Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 10:45 PM EDT

PDB ID	:	3ASV
Title	:	The Closed form of serine dehydrogenase complexed with NADP+
Authors	:	Yamazawa, R.; Nakajima, Y.; Yoshimoto, T.; Ito, K.
Deposited on	:	2010-12-21
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
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:

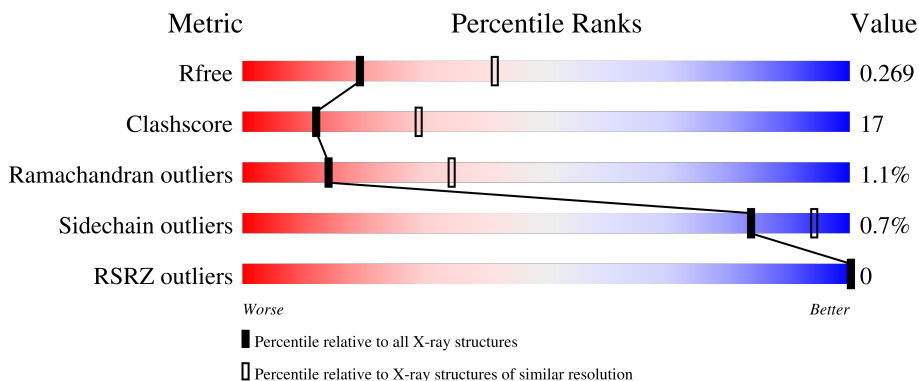|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.269
Clashscore		17
Ramachandran outliers		1.1%
Sidechain outliers		0.7%
RSRZ outliers		0

Worse .... *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	248	76% 23%
1	B	248	77% 22%
1	C	248	71% 28%
1	D	248	64% 35%
1	E	248	58% 40%

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| Mol	Chain	Length	Quality of chain
1	F	248	58% 41%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 12045 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 Short-chain dehydrogenase/reductase SDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	S	0	0	0
			1891	1186	341	354	10			
1	B	248	Total	C	N	O	S	0	0	0
			1911	1196	341	364	10			
1	C	248	Total	C	N	O	S	0	0	0
			1900	1191	340	359	10			
1	D	248	Total	C	N	O	S	0	0	0
			1907	1194	341	362	10			
1	E	248	Total	C	N	O	S	0	0	0
			1891	1185	338	358	10			
1	F	248	Total	C	N	O	S	0	0	0
			1880	1177	334	359	10			

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).
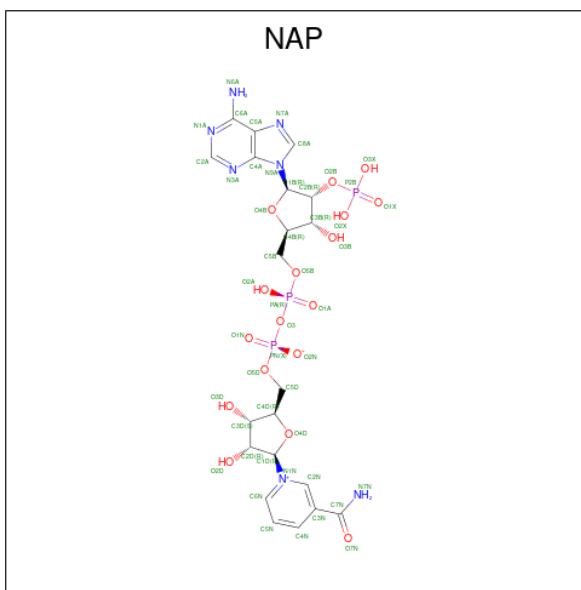
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
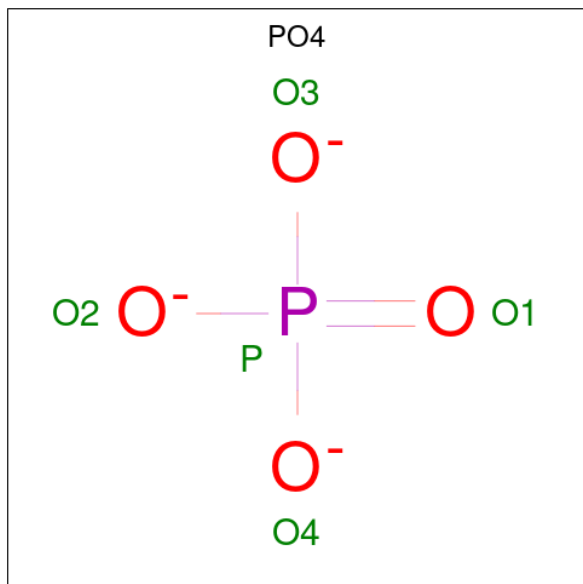
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	F	1	Total	O	P	0	0
			5	4	1		

• Molecule 4 is water.

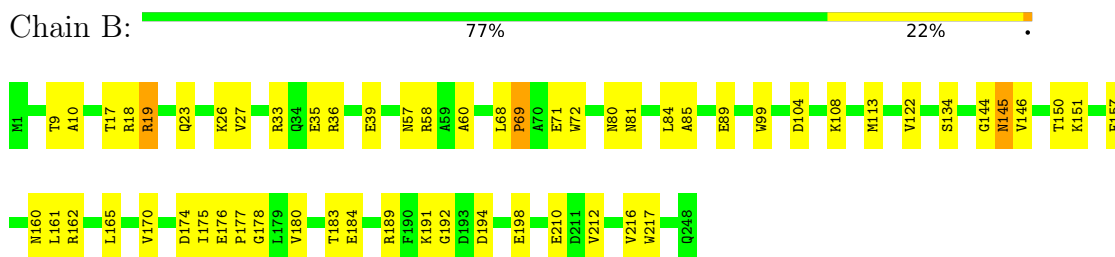| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total 72	O 72	0	0
4	B	66	Total 66	O 66	0	0
4	C	65	Total 65	O 65	0	0
4	D	52	Total 52	O 52	0	0
4	E	47	Total 47	O 47	0	0
4	F	45	Total 45	O 45	0	0

3 Residue-property plots ⓘ

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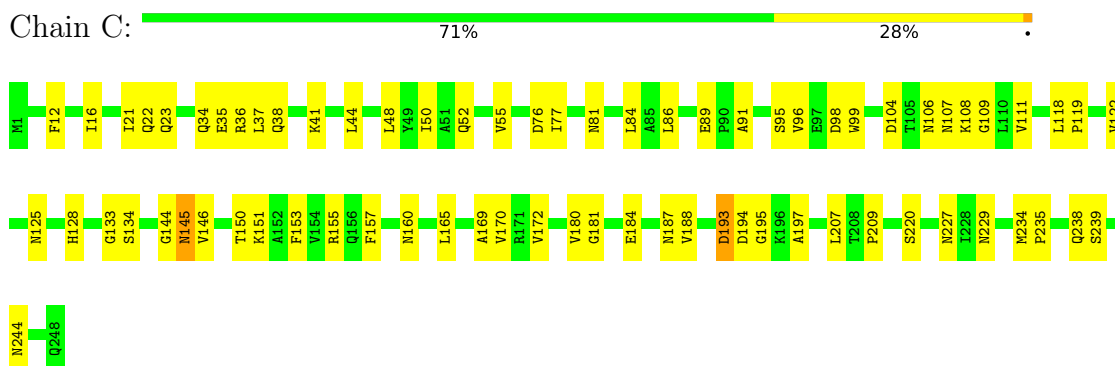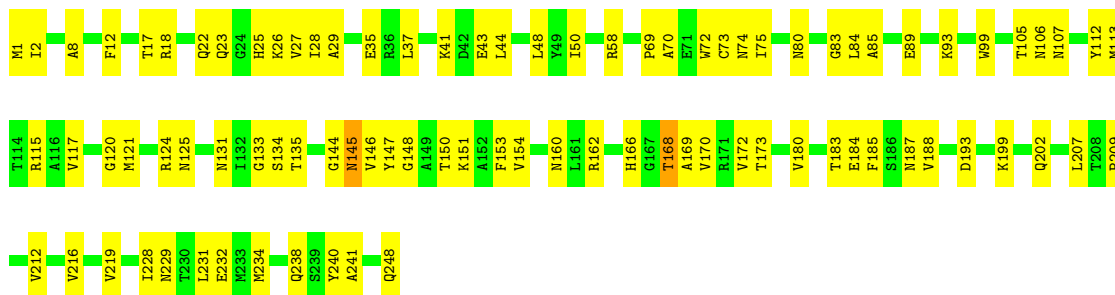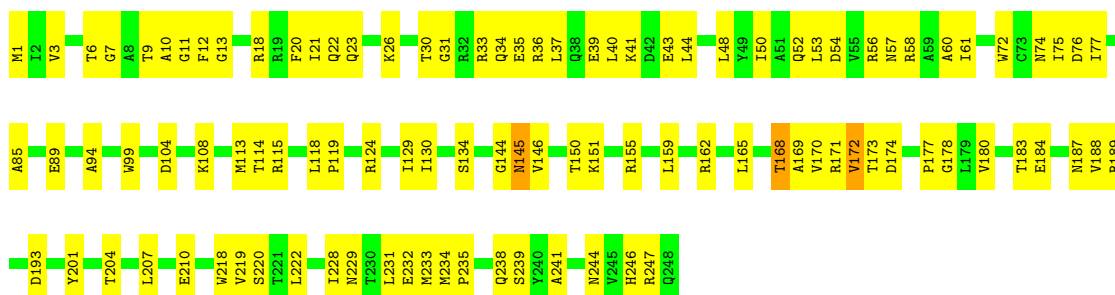
- Molecule 1: Short-chain dehydrogenase/reductase SDR

- Molecule 1: Short-chain dehydrogenase/reductase SDR

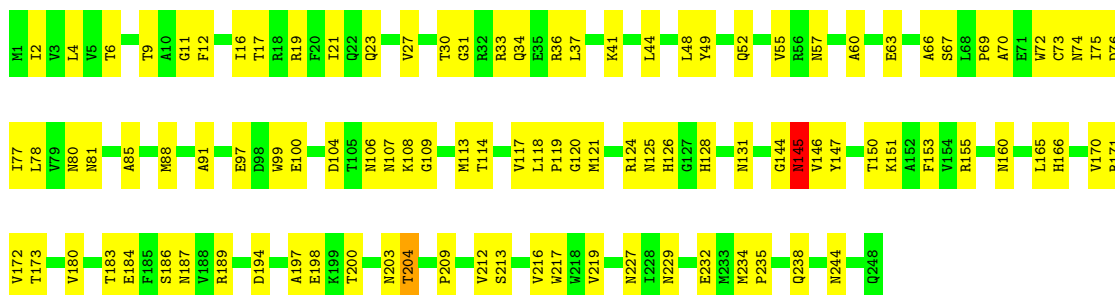- Molecule 1: Short-chain dehydrogenase/reductase SDR

- Molecule 1: Short-chain dehydrogenase/reductase SDR

M1 I2 A8 F12 T17 R18 Q22 Q23 G24 H25 K26 V27 I28 A29 E35 R36 L37 K41 D42 E43 L44 L48 Y49 I50 R58 P69 A70 E71 W72 C73 N74 I75 N80 G83 L84 A85 E89 K93 W99 T105 N106 N107 Y112 M113

T114 R115 A116 V117 G120 M121 R124 N125 N131 I132 G133 S134 T135 G144 N145 V146 Y147 G148 A149 T150 K151 A152 F153 V154 N160 L161 R162 H166 G167 T168 A169 V170 R171 V172 T173 V180 T183 E184 F185 S186 N187 V188 D193 K199 Q202 L207 T208 P209

V212 V216 V219 I228 N229 T230 L231 E232 M233 M234 Q238 S239 Y240 A241 Q248

• Molecule 1: Short-chain dehydrogenase/reductase SDR

Chain E: 58% 40%

M1 I2 V3 T6 G7 A8 T9 A10 G11 F12 G13 R18 R19 F20 I21 Q22 Q23 K26 T30 G31 R32 R33 Q34 E35 R36 L37 Q38 E39 L40 K41 D42 E43 L44 L48 Y49 I50 A51 Q52 L53 D54 V55 R56 N57 R58 A59 A60 I61 W72 C73 N74 I75 D76 I77

A85 E89 A94 W99 D104 K108 M113 T114 R115 L118 P119 R124 I129 I130 S134 G144 N145 V146 T150 K151 R155 L159 R162 L165 T168 A169 V170 R171 V172 T173 D174 P177 G178 L179 V180 T183 E184 N187 V188 R189

D193 Y201 T204 L207 E210 W218 V219 S220 T221 L222 I228 N229 T230 L231 E232 M233 M234 P235 Q238 S239 Y240 A241 N244 V245 H246 R247 Q248

• Molecule 1: Short-chain dehydrogenase/reductase SDR

Chain F: 58% 41%

M1 I2 V3 L4 V5 T6 T9 A10 G11 F12 I16 T17 R18 R19 F20 I21 Q22 Q23 V27 T30 G31 R32 R33 Q34 E35 R36 L37 K41 L44 L48 Y49 Q52 V55 R56 N57 A60 E63 A66 S67 L68 P69 A70 E71 W72 C73 N74 I75 D76

I77 L78 V79 N80 N81 A85 M88 A91 E97 D98 W99 E100 D104 T105 N106 N107 K108 G109 M113 T114 V117 L118 P119 G120 M121 R124 N125 H126 G127 H128 N131 G144 N145 V146 Y147 T150 K151 A152 F153 V154 R155 N160 L165 H166 V170 R171

V172 T173 V180 T183 E184 F185 S186 N187 V188 R189 D194 A197 E198 K199 T200 N203 T204 P209 V212 S213 V216 W217 W218 V219 N227 I228 N229 E232 M233 M234 P235 Q238 N244 Q248

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 64	Depositor
Cell constants a, b, c, α, β, γ	113.86Å 113.86Å 197.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.70 21.53 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.70) 99.8 (21.53-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.71Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.192 , 0.273 0.187 , 0.269	Depositor DCC
R_{free} test set	1991 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 17.2	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.326 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12045	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.47 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.1867e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, PO4

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	0.35	0/1927	0.62	0/2620
1	B	0.36	0/1947	0.61	0/2645
1	C	0.35	0/1936	0.62	0/2631
1	D	0.35	0/1943	0.60	0/2640
1	E	0.34	0/1927	0.60	0/2621
1	F	0.36	0/1916	0.62	0/2609
All	All	0.35	0/11596	0.61	0/15766

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 ⓘ

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	1891	0	1861	53	0
1	B	1911	0	1881	43	0
1	C	1900	0	1869	60	0
1	D	1907	0	1877	87	0
1	E	1891	0	1850	100	0
1	F	1880	0	1818	82	0
2	A	48	0	25	2	0

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W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	25	2	0
2	C	48	0	25	3	0
2	D	48	0	25	2	0
2	E	48	0	25	3	0
2	F	48	0	25	2	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	72	0	0	5	0
4	B	66	0	0	3	0
4	C	65	0	0	6	0
4	D	52	0	0	0	0
4	E	47	0	0	2	0
4	F	45	0	0	4	0
All	All	12045	0	11306	393	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 (393) 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:E:168:THR:HG23	1:E:170:VAL:H	1.12	1.08
1:D:168:THR:HG23	1:D:170:VAL:H	1.30	0.96
1:E:184:GLU:HA	1:E:187:ASN:HD22	1.31	0.93
1:F:41:LYS:HA	1:F:48:LEU:HD23	1.60	0.84
1:F:17:THR:HG23	1:F:27:VAL:HG11	1.59	0.83
1:F:33:ARG:CZ	1:F:36:ARG:HH21	1.92	0.82
1:A:21:ILE:HD12	1:A:44:LEU:HD13	1.60	0.82
1:D:74:ASN:HA	1:D:124:ARG:NH2	1.96	0.81
1:E:37:LEU:HB3	1:E:50:ILE:HD11	1.64	0.80
1:F:34:GLN:HB2	1:F:52:GLN:OE1	1.83	0.79
1:A:35:GLU:O	1:A:39:GLU:HG3	1.85	0.77
1:C:229:ASN:HD21	1:F:234:MET:HG3	1.50	0.77
1:D:44:LEU:HD12	1:D:48:LEU:HD22	1.66	0.77
1:A:17:THR:HG23	1:A:27:VAL:HG11	1.66	0.77
1:B:194:ASP:O	1:B:198:GLU:HG3	1.85	0.77
1:C:35:GLU:HG2	1:C:36:ARG:N	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:ILE:HD11	1:D:231:LEU:HB2	1.68	0.76
1:D:173:THR:HG21	1:D:219:VAL:HG11	1.68	0.75
1:B:17:THR:HG23	1:B:27:VAL:HG11	1.69	0.74
1:A:41:LYS:HA	1:A:48:LEU:HD23	1.70	0.74
1:C:172:VAL:H	1:C:227:ASN:HD21	1.36	0.73
1:F:75:ILE:N	1:F:124:ARG:HH12	1.86	0.73
1:C:184:GLU:HA	1:C:187:ASN:HD22	1.55	0.71
1:B:35:GLU:O	1:B:39:GLU:HG3	1.92	0.70
1:F:172:VAL:H	1:F:227:ASN:HD21	1.40	0.69
1:E:168:THR:HG23	1:E:170:VAL:N	1.97	0.69
1:A:190:PHE:HB3	1:A:196:LYS:HE3	1.74	0.69
1:F:97:GLU:O	1:F:100:GLU:HB3	1.92	0.69
1:D:184:GLU:HA	1:D:187:ASN:HD22	1.57	0.68
1:D:80:ASN:HD22	1:D:131:ASN:HD21	1.40	0.68
1:C:22:GLN:HE21	1:C:23:GLN:NE2	1.92	0.67
1:B:162:ARG:HD2	4:B:1019:HOH:O	1.95	0.67
1:D:22:GLN:NE2	1:D:23:GLN:HE21	1.93	0.67
1:D:17:THR:HG23	1:D:27:VAL:HG11	1.76	0.67
1:E:37:LEU:HB3	1:E:50:ILE:CD1	2.25	0.67
1:F:165:LEU:HD13	1:F:170:VAL:HB	1.76	0.67
1:A:145:ASN:HA	1:B:160:ASN:HB3	1.77	0.67
1:A:180:VAL:HG22	1:A:207:LEU:HB2	1.77	0.67
1:F:212:VAL:O	1:F:216:VAL:HG23	1.96	0.66
1:E:18:ARG:HG2	1:E:18:ARG:HH11	1.60	0.66
1:D:120:GLY:C	1:D:124:ARG:HH11	1.98	0.65
1:E:44:LEU:HD12	1:E:48:LEU:HD22	1.78	0.65
1:B:19:ARG:HH21	1:B:19:ARG:HB2	1.62	0.65
1:E:37:LEU:C	1:E:50:ILE:HD11	2.17	0.65
1:D:80:ASN:HD22	1:D:131:ASN:ND2	1.94	0.65
1:D:134:SER:HB3	1:D:151:LYS:HG3	1.78	0.65
1:A:184:GLU:HA	1:A:187:ASN:HD22	1.62	0.65
1:D:69:PRO:HB2	1:D:72:TRP:HD1	1.60	0.65
1:D:229:ASN:HD21	1:E:234:MET:HG2	1.62	0.64
1:E:3:VAL:HG22	1:E:77:ILE:HB	1.79	0.64
1:F:21:ILE:HG21	1:F:44:LEU:HD13	1.78	0.64
1:D:180:VAL:HG22	1:D:207:LEU:HB2	1.80	0.64
1:B:146:VAL:O	1:B:150:THR:HG23	1.98	0.64
1:E:155:ARG:HA	1:E:174:ASP:OD2	1.97	0.64
1:F:183:THR:HG22	1:F:209:PRO:HG3	1.79	0.64
1:A:14:GLU:O	1:A:18:ARG:HG3	1.98	0.63
1:E:168:THR:CG2	1:E:170:VAL:H	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LYS:HB3	1:A:72:TRP:CZ3	2.34	0.62
1:C:41:LYS:HA	1:C:48:LEU:HD23	1.81	0.62
1:E:115:ARG:HD3	1:F:91:ALA:O	2.00	0.62
1:A:92:HIS:CD2	1:A:92:HIS:H	2.18	0.62
1:B:89:GLU:HG2	4:B:1188:HOH:O	1.99	0.62
1:B:175:ILE:HG22	1:B:177:PRO:HD3	1.82	0.62
1:E:75:ILE:N	1:E:124:ARG:HH12	1.98	0.61
1:E:134:SER:HB3	1:E:151:LYS:HG3	1.81	0.61
1:C:181:GLY:O	1:C:209:PRO:HD3	2.00	0.61
1:B:33:ARG:CZ	1:B:36:ARG:NH1	2.64	0.60
1:A:166:HIS:HA	4:A:1346:HOH:O	2.01	0.60
1:F:184:GLU:HA	1:F:187:ASN:HD22	1.66	0.60
1:D:185:PHE:HB2	2:D:304:NAP:O1N	2.02	0.60
1:F:55:VAL:HG12	1:F:109:GLY:HA3	1.83	0.60
1:C:77:ILE:HG12	1:C:128:HIS:HB3	1.84	0.60
1:A:19:ARG:O	1:A:23:GLN:HG2	2.02	0.59
2:C:303:NAP:H52A	4:C:1322:HOH:O	2.03	0.59
1:C:194:ASP:HA	1:C:197:ALA:HB3	1.83	0.59
1:D:219:VAL:HG22	1:D:228:ILE:HG21	1.84	0.58
1:E:58:ARG:NH1	1:F:100:GLU:OE1	2.37	0.58
1:A:134:SER:HB3	1:A:151:LYS:HG3	1.85	0.58
1:F:19:ARG:HH12	1:F:23:GLN:HG3	1.68	0.58
1:D:37:LEU:HD13	1:D:50:ILE:HG23	1.85	0.57
1:F:114:THR:O	1:F:118:LEU:HB2	2.04	0.57
1:F:104:ASP:HA	1:F:108:LYS:HD3	1.85	0.57
1:A:120:GLY:O	1:A:124:ARG:HG2	2.04	0.57
1:A:4:LEU:HD23	1:A:78:LEU:HD13	1.86	0.57
1:A:33:ARG:HD3	4:A:1300:HOH:O	2.04	0.56
1:C:180:VAL:HG22	1:C:207:LEU:HB2	1.87	0.56
1:F:33:ARG:HG3	2:F:306:NAP:O1X	2.04	0.56
1:D:41:LYS:HA	1:D:48:LEU:HD23	1.86	0.56
1:D:168:THR:CG2	1:D:170:VAL:H	2.12	0.56
1:F:78:LEU:HD22	1:F:117:VAL:HG21	1.86	0.56
1:F:150:THR:O	1:F:153:PHE:HB3	2.05	0.56
1:D:234:MET:HG3	1:E:229:ASN:HD21	1.69	0.56
1:E:207:LEU:HG	1:E:235:PRO:HD3	1.88	0.56
1:D:162:ARG:NH1	1:E:238:GLN:O	2.35	0.56
1:E:219:VAL:HG22	1:E:228:ILE:HG21	1.87	0.56
1:D:41:LYS:HB2	1:D:50:ILE:CD1	2.36	0.56
1:D:146:VAL:O	1:D:150:THR:HG23	2.07	0.55
4:C:1232:HOH:O	1:D:160:ASN:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLY:HA2	1:D:35:GLU:HB2	1.89	0.55
1:E:180:VAL:HG22	1:E:207:LEU:HB2	1.89	0.55
1:E:41:LYS:HA	1:E:48:LEU:HD23	1.89	0.55
1:E:57:ASN:HB3	1:E:60:ALA:HB3	1.86	0.55
1:E:162:ARG:HG2	1:E:172:VAL:CG1	2.37	0.55
1:D:89:GLU:HG3	1:D:93:LYS:O	2.07	0.55
1:F:173:THR:HG21	1:F:219:VAL:HG11	1.88	0.55
1:E:18:ARG:HG2	1:E:18:ARG:NH1	2.22	0.55
1:E:22:GLN:HE21	1:E:23:GLN:HE21	1.53	0.55
1:D:74:ASN:HA	1:D:124:ARG:HH22	1.72	0.55
1:E:104:ASP:O	1:E:108:LYS:HB2	2.06	0.55
1:D:74:ASN:CA	1:D:124:ARG:NH2	2.68	0.54
1:F:80:ASN:HD21	1:F:113:MET:HB2	1.72	0.54
1:D:37:LEU:HB3	1:D:50:ILE:CG2	2.37	0.54
1:D:83:GLY:HA2	1:D:105:THR:HG22	1.90	0.54
1:B:165:LEU:HD13	1:B:170:VAL:HB	1.90	0.54
1:E:35:GLU:H	1:E:35:GLU:CD	2.11	0.54
1:C:50:ILE:O	1:C:50:ILE:HG13	2.07	0.53
1:E:74:ASN:HA	1:E:124:ARG:NH1	2.23	0.53
1:F:17:THR:HG23	1:F:27:VAL:CG1	2.36	0.53
1:C:229:ASN:ND2	1:F:234:MET:HG3	2.22	0.53
1:E:146:VAL:O	1:E:150:THR:HG23	2.08	0.53
1:B:212:VAL:O	1:B:216:VAL:HG23	2.09	0.53
1:E:168:THR:HG23	1:E:169:ALA:N	2.24	0.53
1:E:207:LEU:HD11	1:E:234:MET:HA	1.91	0.53
1:E:6:THR:HA	1:E:30:THR:HB	1.90	0.53
1:E:18:ARG:NH1	1:E:44:LEU:HD21	2.24	0.52
1:E:130:ILE:HD11	1:E:220:SER:HB3	1.91	0.52
1:A:18:ARG:O	1:A:22:GLN:HG3	2.09	0.52
1:A:160:ASN:HB3	4:B:1051:HOH:O	2.08	0.52
1:C:95:SER:HB3	1:C:98:ASP:OD2	2.09	0.52
1:D:248:GLN:O	1:D:248:GLN:HG2	2.09	0.52
1:F:55:VAL:HG12	1:F:109:GLY:CA	2.40	0.52
1:B:85:ALA:O	1:B:189:ARG:HA	2.10	0.52
1:C:22:GLN:HE21	1:C:23:GLN:HE21	1.56	0.52
4:E:1107:HOH:O	1:F:160:ASN:HB3	2.10	0.52
1:F:194:ASP:O	1:F:198:GLU:HG3	2.10	0.52
1:A:92:HIS:CD2	1:A:92:HIS:N	2.75	0.52
1:B:174:ASP:OD2	1:B:176:GLU:OE2	2.28	0.52
1:E:228:ILE:HD11	1:E:231:LEU:HB2	1.90	0.52
1:E:247:ARG:HH11	1:E:247:ARG:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:ASN:HB2	1:F:131:ASN:HD22	1.75	0.52
1:E:22:GLN:O	1:E:22:GLN:HG2	2.10	0.51
1:F:6:THR:HA	1:F:30:THR:OG1	2.09	0.51
1:D:1:MET:N	1:D:25:HIS:ND1	2.48	0.51
1:A:78:LEU:HD22	1:A:117:VAL:HG21	1.92	0.51
1:D:162:ARG:HG2	1:D:172:VAL:HB	1.93	0.51
1:E:173:THR:HG21	1:E:219:VAL:HG11	1.92	0.51
1:E:219:VAL:HG13	1:E:228:ILE:CG2	2.41	0.51
1:C:207:LEU:HG	1:C:235:PRO:HD3	1.93	0.51
1:D:22:GLN:HE21	1:D:23:GLN:NE2	2.09	0.51
1:F:67:SER:HB2	4:F:1138:HOH:O	2.10	0.51
1:F:119:PRO:HG2	4:F:1067:HOH:O	2.10	0.51
1:D:80:ASN:HB2	1:D:131:ASN:HD22	1.75	0.51
1:F:147:TYR:O	1:F:151:LYS:HG2	2.10	0.51
1:E:40:LEU:HD22	1:E:44:LEU:HD11	1.94	0.50
1:D:22:GLN:NE2	1:D:23:GLN:NE2	2.60	0.50
1:F:81:ASN:O	2:F:306:NAP:H4D	2.12	0.50
1:F:9:THR:OG1	1:F:33:ARG:NH2	2.44	0.50
1:C:35:GLU:HG2	1:C:36:ARG:H	1.76	0.50
1:E:162:ARG:HG2	1:E:172:VAL:HG13	1.93	0.50
1:E:145:ASN:HA	1:F:160:ASN:HB3	1.94	0.50
1:E:246:HIS:HB2	1:F:166:HIS:CE1	2.47	0.50
1:C:86:LEU:HB2	1:C:98:ASP:HB3	1.94	0.50
1:C:133:GLY:O	2:C:303:NAP:H6N	2.12	0.50
1:E:53:LEU:HD12	1:E:54:ASP:H	1.76	0.50
1:A:21:ILE:HD12	1:A:44:LEU:CD1	2.39	0.49
1:F:75:ILE:N	1:F:124:ARG:NH1	2.59	0.49
1:C:244:ASN:O	1:E:238:GLN:HA	2.12	0.49
1:E:129:ILE:O	1:E:172:VAL:HA	2.11	0.49
1:D:37:LEU:HB3	1:D:50:ILE:HG21	1.94	0.49
1:E:26:LYS:HE2	1:E:72:TRP:CH2	2.47	0.49
1:B:178:GLY:O	1:B:180:VAL:HG23	2.11	0.49
1:F:85:ALA:O	1:F:189:ARG:HA	2.13	0.49
1:E:35:GLU:O	1:E:39:GLU:HG3	2.12	0.49
1:E:231:LEU:HD23	1:E:231:LEU:C	2.33	0.49
1:B:33:ARG:NH1	1:B:36:ARG:NH1	2.61	0.49
1:C:165:LEU:HD13	1:C:170:VAL:HB	1.94	0.49
1:F:33:ARG:NE	1:F:36:ARG:HH21	2.10	0.49
1:D:58:ARG:HG3	1:D:112:TYR:CE2	2.48	0.49
1:E:21:ILE:HD12	1:E:44:LEU:HD13	1.95	0.49
1:A:12:PHE:HB2	1:A:81:ASN:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:GLY:CA	1:D:35:GLU:HB2	2.42	0.49
1:E:104:ASP:OD2	1:E:108:LYS:HD2	2.13	0.49
1:B:18:ARG:HG2	1:B:18:ARG:HH11	1.77	0.48
1:E:54:ASP:OD1	1:E:56:ARG:HB2	2.12	0.48
1:F:9:THR:CG2	1:F:37:LEU:HG	2.43	0.48
1:B:134:SER:HB3	1:B:151:LYS:HG3	1.94	0.48
1:C:104:ASP:OD2	1:C:108:LYS:HD2	2.13	0.48
1:D:238:GLN:O	1:E:162:ARG:NH1	2.46	0.48
1:B:18:ARG:HG2	1:B:18:ARG:NH1	2.29	0.48
1:B:81:ASN:O	2:B:302:NAP:H4D	2.12	0.48
1:A:175:ILE:O	1:A:177:PRO:HD3	2.13	0.48
1:A:124:ARG:NH2	4:A:1085:HOH:O	2.47	0.48
1:E:9:THR:O	1:E:10:ALA:HB2	2.14	0.48
1:D:12:PHE:N	1:D:12:PHE:CD1	2.80	0.48
1:E:1:MET:HA	1:E:76:ASP:OD2	2.14	0.48
1:E:11:GLY:HA2	1:E:183:THR:HG22	1.96	0.48
1:C:193:ASP:C	1:C:195:GLY:N	2.68	0.48
1:E:30:THR:HG23	1:E:53:LEU:HB3	1.94	0.48
1:B:210:GLU:OE1	1:B:210:GLU:N	2.44	0.47
1:C:119:PRO:HG2	4:C:1299:HOH:O	2.14	0.47
1:D:99:TRP:CD2	1:D:146:VAL:HG21	2.49	0.47
1:D:106:ASN:C	1:D:107:ASN:HD22	2.18	0.47
1:A:99:TRP:CD2	1:A:146:VAL:HG21	2.49	0.47
1:D:37:LEU:C	1:D:50:ILE:HD13	2.34	0.47
1:D:144:GLY:O	1:D:145:ASN:C	2.53	0.47
1:E:162:ARG:HD3	1:E:172:VAL:HG13	1.96	0.47
1:F:77:ILE:HG12	1:F:128:HIS:HB3	1.96	0.47
1:D:228:ILE:CD1	1:E:231:LEU:HG	2.45	0.47
1:E:145:ASN:HA	1:F:160:ASN:CB	2.44	0.47
1:E:184:GLU:HA	1:E:187:ASN:ND2	2.15	0.47
1:D:22:GLN:HG2	1:D:22:GLN:O	2.15	0.47
1:B:23:GLN:HG3	1:B:217:TRP:CH2	2.48	0.47
1:C:81:ASN:O	2:C:303:NAP:H4D	2.15	0.47
1:C:118:LEU:O	1:C:122:VAL:HG23	2.14	0.47
1:E:37:LEU:CB	1:E:50:ILE:HD11	2.39	0.47
1:F:2:ILE:HD12	1:F:74:ASN:O	2.15	0.47
1:F:76:ASP:OD1	1:F:126:HIS:CD2	2.68	0.47
1:A:41:LYS:CA	1:A:48:LEU:HD23	2.43	0.47
1:A:144:GLY:O	1:A:145:ASN:C	2.53	0.47
1:B:33:ARG:NH2	1:B:36:ARG:NH1	2.63	0.47
1:E:61:ILE:HD13	1:E:113:MET:SD	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:155:ARG:NH1	4:F:1091:HOH:O	2.36	0.47
1:A:175:ILE:C	1:A:177:PRO:HD3	2.35	0.47
1:C:229:ASN:HD21	1:F:234:MET:CG	2.25	0.47
1:D:41:LYS:CA	1:D:48:LEU:HD23	2.45	0.47
1:C:244:ASN:ND2	1:E:241:ALA:HA	2.30	0.47
1:E:99:TRP:CD2	1:E:146:VAL:HG21	2.49	0.47
1:F:11:GLY:O	1:F:12:PHE:C	2.54	0.47
1:F:203:ASN:O	1:F:204:THR:HB	2.15	0.47
1:A:190:PHE:CG	1:A:196:LYS:HE3	2.50	0.46
1:C:111:VAL:HG12	1:C:157:PHE:CZ	2.49	0.46
1:D:28:ILE:HD12	1:D:75:ILE:CD1	2.45	0.46
1:D:135:THR:HG22	1:D:232:GLU:HG3	1.97	0.46
1:E:7:GLY:O	1:E:13:GLY:HA3	2.14	0.46
1:E:43:GLU:O	1:E:43:GLU:HG2	2.16	0.46
1:F:4:LEU:HD23	1:F:78:LEU:HD13	1.97	0.46
1:F:186:SER:HA	1:F:189:ARG:HB3	1.98	0.46
1:B:192:GLY:HA2	1:D:35:GLU:OE1	2.14	0.46
1:C:89:GLU:HB2	4:C:1344:HOH:O	2.15	0.46
1:C:144:GLY:O	1:C:145:ASN:C	2.54	0.46
1:C:234:MET:CE	1:F:229:ASN:HD21	2.28	0.46
1:A:44:LEU:HD12	1:A:48:LEU:HD22	1.96	0.46
1:C:12:PHE:O	1:C:16:ILE:HG13	2.15	0.46
1:C:77:ILE:HD13	1:C:220:SER:HB2	1.96	0.46
1:D:199:LYS:O	1:D:202:GLN:HG2	2.15	0.46
1:D:69:PRO:HB2	1:D:72:TRP:CD1	2.46	0.46
1:F:144:GLY:O	1:F:145:ASN:C	2.54	0.46
1:F:99:TRP:HA	1:F:146:VAL:HG21	1.98	0.46
1:A:190:PHE:CB	1:A:196:LYS:HE3	2.45	0.46
1:C:150:THR:O	1:C:153:PHE:HB3	2.16	0.46
1:D:231:LEU:C	1:D:231:LEU:HD23	2.37	0.46
1:C:193:ASP:C	1:C:195:GLY:H	2.18	0.45
1:C:55:VAL:O	1:C:109:GLY:HA2	2.17	0.45
1:C:86:LEU:CB	1:C:98:ASP:HB3	2.47	0.45
1:E:11:GLY:HA3	2:E:305:NAP:O2N	2.16	0.45
1:F:63:GLU:O	1:F:66:ALA:N	2.50	0.45
1:F:106:ASN:C	1:F:107:ASN:HD22	2.19	0.45
1:B:104:ASP:O	1:B:108:LYS:HB2	2.16	0.45
1:D:183:THR:HG22	1:D:209:PRO:HG3	1.98	0.45
1:F:21:ILE:HG12	1:F:27:VAL:CG2	2.47	0.45
1:A:92:HIS:H	1:A:92:HIS:HD2	1.61	0.45
1:A:190:PHE:CD1	1:A:196:LYS:HE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:ASN:HB3	1:F:60:ALA:HB3	1.98	0.45
1:F:70:ALA:C	1:F:72:TRP:H	2.19	0.45
1:B:80:ASN:HD21	1:B:113:MET:HB2	1.82	0.45
1:F:12:PHE:CE1	1:F:180:VAL:HG11	2.52	0.45
1:C:34:GLN:HB2	1:C:52:GLN:OE1	2.17	0.45
1:F:80:ASN:HA	4:F:1306:HOH:O	2.16	0.45
1:B:26:LYS:HB3	1:B:72:TRP:CZ3	2.52	0.45
1:A:12:PHE:CZ	1:A:212:VAL:HG21	2.52	0.44
1:A:96:VAL:HG21	1:B:58:ARG:HD3	1.99	0.44
1:C:238:GLN:HA	1:E:244:ASN:O	2.17	0.44
1:E:33:ARG:HB3	1:E:36:ARG:HG2	1.98	0.44
1:A:102:MET:O	1:A:106:ASN:HB2	2.17	0.44
1:B:57:ASN:HB3	1:B:60:ALA:HB3	1.98	0.44
1:D:240:TYR:OH	1:E:159:LEU:HD22	2.18	0.44
1:E:37:LEU:O	1:E:40:LEU:HB2	2.16	0.44
1:F:235:PRO:HD2	1:F:238:GLN:OE1	2.17	0.44
1:A:21:ILE:CD1	1:A:44:LEU:HD13	2.42	0.44
1:C:99:TRP:CD2	1:C:146:VAL:HG21	2.53	0.44
1:D:113:MET:O	1:D:117:VAL:HG23	2.17	0.44
1:E:34:GLN:HB2	1:E:52:GLN:NE2	2.32	0.44
1:A:81:ASN:O	2:A:301:NAP:H4D	2.18	0.44
1:D:26:LYS:HE3	1:D:72:TRP:CH2	2.52	0.44
1:E:9:THR:HB	1:E:36:ARG:CB	2.48	0.44
1:E:22:GLN:HE21	1:E:23:GLN:NE2	2.16	0.44
1:D:28:ILE:CD1	1:D:75:ILE:HD11	2.48	0.44
1:D:229:ASN:HD21	1:E:234:MET:CG	2.31	0.44
1:C:91:ALA:O	1:D:115:ARG:HD3	2.18	0.44
1:D:125:ASN:O	1:D:169:ALA:HB3	2.17	0.44
1:D:212:VAL:O	1:D:216:VAL:HG23	2.18	0.44
1:A:70:ALA:HA	1:A:73:CYS:SG	2.58	0.44
1:D:70:ALA:HA	1:D:73:CYS:SG	2.58	0.44
1:E:1:MET:HE3	1:E:20:PHE:CE1	2.53	0.44
1:D:133:GLY:O	2:D:304:NAP:H6N	2.18	0.43
1:E:37:LEU:HB3	1:E:50:ILE:CG1	2.49	0.43
1:B:99:TRP:CD2	1:B:146:VAL:HG21	2.53	0.43
1:C:99:TRP:CG	1:C:146:VAL:HG21	2.53	0.43
1:F:16:ILE:HA	1:F:213:SER:HB3	2.00	0.43
1:F:104:ASP:O	1:F:109:GLY:N	2.47	0.43
1:C:21:ILE:HD12	1:C:44:LEU:HD13	2.00	0.43
1:D:8:ALA:HB3	1:D:29:ALA:HB1	2.00	0.43
1:A:47:ASN:O	1:A:72:TRP:HH2	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LEU:O	1:B:69:PRO:O	2.36	0.43
1:C:38:GLN:O	1:C:41:LYS:HB3	2.19	0.43
1:C:155:ARG:NH1	4:C:1200:HOH:O	2.49	0.43
1:F:197:ALA:O	1:F:200:THR:HB	2.18	0.43
1:D:241:ALA:HA	1:F:244:ASN:HD21	1.84	0.43
1:E:31:GLY:O	1:E:52:GLN:HA	2.19	0.43
1:C:37:LEU:HB3	1:C:50:ILE:HB	2.01	0.43
1:C:234:MET:HE3	1:F:229:ASN:HD21	1.84	0.43
1:E:201:TYR:O	1:E:204:THR:HG22	2.19	0.43
1:A:207:LEU:HG	1:A:235:PRO:HD3	2.01	0.43
1:D:26:LYS:HB3	1:D:72:TRP:CZ3	2.54	0.43
1:F:120:GLY:C	1:F:124:ARG:HH21	2.21	0.43
1:D:228:ILE:HG13	1:E:232:GLU:O	2.18	0.42
1:D:229:ASN:HD21	1:E:234:MET:CE	2.32	0.42
1:E:171:ARG:HH22	1:E:222:LEU:C	2.22	0.42
1:B:84:LEU:N	1:B:84:LEU:HD23	2.34	0.42
1:C:77:ILE:CD1	1:C:220:SER:HB2	2.48	0.42
1:C:96:VAL:CG2	1:D:115:ARG:HG2	2.50	0.42
1:D:28:ILE:HD12	1:D:75:ILE:HD11	2.00	0.42
1:E:35:GLU:CD	1:E:35:GLU:N	2.72	0.42
1:E:178:GLY:O	2:E:305:NAP:H4N	2.19	0.42
1:F:31:GLY:O	1:F:52:GLN:HA	2.19	0.42
1:D:75:ILE:N	1:D:124:ARG:HH22	2.16	0.42
1:D:121:MET:N	1:D:124:ARG:HH11	2.17	0.42
1:E:114:THR:O	1:E:118:LEU:HB2	2.20	0.42
1:F:49:TYR:HB2	1:F:72:TRP:CZ2	2.53	0.42
1:B:144:GLY:O	1:B:145:ASN:C	2.58	0.42
1:C:184:GLU:O	1:C:188:VAL:HG23	2.20	0.42
1:D:150:THR:O	1:D:154:VAL:HG23	2.20	0.42
1:E:21:ILE:HD11	1:E:48:LEU:HD13	2.01	0.42
1:E:144:GLY:O	1:E:145:ASN:C	2.58	0.42
1:E:228:ILE:O	1:E:228:ILE:HG23	2.20	0.42
1:F:78:LEU:HD22	1:F:117:VAL:CG2	2.49	0.42
1:A:184:GLU:O	1:A:187:ASN:HB2	2.20	0.42
1:B:157:PHE:O	1:B:161:LEU:HG	2.20	0.42
1:D:85:ALA:HB2	1:D:147:TYR:CE1	2.54	0.42
1:A:146:VAL:O	1:A:150:THR:HG23	2.20	0.42
1:B:26:LYS:HE3	1:B:72:TRP:CZ2	2.55	0.42
1:C:229:ASN:HD22	1:F:232:GLU:HG2	1.84	0.42
1:C:239:SER:OG	1:F:166:HIS:HD2	2.01	0.42
1:E:85:ALA:O	1:E:189:ARG:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ILE:HG12	1:A:128:HIS:HB3	2.02	0.42
1:A:92:HIS:ND1	1:B:122:VAL:HG21	2.35	0.42
1:C:106:ASN:C	1:C:107:ASN:HD22	2.23	0.42
1:E:12:PHE:N	1:E:12:PHE:CD1	2.86	0.42
1:E:89:GLU:OE1	1:E:94:ALA:HA	2.19	0.42
1:A:7:GLY:O	1:A:13:GLY:HA3	2.19	0.42
1:A:78:LEU:HD22	1:A:117:VAL:CG2	2.50	0.42
1:A:150:THR:O	1:A:154:VAL:HG23	2.21	0.41
1:D:18:ARG:NH1	1:D:43:GLU:OE1	2.47	0.41
1:F:23:GLN:HG3	1:F:217:TRP:CH2	2.55	0.41
1:B:9:THR:O	1:B:10:ALA:HB2	2.19	0.41
1:D:2:ILE:HD12	1:D:74:ASN:O	2.20	0.41
1:D:150:THR:O	1:D:153:PHE:HB3	2.20	0.41
1:C:160:ASN:HB3	1:D:145:ASN:HA	2.03	0.41
1:E:165:LEU:HD13	1:E:170:VAL:HB	2.02	0.41
1:F:74:ASN:HA	1:F:124:ARG:NH1	2.34	0.41
1:A:26:LYS:HB3	1:A:72:TRP:CH2	2.55	0.41
1:F:33:ARG:NE	1:F:36:ARG:NH2	2.68	0.41
1:A:192:GLY:O	1:A:194:ASP:N	2.54	0.41
1:C:22:GLN:NE2	1:C:23:GLN:HE21	2.17	0.41
1:C:76:ASP:C	1:C:77:ILE:HG13	2.41	0.41
1:C:146:VAL:O	1:C:150:THR:HG23	2.20	0.41
1:E:218:TRP:O	1:E:222:LEU:HG	2.19	0.41
1:F:75:ILE:H	1:F:124:ARG:HH12	1.64	0.41
1:A:70:ALA:HB1	4:A:1115:HOH:O	2.18	0.41
1:E:118:LEU:N	1:E:119:PRO:CD	2.83	0.41
1:F:19:ARG:HH12	1:F:23:GLN:CG	2.33	0.41
1:D:84:LEU:HD12	1:D:188:VAL:HG11	2.02	0.41
1:E:177:PRO:HA	1:E:233:MET:O	2.21	0.41
1:E:184:GLU:O	1:E:188:VAL:HG23	2.21	0.41
2:E:305:NAP:H52A	4:E:1271:HOH:O	2.21	0.41
1:A:56:ARG:HG2	1:A:104:ASP:HB3	2.03	0.41
1:C:125:ASN:O	1:C:169:ALA:HB3	2.21	0.41
1:C:134:SER:HB3	1:C:151:LYS:HG3	2.03	0.41
4:C:1135:HOH:O	1:D:148:GLY:HA3	2.19	0.41
1:D:41:LYS:HB2	1:D:50:ILE:HD11	2.03	0.41
1:D:168:THR:HG23	1:D:169:ALA:N	2.35	0.41
1:B:84:LEU:HD23	1:B:84:LEU:H	1.86	0.40
1:D:166:HIS:HD2	1:E:239:SER:OG	2.04	0.40
1:F:171:ARG:HB3	1:F:227:ASN:ND2	2.37	0.40
2:A:301:NAP:H8A	4:A:1157:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:GLU:H	1:E:89:GLU:CD	2.25	0.40
1:B:36:ARG:NH1	1:B:184:GLU:OE2	2.53	0.40
1:C:118:LEU:N	1:C:119:PRO:HD2	2.36	0.40
1:B:71:GLU:O	1:B:71:GLU:HG2	2.21	0.40
1:D:37:LEU:HB3	1:D:50:ILE:HG23	2.03	0.40
1:B:183:THR:HB	2:B:302:NAP:O2A	2.21	0.40
1:F:73:CYS:O	1:F:75:ILE:HG13	2.22	0.40
1:F:121:MET:O	1:F:125:ASN:N	2.54	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	246/248 (99%)	222 (90%)	21 (8%)	3 (1%)	13	32
1	B	246/248 (99%)	230 (94%)	13 (5%)	3 (1%)	13	32
1	C	246/248 (99%)	229 (93%)	15 (6%)	2 (1%)	19	43
1	D	246/248 (99%)	226 (92%)	18 (7%)	2 (1%)	19	43
1	E	246/248 (99%)	229 (93%)	15 (6%)	2 (1%)	19	43
1	F	246/248 (99%)	222 (90%)	20 (8%)	4 (2%)	9	24
All	All	1476/1488 (99%)	1358 (92%)	102 (7%)	16 (1%)	14	34

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	B	145	ASN
1	C	145	ASN
1	C	193	ASP

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Mol	Chain	Res	Type
1	D	145	ASN
1	E	145	ASN
1	F	145	ASN
1	D	193	ASP
1	A	69	PRO
1	B	69	PRO
1	B	191	LYS
1	E	193	ASP
1	F	69	PRO
1	A	125	ASN
1	F	88	MET
1	F	204	THR

5.3.2　Protein sidechains ⓘ

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	196/202 (97%)	195 (100%)	1 (0%)	88	96
1	B	201/202 (100%)	200 (100%)	1 (0%)	88	96
1	C	198/202 (98%)	197 (100%)	1 (0%)	88	96
1	D	200/202 (99%)	199 (100%)	1 (0%)	88	96
1	E	196/202 (97%)	193 (98%)	3 (2%)	65	86
1	F	193/202 (96%)	192 (100%)	1 (0%)	88	96
All	All	1184/1212 (98%)	1176 (99%)	8 (1%)	84	94

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	B	19	ARG
1	C	84	LEU
1	D	168	THR
1	E	168	THR
1	E	172	VAL

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Mol	Chain	Res	Type
1	E	210	GLU
1	F	145	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	126	HIS
1	A	166	HIS
1	A	187	ASN
1	B	38	GLN
1	B	80	ASN
1	B	107	ASN
1	B	131	ASN
1	B	156	GLN
1	C	23	GLN
1	C	187	ASN
1	C	227	ASN
1	C	229	ASN
1	C	244	ASN
1	D	22	GLN
1	D	107	ASN
1	D	131	ASN
1	D	166	HIS
1	D	187	ASN
1	D	229	ASN
1	E	23	GLN
1	E	47	ASN
1	E	52	GLN
1	E	107	ASN
1	E	166	HIS
1	E	187	ASN
1	E	246	HIS
1	F	80	ASN
1	F	107	ASN
1	F	131	ASN
1	F	166	HIS
1	F	187	ASN
1	F	227	ASN
1	F	229	ASN
1	F	246	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	PO4	D	314	-	4,4,4	1.60	0	6,6,6	0.43	0
2	NAP	A	301	-	45,52,52	2.17	8 (17%)	56,80,80	1.28	1 (1%)
3	PO4	F	316	-	4,4,4	1.60	0	6,6,6	0.44	0
3	PO4	E	315	-	4,4,4	1.63	0	6,6,6	0.44	0
2	NAP	E	305	-	45,52,52	2.14	7 (15%)	56,80,80	1.25	1 (1%)
2	NAP	C	303	-	45,52,52	2.21	9 (20%)	56,80,80	1.31	2 (3%)
2	NAP	B	302	-	45,52,52	2.25	10 (22%)	56,80,80	1.28	2 (3%)
3	PO4	C	313	-	4,4,4	1.57	0	6,6,6	0.43	0
2	NAP	F	306	-	45,52,52	2.21	8 (17%)	56,80,80	1.34	3 (5%)
2	NAP	D	304	-	45,52,52	2.13	8 (17%)	56,80,80	1.34	1 (1%)
3	PO4	B	312	-	4,4,4	1.60	0	6,6,6	0.45	0
3	PO4	A	311	-	4,4,4	1.58	0	6,6,6	0.44	0

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	NAP	A	301	-	-	10/31/67/67	0/5/5/5
2	NAP	E	305	-	-	12/31/67/67	0/5/5/5
2	NAP	C	303	-	-	12/31/67/67	0/5/5/5
2	NAP	B	302	-	-	12/31/67/67	0/5/5/5
2	NAP	F	306	-	-	12/31/67/67	0/5/5/5
2	NAP	D	304	-	-	12/31/67/67	0/5/5/5

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	NAP	O7N-C7N	9.00	1.41	1.24
2	F	306	NAP	O7N-C7N	8.79	1.41	1.24
2	E	305	NAP	O7N-C7N	8.72	1.40	1.24
2	B	302	NAP	O7N-C7N	8.69	1.40	1.24
2	D	304	NAP	O7N-C7N	8.59	1.40	1.24
2	C	303	NAP	O7N-C7N	8.24	1.39	1.24
2	C	303	NAP	C2N-N1N	6.56	1.43	1.35
2	B	302	NAP	C2N-N1N	6.55	1.42	1.35
2	F	306	NAP	C2N-N1N	6.53	1.42	1.35
2	D	304	NAP	C2N-N1N	5.76	1.42	1.35
2	A	301	NAP	C2N-N1N	5.54	1.41	1.35
2	E	305	NAP	C2A-N3A	5.50	1.41	1.32
2	C	303	NAP	C2A-N3A	5.39	1.40	1.32
2	E	305	NAP	C2N-N1N	5.38	1.41	1.35
2	B	302	NAP	C2A-N3A	5.25	1.40	1.32
2	D	304	NAP	C2A-N3A	5.24	1.40	1.32
2	F	306	NAP	C2A-N3A	5.17	1.40	1.32
2	A	301	NAP	C2A-N3A	5.07	1.40	1.32
2	B	302	NAP	C2A-N1A	4.23	1.41	1.33
2	A	301	NAP	C2A-N1A	4.21	1.41	1.33
2	E	305	NAP	C2A-N1A	4.17	1.41	1.33
2	C	303	NAP	C2A-N1A	4.16	1.41	1.33
2	D	304	NAP	C2A-N1A	3.98	1.41	1.33
2	F	306	NAP	C2A-N1A	3.87	1.41	1.33
2	F	306	NAP	C2N-C3N	3.10	1.43	1.39
2	A	301	NAP	C4A-N3A	3.04	1.39	1.35
2	C	303	NAP	C2N-C3N	2.96	1.43	1.39
2	D	304	NAP	C4A-N3A	2.95	1.39	1.35
2	E	305	NAP	C4A-N3A	2.92	1.39	1.35
2	F	306	NAP	C4A-N3A	2.80	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	304	NAP	C2N-C3N	2.76	1.43	1.39
2	B	302	NAP	C2N-C3N	2.69	1.43	1.39
2	B	302	NAP	C4N-C3N	2.62	1.43	1.39
2	C	303	NAP	C4N-C3N	2.60	1.43	1.39
2	E	305	NAP	C4N-C3N	2.56	1.43	1.39
2	C	303	NAP	C4A-N3A	2.55	1.39	1.35
2	F	306	NAP	C4N-C3N	2.54	1.43	1.39
2	C	303	NAP	C6N-N1N	2.54	1.41	1.35
2	E	305	NAP	C6N-N1N	2.52	1.41	1.35
2	F	306	NAP	C6N-N1N	2.51	1.41	1.35
2	A	301	NAP	C2N-C3N	2.35	1.42	1.39
2	B	302	NAP	C4A-N3A	2.34	1.38	1.35
2	A	301	NAP	C6N-N1N	2.34	1.41	1.35
2	B	302	NAP	C6N-N1N	2.31	1.41	1.35
2	B	302	NAP	C2D-C1D	-2.19	1.50	1.53
2	D	304	NAP	C6N-N1N	2.16	1.40	1.35
2	B	302	NAP	C5N-C4N	2.08	1.43	1.38
2	C	303	NAP	C5N-C4N	2.03	1.43	1.38
2	A	301	NAP	C4N-C3N	2.02	1.42	1.39
2	D	304	NAP	C4N-C3N	2.01	1.42	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	304	NAP	N3A-C2A-N1A	-6.78	118.08	128.68
2	A	301	NAP	N3A-C2A-N1A	-6.65	118.28	128.68
2	E	305	NAP	N3A-C2A-N1A	-6.61	118.34	128.68
2	C	303	NAP	N3A-C2A-N1A	-6.57	118.41	128.68
2	F	306	NAP	N3A-C2A-N1A	-6.54	118.45	128.68
2	B	302	NAP	N3A-C2A-N1A	-6.41	118.66	128.68
2	F	306	NAP	C1B-N9A-C4A	-2.37	122.48	126.64
2	F	306	NAP	O5B-C5B-C4B	2.30	116.92	108.99
2	C	303	NAP	C1B-N9A-C4A	-2.27	122.66	126.64
2	B	302	NAP	O5B-C5B-C4B	2.08	116.14	108.99

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	NAP	C5B-O5B-PA-O1A
2	A	301	NAP	C5B-O5B-PA-O2A
2	A	301	NAP	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
2	A	301	NAP	O4B-C4B-C5B-O5B
2	A	301	NAP	C2B-O2B-P2B-O1X
2	B	302	NAP	C5B-O5B-PA-O1A
2	B	302	NAP	C5B-O5B-PA-O2A
2	B	302	NAP	C5B-O5B-PA-O3
2	B	302	NAP	O4B-C4B-C5B-O5B
2	B	302	NAP	C2B-O2B-P2B-O1X
2	B	302	NAP	O4D-C1D-N1N-C2N
2	C	303	NAP	C5B-O5B-PA-O1A
2	C	303	NAP	C5B-O5B-PA-O2A
2	C	303	NAP	C5B-O5B-PA-O3
2	C	303	NAP	O4B-C4B-C5B-O5B
2	C	303	NAP	C2B-O2B-P2B-O1X
2	C	303	NAP	O4D-C1D-N1N-C2N
2	D	304	NAP	C5B-O5B-PA-O1A
2	D	304	NAP	C5B-O5B-PA-O2A
2	D	304	NAP	C5B-O5B-PA-O3
2	D	304	NAP	O4B-C4B-C5B-O5B
2	D	304	NAP	C2B-O2B-P2B-O1X
2	D	304	NAP	O4D-C1D-N1N-C2N
2	E	305	NAP	C5B-O5B-PA-O1A
2	E	305	NAP	C5B-O5B-PA-O2A
2	E	305	NAP	C5B-O5B-PA-O3
2	E	305	NAP	O4B-C4B-C5B-O5B
2	E	305	NAP	C2B-O2B-P2B-O1X
2	E	305	NAP	O4D-C1D-N1N-C2N
2	F	306	NAP	C5B-O5B-PA-O1A
2	F	306	NAP	C5B-O5B-PA-O2A
2	F	306	NAP	C5B-O5B-PA-O3
2	F	306	NAP	O4B-C4B-C5B-O5B
2	F	306	NAP	C2B-O2B-P2B-O1X
2	F	306	NAP	O4D-C1D-N1N-C2N
2	A	301	NAP	C3B-C4B-C5B-O5B
2	B	302	NAP	C3B-C4B-C5B-O5B
2	C	303	NAP	C3B-C4B-C5B-O5B
2	D	304	NAP	C3B-C4B-C5B-O5B
2	E	305	NAP	C3B-C4B-C5B-O5B
2	F	306	NAP	C3B-C4B-C5B-O5B
2	B	302	NAP	O4D-C4D-C5D-O5D
2	B	302	NAP	C3D-C4D-C5D-O5D
2	F	306	NAP	O4D-C4D-C5D-O5D
2	C	303	NAP	O4D-C4D-C5D-O5D

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Mol	Chain	Res	Type	Atoms
2	D	304	NAP	O4D-C4D-C5D-O5D
2	B	302	NAP	C2B-O2B-P2B-O3X
2	C	303	NAP	C2B-O2B-P2B-O3X
2	D	304	NAP	C2B-O2B-P2B-O3X
2	E	305	NAP	C2B-O2B-P2B-O3X
2	F	306	NAP	C2B-O2B-P2B-O3X
2	A	301	NAP	O4D-C4D-C5D-O5D
2	A	301	NAP	PN-O3-PA-O2A
2	B	302	NAP	PN-O3-PA-O2A
2	C	303	NAP	PN-O3-PA-O2A
2	D	304	NAP	PN-O3-PA-O2A
2	E	305	NAP	PN-O3-PA-O2A
2	F	306	NAP	PN-O3-PA-O2A
2	E	305	NAP	O4D-C4D-C5D-O5D
2	F	306	NAP	C3D-C4D-C5D-O5D
2	C	303	NAP	C3D-C4D-C5D-O5D
2	A	301	NAP	C3D-C4D-C5D-O5D
2	D	304	NAP	C3D-C4D-C5D-O5D
2	A	301	NAP	PN-O3-PA-O1A
2	B	302	NAP	PN-O3-PA-O1A
2	C	303	NAP	PN-O3-PA-O1A
2	D	304	NAP	PN-O3-PA-O1A
2	E	305	NAP	PN-O3-PA-O1A
2	F	306	NAP	PN-O3-PA-O1A
2	E	305	NAP	C3D-C4D-C5D-O5D

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	NAP	2	0
2	E	305	NAP	3	0
2	C	303	NAP	3	0
2	B	302	NAP	2	0
2	F	306	NAP	2	0
2	D	304	NAP	2	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.
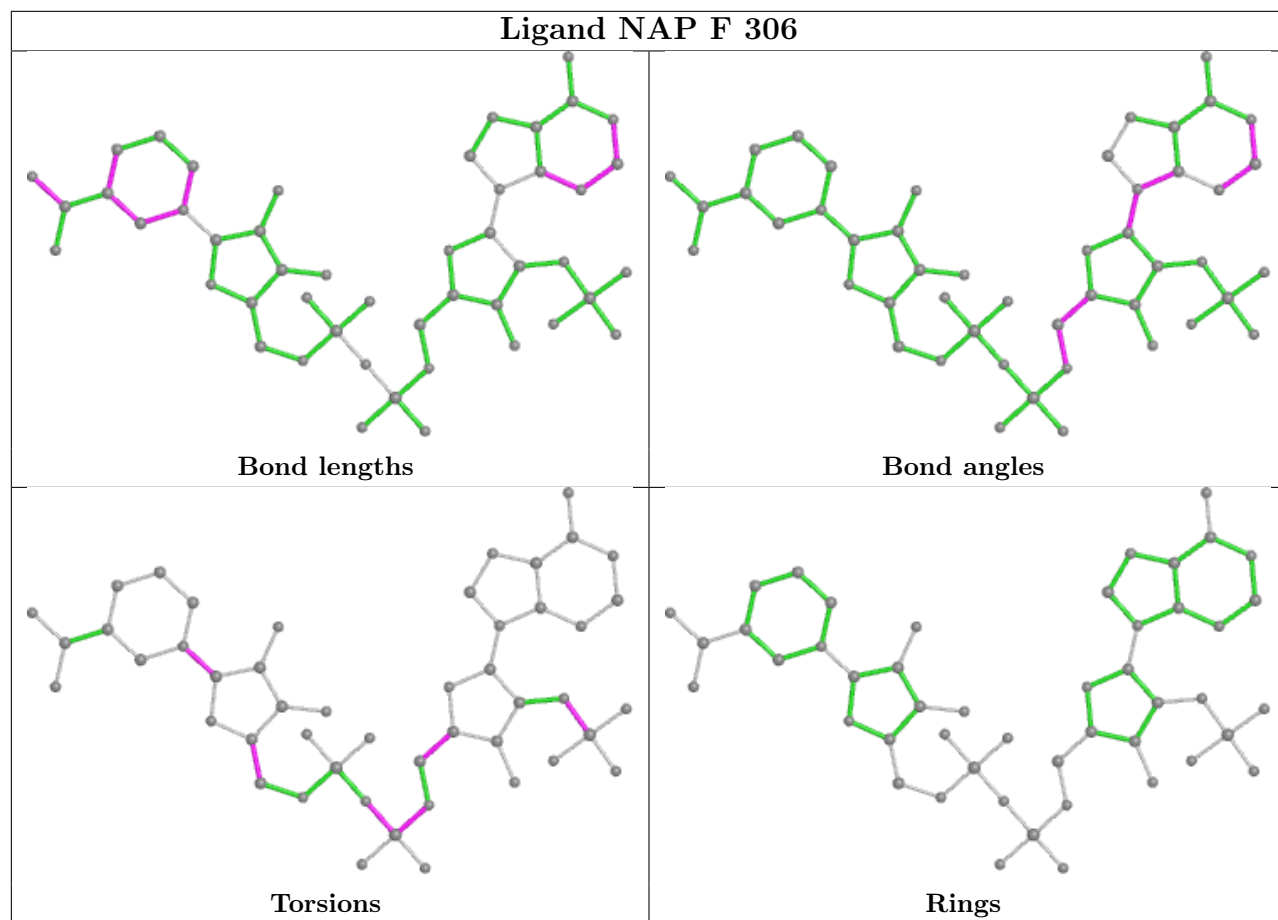
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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 NAP A 301

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP E 305

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP C 303

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP B 302

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP F 306

Bond lengths

Bond angles

Torsions

Rings

Ligand NAP D 304

Bond lengths

Bond angles

Torsions

Rings
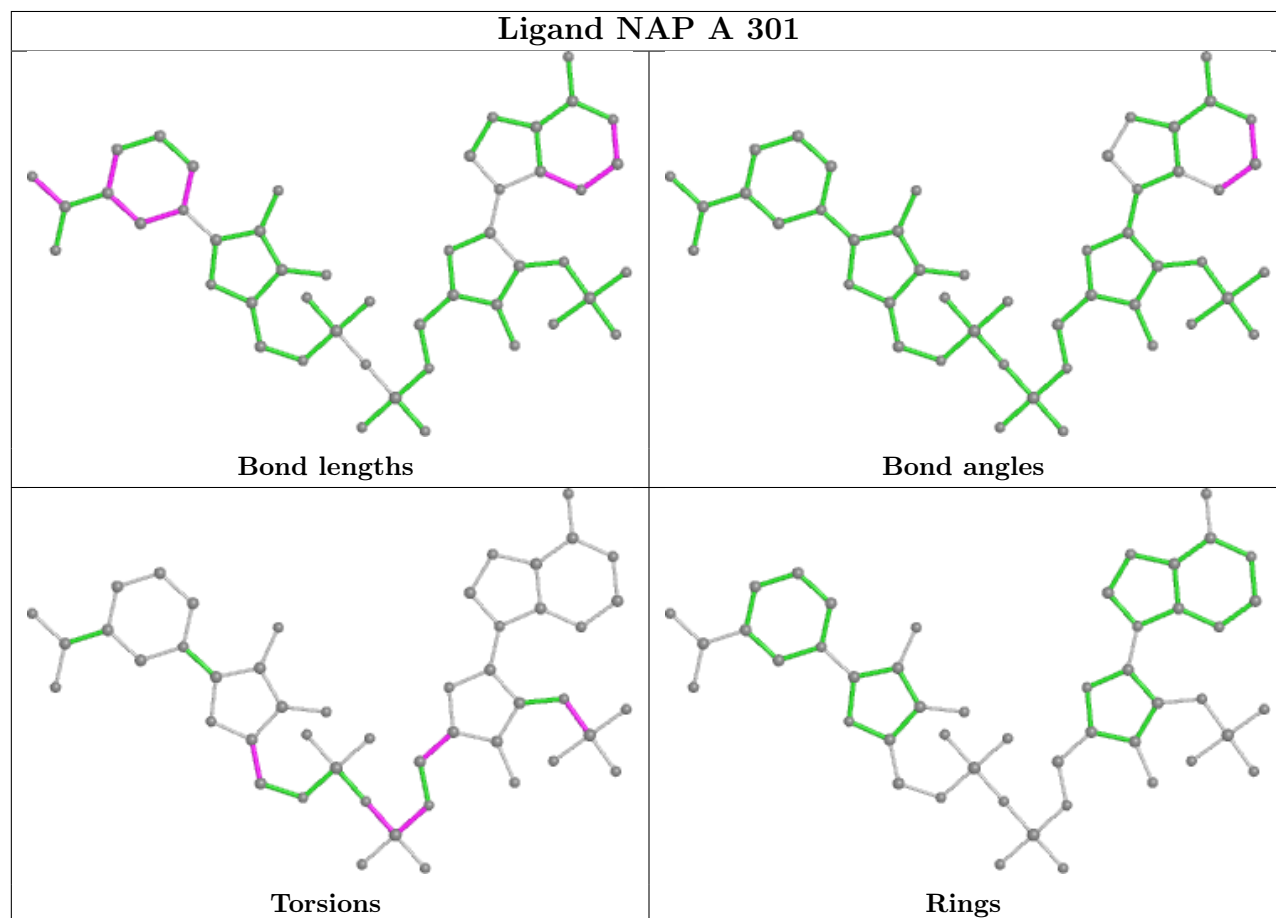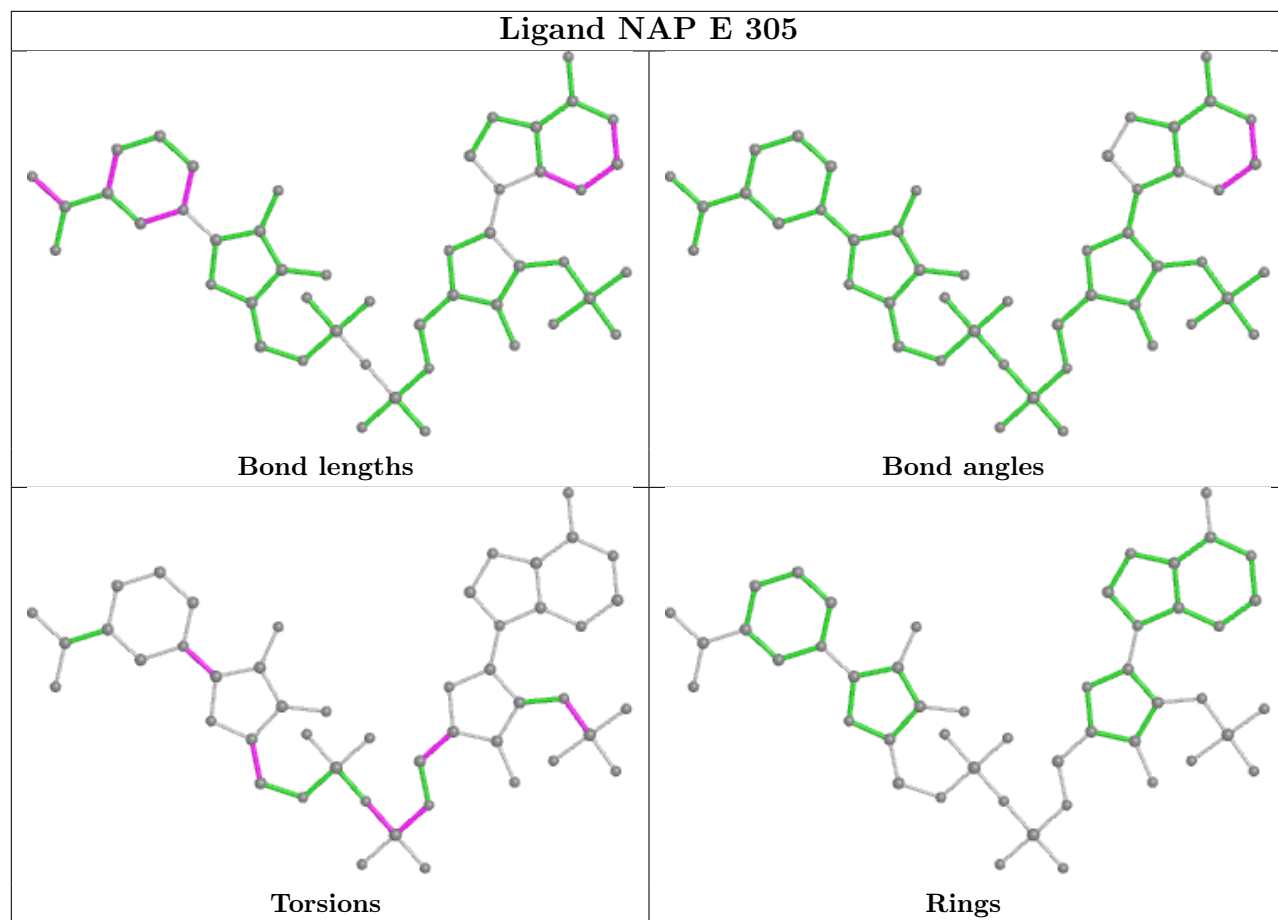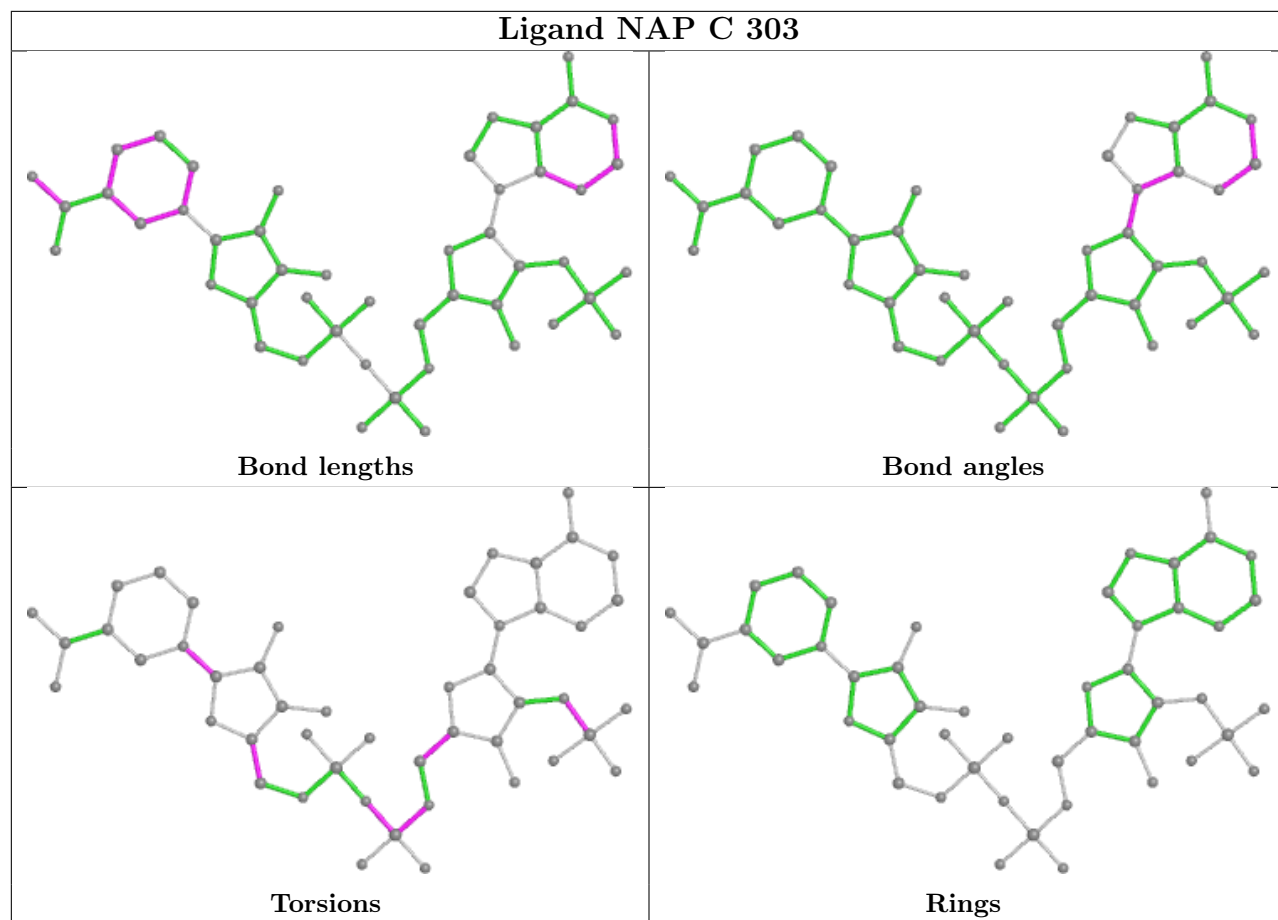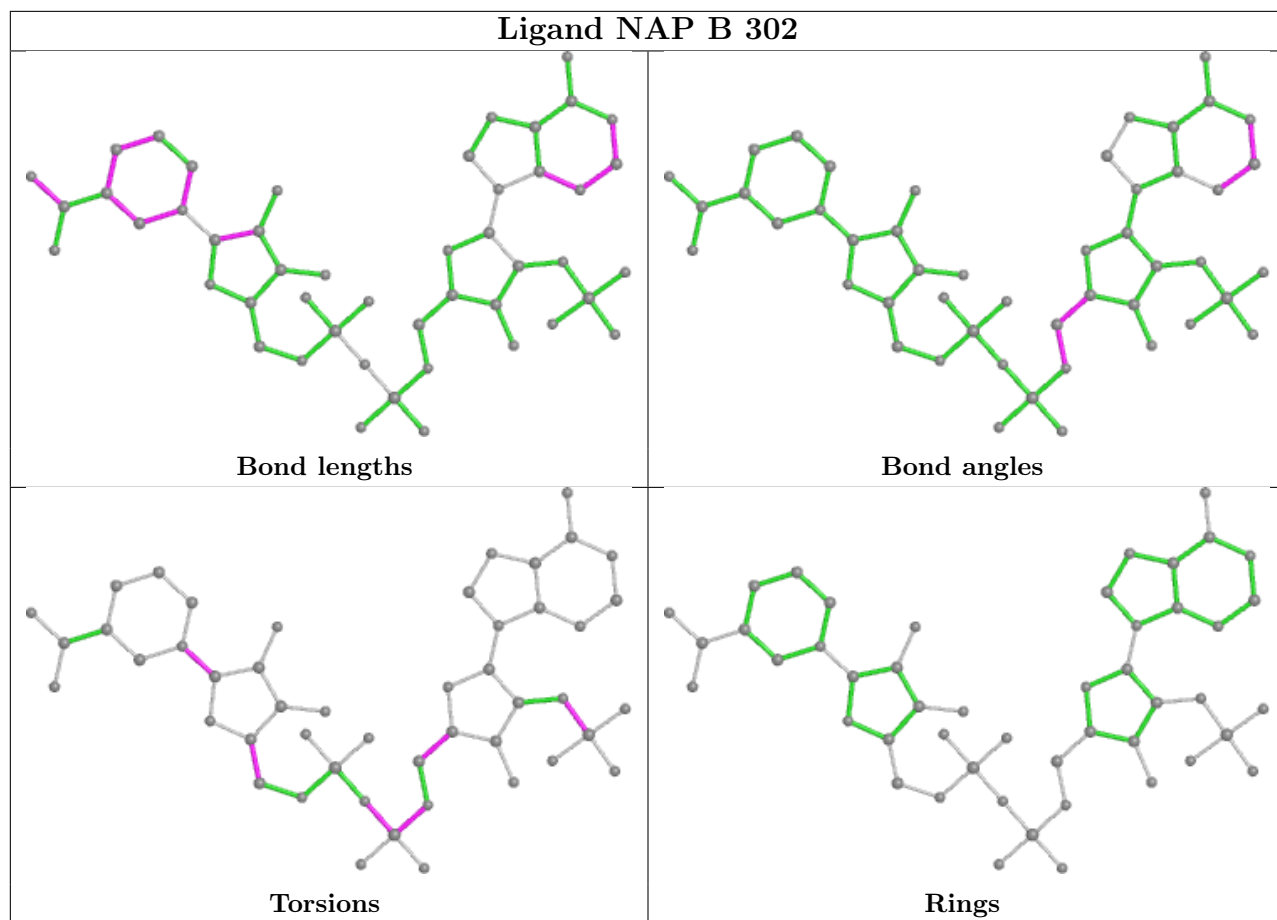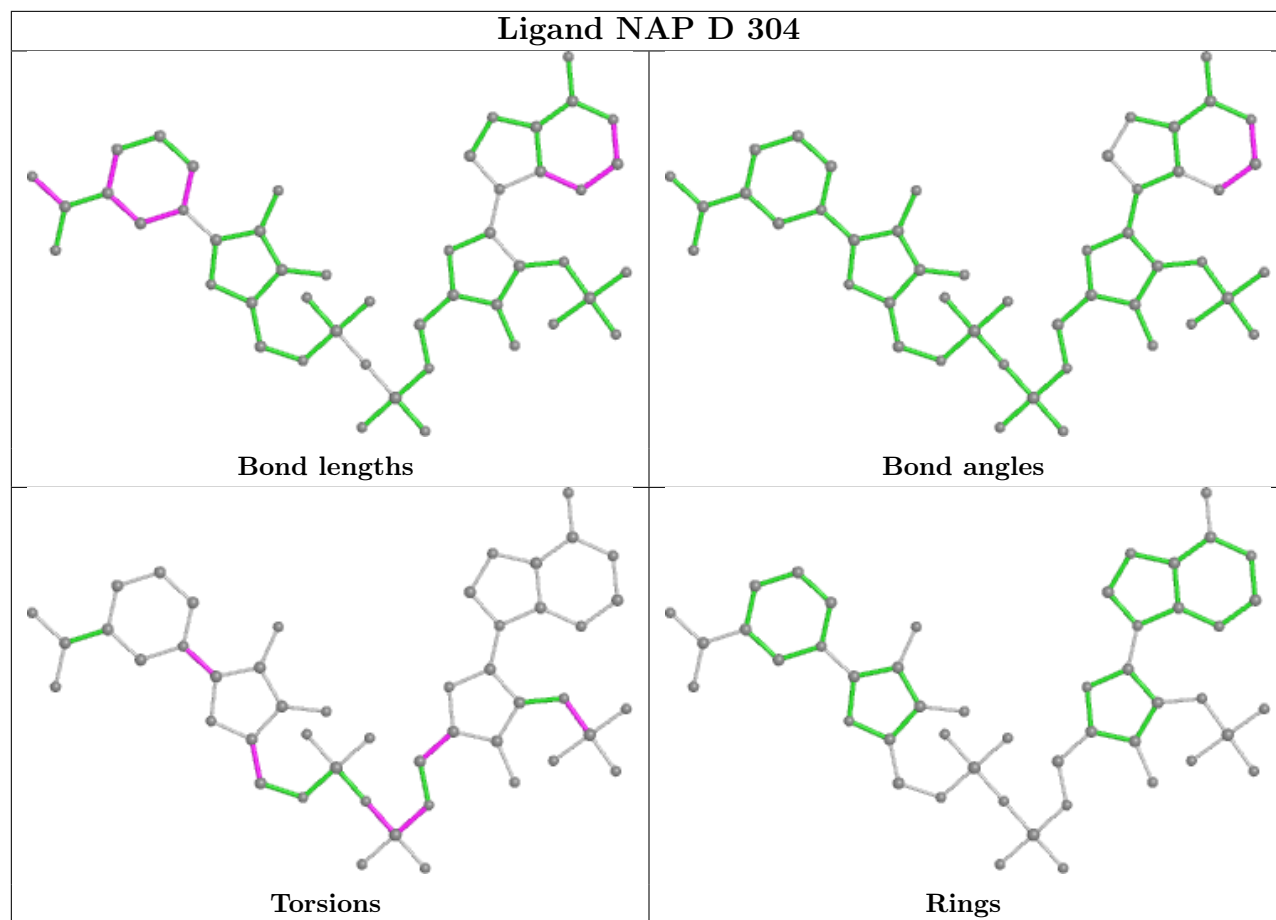
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 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	248/248 (100%)	-0.51	0	100	100	18, 30, 48, 55	0
1	B	248/248 (100%)	-0.53	0	100	100	18, 30, 44, 52	0
1	C	248/248 (100%)	-0.46	0	100	100	20, 32, 46, 55	0
1	D	248/248 (100%)	-0.38	0	100	100	21, 32, 50, 58	0
1	E	248/248 (100%)	-0.36	0	100	100	23, 36, 52, 60	0
1	F	248/248 (100%)	-0.34	0	100	100	26, 36, 53, 61	0
All	All	1488/1488 (100%)	-0.43	0	100	100	18, 32, 50, 61	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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.
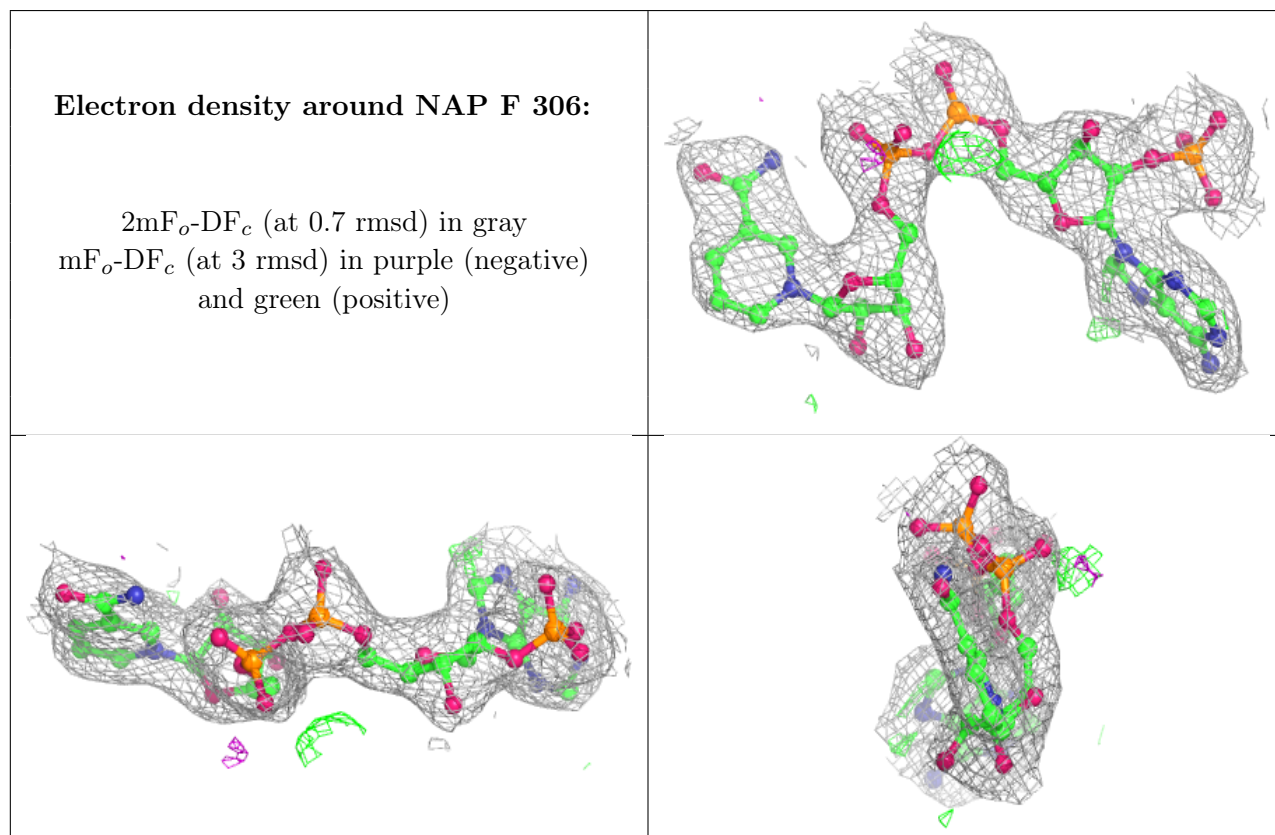
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	E	315	5/5	0.93	0.19	71,71,72,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	PO4	C	313	5/5	0.95	0.19	72,73,73,74	0
3	PO4	B	312	5/5	0.95	0.21	61,62,63,64	0
3	PO4	A	311	5/5	0.97	0.14	43,43,45,45	0
3	PO4	D	314	5/5	0.97	0.14	66,66,67,67	0
2	NAP	F	306	48/48	0.97	0.15	29,40,45,46	0
3	PO4	F	316	5/5	0.97	0.18	60,61,62,62	0
2	NAP	C	303	48/48	0.98	0.13	22,29,36,38	0
2	NAP	D	304	48/48	0.98	0.14	26,32,36,38	0
2	NAP	E	305	48/48	0.98	0.12	31,37,42,43	0
2	NAP	A	301	48/48	0.98	0.12	21,26,33,34	0
2	NAP	B	302	48/48	0.98	0.13	19,28,33,34	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 F 306:

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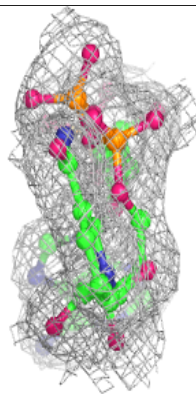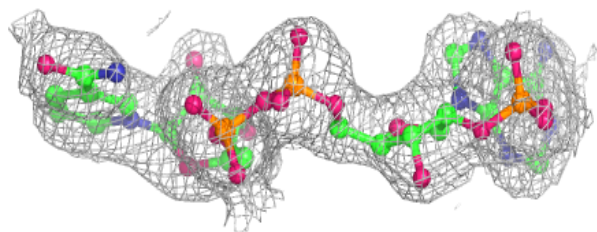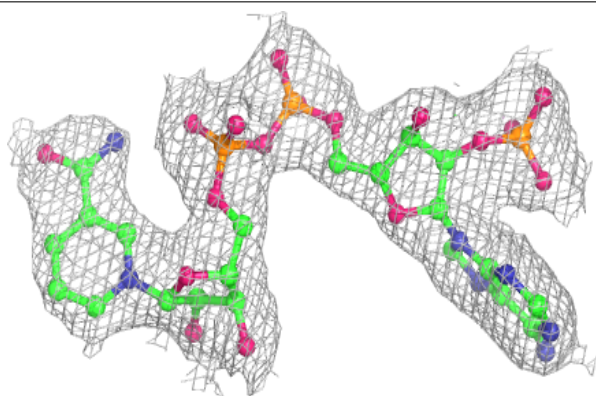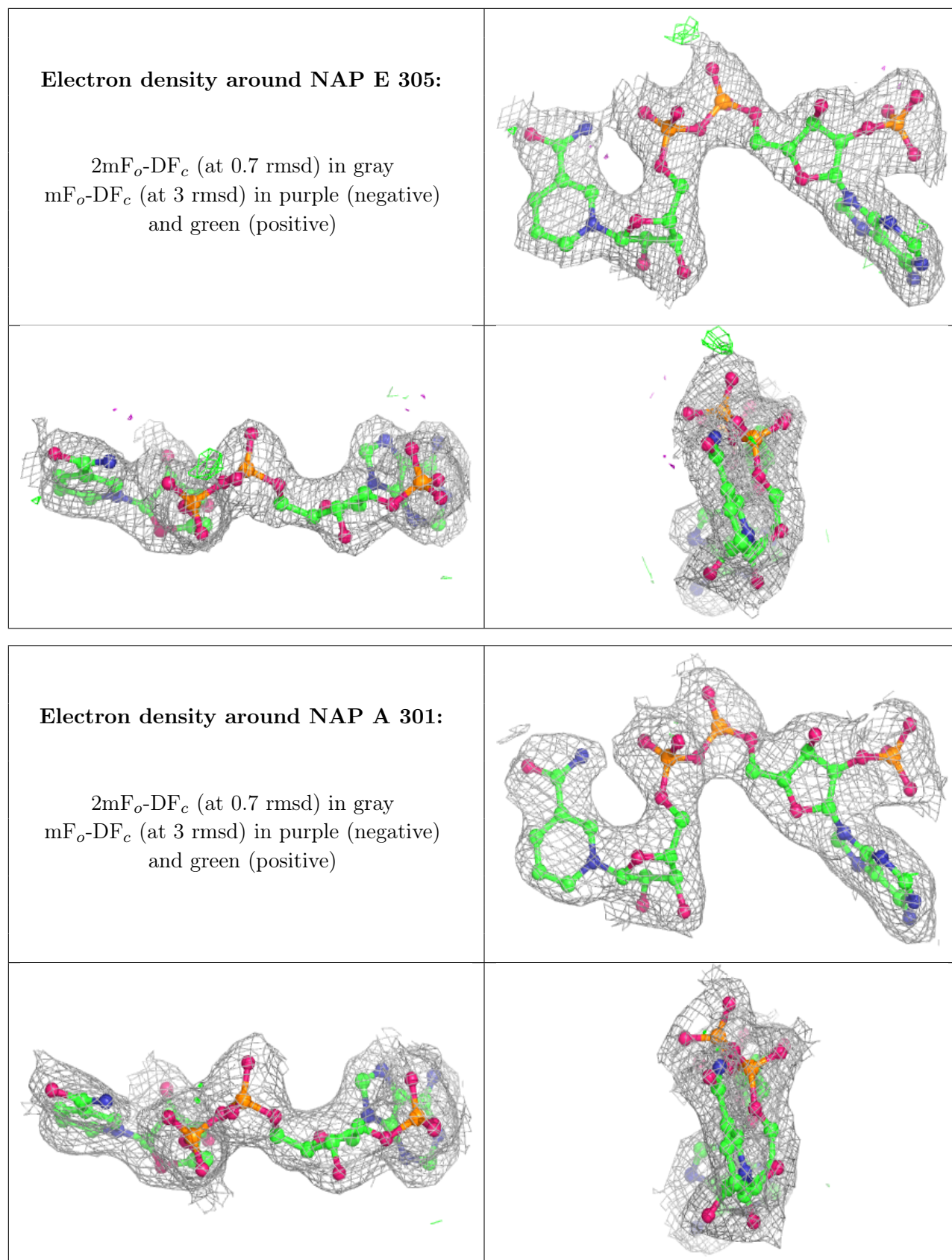mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around NAP C 303:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
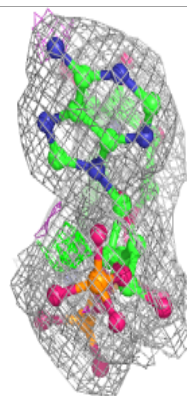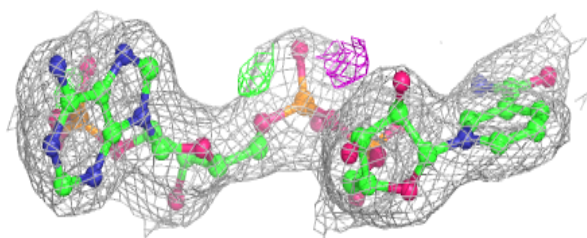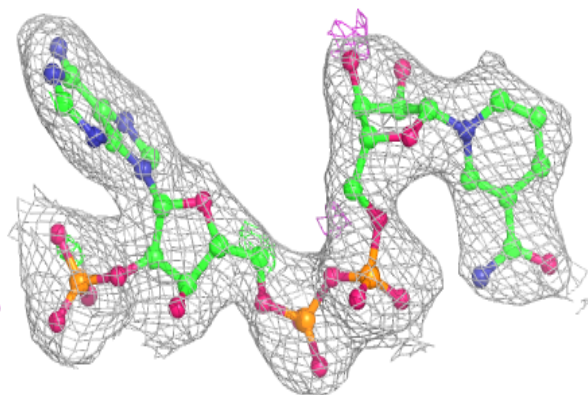
Electron density around NAP D 304:

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

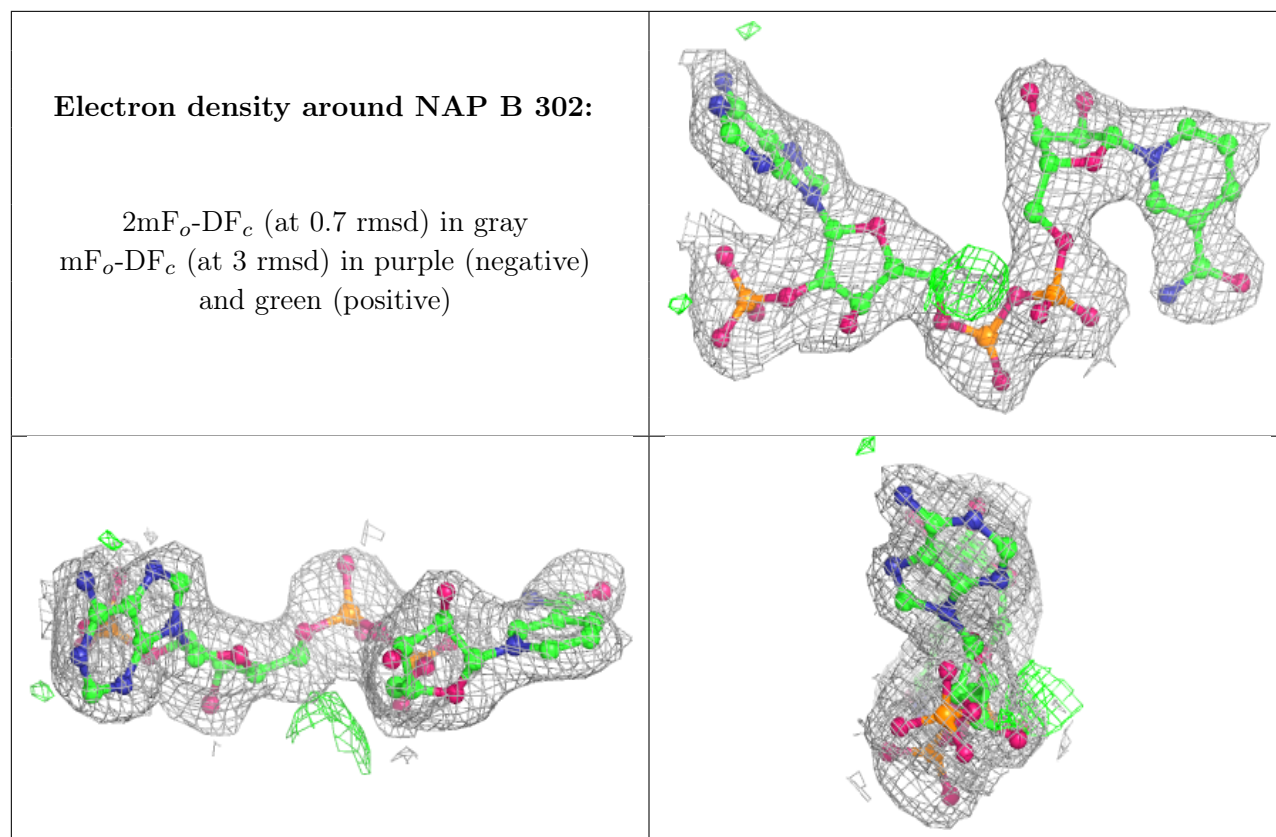**Electron density around NAP E 305:**

$2mF_o$-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 301:

$2mF_o$-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 302:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.