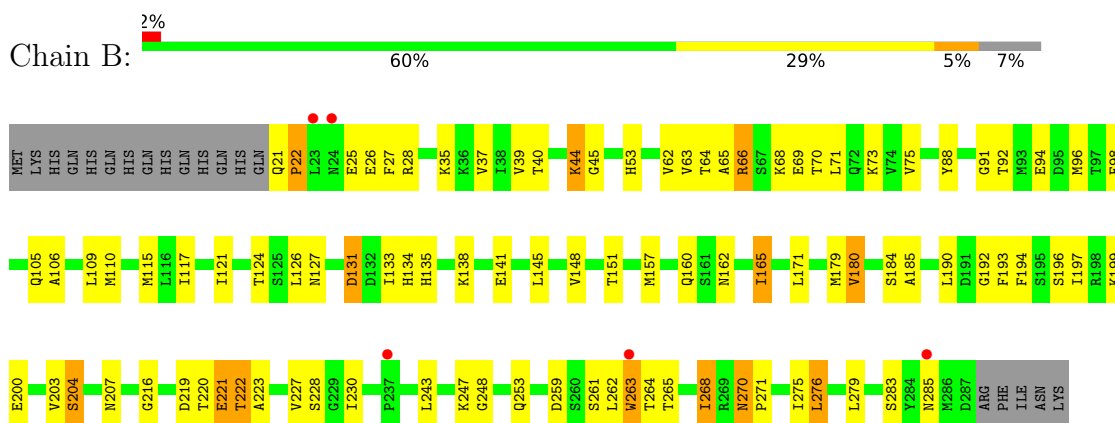
### 3 Residue-property plots i

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.

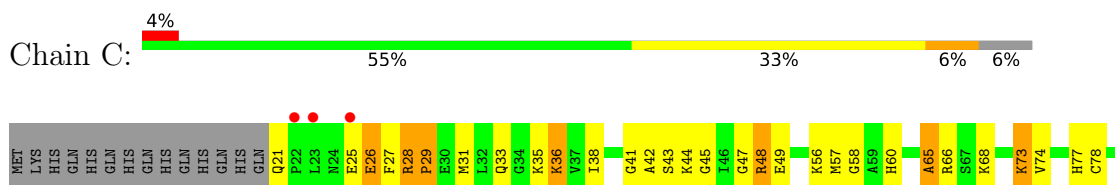
- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

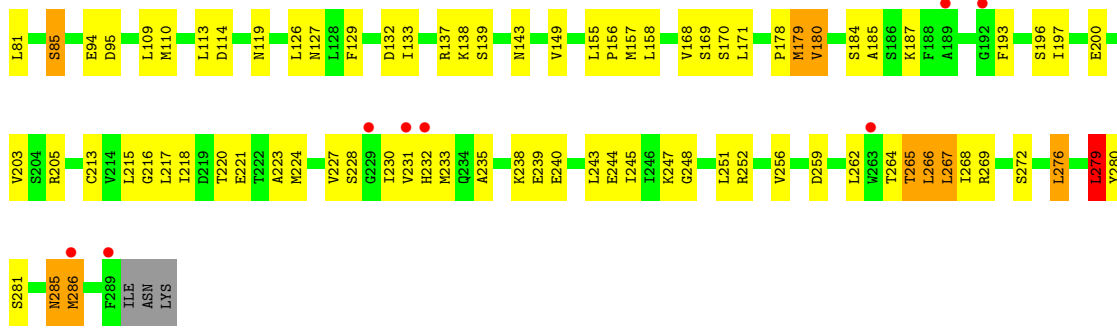


- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

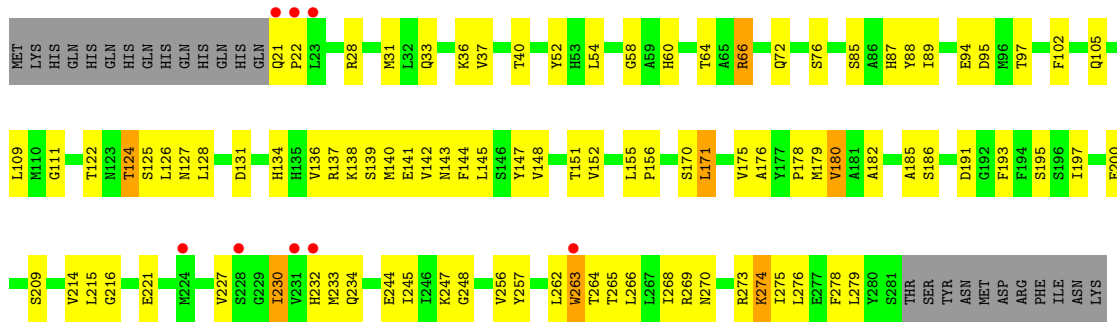


- Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1





• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.30Å 153.40Å 73.59Å 90.00° 92.40° 90.00°	Depositor
Resolution (Å)	38.00 – 2.60 38.04 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.2 (38.00-2.60) 96.2 (38.04-2.60)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 2.61Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.220 , 0.308 0.221 , 0.304	Depositor DCC
$R_{free}$ test set	1843 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.2	Xtrriage
Anisotropy	0.357	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8469	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3OQ, NAP

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	0.65	0/2035	0.76	0/2748
1	B	0.73	0/2096	0.84	1/2831 (0.0%)
1	C	0.69	0/2108	0.78	1/2846 (0.0%)
1	D	0.78	0/2046	0.82	0/2763
All	All	0.71	0/8285	0.80	2/11188 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ARG	NE-CZ-NH1	-6.19	117.21	120.30
1	C	276	LEU	CA-CB-CG	5.38	127.69	115.30

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2001	0	2051	96	0
1	B	2057	0	2098	75	0
1	C	2072	0	2113	75	0
1	D	2008	0	2058	61	0
2	A	48	0	25	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	25	5	0
2	C	48	0	25	4	0
2	D	48	0	25	3	0
3	A	27	0	15	0	0
3	B	27	0	15	0	0
3	C	27	0	15	3	0
3	D	27	0	15	3	0
4	A	2	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	2	0
4	D	9	0	0	1	0
All	All	8469	0	8480	288	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 17.

All (288) 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:62:VAL:HG23	1:A:110:MET:HE3	1.23	1.09
1:C:44:LYS:O	1:C:48:ARG:HB3	1.63	0.99
1:B:126:LEU:O	1:B:127:ASN:ND2	2.00	0.94
1:C:60:HIS:HD1	1:C:85:SER:HG	1.24	0.84
1:A:206:VAL:HG12	1:A:208:VAL:HG23	1.61	0.82
1:A:32:LEU:O	1:A:35:LYS:HG2	1.79	0.82
1:C:43:SER:HB3	2:C:3:NAP:O3B	1.80	0.80
1:B:248:GLY:HA2	1:B:253:GLN:HE21	1.47	0.79
1:D:140:MET:HE1	1:D:186:SER:HA	1.66	0.78
1:A:271:PRO:O	1:A:275:ILE:HD12	1.82	0.78
1:A:273:ARG:HG3	1:D:175:VAL:HG12	1.67	0.77
1:B:259:ASP:OD1	1:B:264:THR:HG21	1.84	0.76
1:A:129:PHE:CD2	1:D:197:ILE:HD11	2.21	0.75
1:C:60:HIS:ND1	1:C:85:SER:OG	2.20	0.75
1:C:179:MET:O	1:C:180:VAL:HG23	1.86	0.74
1:A:269:ARG:HH21	1:A:269:ARG:HB2	1.51	0.74
1:D:233:MET:HG3	3:D:293:3OQ:N6	2.01	0.73
1:B:44:LYS:HG3	2:B:2:NAP:H3B	1.70	0.72
1:B:216:GLY:HA3	1:B:259:ASP:OD2	1.90	0.72
1:B:40:THR:HA	1:B:64:THR:HG22	1.71	0.71
1:B:276:LEU:HD13	1:C:267:LEU:HD12	1.70	0.71
1:D:140:MET:CE	1:D:186:SER:HA	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ALA:HB2	1:D:193:PHE:HB2	1.73	0.69
1:B:27:PHE:CD2	1:B:247:LYS:HE2	2.27	0.69
1:D:171:LEU:HD12	1:D:216:GLY:HA2	1.74	0.69
1:A:62:VAL:HG23	1:A:110:MET:CE	2.13	0.68
1:B:66:ARG:HB2	2:B:2:NAP:O2X	1.93	0.68
1:B:92:THR:OG1	1:B:94:GLU:HB2	1.93	0.68
1:C:279:LEU:HD13	1:D:263:TRP:CZ2	2.29	0.68
1:D:275:ILE:O	1:D:279:LEU:HG	1.94	0.67
1:D:137:ARG:O	1:D:141:GLU:HG3	1.95	0.67
1:D:270:ASN:ND2	1:D:273:ARG:H	1.93	0.67
1:B:179:MET:CE	1:C:286:MET:HB3	2.25	0.66
1:B:200:GLU:O	1:B:204:SER:HB2	1.95	0.66
1:A:200:GLU:O	1:A:204:SER:HB2	1.97	0.65
1:D:178:PRO:O	1:D:179:MET:HB2	1.96	0.64
1:D:248:GLY:HA3	1:D:256:VAL:HG21	1.80	0.64
1:D:37:VAL:HG11	1:D:54:LEU:HD13	1.79	0.64
1:A:35:LYS:O	1:A:59:ALA:HB1	1.98	0.63
1:B:126:LEU:C	1:B:127:ASN:HD22	2.00	0.63
1:D:136:VAL:HG22	1:D:182:ALA:HB2	1.79	0.63
1:B:148:VAL:HG22	1:B:193:PHE:CE1	2.33	0.63
2:D:4:NAP:N7N	2:D:4:NAP:O2N	2.32	0.63
1:C:239:GLU:CD	1:C:239:GLU:H	2.00	0.63
1:C:94:GLU:OE2	1:C:138:LYS:HE3	1.99	0.63
1:A:121:ILE:HG13	1:A:143:ASN:ND2	2.14	0.62
3:C:293:3OQ:H15	3:C:293:3OQ:C16	2.29	0.62
3:C:293:3OQ:H15	3:C:293:3OQ:H11	1.82	0.62
1:C:113:LEU:CD2	1:C:158:LEU:HD21	2.30	0.62
1:D:124:THR:HG22	3:D:293:3OQ:F23	1.91	0.61
1:B:262:LEU:H	1:B:263:TRP:HE3	1.47	0.61
1:A:202:SER:O	1:A:204:SER:N	2.33	0.60
1:C:139:SER:O	1:C:143:ASN:HB2	2.00	0.60
1:B:261:SER:HG	1:B:263:TRP:HE3	1.50	0.60
1:D:28:ARG:O	1:D:31:MET:HG3	2.02	0.60
1:B:270:ASN:C	1:B:270:ASN:HD22	2.05	0.60
1:B:151:THR:HG23	1:B:165:ILE:HD12	1.83	0.59
1:D:60:HIS:ND1	1:D:85:SER:HB2	2.17	0.59
1:A:243:LEU:O	1:A:247:LYS:HG3	2.03	0.59
1:A:272:SER:O	1:A:276:LEU:HD23	2.03	0.59
1:C:215:LEU:O	2:C:3:NAP:H5N	2.03	0.59
1:B:193:PHE:HB2	1:C:185:ALA:HB2	1.85	0.59
1:D:66:ARG:HD3	2:D:4:NAP:C6A	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:SER:OG	2:A:1:NAP:H6N	2.04	0.58
1:B:268:ILE:HG23	1:C:276:LEU:HD21	1.84	0.58
1:B:133:ILE:HD13	1:C:149:VAL:HG22	1.84	0.58
1:B:270:ASN:C	1:B:270:ASN:ND2	2.57	0.58
1:A:263:TRP:C	1:A:263:TRP:HE3	2.07	0.58
1:B:261:SER:OG	1:B:264:THR:HG22	2.04	0.58
1:B:27:PHE:CE2	1:B:247:LYS:HE2	2.39	0.58
1:D:264:THR:O	1:D:268:ILE:HG13	2.02	0.58
1:A:176:ALA:HB2	1:D:195:SER:HB3	1.84	0.57
1:C:215:LEU:HD11	1:C:245:ILE:HD11	1.86	0.57
1:C:220:THR:O	1:C:224:MET:HG2	2.04	0.57
1:A:262:LEU:HA	1:A:265:THR:OG1	2.04	0.56
1:C:227:VAL:CG1	1:C:231:VAL:HG22	2.34	0.56
1:B:223:ALA:O	1:B:227:VAL:HG22	2.05	0.56
1:C:25:GLU:HG2	1:C:26:GLU:H	1.71	0.56
1:C:33:GLN:HB2	1:C:57:MET:O	2.05	0.56
1:A:62:VAL:CG2	1:A:110:MET:HE3	2.15	0.56
1:D:139:SER:O	1:D:143:ASN:HB2	2.06	0.56
1:C:35:LYS:HD2	1:C:114:ASP:OD1	2.05	0.56
1:D:95:ASP:OD1	1:D:97:THR:HB	2.07	0.55
1:A:37:VAL:HG22	1:A:115:MET:HB3	1.88	0.55
1:C:28:ARG:O	1:C:31:MET:HG3	2.05	0.55
1:B:94:GLU:OE2	1:B:138:LYS:HE2	2.07	0.55
1:B:262:LEU:HA	1:B:265:THR:OG1	2.06	0.55
1:A:197:ILE:HA	1:A:200:GLU:HG3	1.88	0.55
1:C:216:GLY:HA3	1:C:259:ASP:OD2	2.07	0.55
1:A:39:VAL:HB	1:A:63:VAL:HG12	1.87	0.55
1:C:227:VAL:HG13	1:C:231:VAL:HG22	1.89	0.55
1:A:276:LEU:O	1:A:280:TYR:HD1	1.90	0.55
1:D:180:VAL:O	1:D:180:VAL:HG13	2.07	0.55
1:B:162:ASN:OD1	1:B:207:ASN:ND2	2.39	0.54
1:A:58:GLY:HA2	1:A:83:ALA:HA	1.89	0.54
1:A:124:THR:HG23	1:A:135:HIS:NE2	2.22	0.54
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.89	0.54
1:C:33:GLN:HA	1:C:58:GLY:O	2.07	0.54
1:D:33:GLN:HA	1:D:58:GLY:O	2.08	0.54
1:A:198:ARG:NE	1:A:254:GLU:HG2	2.22	0.54
1:A:244:GLU:HG3	1:A:258:TYR:CD2	2.43	0.54
1:C:38:ILE:HD12	1:C:113:LEU:HD11	1.90	0.54
1:D:87:HIS:CG	1:D:109:LEU:HD22	2.43	0.54
1:B:126:LEU:HD13	1:B:179:MET:HG3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:214:VAL:HG11	1:D:268:ILE:HG21	1.90	0.54
1:A:240:GLU:O	1:A:244:GLU:HG2	2.08	0.53
1:A:27:PHE:CD2	1:A:247:LYS:HG2	2.44	0.53
1:C:178:PRO:O	1:C:179:MET:HB2	2.09	0.53
1:D:40:THR:HA	1:D:64:THR:HG22	1.90	0.53
1:A:276:LEU:O	1:A:280:TYR:CD1	2.62	0.53
1:D:145:LEU:O	1:D:148:VAL:HB	2.08	0.53
1:D:270:ASN:HD22	1:D:273:ARG:CB	2.21	0.52
1:B:141:GLU:OE1	1:B:145:LEU:HD23	2.10	0.52
1:D:215:LEU:HD11	1:D:245:ILE:HD11	1.90	0.52
1:A:144:PHE:O	1:A:148:VAL:HG23	2.10	0.52
1:A:180:VAL:O	1:A:183:TYR:HB3	2.09	0.52
1:A:198:ARG:HA	1:A:210:ILE:HD12	1.92	0.52
1:A:263:TRP:C	1:A:263:TRP:CE3	2.83	0.51
1:D:64:THR:HB	1:D:102:PHE:CE1	2.45	0.51
1:B:264:THR:HG23	1:B:265:THR:N	2.25	0.51
1:D:244:GLU:OE1	1:D:247:LYS:HE2	2.10	0.51
1:D:151:THR:O	1:D:152:VAL:C	2.48	0.51
1:A:192:GLY:O	1:A:196:SER:HB3	2.11	0.51
1:A:212:LEU:HB3	1:A:255:GLU:HG3	1.93	0.51
1:B:179:MET:HE1	1:C:286:MET:HB3	1.92	0.51
1:A:223:ALA:CB	2:A:1:NAP:H72N	2.24	0.51
1:C:203:VAL:HG11	1:C:286:MET:CE	2.41	0.51
1:A:193:PHE:HB2	1:D:185:ALA:HB2	1.93	0.50
1:C:113:LEU:HD23	1:C:158:LEU:HD21	1.92	0.50
1:A:62:VAL:HG11	1:A:106:ALA:HB2	1.93	0.50
1:C:36:LYS:HG2	1:C:110:MET:HB3	1.93	0.50
1:C:73:LYS:HE3	4:C:5:HOH:O	2.11	0.50
1:B:219:ASP:O	1:B:219:ASP:OD2	2.30	0.50
1:B:63:VAL:HG23	1:B:71:LEU:HD22	1.94	0.50
1:A:95:ASP:HB3	1:A:98:PHE:HB3	1.94	0.50
1:A:128:LEU:HA	1:D:200:GLU:OE2	2.11	0.50
1:A:257:TYR:O	1:A:258:TYR:HB2	2.12	0.50
1:D:215:LEU:O	2:D:4:NAP:H5N	2.12	0.49
1:C:49:GLU:HG3	1:C:238:LYS:HG3	1.95	0.49
1:C:171:LEU:HD23	1:C:268:ILE:HD11	1.94	0.49
1:D:88:TYR:O	1:D:89:ILE:HG13	2.12	0.49
1:B:185:ALA:HB2	1:C:193:PHE:HB2	1.94	0.49
1:A:218:ILE:C	1:A:235:ALA:HB1	2.33	0.49
1:A:64:THR:O	1:A:65:ALA:HB2	2.13	0.49
1:D:227:VAL:HB	1:D:230:ILE:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PRO:HB3	1:A:57:MET:HG2	1.95	0.49
1:B:131:ASP:CG	1:B:131:ASP:O	2.50	0.49
1:C:227:VAL:HG12	1:C:228:SER:N	2.28	0.48
1:B:39:VAL:HG22	1:B:117:ILE:HD12	1.94	0.48
1:C:180:VAL:O	1:C:180:VAL:CG1	2.60	0.48
1:C:259:ASP:HB3	1:C:265:THR:HG23	1.95	0.48
1:D:274:LYS:NZ	4:D:300:HOH:O	2.38	0.48
1:A:201:TYR:O	1:A:204:SER:CB	2.62	0.48
1:A:61:VAL:HG23	1:A:61:VAL:O	2.13	0.48
1:A:64:THR:HG22	1:A:65:ALA:H	1.79	0.48
1:C:43:SER:HB2	1:C:65:ALA:CB	2.44	0.48
1:B:62:VAL:HG23	1:B:110:MET:SD	2.53	0.48
1:B:261:SER:OG	1:B:263:TRP:HE3	1.97	0.48
1:A:220:THR:OG1	1:A:223:ALA:HB3	2.14	0.48
1:A:121:ILE:HG23	1:A:122:THR:N	2.29	0.47
1:A:219:ASP:OD2	1:A:237:PRO:HA	2.14	0.47
1:B:44:LYS:HD2	2:B:2:NAP:H51A	1.95	0.47
1:A:248:GLY:HA2	1:A:251:LEU:HB2	1.96	0.47
1:D:37:VAL:HG11	1:D:54:LEU:CD1	2.43	0.47
1:B:126:LEU:HD22	1:B:180:VAL:HG13	1.96	0.47
1:C:217:LEU:HD23	1:C:235:ALA:HB2	1.96	0.47
1:A:75:VAL:HG21	1:A:88:TYR:HB3	1.96	0.47
1:C:230:ILE:HG22	1:C:231:VAL:HG12	1.97	0.47
1:A:275:ILE:O	1:A:279:LEU:HG	2.15	0.47
1:B:263:TRP:HE3	1:B:263:TRP:H	1.57	0.47
1:B:192:GLY:O	1:B:196:SER:HB3	2.15	0.47
1:A:37:VAL:HG11	1:A:54:LEU:HD13	1.97	0.47
1:A:88:TYR:CD1	1:A:88:TYR:C	2.88	0.46
1:A:27:PHE:HB2	1:A:251:LEU:HD21	1.97	0.46
1:A:70:THR:O	1:A:73:LYS:HB2	2.15	0.46
1:B:157:MET:O	1:B:160:GLN:HG2	2.15	0.46
1:A:89:ILE:HD12	1:A:102:PHE:HD1	1.81	0.46
1:D:88:TYR:C	1:D:89:ILE:HG13	2.35	0.46
1:D:178:PRO:O	1:D:179:MET:CB	2.62	0.46
1:C:279:LEU:HD12	1:C:279:LEU:C	2.36	0.46
1:A:267:LEU:HD13	1:B:275:ILE:CD1	2.46	0.46
1:C:26:GLU:HG2	1:C:27:PHE:N	2.31	0.45
1:C:155:LEU:HB3	1:C:156:PRO:HD3	1.98	0.45
1:C:38:ILE:CD1	1:C:113:LEU:HD11	2.46	0.45
1:D:36:LYS:HE3	1:D:111:GLY:O	2.16	0.45
1:B:37:VAL:HG22	1:B:115:MET:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:THR:O	1:A:266:LEU:N	2.49	0.45
1:C:66:ARG:HB2	2:C:3:NAP:O2X	2.16	0.45
1:A:243:LEU:HD12	1:A:243:LEU:HA	1.76	0.45
1:B:45:GLY:HA2	1:B:220:THR:HG23	1.99	0.45
1:B:199:LYS:O	1:B:200:GLU:C	2.54	0.45
1:D:94:GLU:HG3	1:D:142:VAL:HG22	1.99	0.45
1:C:223:ALA:HB2	2:C:3:NAP:H72N	1.82	0.45
1:D:270:ASN:ND2	1:D:273:ARG:HB2	2.32	0.45
1:A:175:VAL:HG12	1:D:273:ARG:HG3	1.96	0.45
1:B:220:THR:O	1:B:221:GLU:C	2.54	0.45
1:D:88:TYR:C	1:D:88:TYR:CD1	2.90	0.45
1:A:118:LEU:HB3	1:A:147:TYR:CD2	2.52	0.45
1:A:196:SER:O	1:A:200:GLU:HG3	2.17	0.45
1:B:66:ARG:N	2:B:2:NAP:O2X	2.48	0.45
1:C:27:PHE:HB2	1:C:251:LEU:HD11	1.97	0.45
1:D:21:GLN:N	1:D:22:PRO:HD3	2.32	0.45
1:A:212:LEU:HD23	1:A:255:GLU:OE1	2.18	0.44
1:B:179:MET:HE2	1:B:230:ILE:HG21	1.98	0.44
1:B:197:ILE:HD11	1:C:129:PHE:HB3	1.99	0.44
1:D:227:VAL:O	1:D:230:ILE:HG22	2.16	0.44
1:B:220:THR:HG22	1:B:222:THR:H	1.83	0.44
1:C:77:HIS:ND1	1:C:81:LEU:HD11	2.33	0.44
1:D:140:MET:HE3	1:D:186:SER:HA	1.99	0.44
1:A:191:ASP:O	1:A:192:GLY:C	2.55	0.44
1:A:200:GLU:HB3	1:D:128:LEU:HD22	1.98	0.44
1:A:201:TYR:O	1:A:202:SER:C	2.54	0.44
1:A:198:ARG:NH2	1:A:254:GLU:O	2.50	0.44
1:B:179:MET:HE3	1:C:286:MET:HB3	2.00	0.44
1:B:270:ASN:HA	1:B:271:PRO:HD3	1.79	0.44
1:C:25:GLU:HG2	1:C:26:GLU:N	2.32	0.44
1:C:41:GLY:O	1:C:47:GLY:HA3	2.18	0.44
1:A:89:ILE:HD12	1:A:102:PHE:CD1	2.53	0.44
1:B:259:ASP:CG	1:B:264:THR:HG21	2.39	0.44
1:A:267:LEU:HD13	1:B:275:ILE:HD11	1.99	0.44
1:B:268:ILE:H	1:B:268:ILE:HG12	1.57	0.44
1:C:95:ASP:C	1:C:95:ASP:OD1	2.56	0.44
1:B:96:MET:HG3	1:C:137:ARG:HH22	1.83	0.43
1:D:193:PHE:CZ	1:D:197:ILE:HD12	2.53	0.43
1:A:49:GLU:HG3	1:A:238:LYS:HB2	1.99	0.43
1:B:106:ALA:HA	1:B:109:LEU:HD12	1.99	0.43
1:C:264:THR:C	1:C:266:LEU:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:TYR:O	1:A:204:SER:HB2	2.18	0.43
1:C:26:GLU:HG2	1:C:27:PHE:H	1.83	0.43
1:C:197:ILE:O	1:C:200:GLU:HB2	2.19	0.43
1:B:190:LEU:CD2	1:B:194:PHE:HE1	2.31	0.43
3:C:293:3OQ:H4	3:C:293:3OQ:F25	2.08	0.43
1:A:129:PHE:CD2	1:D:197:ILE:CD1	2.98	0.43
1:A:273:ARG:HH21	1:D:176:ALA:HB2	1.83	0.43
1:A:32:LEU:O	1:A:35:LYS:CG	2.58	0.42
1:A:43:SER:HG	2:A:1:NAP:P2B	2.42	0.42
1:A:53:HIS:CG	1:A:243:LEU:HD13	2.53	0.42
1:A:72:GLN:O	1:A:73:LYS:C	2.58	0.42
1:C:243:LEU:O	1:C:247:LYS:HG3	2.20	0.42
1:C:197:ILE:HD13	1:C:197:ILE:HA	1.83	0.42
1:D:257:TYR:CE1	1:D:269:ARG:HG2	2.54	0.42
1:C:42:ALA:HA	1:C:47:GLY:HA3	2.02	0.42
1:C:180:VAL:HG12	1:C:184:SER:HB2	2.02	0.42
1:C:74:VAL:O	1:C:78:CYS:SG	2.71	0.42
1:B:44:LYS:CG	2:B:2:NAP:H3B	2.44	0.42
1:C:77:HIS:CE1	1:C:81:LEU:HD11	2.54	0.42
1:A:217:LEU:HG	1:A:235:ALA:HB2	2.01	0.42
1:D:191:ASP:O	1:D:195:SER:HB2	2.19	0.42
1:B:261:SER:CB	1:B:264:THR:HG22	2.50	0.42
1:D:144:PHE:O	1:D:147:TYR:HB2	2.20	0.42
1:C:28:ARG:HA	1:C:29:PRO:HD2	1.83	0.42
1:C:73:LYS:CE	4:C:5:HOH:O	2.66	0.42
1:C:133:ILE:H	1:C:133:ILE:HG13	1.60	0.42
1:C:217:LEU:O	1:C:218:ILE:HD13	2.20	0.42
1:C:252:ARG:NH1	1:C:252:ARG:HG2	2.35	0.42
1:D:40:THR:HA	1:D:64:THR:CG2	2.50	0.41
1:B:264:THR:HG23	1:B:265:THR:H	1.85	0.41
1:A:83:ALA:C	1:A:85:SER:H	2.23	0.41
1:C:169:SER:N	1:C:213:CYS:O	2.51	0.41
1:A:46:ILE:HD12	2:A:1:NAP:PN	2.61	0.41
1:A:121:ILE:HG23	1:A:122:THR:H	1.86	0.41
1:A:197:ILE:O	1:A:198:ARG:C	2.59	0.41
1:B:21:GLN:N	1:B:22:PRO:HD3	2.36	0.41
1:A:272:SER:O	1:A:276:LEU:CD2	2.67	0.41
1:D:233:MET:CG	3:D:293:3OQ:N6	2.79	0.41
1:B:53:HIS:HD2	1:B:243:LEU:HD13	1.86	0.41
1:A:217:LEU:HD22	1:A:232:HIS:HB2	2.02	0.41
1:A:223:ALA:HB2	2:A:1:NAP:H72N	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLY:HA3	1:B:98:PHE:CZ	2.56	0.41
1:B:134:HIS:O	1:B:138:LYS:HB2	2.21	0.41
1:B:261:SER:OG	1:B:262:LEU:N	2.53	0.41
1:C:252:ARG:HG2	1:C:252:ARG:HH11	1.86	0.41
1:C:285:ASN:O	1:C:285:ASN:ND2	2.54	0.41
1:A:171:LEU:HD23	1:A:268:ILE:HD13	2.03	0.41
1:B:75:VAL:HG21	1:B:88:TYR:HD2	1.85	0.41
1:A:44:LYS:HB2	2:A:1:NAP:H3B	2.03	0.40
1:A:119:ASN:HD22	1:A:168:VAL:HG21	1.86	0.40
1:A:202:SER:OG	1:A:203:VAL:N	2.54	0.40
1:A:115:MET:HE3	1:A:115:MET:HB2	2.00	0.40
1:B:105:GLN:HE21	1:B:105:GLN:HB2	1.64	0.40
1:B:221:GLU:H	1:B:221:GLU:HG3	1.63	0.40
1:A:84:ALA:O	1:A:85:SER:CB	2.68	0.40
1:B:121:ILE:O	1:B:121:ILE:HG13	2.21	0.40
1:B:124:THR:HG23	1:B:135:HIS:CE1	2.57	0.40
1:C:168:VAL:O	1:C:187:LYS:NZ	2.55	0.40
1:A:37:VAL:HA	1:A:115:MET:O	2.21	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	259/286 (91%)	205 (79%)	40 (15%)	14 (5%)	<b>2</b> <b>2</b>
1	B	266/286 (93%)	232 (87%)	29 (11%)	5 (2%)	<b>8</b> <b>15</b>
1	C	267/286 (93%)	229 (86%)	31 (12%)	7 (3%)	<b>5</b> <b>9</b>
1	D	260/286 (91%)	225 (86%)	32 (12%)	3 (1%)	<b>13</b> <b>27</b>
All	All	1052/1144 (92%)	891 (85%)	132 (12%)	29 (3%)	<b>5</b> <b>7</b>

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	SER
1	A	228	SER
1	A	265	THR
1	C	180	VAL
1	A	33	GLN
1	A	45	GLY
1	A	65	ALA
1	A	203	VAL
1	A	204	SER
1	A	258	TYR
1	B	69	GLU
1	C	45	GLY
1	D	52	TYR
1	D	180	VAL
1	A	109	LEU
1	A	263	TRP
1	C	65	ALA
1	C	279	LEU
1	B	22	PRO
1	B	65	ALA
1	B	70	THR
1	C	29	PRO
1	A	80	GLU
1	C	280	TYR
1	A	202	SER
1	B	279	LEU
1	C	265	THR
1	D	156	PRO
1	A	121	ILE

### 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	218/243 (90%)	197 (90%)	21 (10%)	8 16
1	B	225/243 (93%)	202 (90%)	23 (10%)	7 14
1	C	226/243 (93%)	193 (85%)	33 (15%)	3 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	219/243 (90%)	193 (88%)	26 (12%)	5 9
All	All	888/972 (91%)	785 (88%)	103 (12%)	5 10

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	33	GLN
1	A	36	LYS
1	A	56	LYS
1	A	64	THR
1	A	67	SER
1	A	70	THR
1	A	80	GLU
1	A	124	THR
1	A	126	LEU
1	A	145	LEU
1	A	152	VAL
1	A	180	VAL
1	A	204	SER
1	A	221	GLU
1	A	238	LYS
1	A	251	LEU
1	A	262	LEU
1	A	263	TRP
1	A	269	ARG
1	A	277	GLU
1	B	25	GLU
1	B	26	GLU
1	B	28	ARG
1	B	35	LYS
1	B	44	LYS
1	B	68	LYS
1	B	73	LYS
1	B	131	ASP
1	B	165	ILE
1	B	171	LEU
1	B	180	VAL
1	B	184	SER
1	B	203	VAL
1	B	204	SER
1	B	221	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	222	THR
1	B	228	SER
1	B	263	TRP
1	B	268	ILE
1	B	270	ASN
1	B	276	LEU
1	B	283	SER
1	B	285	ASN
1	C	21	GLN
1	C	26	GLU
1	C	28	ARG
1	C	36	LYS
1	C	48	ARG
1	C	56	LYS
1	C	68	LYS
1	C	73	LYS
1	C	85	SER
1	C	109	LEU
1	C	119	ASN
1	C	126	LEU
1	C	127	ASN
1	C	132	ASP
1	C	157	MET
1	C	170	SER
1	C	179	MET
1	C	196	SER
1	C	205	ARG
1	C	221	GLU
1	C	232	HIS
1	C	233	MET
1	C	240	GLU
1	C	244	GLU
1	C	262	LEU
1	C	266	LEU
1	C	267	LEU
1	C	269	ARG
1	C	272	SER
1	C	279	LEU
1	C	281	SER
1	C	285	ASN
1	C	286	MET
1	D	66	ARG

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Mol	Chain	Res	Type
1	D	72	GLN
1	D	76	SER
1	D	105	GLN
1	D	122	THR
1	D	124	THR
1	D	125	SER
1	D	126	LEU
1	D	127	ASN
1	D	134	HIS
1	D	138	LYS
1	D	155	LEU
1	D	170	SER
1	D	171	LEU
1	D	209	SER
1	D	221	GLU
1	D	230	ILE
1	D	232	HIS
1	D	234	GLN
1	D	262	LEU
1	D	263	TRP
1	D	265	THR
1	D	266	LEU
1	D	274	LYS
1	D	276	LEU
1	D	278	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	119	ASN
1	A	130	HIS
1	A	160	GLN
1	A	162	ASN
1	A	253	GLN
1	B	33	GLN
1	B	105	GLN
1	B	135	HIS
1	B	253	GLN
1	B	270	ASN
1	C	53	HIS
1	C	127	ASN

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Mol	Chain	Res	Type
1	C	232	HIS
1	D	72	GLN
1	D	101	GLN
1	D	105	GLN
1	D	160	GLN
1	D	232	HIS
1	D	270	ASN

### 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](#)

8 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	3OQ	D	293	-	27,28,28	2.21	4 (14%)	38,43,43	2.23	7 (18%)
2	NAP	A	1	-	45,52,52	1.69	3 (6%)	56,80,80	1.26	3 (5%)
3	3OQ	A	293	-	27,28,28	1.49	4 (14%)	38,43,43	1.76	7 (18%)
2	NAP	D	4	-	45,52,52	1.75	5 (11%)	56,80,80	1.76	10 (17%)
3	3OQ	C	293	-	27,28,28	1.13	3 (11%)	38,43,43	1.94	10 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAP	C	3	-	45,52,52	1.83	4 (8%)	56,80,80	1.27	4 (7%)
3	3OQ	B	293	-	27,28,28	1.37	5 (18%)	38,43,43	1.76	6 (15%)
2	NAP	B	2	-	45,52,52	1.71	4 (8%)	56,80,80	1.43	8 (14%)

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	3OQ	D	293	-	-	14/31/32/32	0/2/2/2
2	NAP	A	1	-	-	4/31/67/67	0/5/5/5
3	3OQ	A	293	-	-	4/31/32/32	0/2/2/2
2	NAP	D	4	-	-	7/31/67/67	0/5/5/5
3	3OQ	C	293	-	-	8/31/32/32	0/2/2/2
2	NAP	C	3	-	-	3/31/67/67	0/5/5/5
3	3OQ	B	293	-	-	2/31/32/32	0/2/2/2
2	NAP	B	2	-	-	10/31/67/67	0/5/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	NAP	O7N-C7N	9.26	1.41	1.24
2	A	1	NAP	O7N-C7N	8.97	1.41	1.24
2	B	2	NAP	O7N-C7N	8.81	1.41	1.24
2	D	4	NAP	O7N-C7N	8.53	1.40	1.24
3	D	293	3OQ	C1-S12	-8.50	1.66	1.78
3	D	293	3OQ	C15-S12	-4.89	1.69	1.77
3	A	293	3OQ	C1-S12	-4.45	1.72	1.78
2	D	4	NAP	C2N-N1N	4.36	1.40	1.35
2	C	3	NAP	C2A-N3A	3.96	1.38	1.32
3	B	293	3OQ	O14-S12	3.85	1.51	1.44
3	A	293	3OQ	O14-S12	3.81	1.51	1.44
2	A	1	NAP	C2A-N3A	3.80	1.38	1.32
3	D	293	3OQ	O13-S12	3.77	1.51	1.44
2	B	2	NAP	C2A-N3A	3.74	1.38	1.32
2	C	3	NAP	C2N-N1N	3.69	1.39	1.35
3	D	293	3OQ	O14-S12	3.51	1.50	1.44
3	B	293	3OQ	O13-S12	3.50	1.50	1.44
3	C	293	3OQ	O14-S12	3.00	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	293	3OQ	C15-S12	-2.99	1.72	1.77
3	A	293	3OQ	O13-S12	2.90	1.49	1.44
3	C	293	3OQ	C1-S12	-2.75	1.74	1.78
3	B	293	3OQ	C1-S12	-2.72	1.74	1.78
3	C	293	3OQ	O13-S12	2.71	1.49	1.44
2	C	3	NAP	C2A-N1A	2.49	1.38	1.33
2	D	4	NAP	C3N-C7N	2.40	1.54	1.50
2	B	2	NAP	C2N-N1N	2.39	1.37	1.35
2	B	2	NAP	C2A-N1A	2.38	1.38	1.33
3	B	293	3OQ	O20-C19	-2.37	1.39	1.43
2	D	4	NAP	C2A-N3A	2.25	1.35	1.32
2	D	4	NAP	C2A-N1A	2.21	1.38	1.33
2	A	1	NAP	C2A-N1A	2.19	1.38	1.33
3	B	293	3OQ	C15-S12	-2.03	1.73	1.77

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	293	3OQ	C15-S12-C1	8.34	117.06	105.28
3	C	293	3OQ	O14-S12-O13	-7.01	105.84	119.23
2	B	2	NAP	N3A-C2A-N1A	-6.93	117.84	128.68
3	B	293	3OQ	O14-S12-O13	-6.88	106.10	119.23
3	A	293	3OQ	O14-S12-O13	-6.22	107.35	119.23
2	A	1	NAP	N3A-C2A-N1A	-5.93	119.41	128.68
3	D	293	3OQ	O14-S12-O13	-5.92	107.93	119.23
2	D	4	NAP	C3N-C7N-N7N	5.56	124.42	117.75
3	D	293	3OQ	O13-S12-C15	5.21	113.85	107.97
2	C	3	NAP	N3A-C2A-N1A	-5.05	120.78	128.68
2	D	4	NAP	O4D-C1D-C2D	-4.59	100.22	106.93
3	C	293	3OQ	C26-C18-C19	-4.06	117.00	121.46
2	D	4	NAP	N3A-C2A-N1A	-4.03	122.38	128.68
2	D	4	NAP	O7N-C7N-N7N	-3.97	116.94	122.58
3	B	293	3OQ	O13-S12-C15	3.73	112.18	107.97
3	A	293	3OQ	C15-S12-C1	3.42	110.10	105.28
2	D	4	NAP	C4A-C5A-N7A	-3.17	106.10	109.40
3	D	293	3OQ	O14-S12-C15	-3.16	104.41	107.97
2	C	3	NAP	C3N-C7N-N7N	3.10	121.47	117.75
3	C	293	3OQ	C15-S12-C1	3.08	109.62	105.28
3	A	293	3OQ	O13-S12-C15	3.04	111.40	107.97
3	C	293	3OQ	C16-C15-S12	2.97	123.30	119.52
3	A	293	3OQ	C3-C4-C5	-2.91	115.13	119.99
3	C	293	3OQ	C17-C18-C19	2.90	124.64	121.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	293	3OQ	C17-C18-C19	-2.89	118.28	121.46
3	D	293	3OQ	C7-C4-C5	2.81	123.28	119.54
3	C	293	3OQ	O13-S12-C15	2.78	111.11	107.97
2	D	4	NAP	C5A-C6A-N6A	2.78	124.58	120.35
3	D	293	3OQ	C3-C4-C5	-2.78	115.36	119.99
2	B	2	NAP	C4A-C5A-N7A	-2.76	106.52	109.40
3	A	293	3OQ	C7-C4-C5	2.72	123.16	119.54
2	A	1	NAP	C1B-N9A-C4A	-2.69	121.91	126.64
3	B	293	3OQ	O14-S12-C15	2.56	110.86	107.97
2	A	1	NAP	O7N-C7N-C3N	-2.54	116.59	119.63
2	D	4	NAP	C3N-C2N-N1N	2.51	122.88	120.43
3	C	293	3OQ	C7-C8-C1	2.50	118.83	117.21
2	D	4	NAP	O2B-C2B-C1B	2.43	118.86	110.10
2	B	2	NAP	C3N-C7N-N7N	2.42	120.65	117.75
3	B	293	3OQ	O20-C19-C18	-2.41	103.17	108.01
3	B	293	3OQ	C9-C8-C7	-2.34	114.70	119.41
2	B	2	NAP	C5A-C6A-N6A	2.33	123.89	120.35
2	C	3	NAP	O4B-C4B-C3B	2.28	109.63	105.11
2	D	4	NAP	C5B-C4B-C3B	-2.24	106.78	115.18
2	C	3	NAP	C1B-N9A-C4A	-2.23	122.73	126.64
2	D	4	NAP	PN-O3-PA	-2.19	125.30	132.83
3	C	293	3OQ	C8-C1-S12	-2.12	119.52	124.07
3	A	293	3OQ	C27-C15-S12	2.12	122.22	119.52
3	D	293	3OQ	C2-C1-C8	2.09	123.23	121.31
2	B	2	NAP	O2N-PN-O1N	2.09	122.57	112.24
3	B	293	3OQ	O20-C19-C22	2.05	109.22	106.18
3	C	293	3OQ	O14-S12-C15	2.04	110.27	107.97
2	B	2	NAP	C5B-C4B-C3B	-2.03	107.56	115.18
2	B	2	NAP	O4D-C1D-C2D	-2.02	103.97	106.93
3	C	293	3OQ	C2-C1-S12	2.02	119.44	116.40
2	B	2	NAP	O7N-C7N-C3N	-2.02	117.22	119.63

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	NAP	C2B-O2B-P2B-O2X
2	B	2	NAP	C5B-O5B-PA-O2A
2	B	2	NAP	O4B-C4B-C5B-O5B
2	B	2	NAP	C3B-C4B-C5B-O5B
2	B	2	NAP	C2B-O2B-P2B-O1X
2	B	2	NAP	C5D-O5D-PN-O1N

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Mol	Chain	Res	Type	Atoms
2	C	3	NAP	C2B-O2B-P2B-O1X
2	D	4	NAP	O4D-C4D-C5D-O5D
3	C	293	3OQ	C7-C8-C9-C10
3	C	293	3OQ	C21-C19-C22-F25
3	C	293	3OQ	C17-C18-C19-C21
3	C	293	3OQ	C26-C18-C19-C21
3	C	293	3OQ	C17-C18-C19-C22
3	C	293	3OQ	C26-C18-C19-C22
3	D	293	3OQ	C21-C19-C22-F23
3	D	293	3OQ	O20-C19-C22-F23
3	D	293	3OQ	C18-C19-C22-F23
3	D	293	3OQ	C21-C19-C22-F24
3	D	293	3OQ	O20-C19-C22-F24
3	D	293	3OQ	C18-C19-C22-F24
3	D	293	3OQ	C21-C19-C22-F25
3	D	293	3OQ	O20-C19-C22-F25
3	D	293	3OQ	C18-C19-C22-F25
2	D	4	NAP	C3D-C4D-C5D-O5D
3	D	293	3OQ	C1-C8-C9-C10
3	A	293	3OQ	C27-C15-S12-O14
3	D	293	3OQ	C16-C15-S12-O14
3	D	293	3OQ	C27-C15-S12-O14
3	A	293	3OQ	C16-C15-S12-O14
2	A	1	NAP	C5D-O5D-PN-O3
2	B	2	NAP	C5B-O5B-PA-O3
2	B	2	NAP	C5D-O5D-PN-O3
2	D	4	NAP	C2B-O2B-P2B-O3X
2	A	1	NAP	C5D-O5D-PN-O1N
2	B	2	NAP	C5B-O5B-PA-O1A
2	B	2	NAP	C5D-O5D-PN-O2N
3	C	293	3OQ	C21-C19-C22-F24
3	D	293	3OQ	C16-C15-S12-C1
2	D	4	NAP	O4B-C4B-C5B-O5B
3	C	293	3OQ	O20-C19-C22-F25
3	D	293	3OQ	C27-C15-S12-C1
2	C	3	NAP	PN-O3-PA-O1A
3	A	293	3OQ	C27-C15-S12-C1
2	B	2	NAP	C2B-O2B-P2B-O3X
2	A	1	NAP	O4B-C4B-C5B-O5B
2	D	4	NAP	PN-O3-PA-O1A
2	D	4	NAP	PN-O3-PA-O2A
3	B	293	3OQ	C16-C15-S12-O14

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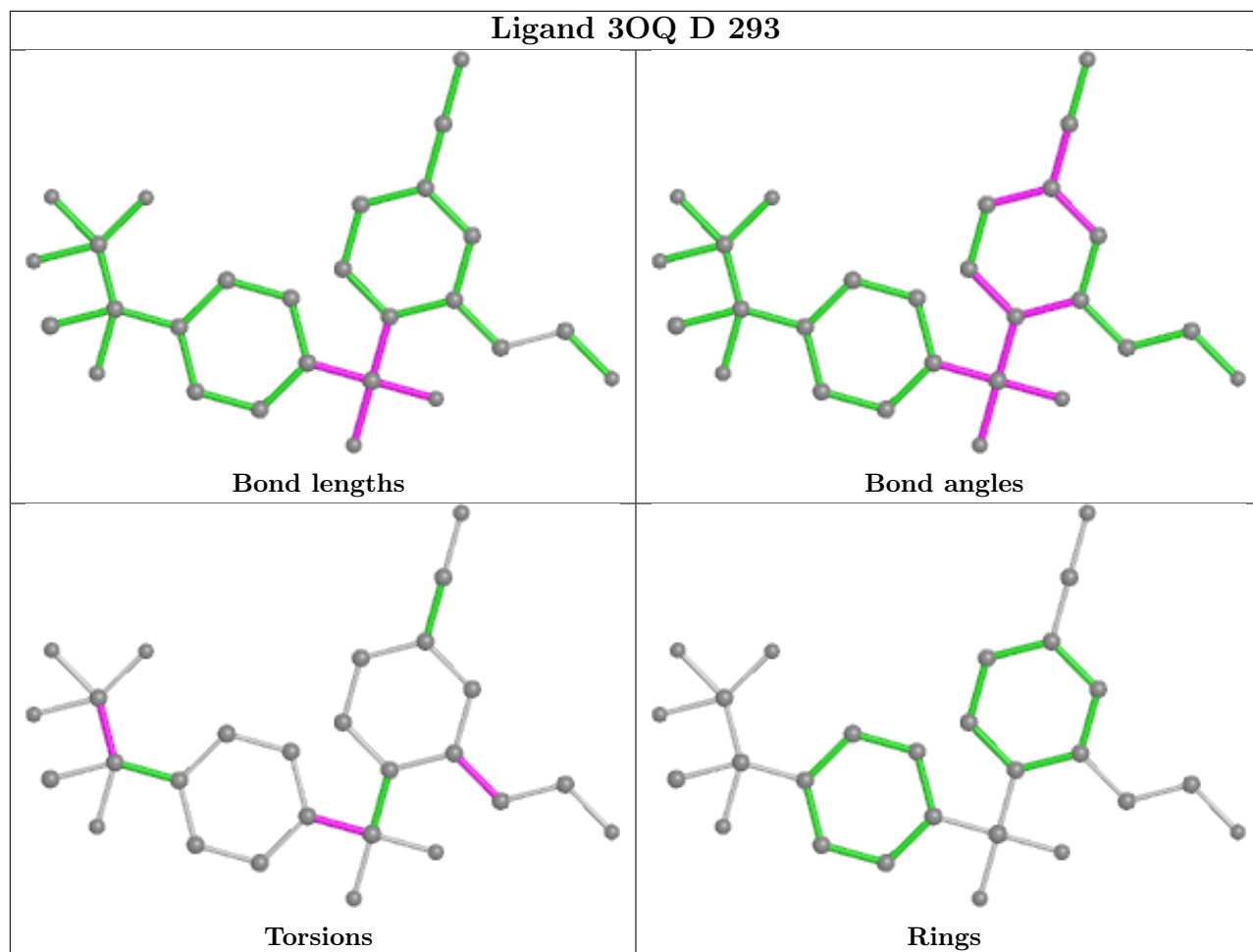
Mol	Chain	Res	Type	Atoms
2	D	4	NAP	C5D-O5D-PN-O1N
2	C	3	NAP	O4B-C4B-C5B-O5B
3	A	293	3OQ	C16-C15-S12-C1
3	B	293	3OQ	C27-C15-S12-O14

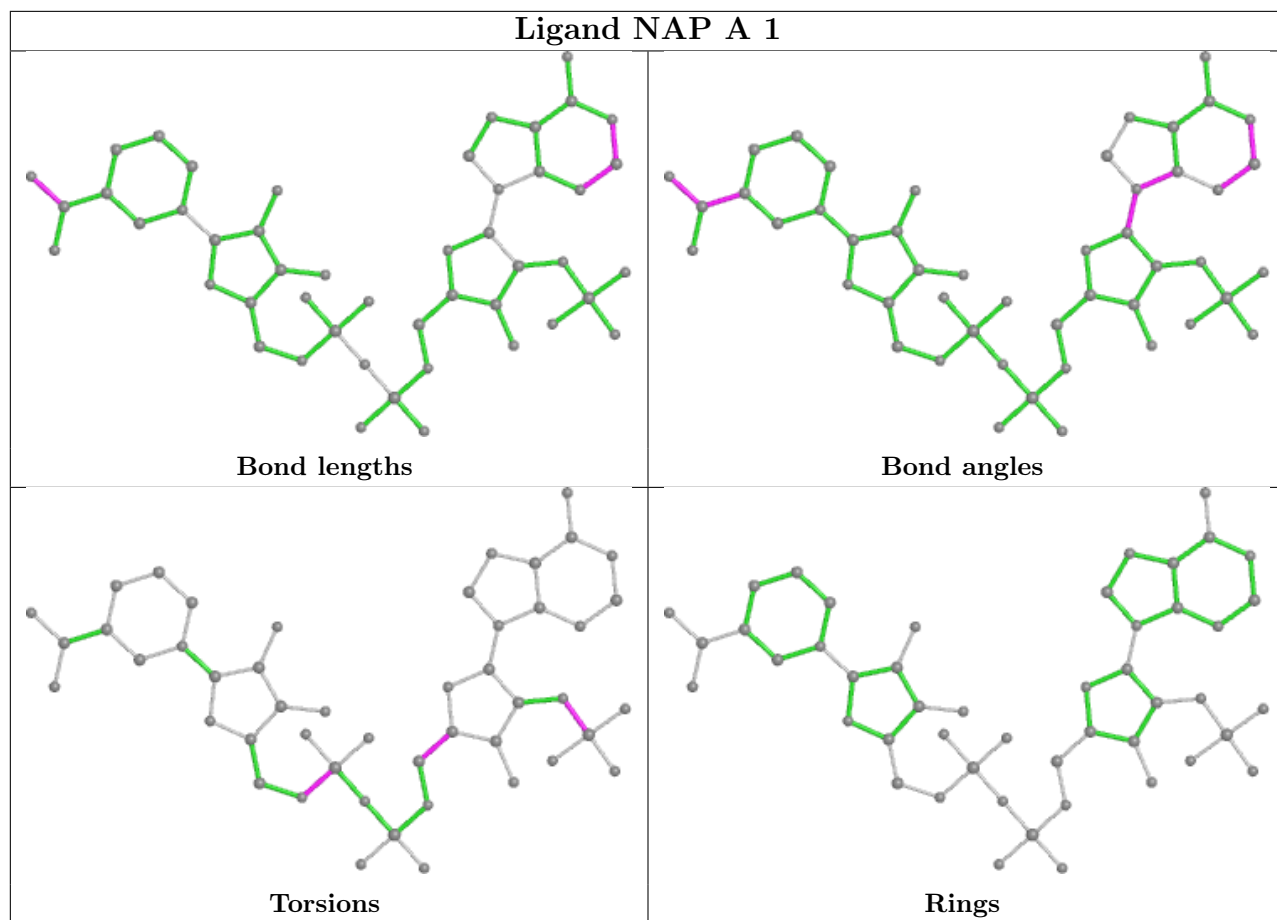
There are no ring outliers.

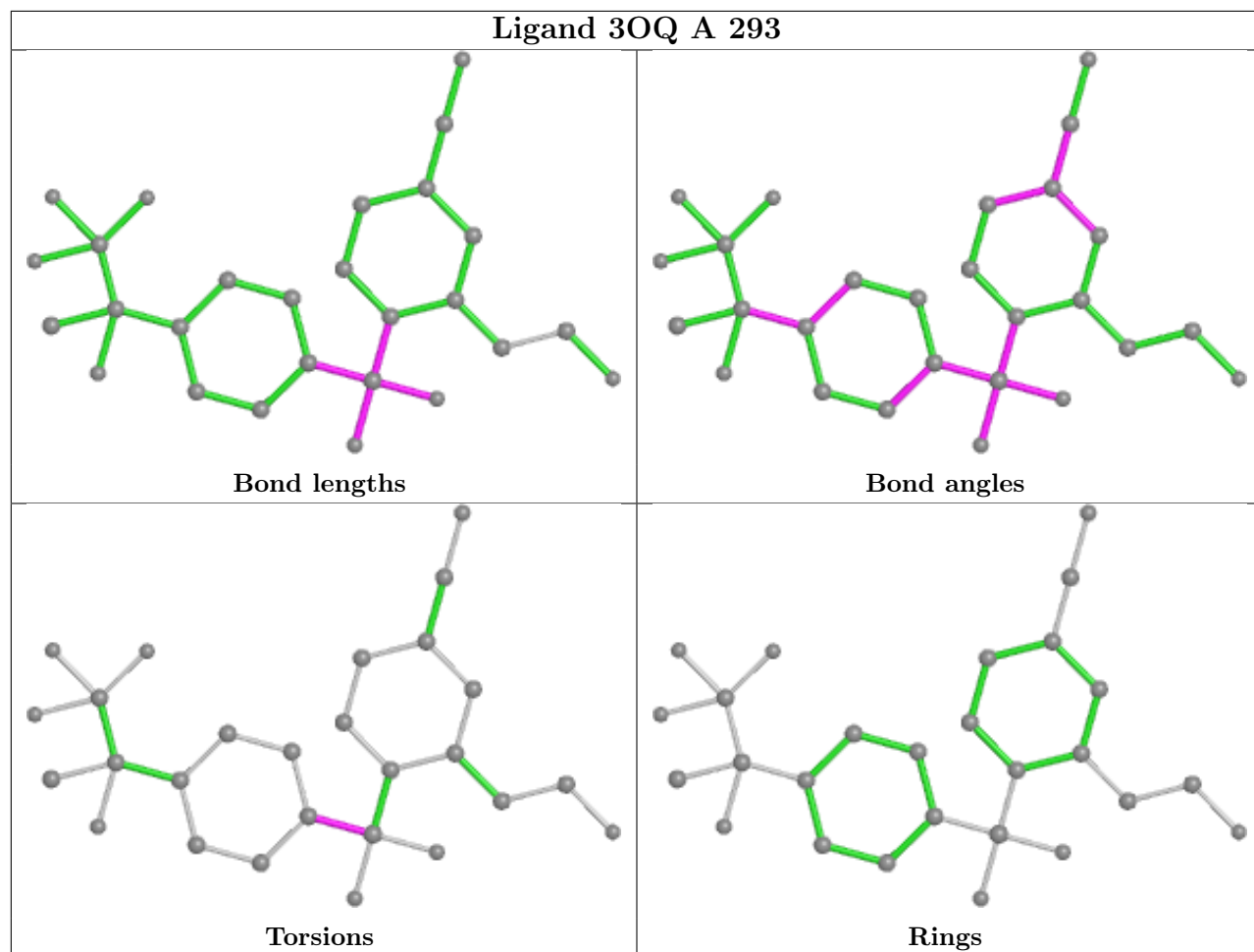
6 monomers are involved in 24 short contacts:

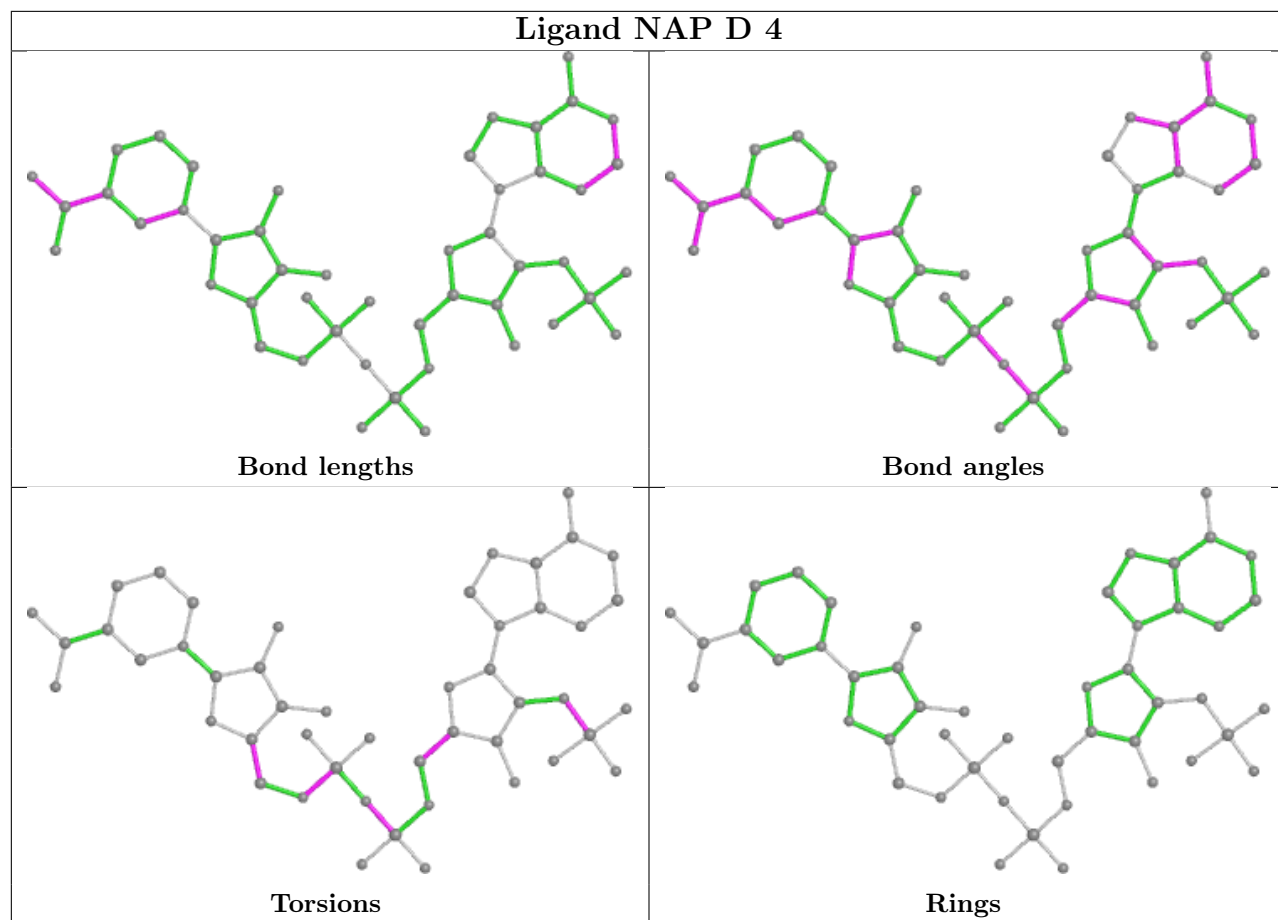
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	293	3OQ	3	0
2	A	1	NAP	6	0
2	D	4	NAP	3	0
3	C	293	3OQ	3	0
2	C	3	NAP	4	0
2	B	2	NAP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

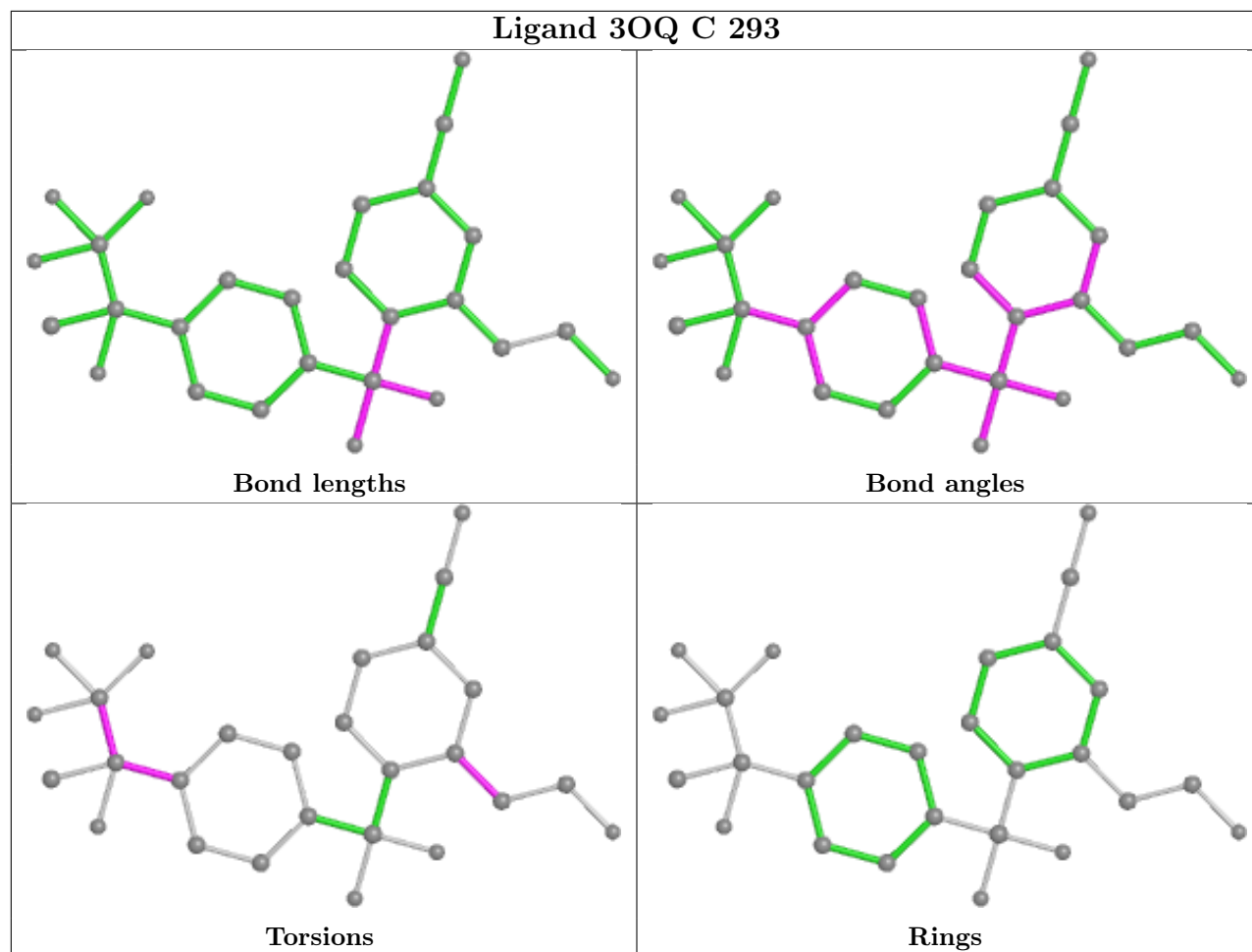


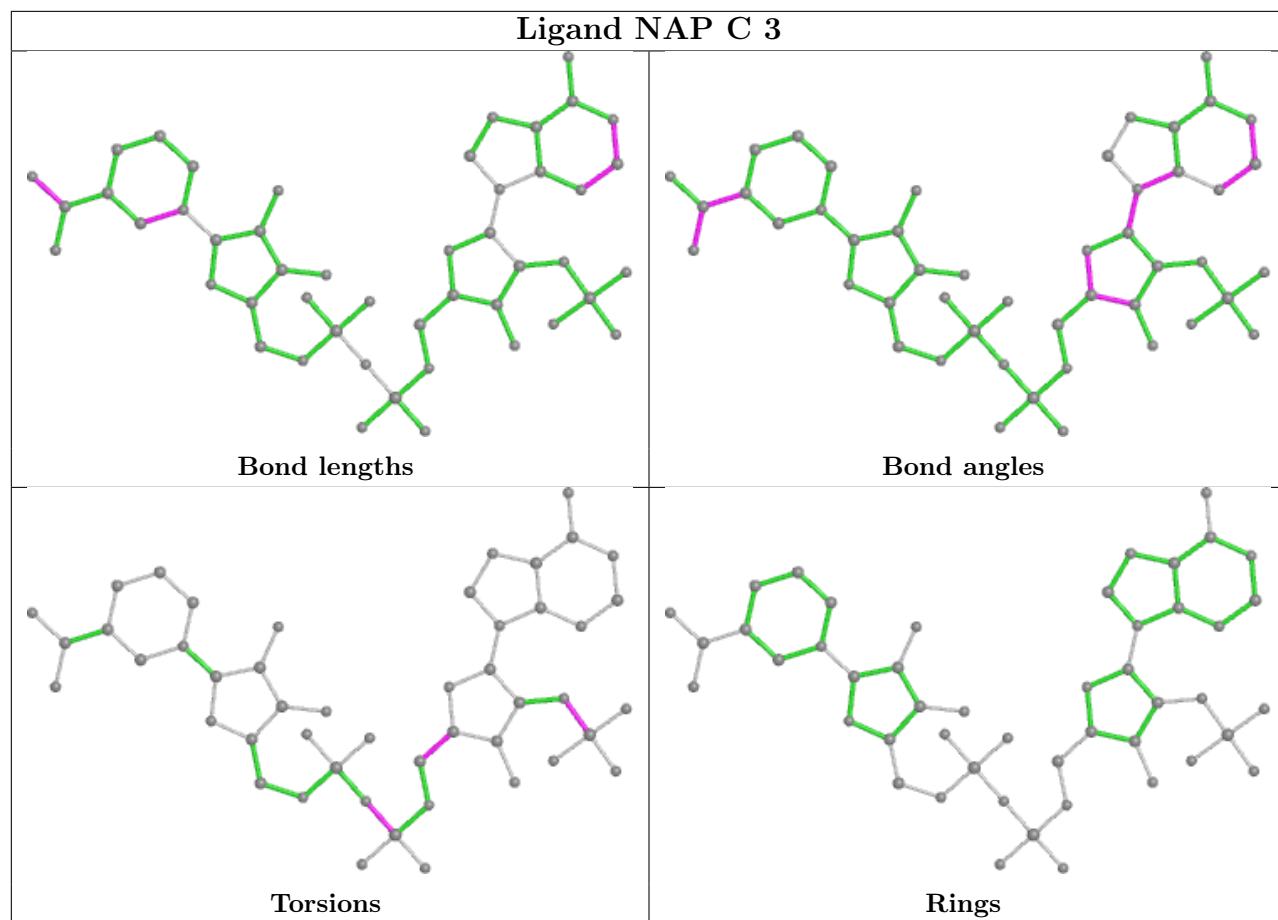


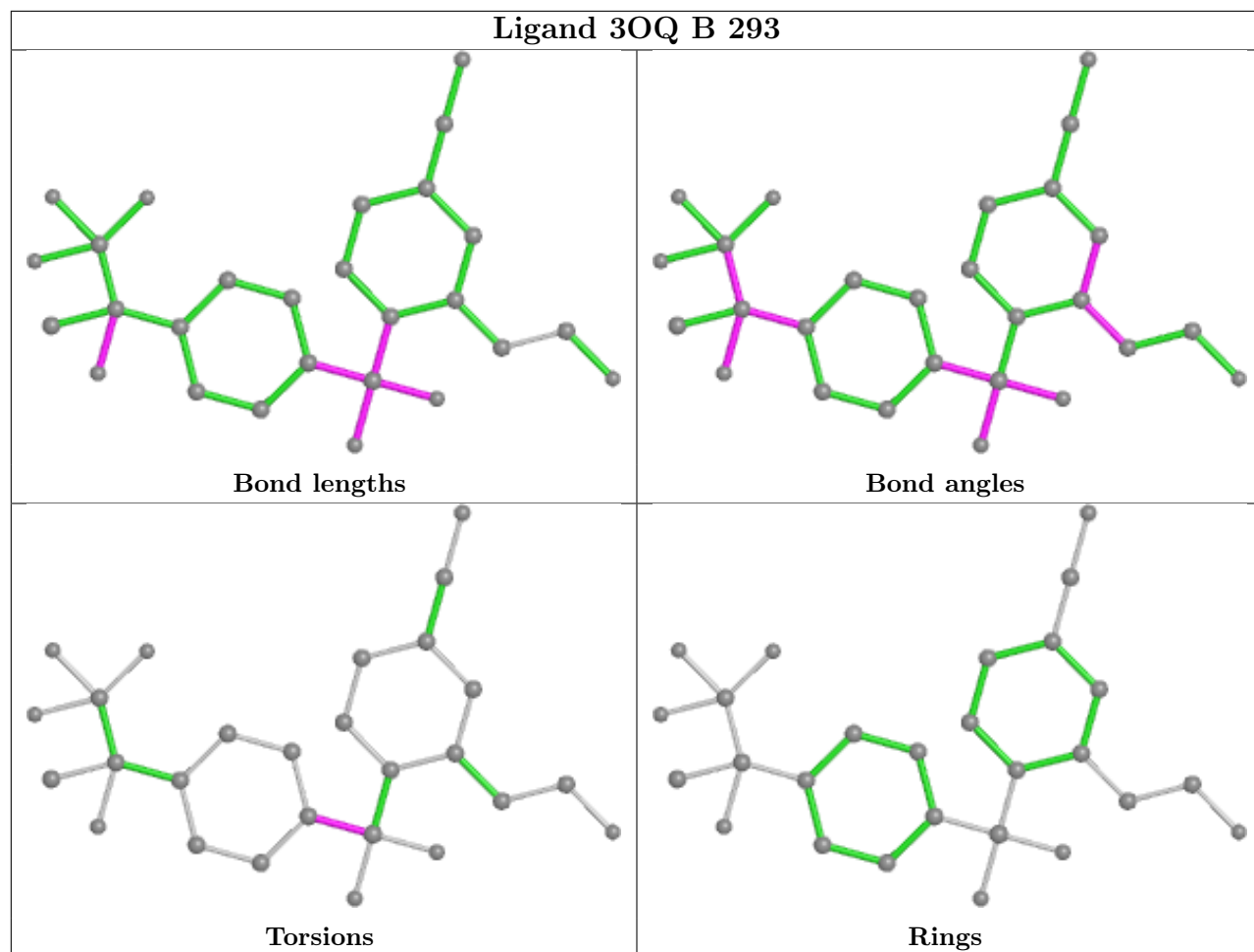


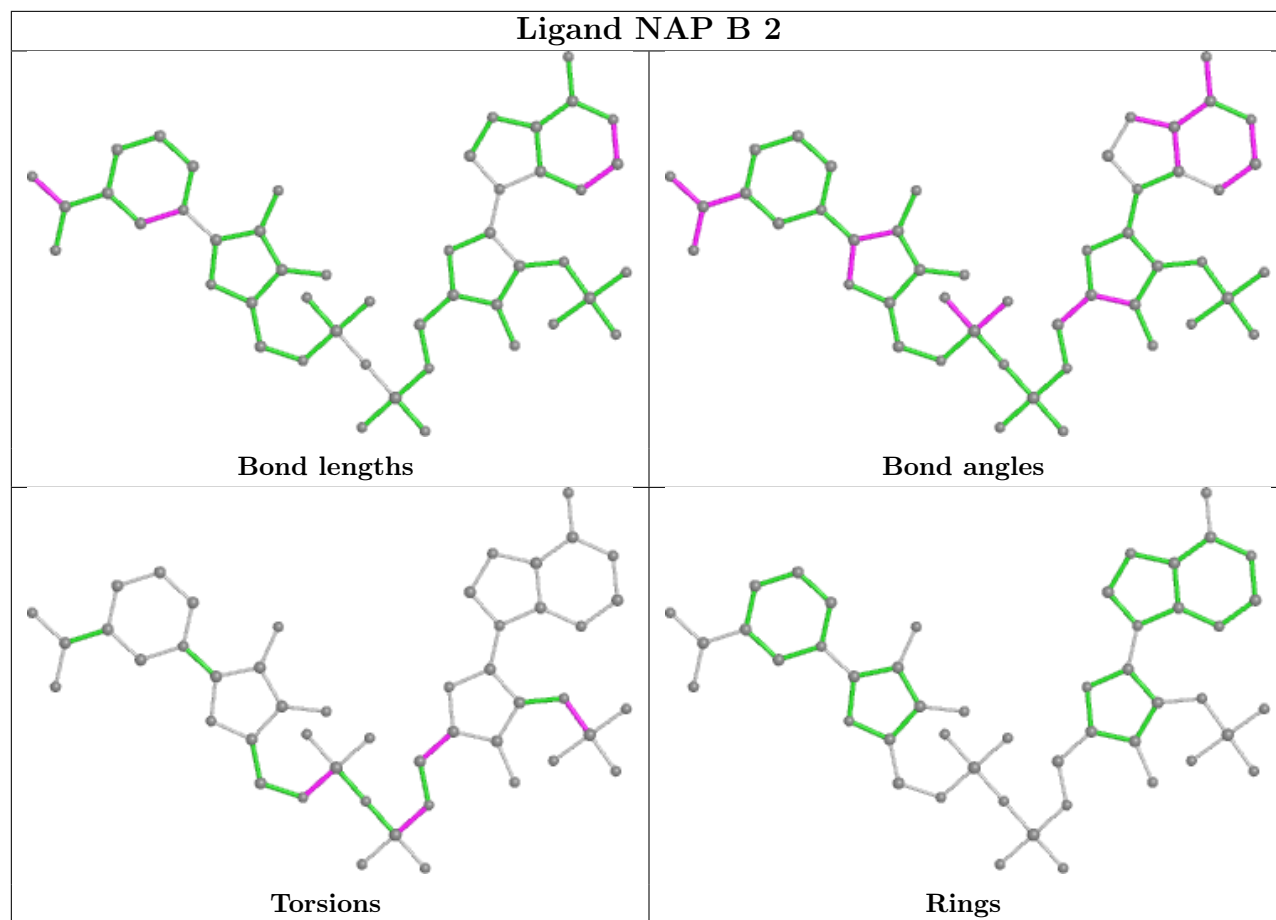












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	261/286 (91%)	0.35	16 (6%) 21 16	33, 74, 100, 115	0
1	B	267/286 (93%)	0.02	5 (1%) 66 62	37, 58, 91, 109	0
1	C	269/286 (94%)	0.11	11 (4%) 37 30	42, 63, 96, 112	0
1	D	261/286 (91%)	-0.10	8 (3%) 49 42	34, 57, 89, 103	0
All	All	1058/1144 (92%)	0.10	40 (3%) 40 33	33, 62, 97, 115	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	24	ASN	5.6
1	C	289	PHE	5.0
1	A	23	LEU	4.7
1	B	285	ASN	4.5
1	D	232	HIS	4.3
1	D	22	PRO	3.9
1	A	22	PRO	3.6
1	C	263	TRP	3.6
1	A	231	VAL	3.6
1	D	21	GLN	3.4
1	C	25	GLU	3.4
1	A	237	PRO	3.2
1	B	263	TRP	3.2
1	A	233	MET	3.0
1	C	286	MET	3.0
1	D	23	LEU	2.9
1	C	23	LEU	2.9
1	A	68	LYS	2.7
1	D	263	TRP	2.7
1	A	166	VAL	2.7
1	C	231	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	22	PRO	2.5
1	D	228	SER	2.5
1	D	231	VAL	2.4
1	A	263	TRP	2.4
1	A	232	HIS	2.4
1	A	211	THR	2.3
1	C	189	ALA	2.3
1	B	24	ASN	2.3
1	C	229	GLY	2.2
1	A	21	GLN	2.1
1	B	23	LEU	2.1
1	A	278	PHE	2.1
1	A	167	VAL	2.1
1	A	40	THR	2.1
1	D	224	MET	2.1
1	C	192	GLY	2.1
1	C	232	HIS	2.0
1	A	226	ALA	2.0
1	B	237	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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

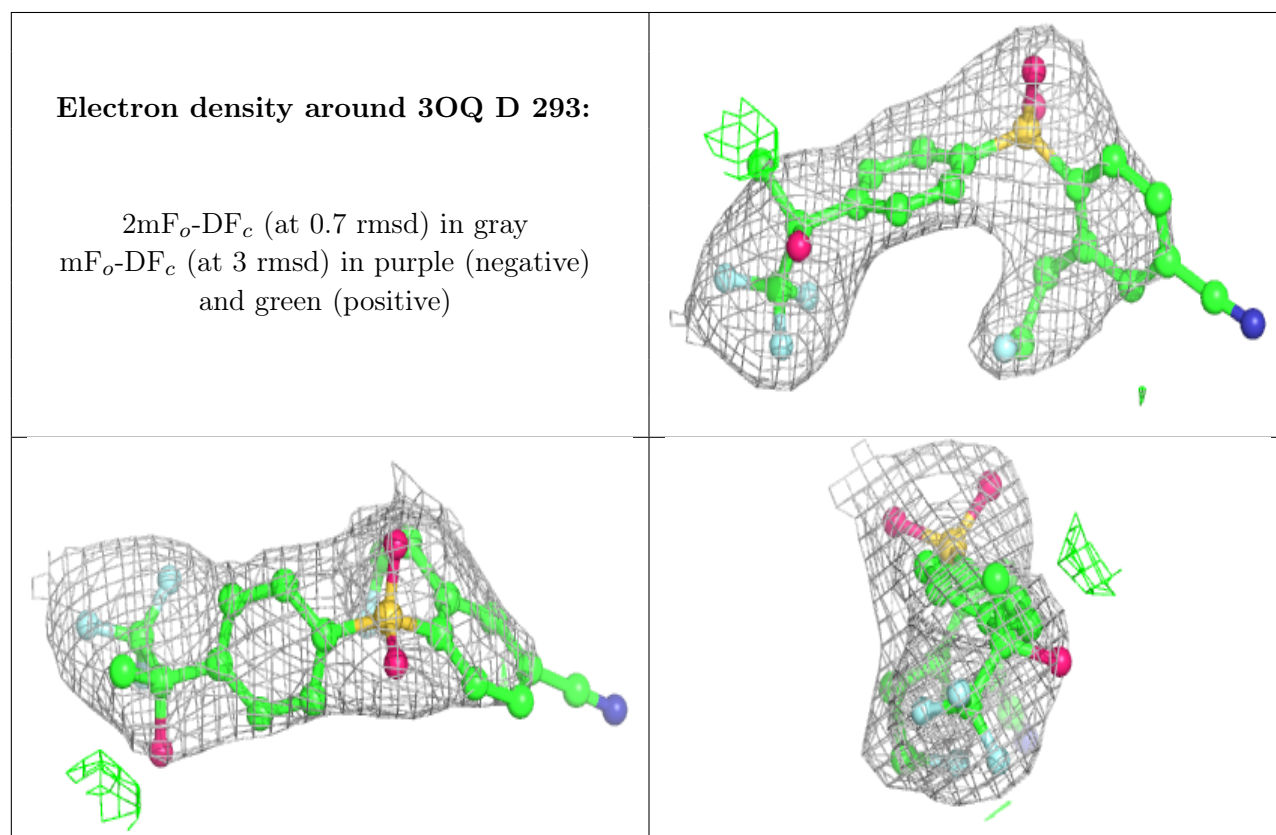
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	3OQ	D	293	27/27	0.92	0.21	80,84,91,95	0
3	3OQ	B	293	27/27	0.94	0.23	62,70,78,83	0
3	3OQ	C	293	27/27	0.94	0.19	63,66,72,74	0
3	3OQ	A	293	27/27	0.94	0.15	69,72,75,78	0

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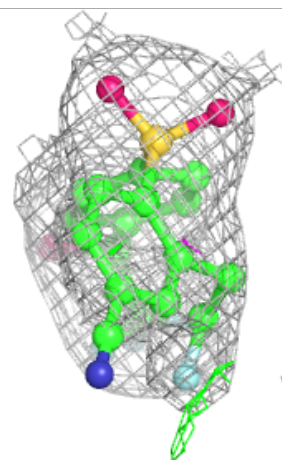
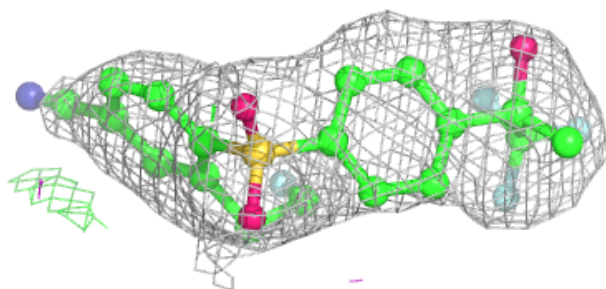
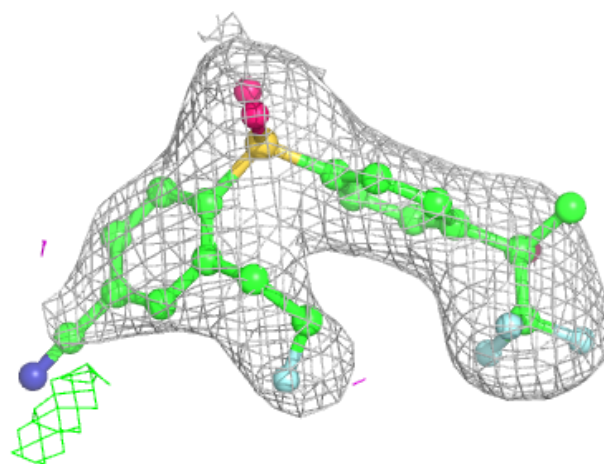
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAP	A	1	48/48	0.95	0.13	64,70,74,76	0
2	NAP	B	2	48/48	0.96	0.13	40,52,59,60	0
2	NAP	C	3	48/48	0.96	0.12	44,53,63,65	0
2	NAP	D	4	48/48	0.97	0.12	36,47,51,55	0

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 3OQ B 293:**

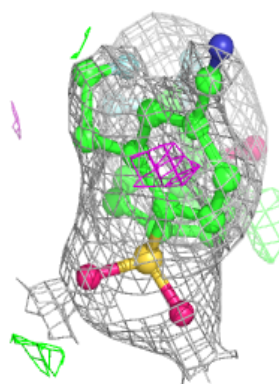
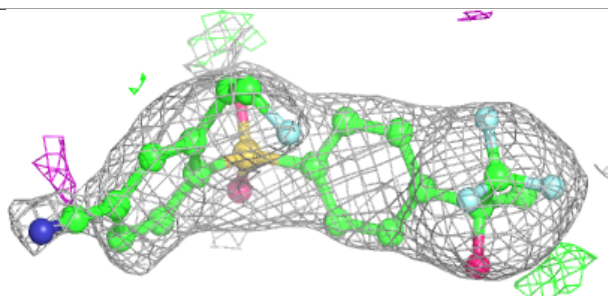
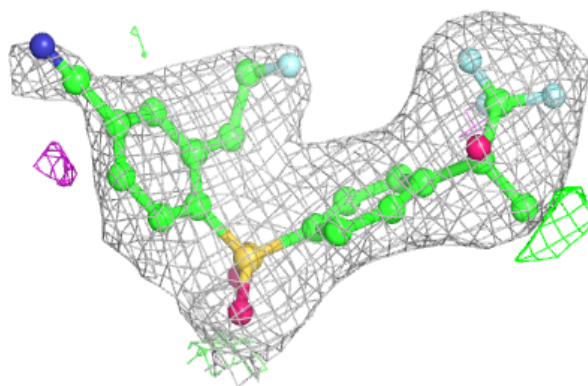
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



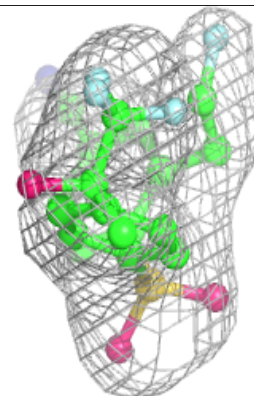
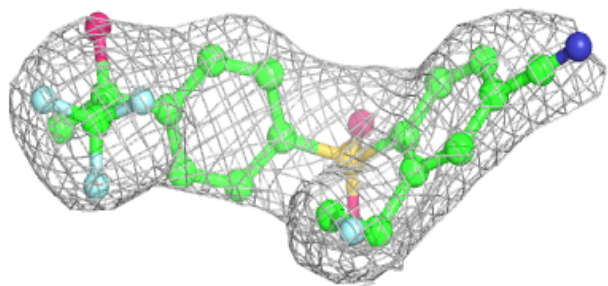
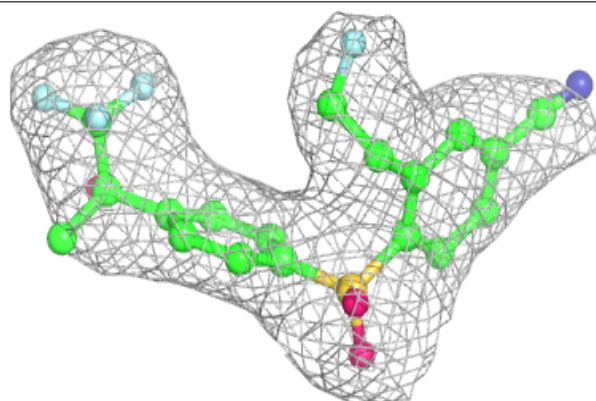


**Electron density around 3OQ C 293:**

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

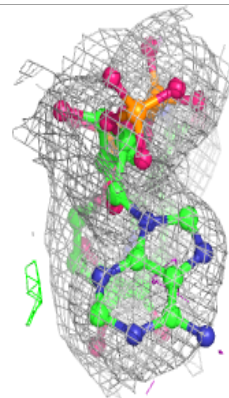
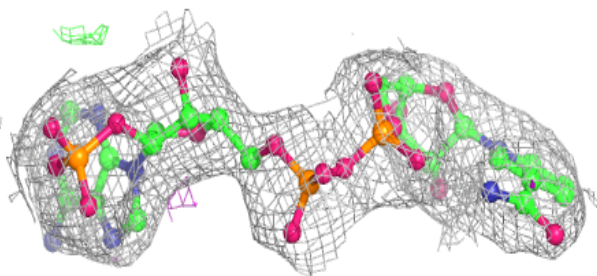
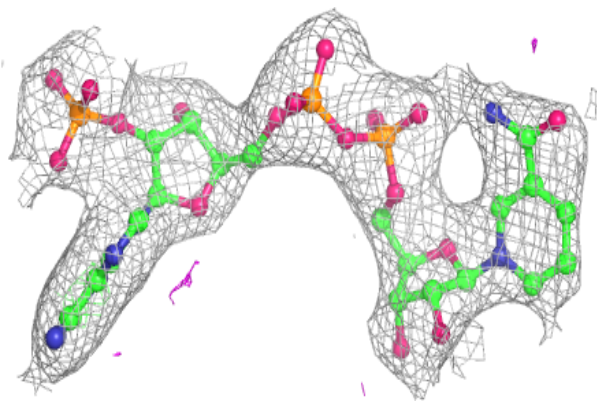
**Electron density around 3OQ A 293:**

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

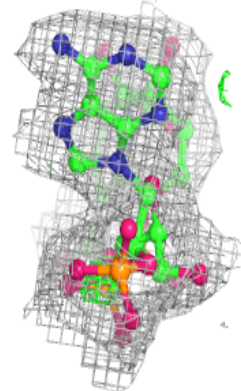
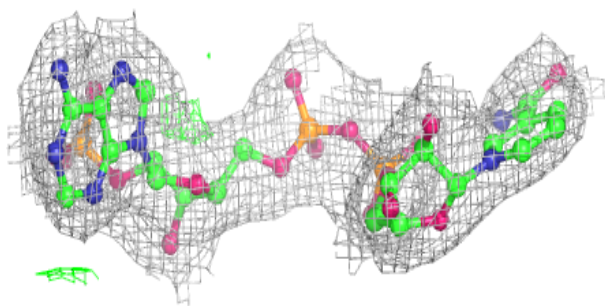
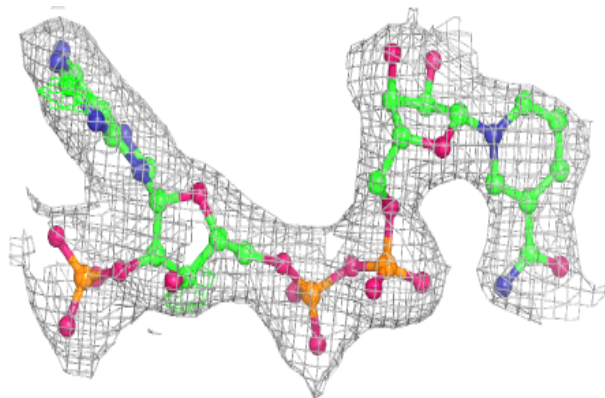


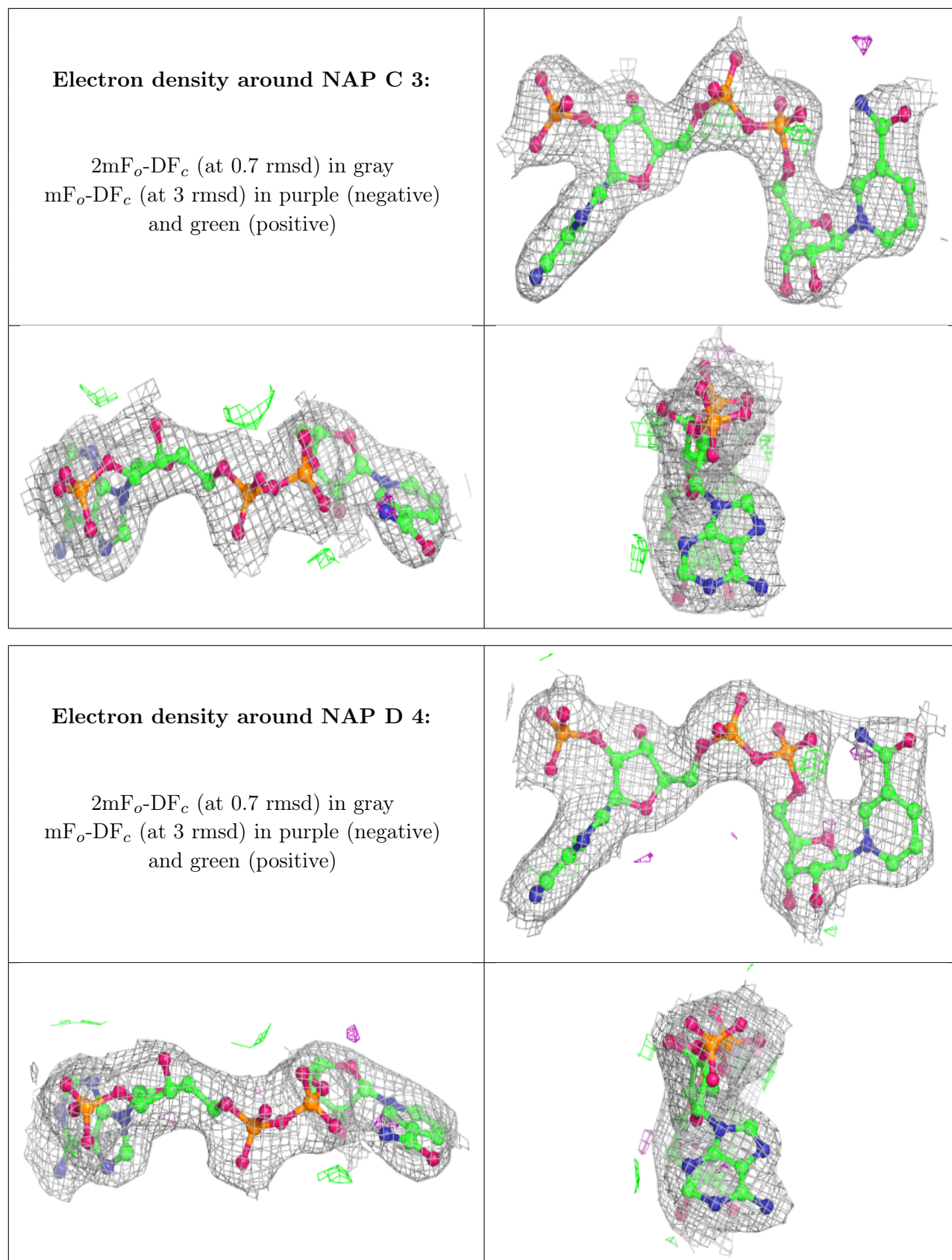
**Electron density around NAP A 1:**

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

**Electron density around NAP B 2:**

$2mF_o-DF_c$  (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.