Full wwPDB X-ray Structure Validation Report ⓘ

Aug 14, 2023 – 06:12 PM EDT

PDB ID	:	1R0L
Title	:	1-deoxy-D-xylulose 5-phosphate reductoisomerase from zymomonas mobilis in complex with NADPH
Authors	:	Ricagno, S.; Grolle, S.; Bringer-Meyer, S.; Sahm, H.; Lindqvist, Y.; Schneider, G.
Deposited on	:	2003-09-22
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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

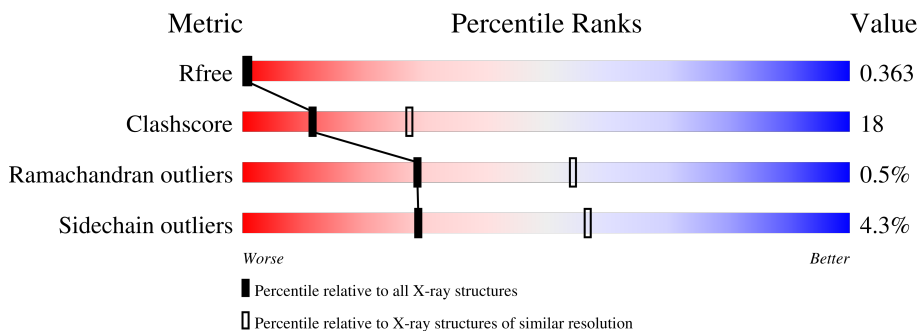|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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		0.363
Clashscore		18
Ramachandran outliers		0.5%
Sidechain outliers		4.3%

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)

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%

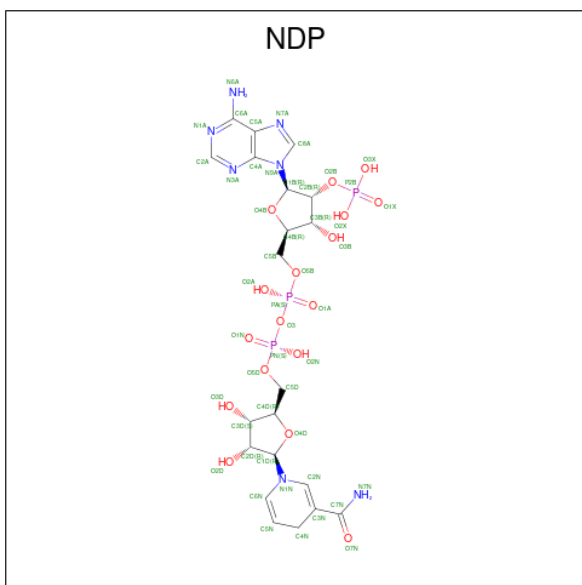| Mol	Chain	Length	Quality of chain
1	A	388	63% 32% • •
1	B	388	66% 30% • •
1	C	388	66% 29% • •
1	D	388	66% 30% • • •

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 11652 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 1-deoxy-D-xylulose 5-phosphate reductoisomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2854	1798	496	544	16			
1	B	379	Total	C	N	O	S	0	0	0
			2867	1807	499	545	16			
1	C	378	Total	C	N	O	S	0	0	0
			2855	1799	495	544	17			
1	D	378	Total	C	N	O	S	0	0	0
			2860	1802	498	544	16			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

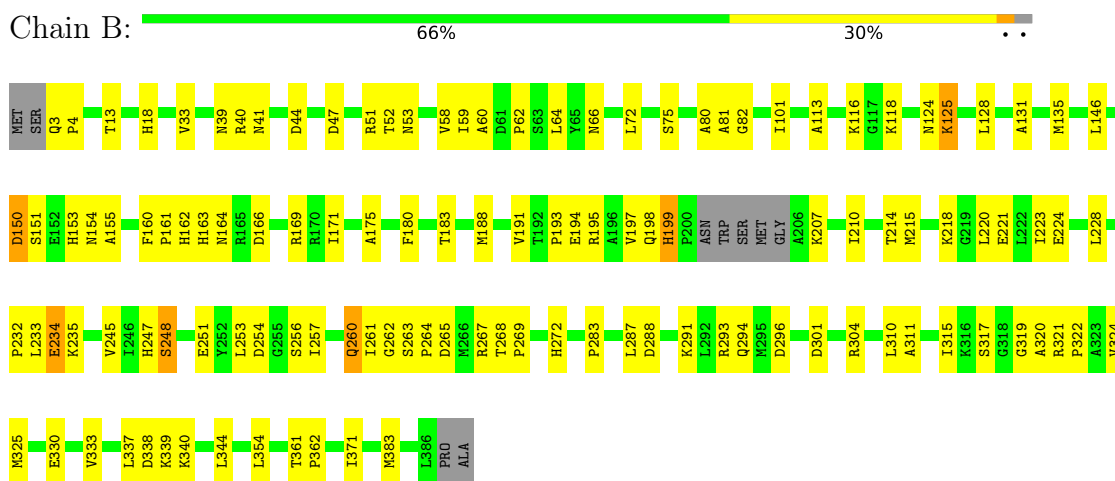| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	36	Total	O	0	0
			36	36		
3	C	22	Total	O	0	0
			22	22		
3	D	20	Total	O	0	0
			20	20		

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. 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. 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.
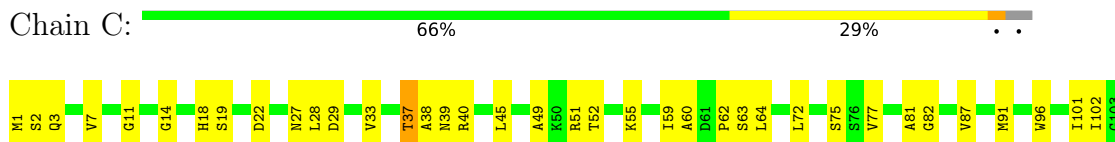
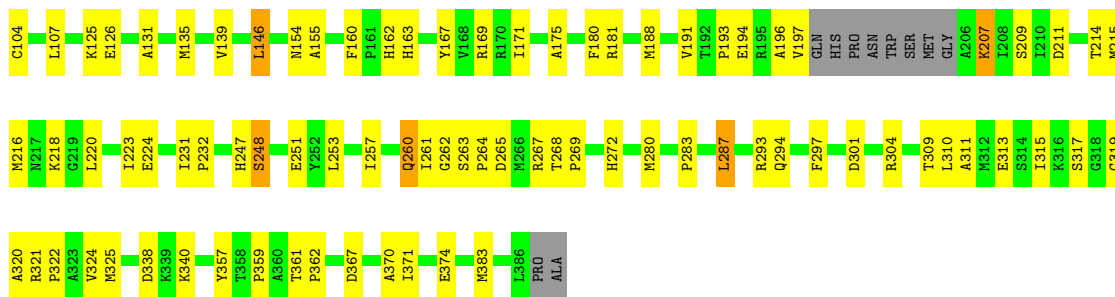- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain A:

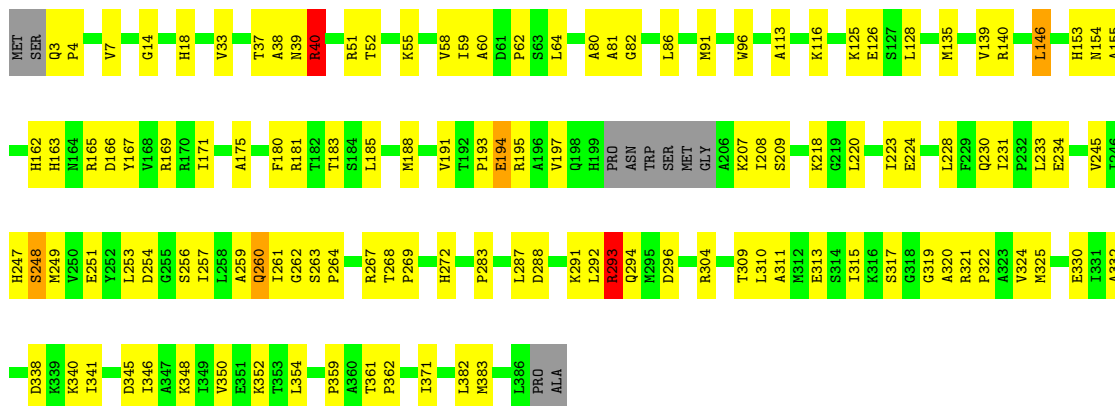- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain B:

- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain C:

C104 L107 K125 E126 A131 M135 V139 L146 N154 A155 F160 P161 H162 H163 Y167 V168 R169 R170 I171 A175 F180 R181 M188 V191 T192 P193 E194 R195 A196 V197 GLN HIS PRO ASN TRP SER MET GLY A206 K207 I208 S209 I210 D211 T214 M215

M216 N217 K218 G219 L220 I223 E224 I231 P232 H247 S248 E251 Y252 L253 I257 Q260 I261 G262 S263 P264 D265 M266 R267 T268 P269 H272 M280 P283 L287 R293 Q294 F297 D301 R304 T309 L310 A311 M312 E313 S314 I315 K316 S317 G318 G319

A320 R321 P322 A323 V324 M325 D338 K339 K340 Y357 T358 P359 A360 T361 P362 D367 A370 I371 E374 M383 L386 PRO ALA

- Molecule 1: 1-deoxy-D-xylulose 5-phosphate reductoisomerase

Chain D:

MET SER Q3 P4 V7 G14 H18 V33 T37 A38 N39 R40 R51 T52 K55 V58 I59 A60 D61 P62 S63 L64 A80 A81 G82 L86 M91 W96 A113 K116 K125 E126 S127 L128 M135 V139 R140 L146 H153 N154 A155

H162 H163 N164 R165 D166 Y167 V168 R169 R170 I171 A175 F180 R181 T182 T183 S184 L185 M188 V191 T192 P193 E194 R195 A196 V197 Q198 H199 PRO ASN TRP SER MET GLY A206 K207 I208 S209 K218 G219 L220 I223 E224 L228 F229 Q230 I231 P232 L233 E234 V245 I246

H247 S248 M249 V250 E251 Y252 L253 D254 G255 S256 I257 L258 A259 Q260 I261 G262 S263 P264 R267 T268 P269 H272 P283 L287 D288 K291 L292 R293 Q294 M295 D296 R304 T309 L310 A311 M312 E313 S314 I315 K316 S317 G318 G319 A320 R321 P322 A323 V324 M325 E330 I331 A332

D338 K339 K340 I341 D345 I346 A347 K348 I349 V350 E351 K352 T353 L354 P359 A360 T361 P362 I371 L382 M383 L386 PRO ALA

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.70Å 93.20Å 98.60Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	29.63 – 2.70 29.63 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.63-2.70) 98.3 (29.63-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.68Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.269 0.361 , 0.363	Depositor DCC
R_{free} test set	493 reflections (1.13%)	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 40.1	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	11652	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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 53.88 % 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 3.9583e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

---

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.45	0/2901	0.65	0/3933
1	B	0.46	1/2916 (0.0%)	0.73	2/3955 (0.1%)
1	C	0.41	0/2902	0.62	0/3934
1	D	0.41	0/2908	0.64	2/3943 (0.1%)
All	All	0.43	1/11627 (0.0%)	0.66	4/15765 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	HIS	C-O	-5.95	1.12	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	HIS	C-N-CD	-17.40	82.32	120.60
1	B	199	HIS	C-N-CA	6.81	150.59	122.00
1	D	40	ARG	NE-CZ-NH1	-5.19	117.70	120.30
1	D	126	GLU	CA-CB-CG	-5.09	102.19	113.40

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	2854	0	2891	113	0
1	B	2867	0	2902	98	14
1	C	2855	0	2897	103	15
1	D	2860	0	2895	101	0
2	A	27	0	11	1	0
2	B	27	0	11	3	0
2	C	27	0	11	1	0
2	D	27	0	11	3	0
3	A	30	0	0	3	0
3	B	36	0	0	6	1
3	C	22	0	0	4	0
3	D	20	0	0	2	0
All	All	11652	0	11629	407	15

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 18.

All (407) 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:C:125:LYS:HB2	1:C:224:GLU:OE2	1.50	1.11
1:D:40:ARG:HG2	1:D:64:LEU:HD11	1.48	0.95
1:C:126:GLU:HA	1:C:126:GLU:OE1	1.74	0.87
1:A:3:GLN:HB3	1:A:4:PRO:HD3	1.59	0.84
1:A:247:HIS:HD2	1:A:260:GLN:HE22	1.25	0.82
1:C:207:LYS:HE2	1:C:211:ASP:OD2	1.81	0.80
1:B:47:ASP:CG	1:B:51:ARG:HH22	1.85	0.80
1:D:220:LEU:O	1:D:224:GLU:HG3	1.81	0.79
1:C:251:GLU:HG3	1:C:257:ILE:HG12	1.63	0.79
1:C:294:GLN:NE2	1:D:294:GLN:HE22	1.80	0.79
1:A:125:LYS:HG3	1:A:126:GLU:N	1.95	0.79
1:B:154:ASN:HD21	1:B:272:HIS:CD2	2.03	0.77
1:A:124:ASN:ND2	1:A:126:GLU:HB2	2.01	0.76
1:B:51:ARG:HH21	1:B:51:ARG:HG3	1.49	0.76
1:D:154:ASN:HD21	1:D:272:HIS:CD2	2.04	0.76
1:A:124:ASN:HD21	1:A:126:GLU:HB2	1.51	0.75
1:C:220:LEU:O	1:C:224:GLU:HG3	1.87	0.75
1:B:154:ASN:HD21	1:B:272:HIS:HD2	1.37	0.73
1:A:247:HIS:CD2	1:A:260:GLN:HE22	2.05	0.73
1:B:267:ARG:CZ	1:B:283:PRO:HG2	2.19	0.73
1:C:125:LYS:CB	1:C:224:GLU:OE2	2.36	0.72
1:D:125:LYS:HB3	1:D:224:GLU:OE2	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:O	1:A:25:GLU:HG3	1.90	0.72
1:A:374:GLU:O	1:A:377:ILE:HG12	1.89	0.71
1:D:3:GLN:N	1:D:4:PRO:HD3	2.05	0.71
1:C:223:ILE:HG12	1:C:315:ILE:HG12	1.72	0.71
1:B:207:LYS:HE3	1:B:330:GLU:OE1	1.90	0.71
1:B:223:ILE:HG12	1:B:315:ILE:HG12	1.71	0.70
1:C:297:PHE:O	1:D:293:ARG:HG2	1.93	0.69
1:D:309:THR:O	1:D:313:GLU:HG3	1.92	0.69
1:D:362:PRO:HG3	1:D:371:ILE:HD12	1.76	0.68
1:C:319:GLY:HA2	1:C:361:THR:HG22	1.76	0.68
1:D:39:ASN:HD22	1:D:60:ALA:HB3	1.59	0.68
1:A:362:PRO:HG3	1:A:371:ILE:HD12	1.75	0.68
1:A:154:ASN:HD21	1:A:272:HIS:CD2	2.10	0.68
1:D:7:VAL:HG13	1:D:96:TRP:HE3	1.59	0.68
1:A:223:ILE:HG12	1:A:315:ILE:CG1	2.24	0.68
1:A:301:ASP:OD2	1:A:304:ARG:HD3	1.93	0.67
1:B:40:ARG:HG2	1:B:40:ARG:HH11	1.60	0.67
1:B:39:ASN:HB2	2:B:401:NDP:C4A	2.24	0.67
1:C:37:THR:HG21	1:C:101:ILE:HD11	1.77	0.67
1:C:180:PHE:HZ	1:C:191:VAL:HG11	1.58	0.66
1:D:59:ILE:O	1:D:81:ALA:HA	1.95	0.66
1:D:233:LEU:HD21	1:D:315:ILE:HG21	1.78	0.66
1:C:319:GLY:CA	1:C:361:THR:HG22	2.26	0.66
1:C:126:GLU:OE1	1:C:126:GLU:CA	2.43	0.66
1:D:154:ASN:HD21	1:D:272:HIS:HD2	1.43	0.66
1:B:362:PRO:HG3	1:B:371:ILE:HD12	1.78	0.65
1:A:317:SER:HB3	1:A:321:ARG:HG3	1.77	0.65
1:D:251:GLU:HG3	1:D:257:ILE:HG12	1.78	0.65
1:C:267:ARG:CZ	1:C:283:PRO:HG2	2.25	0.65
1:A:223:ILE:CG1	1:A:315:ILE:HD11	2.26	0.65
1:B:47:ASP:CG	1:B:51:ARG:NH2	2.50	0.65
1:C:338:ASP:OD1	1:C:340:LYS:HE3	1.97	0.65
1:A:7:VAL:HG13	1:A:96:TRP:HE3	1.63	0.64
1:B:233:LEU:HD21	1:B:315:ILE:HG21	1.80	0.64
1:A:207:LYS:HD2	1:A:333:VAL:HG11	1.79	0.64
1:A:223:ILE:HG12	1:A:315:ILE:HD11	1.78	0.64
1:A:357:TYR:CZ	1:A:374:GLU:HG2	2.31	0.64
1:C:311:ALA:N	1:C:325:MET:HE1	2.13	0.64
1:B:338:ASP:OD1	1:B:340:LYS:HE3	1.97	0.64
1:A:309:THR:O	1:A:313:GLU:HG3	1.98	0.64
1:C:301:ASP:OD2	1:C:304:ARG:HD3	1.97	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:HIS:ND1	3:B:434:HOH:O	2.30	0.63
1:C:39:ASN:HA	1:C:60:ALA:HB3	1.79	0.63
1:B:59:ILE:O	1:B:81:ALA:HA	1.99	0.63
1:B:223:ILE:HG12	1:B:315:ILE:CG1	2.28	0.63
1:B:267:ARG:NH1	1:B:283:PRO:HG2	2.14	0.62
1:A:125:LYS:HD3	3:A:407:HOH:O	1.98	0.62
1:C:55:LYS:NZ	1:C:55:LYS:HB3	2.14	0.62
1:B:51:ARG:HG3	1:B:51:ARG:NH2	2.13	0.62
1:C:223:ILE:HG12	1:C:315:ILE:CG1	2.29	0.62
1:A:268:THR:HB	1:A:269:PRO:CD	2.30	0.62
1:C:197:VAL:HA	1:C:209:SER:HB3	1.82	0.62
1:D:39:ASN:HB2	2:D:403:NDP:C4A	2.30	0.62
1:A:345:ASP:HA	1:A:348:LYS:HD2	1.82	0.61
1:C:180:PHE:CZ	1:C:191:VAL:HG11	2.35	0.61
1:A:62:PRO:HG3	1:A:82:GLY:HA2	1.81	0.61
1:B:194:GLU:N	1:B:194:GLU:OE1	2.34	0.61
1:A:207:LYS:CD	1:A:333:VAL:HG11	2.31	0.61
1:A:338:ASP:OD1	1:A:340:LYS:HE3	2.00	0.61
1:A:125:LYS:CG	1:A:126:GLU:N	2.63	0.61
1:D:86:LEU:HD11	2:D:403:NDP:H2A	1.82	0.60
1:D:345:ASP:HA	1:D:348:LYS:HD2	1.83	0.60
1:A:311:ALA:N	1:A:325:MET:HE1	2.17	0.60
1:B:251:GLU:HG3	1:B:257:ILE:HG12	1.84	0.60
1:D:39:ASN:HA	1:D:60:ALA:HB3	1.83	0.60
1:A:103:GLY:HA2	1:A:126:GLU:HG3	1.83	0.60
1:B:193:PRO:O	1:B:197:VAL:HG22	2.02	0.60
1:B:150:ASP:OD2	1:B:153:HIS:ND1	2.35	0.60
1:D:193:PRO:O	1:D:197:VAL:HG22	2.02	0.60
1:A:221:GLU:HA	1:A:224:GLU:HG3	1.83	0.60
1:B:47:ASP:OD2	1:B:51:ARG:NH2	2.30	0.59
1:A:30:ARG:HB2	3:A:404:HOH:O	2.02	0.59
1:C:362:PRO:HG3	1:C:371:ILE:HD12	1.84	0.59
1:A:294:GLN:NE2	1:B:294:GLN:NE2	2.50	0.59
1:A:162:HIS:O	1:A:163:HIS:HB2	2.03	0.59
1:B:118:LYS:HE3	3:B:430:HOH:O	2.03	0.59
1:A:135:MET:O	1:A:139:VAL:HG23	2.03	0.59
1:A:220:LEU:O	1:A:224:GLU:CG	2.51	0.59
1:A:223:ILE:HG12	1:A:315:ILE:CD1	2.33	0.59
1:C:7:VAL:HG13	1:C:96:TRP:HE3	1.68	0.59
1:B:3:GLN:HB2	1:B:4:PRO:HD3	1.85	0.59
1:A:223:ILE:HG12	1:A:315:ILE:HG12	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ALA:CB	1:C:218:LYS:HE3	2.33	0.58
1:D:185:LEU:HA	1:D:188:MET:HE2	1.85	0.58
1:C:62:PRO:HG3	1:C:82:GLY:HA2	1.85	0.58
1:A:207:LYS:HE2	1:A:333:VAL:HG21	1.85	0.57
1:D:223:ILE:HG12	1:D:315:ILE:HG12	1.86	0.57
1:C:72:LEU:O	1:C:75:SER:HB3	2.03	0.57
1:A:319:GLY:HA2	1:A:361:THR:HG22	1.85	0.57
1:B:40:ARG:HA	1:B:64:LEU:CD1	2.34	0.57
1:D:58:VAL:HG22	1:D:80:ALA:HB3	1.86	0.57
1:C:223:ILE:HG12	1:C:315:ILE:CD1	2.34	0.57
1:D:207:LYS:HE3	1:D:330:GLU:OE1	2.05	0.57
1:D:267:ARG:CZ	1:D:283:PRO:HG2	2.34	0.57
1:B:47:ASP:OD1	1:B:51:ARG:NH2	2.37	0.56
1:D:338:ASP:OD1	1:D:340:LYS:HE3	2.05	0.56
1:A:180:PHE:CZ	1:A:191:VAL:HG11	2.40	0.56
1:B:311:ALA:O	1:B:315:ILE:HG13	2.05	0.56
1:D:40:ARG:HA	1:D:64:LEU:CD1	2.35	0.56
1:A:216:MET:SD	1:A:325:MET:HE2	2.46	0.56
1:D:175:ALA:CB	1:D:218:LYS:HE3	2.36	0.56
1:A:220:LEU:O	1:A:224:GLU:HG3	2.06	0.56
1:C:309:THR:O	1:C:313:GLU:HG3	2.05	0.56
1:B:39:ASN:HA	1:B:60:ALA:HB3	1.88	0.56
1:B:220:LEU:O	1:B:224:GLU:HG3	2.07	0.55
1:C:40:ARG:HA	1:C:64:LEU:CD1	2.35	0.55
1:D:362:PRO:HG3	1:D:371:ILE:CD1	2.37	0.55
1:B:320:ALA:O	1:B:324:VAL:HG23	2.07	0.55
1:D:325:MET:HB2	1:D:354:LEU:HD21	1.88	0.55
1:A:332:ALA:O	1:A:341:ILE:HD11	2.06	0.55
1:D:310:LEU:CB	1:D:325:MET:HE3	2.36	0.55
1:D:268:THR:HB	1:D:269:PRO:CD	2.37	0.54
1:C:162:HIS:O	1:C:163:HIS:HB2	2.08	0.54
1:C:311:ALA:O	1:C:315:ILE:HG13	2.07	0.54
1:D:3:GLN:N	1:D:4:PRO:CD	2.71	0.54
1:B:338:ASP:HA	3:B:409:HOH:O	2.06	0.54
1:C:154:ASN:HD21	1:C:272:HIS:CD2	2.26	0.54
1:D:223:ILE:HG12	1:D:315:ILE:CG1	2.38	0.54
1:B:311:ALA:N	1:B:325:MET:HE3	2.23	0.53
1:C:59:ILE:O	1:C:81:ALA:HA	2.09	0.53
1:C:317:SER:HB3	1:C:321:ARG:HG3	1.90	0.53
1:A:175:ALA:HB2	1:A:218:LYS:HE2	1.89	0.53
1:A:292:LEU:HD22	1:A:294:GLN:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:GLY:CA	1:A:361:THR:HG22	2.39	0.53
1:C:155:ALA:HB1	1:C:260:GLN:HB3	1.89	0.53
1:B:39:ASN:ND2	1:B:40:ARG:HG3	2.24	0.53
1:B:58:VAL:HG22	1:B:80:ALA:HB3	1.90	0.53
1:B:254:ASP:OD1	1:B:256:SER:HB3	2.09	0.53
1:C:294:GLN:NE2	1:D:294:GLN:NE2	2.52	0.53
1:D:332:ALA:O	1:D:341:ILE:HD11	2.08	0.53
1:C:223:ILE:HG12	1:C:315:ILE:HD11	1.91	0.53
1:B:234:GLU:H	1:B:234:GLU:CD	2.11	0.52
1:A:154:ASN:HD21	1:A:272:HIS:HD2	1.55	0.52
1:A:59:ILE:O	1:A:81:ALA:HA	2.09	0.52
1:B:188:MET:HA	1:B:191:VAL:HG23	1.90	0.52
1:C:51:ARG:HH21	1:C:51:ARG:HG2	1.75	0.52
1:A:234:GLU:CD	1:A:234:GLU:H	2.13	0.52
1:A:294:GLN:HG2	1:B:296:ASP:OD1	2.10	0.52
1:D:311:ALA:O	1:D:315:ILE:HG13	2.09	0.52
1:D:55:LYS:NZ	1:D:55:LYS:HB3	2.25	0.52
1:D:254:ASP:OD1	1:D:256:SER:HB3	2.10	0.52
1:C:27:ASN:C	1:C:29:ASP:H	2.11	0.52
1:A:40:ARG:HA	1:A:64:LEU:CD1	2.40	0.51
1:A:169:ARG:NH2	1:A:253:LEU:O	2.43	0.51
1:A:175:ALA:CB	1:A:218:LYS:HE2	2.40	0.51
1:C:197:VAL:HG12	1:C:197:VAL:O	2.10	0.51
1:A:39:ASN:HA	1:A:60:ALA:HB3	1.91	0.51
1:C:135:MET:O	1:C:139:VAL:HG23	2.10	0.51
1:A:40:ARG:HA	1:A:64:LEU:HD12	1.92	0.51
1:A:180:PHE:HZ	1:A:191:VAL:HG11	1.74	0.51
1:C:362:PRO:HG3	1:C:371:ILE:CD1	2.39	0.51
1:B:268:THR:HB	1:B:269:PRO:CD	2.41	0.51
1:D:263:SER:HB2	1:D:264:PRO:HD2	1.91	0.51
1:A:188:MET:HA	1:A:191:VAL:HG23	1.92	0.51
1:C:251:GLU:HG3	1:C:257:ILE:CG1	2.39	0.51
1:D:223:ILE:HG12	1:D:315:ILE:HD11	1.93	0.51
1:C:27:ASN:C	1:C:29:ASP:N	2.63	0.51
1:D:188:MET:HA	1:D:191:VAL:HG23	1.92	0.51
1:B:310:LEU:HB2	1:B:325:MET:HE3	1.92	0.50
1:C:33:VAL:HG21	1:C:52:THR:HB	1.93	0.50
1:A:245:VAL:O	1:A:261:ILE:HG23	2.11	0.50
1:A:254:ASP:OD1	1:A:256:SER:HB3	2.11	0.50
1:D:319:GLY:HA2	1:D:361:THR:HG22	1.93	0.50
1:B:162:HIS:O	1:B:163:HIS:HB2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:ARG:HG2	1:D:51:ARG:HH21	1.77	0.50
1:B:221:GLU:HA	1:B:224:GLU:OE1	2.11	0.50
1:C:55:LYS:HB3	1:C:55:LYS:HZ3	1.75	0.50
1:A:357:TYR:CE1	1:A:359:PRO:HD3	2.46	0.50
1:B:310:LEU:CB	1:B:325:MET:HE3	2.42	0.50
1:D:320:ALA:O	1:D:324:VAL:HG23	2.12	0.50
1:A:126:GLU:HA	1:A:126:GLU:OE1	2.11	0.49
1:C:40:ARG:HA	1:C:64:LEU:HD12	1.94	0.49
1:A:34:ILE:O	1:A:55:LYS:HB2	2.13	0.49
1:C:125:LYS:HE2	1:C:224:GLU:OE1	2.12	0.49
1:C:223:ILE:CG1	1:C:315:ILE:HD11	2.41	0.49
1:D:162:HIS:O	1:D:163:HIS:HB2	2.12	0.49
1:A:357:TYR:CE1	1:A:374:GLU:HG2	2.47	0.49
1:B:66:ASN:ND2	3:B:429:HOH:O	2.40	0.49
1:B:223:ILE:HG12	1:B:315:ILE:CD1	2.41	0.49
1:D:153:HIS:HE1	1:D:224:GLU:OE1	1.96	0.49
1:C:11:GLY:H	1:C:37:THR:HG22	1.78	0.49
1:D:249:MET:HG2	1:D:259:ALA:HB2	1.94	0.49
1:B:267:ARG:NH1	1:B:283:PRO:CG	2.76	0.49
1:D:39:ASN:ND2	1:D:60:ALA:HB3	2.28	0.49
1:A:357:TYR:CD1	1:A:359:PRO:HD3	2.48	0.48
1:C:357:TYR:CE1	1:C:374:GLU:HG2	2.49	0.48
1:A:7:VAL:HG13	1:A:96:TRP:CE3	2.47	0.48
1:A:189:ALA:HB2	1:A:344:LEU:HD12	1.93	0.48
1:B:40:ARG:HA	1:B:64:LEU:HD12	1.93	0.48
1:C:101:ILE:HB	3:C:411:HOH:O	2.13	0.48
1:C:216:MET:SD	1:C:325:MET:HE2	2.53	0.48
1:B:101:ILE:O	1:B:124:ASN:ND2	2.46	0.48
1:B:261:ILE:HG22	1:B:262:GLY:N	2.28	0.48
1:C:207:LYS:CE	1:C:211:ASP:OD2	2.57	0.48
1:D:180:PHE:HB3	1:D:183:THR:HB	1.96	0.48
1:A:196:ALA:O	1:A:209:SER:HB3	2.14	0.48
1:A:362:PRO:HG3	1:A:371:ILE:CD1	2.43	0.48
1:B:321:ARG:HB2	1:B:322:PRO:CD	2.43	0.48
1:B:362:PRO:HG3	1:B:371:ILE:CD1	2.42	0.48
1:D:139:VAL:HG21	1:D:146:LEU:HD12	1.96	0.48
1:A:155:ALA:HB1	1:A:260:GLN:HB3	1.95	0.48
1:D:169:ARG:NH2	1:D:253:LEU:O	2.46	0.48
1:D:175:ALA:HA	1:D:218:LYS:HE3	1.96	0.48
1:B:175:ALA:HB1	3:B:417:HOH:O	2.14	0.48
1:B:247:HIS:ND1	1:B:260:GLN:NE2	2.59	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PHE:HE1	1:C:171:ILE:HD11	1.78	0.48
1:B:265:ASP:OD1	1:B:267:ARG:HB2	2.14	0.48
1:C:37:THR:HG23	3:C:424:HOH:O	2.13	0.48
1:D:62:PRO:HG3	1:D:82:GLY:HA2	1.94	0.47
1:A:193:PRO:HB3	1:A:337:LEU:HD23	1.95	0.47
1:C:39:ASN:HB2	2:C:402:NDP:C4A	2.45	0.47
1:D:317:SER:HB3	1:D:321:ARG:HG3	1.95	0.47
1:A:3:GLN:OE1	1:A:3:GLN:HA	2.14	0.47
1:B:263:SER:HB2	1:B:264:PRO:HD2	1.95	0.47
1:C:154:ASN:HD21	1:C:272:HIS:HD2	1.63	0.47
1:D:223:ILE:HG12	1:D:315:ILE:CD1	2.44	0.47
1:C:357:TYR:CZ	1:C:374:GLU:HG2	2.48	0.47
1:D:167:TYR:O	1:D:253:LEU:HG	2.15	0.47
1:A:220:LEU:O	1:A:224:GLU:HG2	2.13	0.47
1:A:245:VAL:HG21	1:A:292:LEU:HD11	1.97	0.47
1:C:27:ASN:O	1:C:29:ASP:N	2.48	0.47
1:D:7:VAL:HG13	1:D:96:TRP:CE3	2.44	0.47
1:D:251:GLU:HG3	1:D:257:ILE:CG1	2.45	0.47
1:D:319:GLY:CA	1:D:361:THR:HG22	2.45	0.47
1:A:4:PRO:HA	1:A:30:ARG:O	2.14	0.47
1:C:214:THR:O	1:C:215:MET:HB2	2.14	0.47
1:B:180:PHE:CZ	1:B:191:VAL:HG11	2.50	0.47
1:A:223:ILE:HA	1:A:315:ILE:CD1	2.45	0.47
1:B:160:PHE:HE1	1:B:171:ILE:HD11	1.80	0.47
1:C:7:VAL:HG13	1:C:96:TRP:CE3	2.48	0.47
1:C:181:ARG:C	1:C:304:ARG:HH22	2.15	0.47
1:C:251:GLU:CG	1:C:257:ILE:HG12	2.41	0.47
1:A:223:ILE:HA	1:A:315:ILE:HD13	1.95	0.46
1:C:247:HIS:O	1:C:248:SER:CB	2.62	0.46
1:D:247:HIS:ND1	1:D:260:GLN:NE2	2.52	0.46
1:A:310:LEU:HB2	1:A:325:MET:HE1	1.97	0.46
1:A:320:ALA:O	1:A:324:VAL:HG23	2.16	0.46
1:A:367:ASP:O	1:A:370:ALA:HB3	2.15	0.46
1:A:167:TYR:O	1:A:253:LEU:HG	2.14	0.46
1:B:232:PRO:HD2	1:B:235:LYS:HD2	1.96	0.46
1:C:38:ALA:HB3	1:C:45:LEU:HD22	1.96	0.46
1:C:265:ASP:OD1	1:C:267:ARG:HB2	2.15	0.46
1:B:72:LEU:O	1:B:75:SER:HB3	2.16	0.46
1:B:125:LYS:HB2	1:B:224:GLU:OE2	2.16	0.46
1:B:40:ARG:HG2	1:B:40:ARG:NH1	2.28	0.46
1:B:169:ARG:HD2	1:B:251:GLU:OE2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLU:HG3	1:A:257:ILE:HG12	1.98	0.46
1:D:310:LEU:HB2	1:D:325:MET:HE3	1.98	0.46
1:A:195:ARG:O	1:A:195:ARG:HG2	2.15	0.46
1:C:131:ALA:O	1:C:135:MET:HG2	2.16	0.46
1:A:294:GLN:HE22	1:B:294:GLN:NE2	2.14	0.46
1:B:155:ALA:HB1	1:B:260:GLN:HB3	1.97	0.46
1:B:223:ILE:HG12	1:B:315:ILE:HD11	1.97	0.46
1:D:249:MET:HG2	1:D:259:ALA:CB	2.46	0.45
1:C:268:THR:HB	1:C:269:PRO:CD	2.47	0.45
1:C:310:LEU:C	1:C:325:MET:HE1	2.37	0.45
1:C:359:PRO:HG3	1:C:371:ILE:HG23	1.98	0.45
1:D:128:LEU:HD13	1:D:228:LEU:HG	1.99	0.45
1:B:125:LYS:CB	1:B:224:GLU:OE2	2.65	0.45
1:B:169:ARG:NH2	1:B:253:LEU:O	2.49	0.45
1:A:128:LEU:HA	1:A:132:GLY:HA2	1.98	0.45
1:C:193:PRO:O	1:C:197:VAL:HG23	2.16	0.45
1:C:191:VAL:HG11	1:C:196:ALA:HB2	1.99	0.45
1:D:169:ARG:HD2	1:D:251:GLU:OE2	2.17	0.45
1:A:139:VAL:HG21	1:A:146:LEU:HD12	1.99	0.45
1:B:223:ILE:CG1	1:B:315:ILE:HD11	2.47	0.45
1:D:171:ILE:HD11	1:D:231:ILE:HD12	1.99	0.45
1:B:223:ILE:HD13	1:B:322:PRO:HB3	1.99	0.45
1:D:207:LYS:HD2	1:D:207:LYS:O	2.16	0.45
1:A:357:TYR:CZ	1:A:374:GLU:CG	2.99	0.45
1:C:263:SER:HB2	1:C:264:PRO:HD2	1.98	0.45
1:A:6:THR:HG21	3:A:410:HOH:O	2.15	0.45
1:B:175:ALA:CB	1:B:218:LYS:HE3	2.47	0.45
1:B:33:VAL:HG21	1:B:52:THR:HB	1.99	0.44
1:B:62:PRO:HG3	1:B:82:GLY:HA2	1.99	0.44
1:C:59:ILE:O	1:C:59:ILE:HG23	2.17	0.44
1:C:321:ARG:HB2	1:C:322:PRO:CD	2.47	0.44
1:B:245:VAL:O	1:B:261:ILE:HG23	2.17	0.44
1:B:317:SER:HB3	1:B:321:ARG:HG3	1.99	0.44
1:C:139:VAL:HG21	1:C:146:LEU:HD12	1.98	0.44
1:C:261:ILE:HG22	1:C:262:GLY:N	2.33	0.44
1:D:245:VAL:O	1:D:261:ILE:HG23	2.17	0.44
1:D:269:PRO:O	1:D:272:HIS:HB3	2.17	0.44
1:A:247:HIS:O	1:A:248:SER:CB	2.64	0.44
1:A:233:LEU:HD21	1:A:315:ILE:HG21	1.98	0.44
1:B:198:GLN:O	1:B:199:HIS:HB3	2.17	0.44
1:B:210:ILE:HG21	1:B:333:VAL:HG13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ILE:HG23	1:C:232:PRO:HD2	2.00	0.44
1:D:18:HIS:ND1	3:D:411:HOH:O	2.36	0.44
1:D:288:ASP:CG	1:D:291:LYS:HG2	2.38	0.44
1:C:14:GLY:O	1:C:18:HIS:HB2	2.18	0.44
1:A:321:ARG:HB2	1:A:322:PRO:CD	2.48	0.43
1:C:167:TYR:O	1:C:253:LEU:HG	2.18	0.43
1:C:367:ASP:O	1:C:370:ALA:HB3	2.17	0.43
1:D:165:ARG:HD2	1:D:230:GLN:O	2.19	0.43
1:C:19:SER:O	1:C:22:ASP:HB3	2.18	0.43
1:A:59:ILE:O	1:A:59:ILE:HG23	2.18	0.43
1:B:128:LEU:HD13	1:B:228:LEU:HG	2.00	0.43
1:B:319:GLY:HA2	1:B:361:THR:HG22	2.00	0.43
1:A:3:GLN:HB3	1:A:4:PRO:CD	2.41	0.43
1:A:22:ASP:O	1:A:26:ARG:HG3	2.19	0.43
1:A:288:ASP:CG	1:A:291:LYS:HG3	2.39	0.43
1:C:175:ALA:HA	1:C:218:LYS:HE3	2.01	0.43
1:A:192:THR:OG1	1:A:194:GLU:HG2	2.18	0.43
1:B:288:ASP:CG	1:B:291:LYS:HG2	2.39	0.43
1:B:113:ALA:O	1:B:116:LYS:HB2	2.19	0.43
1:C:169:ARG:NH2	1:C:253:LEU:O	2.52	0.43
1:D:310:LEU:C	1:D:325:MET:HE3	2.39	0.43
1:C:104:CYS:HA	1:C:107:LEU:HG	2.00	0.42
1:C:320:ALA:O	1:C:324:VAL:HG23	2.19	0.42
1:D:292:LEU:O	1:D:294:GLN:N	2.48	0.42
1:A:37:THR:HG21	1:A:101:ILE:HD11	2.01	0.42
1:A:39:ASN:HB2	2:A:400:NDP:C4A	2.49	0.42
1:C:218:LYS:HA	1:C:218:LYS:HD3	1.86	0.42
1:C:293:ARG:O	1:D:296:ASP:HA	2.18	0.42
1:D:194:GLU:H	1:D:194:GLU:HG2	1.26	0.42
1:A:19:SER:O	1:A:22:ASP:HB3	2.19	0.42
1:B:337:LEU:C	1:B:339:LYS:H	2.21	0.42
1:C:37:THR:CG2	3:C:424:HOH:O	2.66	0.42
1:C:261:ILE:HG22	1:C:287:LEU:HD12	2.01	0.42
1:D:185:LEU:HD23	1:D:188:MET:HE3	2.02	0.42
1:A:216:MET:O	1:A:220:LEU:HG	2.19	0.42
1:A:294:GLN:NE2	1:B:294:GLN:CD	2.73	0.42
1:C:1:MET:O	1:C:2:SER:HB2	2.19	0.42
1:D:33:VAL:HG21	1:D:52:THR:HB	2.02	0.42
1:B:214:THR:O	1:B:215:MET:HB2	2.20	0.42
1:D:165:ARG:CD	1:D:230:GLN:O	2.68	0.42
1:A:150:ASP:OD2	1:A:153:HIS:ND1	2.36	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PRO:HB3	1:A:234:GLU:OE2	2.19	0.42
1:A:268:THR:HB	1:A:269:PRO:HD2	2.02	0.42
1:A:308:LEU:O	1:A:312:MET:HG3	2.20	0.42
1:C:181:ARG:O	1:C:304:ARG:NH2	2.42	0.42
1:D:293:ARG:HE	1:D:293:ARG:HB3	1.28	0.42
1:A:181:ARG:C	1:A:304:ARG:HH22	2.24	0.42
1:A:261:ILE:HG22	1:A:262:GLY:N	2.34	0.42
1:B:319:GLY:CA	1:B:361:THR:HG22	2.50	0.42
1:D:14:GLY:O	1:D:18:HIS:HB2	2.20	0.42
1:A:263:SER:HB2	1:A:264:PRO:HD2	2.01	0.41
1:B:41:ASN:ND2	1:B:44:ASP:OD2	2.53	0.41
1:B:160:PHE:CG	1:B:161:PRO:HD2	2.55	0.41
1:C:188:MET:HA	1:C:191:VAL:HG23	2.02	0.41
1:D:346:ILE:O	1:D:350:VAL:HG23	2.20	0.41
1:D:352:LYS:HB3	1:D:382:LEU:HD13	2.02	0.41
1:B:13:THR:HG1	2:B:401:NDP:P2B	2.43	0.41
1:B:39:ASN:HB2	2:B:401:NDP:C5A	2.50	0.41
1:B:325:MET:HB2	1:B:354:LEU:HD21	2.02	0.41
1:D:128:LEU:CD1	1:D:228:LEU:HG	2.50	0.41
1:D:261:ILE:HG22	1:D:262:GLY:N	2.35	0.41
1:A:313:GLU:O	1:A:316:LYS:HB3	2.20	0.41
1:D:181:ARG:C	1:D:304:ARG:HH22	2.23	0.41
1:D:113:ALA:O	1:D:116:LYS:HB2	2.21	0.41
1:D:218:LYS:HD3	1:D:218:LYS:HA	1.87	0.41
1:D:321:ARG:HB2	1:D:322:PRO:CD	2.50	0.41
1:A:38:ALA:HB3	1:A:45:LEU:HD22	2.03	0.41
1:D:208:ILE:HG23	1:D:209:SER:N	2.36	0.41
1:D:359:PRO:HG3	1:D:371:ILE:HG23	2.02	0.41
1:D:38:ALA:HB1	2:D:403:NDP:O3X	2.20	0.41
1:B:344:LEU:HB2	3:B:428:HOH:O	2.19	0.41
1:A:72:LEU:O	1:A:75:SER:HB3	2.20	0.41
1:A:345:ASP:O	1:A:348:LYS:HB2	2.21	0.41
1:B:131:ALA:O	1:B:135:MET:HG2	2.21	0.41
1:C:280:MET:HG2	3:C:406:HOH:O	2.21	0.41
1:D:91:MET:O	1:D:116:LYS:HE3	2.21	0.41
1:D:223:ILE:CG1	1:D:315:ILE:HD11	2.50	0.41
1:D:224:GLU:OE2	3:D:404:HOH:O	2.22	0.41
1:D:251:GLU:CG	1:D:257:ILE:HG12	2.49	0.41
1:D:267:ARG:NH1	1:D:283:PRO:HG2	2.35	0.41
1:A:14:GLY:O	1:A:18:HIS:HB2	2.20	0.41
1:A:156:ILE:HG13	1:A:248:SER:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:O	1:A:293:ARG:CB	2.66	0.41
1:B:310:LEU:C	1:B:325:MET:HE3	2.42	0.41
1:D:155:ALA:HB3	1:D:248:SER:HB2	2.03	0.40
1:C:49:ALA:HB1	1:C:77:VAL:HG11	2.03	0.40
1:C:87:VAL:O	1:C:91:MET:HG3	2.21	0.40
1:B:51:ARG:NH2	1:B:51:ARG:CG	2.76	0.40
1:B:180:PHE:HB3	1:B:183:THR:HB	2.02	0.40
1:B:301:ASP:OD2	1:B:304:ARG:HD3	2.21	0.40
1:C:223:ILE:HA	1:C:315:ILE:HD13	2.03	0.40
1:C:319:GLY:HA3	1:C:361:THR:HG22	1.99	0.40
1:D:135:MET:O	1:D:139:VAL:HG23	2.22	0.40
1:D:361:THR:HA	1:D:362:PRO:HD3	1.93	0.40
1:B:361:THR:HA	1:B:362:PRO:HD3	1.92	0.40
1:C:102:ILE:HD12	1:C:102:ILE:O	2.22	0.40
1:C:361:THR:HA	1:C:362:PRO:HD3	1.91	0.40
1:D:40:ARG:HA	1:D:64:LEU:HD12	2.02	0.40

All (15) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:ASN:N	1:C:1:MET:O[2_656]	0.73	1.47
1:B:164:ASN:N	1:C:1:MET:C[2_656]	1.46	0.74
1:B:163:HIS:C	1:C:1:MET:C[2_656]	1.50	0.70
1:B:164:ASN:CA	1:C:1:MET:O[2_656]	1.55	0.65
1:B:163:HIS:N	1:C:1:MET:CA[2_656]	1.59	0.61
1:B:163:HIS:CA	1:C:1:MET:CA[2_656]	1.81	0.39
1:B:163:HIS:C	1:C:1:MET:O[2_656]	1.82	0.38
1:B:162:HIS:CA	1:C:1:MET:SD[2_656]	1.85	0.35
1:B:163:HIS:C	1:C:2:SER:N[2_656]	1.87	0.33
1:B:163:HIS:O	1:C:2:SER:N[2_656]	1.99	0.21
1:B:163:HIS:CA	1:C:1:MET:C[2_656]	2.06	0.14
1:B:163:HIS:O	1:C:2:SER:CA[2_656]	2.08	0.12
1:B:163:HIS:CA	1:C:1:MET:N[2_656]	2.14	0.06
1:B:164:ASN:C	1:C:1:MET:O[2_656]	2.15	0.05
1:C:3:GLN:N	3:B:412:HOH:O[2_646]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	374/388 (96%)	355 (95%)	17 (4%)	2 (0%)	29	54
1	B	375/388 (97%)	355 (95%)	19 (5%)	1 (0%)	41	66
1	C	374/388 (96%)	353 (94%)	19 (5%)	2 (0%)	29	54
1	D	374/388 (96%)	360 (96%)	12 (3%)	2 (0%)	29	54
All	All	1497/1552 (96%)	1423 (95%)	67 (4%)	7 (0%)	29	54

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	248	SER
1	B	248	SER
1	C	248	SER
1	D	248	SER
1	D	293	ARG
1	A	127	SER
1	C	28	LEU

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	299/308 (97%)	281 (94%)	18 (6%)	19	42
1	B	301/308 (98%)	287 (95%)	14 (5%)	26	54
1	C	300/308 (97%)	292 (97%)	8 (3%)	44	74

Continued on next page...

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

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	300/308 (97%)	288 (96%)	12 (4%)	31	60
All	All	1200/1232 (97%)	1148 (96%)	52 (4%)	29	57

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	61	ASP
1	A	63	SER
1	A	126	GLU
1	A	146	LEU
1	A	165	ARG
1	A	166	ASP
1	A	185	LEU
1	A	194	GLU
1	A	197	VAL
1	A	224	GLU
1	A	248	SER
1	A	260	GLN
1	A	287	LEU
1	A	292	LEU
1	A	293	ARG
1	A	351	GLU
1	A	383	MET
1	B	18	HIS
1	B	53	ASN
1	B	125	LYS
1	B	146	LEU
1	B	150	ASP
1	B	151	SER
1	B	166	ASP
1	B	195	ARG
1	B	234	GLU
1	B	248	SER
1	B	260	GLN
1	B	287	LEU
1	B	293	ARG
1	B	383	MET
1	C	37	THR
1	C	63	SER
1	C	146	LEU
1	C	194	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	207	LYS
1	C	260	GLN
1	C	287	LEU
1	C	383	MET
1	D	37	THR
1	D	40	ARG
1	D	140	ARG
1	D	146	LEU
1	D	166	ASP
1	D	194	GLU
1	D	195	ARG
1	D	234	GLU
1	D	260	GLN
1	D	287	LEU
1	D	293	ARG
1	D	383	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	247	HIS
1	A	260	GLN
1	A	272	HIS
1	A	294	GLN
1	B	53	ASN
1	B	260	GLN
1	B	272	HIS
1	B	294	GLN
1	C	53	ASN
1	C	260	GLN
1	C	272	HIS
1	C	294	GLN
1	D	39	ASN
1	D	53	ASN
1	D	142	HIS
1	D	153	HIS
1	D	260	GLN
1	D	272	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 ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	NDP	C	402	-	25,29,52	1.58	3 (12%)	31,45,80	1.88	9 (29%)
2	NDP	D	403	-	25,29,52	3.65	10 (40%)	31,45,80	4.12	19 (61%)
2	NDP	B	401	-	25,29,52	1.77	7 (28%)	31,45,80	2.88	14 (45%)
2	NDP	A	400	-	25,29,52	1.82	8 (32%)	31,45,80	2.74	15 (48%)

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	NDP	C	402	-	-	5/11/31/77	0/3/3/5
2	NDP	D	403	-	-	5/11/31/77	0/3/3/5
2	NDP	B	401	-	-	4/11/31/77	0/3/3/5
2	NDP	A	400	-	-	4/11/31/77	0/3/3/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	403	NDP	O4B-C1B	9.15	1.53	1.41
2	D	403	NDP	O5B-C5B	-7.79	1.14	1.44
2	D	403	NDP	C3B-C4B	-7.23	1.34	1.53
2	D	403	NDP	C8A-N7A	-6.15	1.23	1.34
2	D	403	NDP	C5B-C4B	-5.82	1.33	1.51
2	A	400	NDP	O3B-C3B	4.60	1.53	1.43
2	C	402	NDP	O3B-C3B	3.82	1.52	1.43
2	D	403	NDP	C2A-N3A	3.55	1.37	1.32
2	C	402	NDP	PA-O1A	-3.52	1.39	1.50
2	B	401	NDP	O3B-C3B	3.47	1.51	1.43
2	A	400	NDP	P2B-O2B	-3.45	1.52	1.59
2	B	401	NDP	C3B-C4B	3.44	1.61	1.53
2	D	403	NDP	PA-O5B	3.43	1.71	1.60
2	B	401	NDP	PA-O1A	-3.34	1.39	1.50
2	D	403	NDP	O3B-C3B	3.25	1.50	1.43
2	B	401	NDP	C8A-N7A	-3.17	1.29	1.34
2	D	403	NDP	O4B-C4B	3.17	1.52	1.45
2	C	402	NDP	C8A-N7A	-2.97	1.29	1.34
2	A	400	NDP	PA-O1A	-2.91	1.41	1.50
2	A	400	NDP	C2A-N3A	2.67	1.36	1.32
2	B	401	NDP	C5B-C4B	-2.65	1.43	1.51
2	A	400	NDP	C8A-N7A	-2.64	1.30	1.34
2	A	400	NDP	O4B-C1B	2.52	1.44	1.41
2	B	401	NDP	P2B-O2B	-2.25	1.55	1.59
2	A	400	NDP	C3B-C4B	2.21	1.58	1.53
2	A	400	NDP	C5B-C4B	-2.18	1.44	1.51
2	D	403	NDP	C2A-N1A	2.08	1.37	1.33
2	B	401	NDP	O5B-C5B	-2.07	1.36	1.44

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	NDP	O3-PA-O2A	-9.98	69.50	107.64
2	D	403	NDP	PA-O5B-C5B	-9.25	92.81	118.30
2	B	401	NDP	O3X-P2B-O1X	-7.55	81.14	110.68
2	A	400	NDP	O3X-P2B-O1X	-7.51	81.30	110.68
2	D	403	NDP	O3X-P2B-O1X	-7.05	83.07	110.68
2	B	401	NDP	O3X-P2B-O2X	-6.53	82.69	107.64
2	D	403	NDP	O5B-PA-O1A	-6.16	89.20	106.47
2	D	403	NDP	O3X-P2B-O2X	-5.80	85.48	107.64
2	D	403	NDP	O3-PA-O1A	5.79	133.33	110.68
2	B	401	NDP	PA-O5B-C5B	-5.70	102.59	118.30

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	NDP	O3X-P2B-O2X	-5.31	87.35	107.64
2	D	403	NDP	O3-PA-O5B	5.12	120.35	106.73
2	A	400	NDP	O3X-P2B-O2B	-5.10	83.15	105.99
2	C	402	NDP	PA-O5B-C5B	-5.01	104.50	118.30
2	D	403	NDP	O2A-PA-O5B	4.96	119.94	106.73
2	D	403	NDP	O2A-PA-O1A	4.62	128.77	110.68
2	D	403	NDP	C1B-N9A-C4A	4.47	134.50	126.64
2	B	401	NDP	O3X-P2B-O2B	-4.34	86.54	105.99
2	A	400	NDP	PA-O5B-C5B	-4.23	106.65	118.30
2	D	403	NDP	O3X-P2B-O2B	-4.22	87.07	105.99
2	C	402	NDP	O4B-C4B-C5B	-4.02	96.13	109.37
2	A	400	NDP	O4B-C4B-C5B	-3.96	96.34	109.37
2	B	401	NDP	O2X-P2B-O1X	3.69	125.11	110.68
2	B	401	NDP	O5B-C5B-C4B	-3.65	96.42	108.99
2	B	401	NDP	O4B-C4B-C5B	-3.65	97.38	109.37
2	D	403	NDP	O5B-C5B-C4B	3.50	121.03	108.99
2	A	400	NDP	O2X-P2B-O1X	3.42	124.07	110.68
2	C	402	NDP	O5B-C5B-C4B	-3.37	97.40	108.99
2	D	403	NDP	N3A-C2A-N1A	-3.35	123.44	128.68
2	D	403	NDP	O2X-P2B-O1X	3.34	123.75	110.68
2	A	400	NDP	O2A-PA-O1A	3.26	123.45	110.68
2	A	400	NDP	N3A-C2A-N1A	-3.21	123.66	128.68
2	B	401	NDP	O2A-PA-O1A	3.20	123.21	110.68
2	C	402	NDP	O2A-PA-O1A	3.11	122.84	110.68
2	A	400	NDP	O5B-C5B-C4B	-2.79	99.37	108.99
2	D	403	NDP	O2X-P2B-O2B	2.64	117.83	105.99
2	D	403	NDP	O3B-C3B-C4B	-2.62	103.49	111.05
2	B	401	NDP	O2B-C2B-C3B	2.55	120.92	111.68
2	C	402	NDP	N3A-C2A-N1A	-2.53	124.73	128.68
2	B	401	NDP	O2A-PA-O5B	-2.52	100.01	106.73
2	D	403	NDP	C3B-C2B-C1B	-2.48	98.23	102.89
2	A	400	NDP	O2B-C2B-C1B	2.42	118.83	110.10
2	A	400	NDP	O2A-PA-O5B	-2.40	100.34	106.73
2	B	401	NDP	O2B-C2B-C1B	2.40	118.75	110.10
2	C	402	NDP	O2B-C2B-C1B	2.38	118.68	110.10
2	A	400	NDP	C1B-N9A-C4A	2.37	130.80	126.64
2	B	401	NDP	C1B-N9A-C4A	2.35	130.78	126.64
2	B	401	NDP	N3A-C2A-N1A	-2.31	125.07	128.68
2	A	400	NDP	O2B-C2B-C3B	2.23	119.76	111.68
2	A	400	NDP	C3B-C2B-C1B	-2.23	98.70	102.89
2	C	402	NDP	O2A-PA-O5B	-2.22	100.83	106.73
2	D	403	NDP	C2B-C3B-C4B	2.20	106.76	101.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	NDP	O2X-P2B-O2B	2.19	115.79	105.99
2	C	402	NDP	C3B-C2B-C1B	-2.16	98.82	102.89
2	C	402	NDP	O2B-C2B-C3B	2.14	119.44	111.68
2	D	403	NDP	O2B-C2B-C1B	2.01	117.35	110.10
2	B	401	NDP	O2B-P2B-O1X	2.01	117.14	109.39

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	NDP	C3B-C2B-O2B-P2B
2	C	402	NDP	C2B-O2B-P2B-O1X
2	B	401	NDP	C3B-C2B-O2B-P2B
2	C	402	NDP	C3B-C2B-O2B-P2B
2	A	400	NDP	C1B-C2B-O2B-P2B
2	D	403	NDP	C1B-C2B-O2B-P2B
2	D	403	NDP	C3B-C2B-O2B-P2B
2	B	401	NDP	C1B-C2B-O2B-P2B
2	C	402	NDP	C1B-C2B-O2B-P2B
2	A	400	NDP	C2B-O2B-P2B-O3X
2	C	402	NDP	C2B-O2B-P2B-O3X
2	D	403	NDP	C2B-O2B-P2B-O2X
2	B	401	NDP	C2B-O2B-P2B-O1X
2	D	403	NDP	C2B-O2B-P2B-O3X
2	A	400	NDP	O4B-C4B-C5B-O5B
2	C	402	NDP	O4B-C4B-C5B-O5B
2	D	403	NDP	O4B-C4B-C5B-O5B
2	B	401	NDP	O4B-C4B-C5B-O5B

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	402	NDP	1	0
2	D	403	NDP	3	0
2	B	401	NDP	3	0
2	A	400	NDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand NDP C 402

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP D 403

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP B 401

Bond lengths

Bond angles

Torsions

Rings

Ligand NDP A 400

Bond lengths

Bond angles

Torsions

Rings
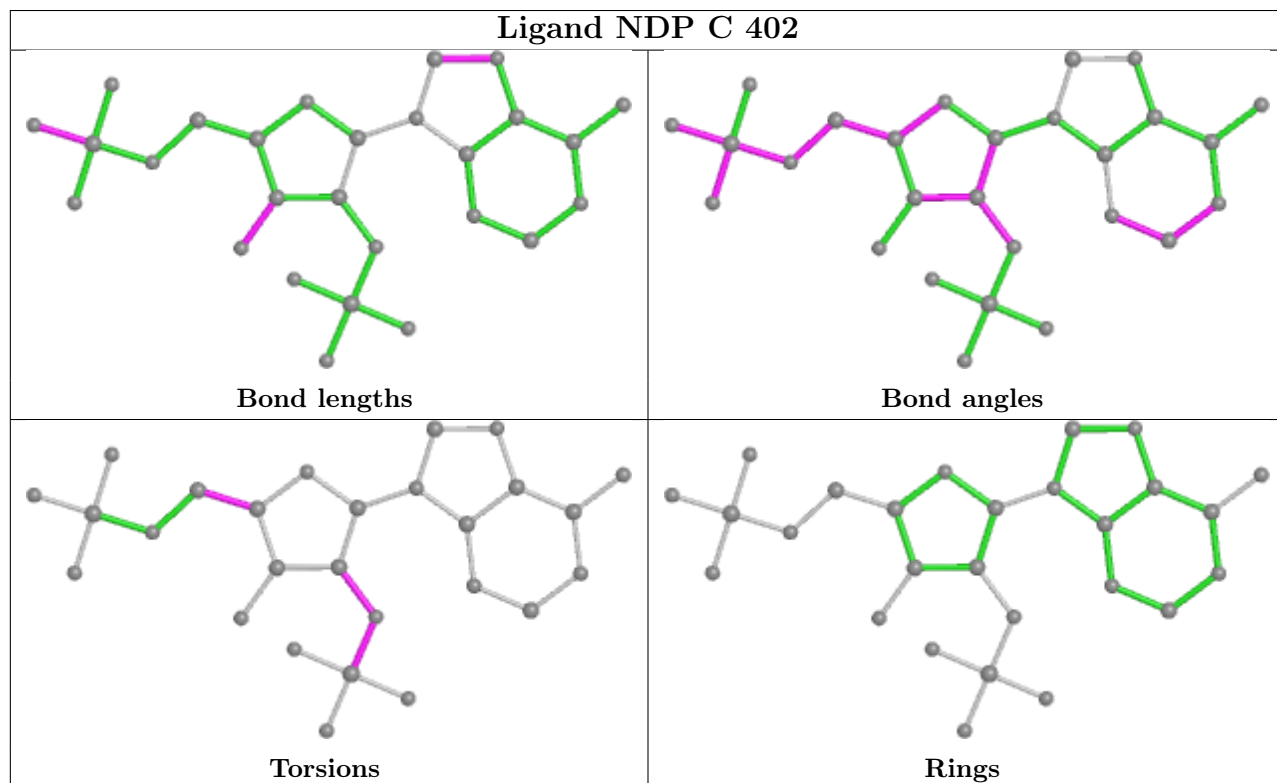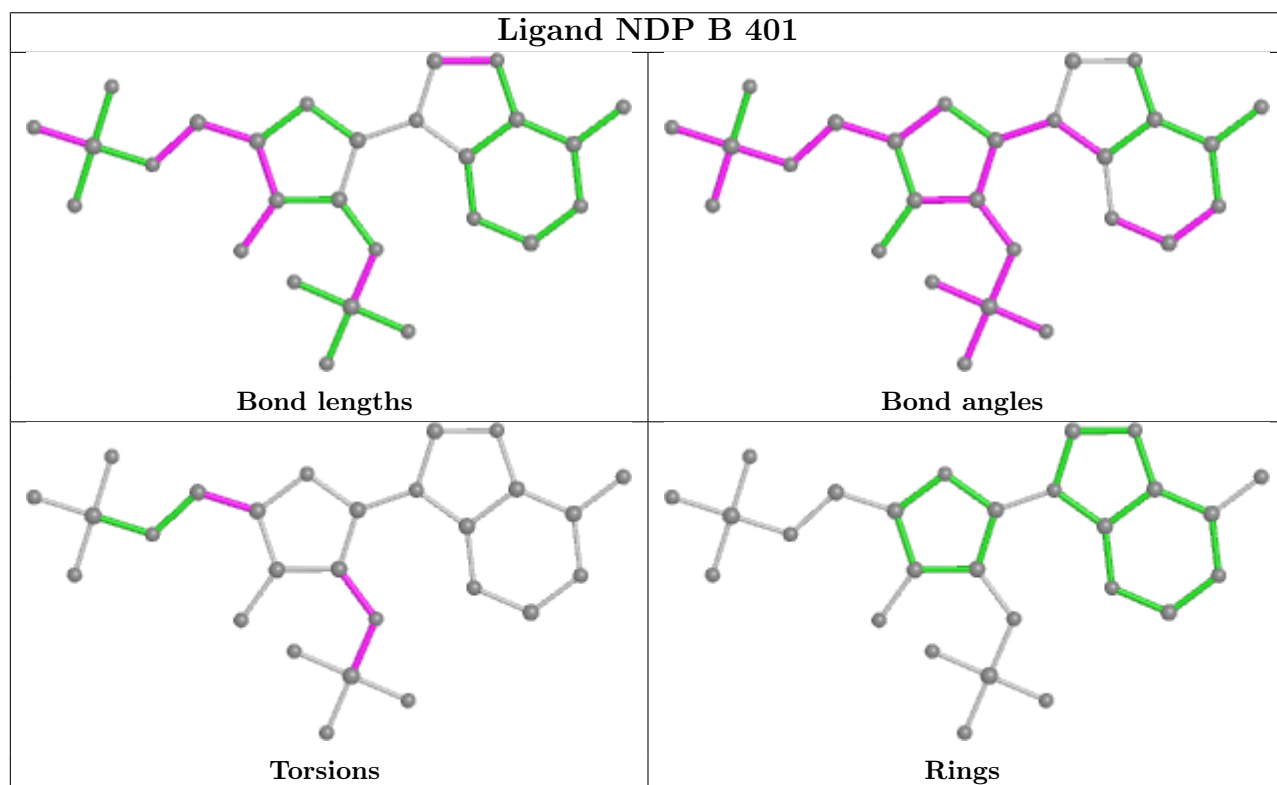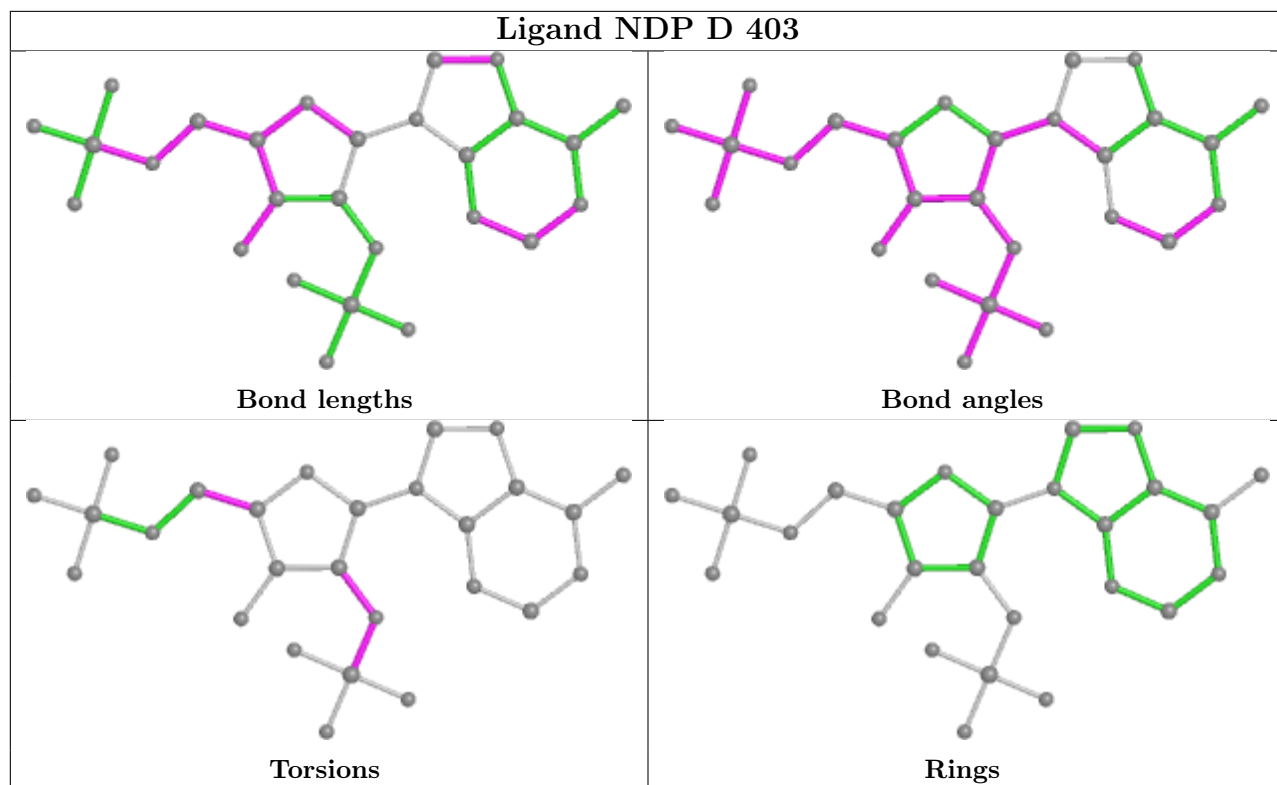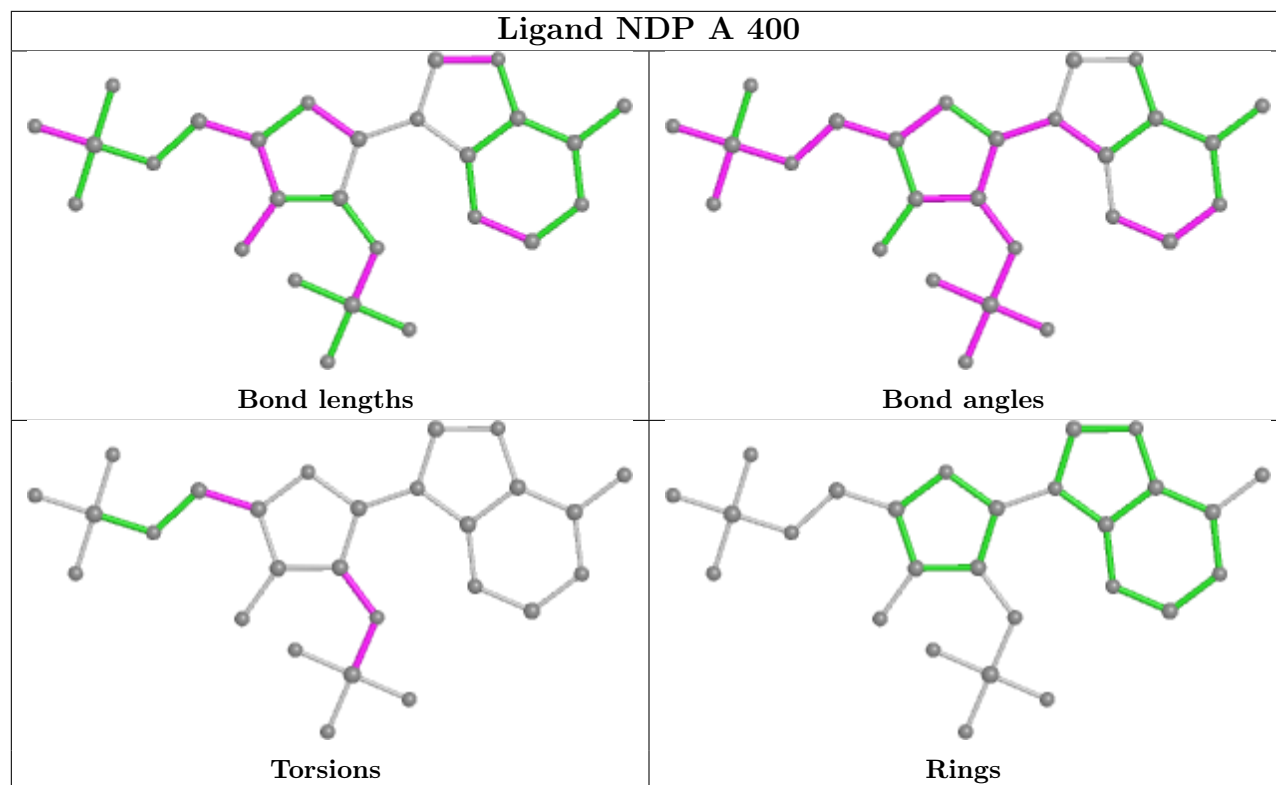
5.7 Other polymers (i)

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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 NDP A 400:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
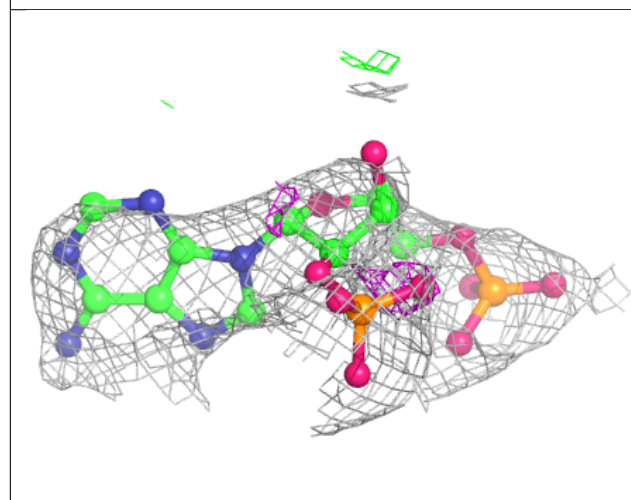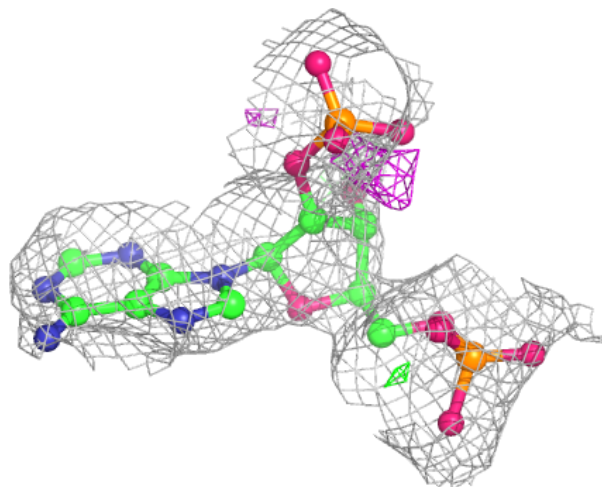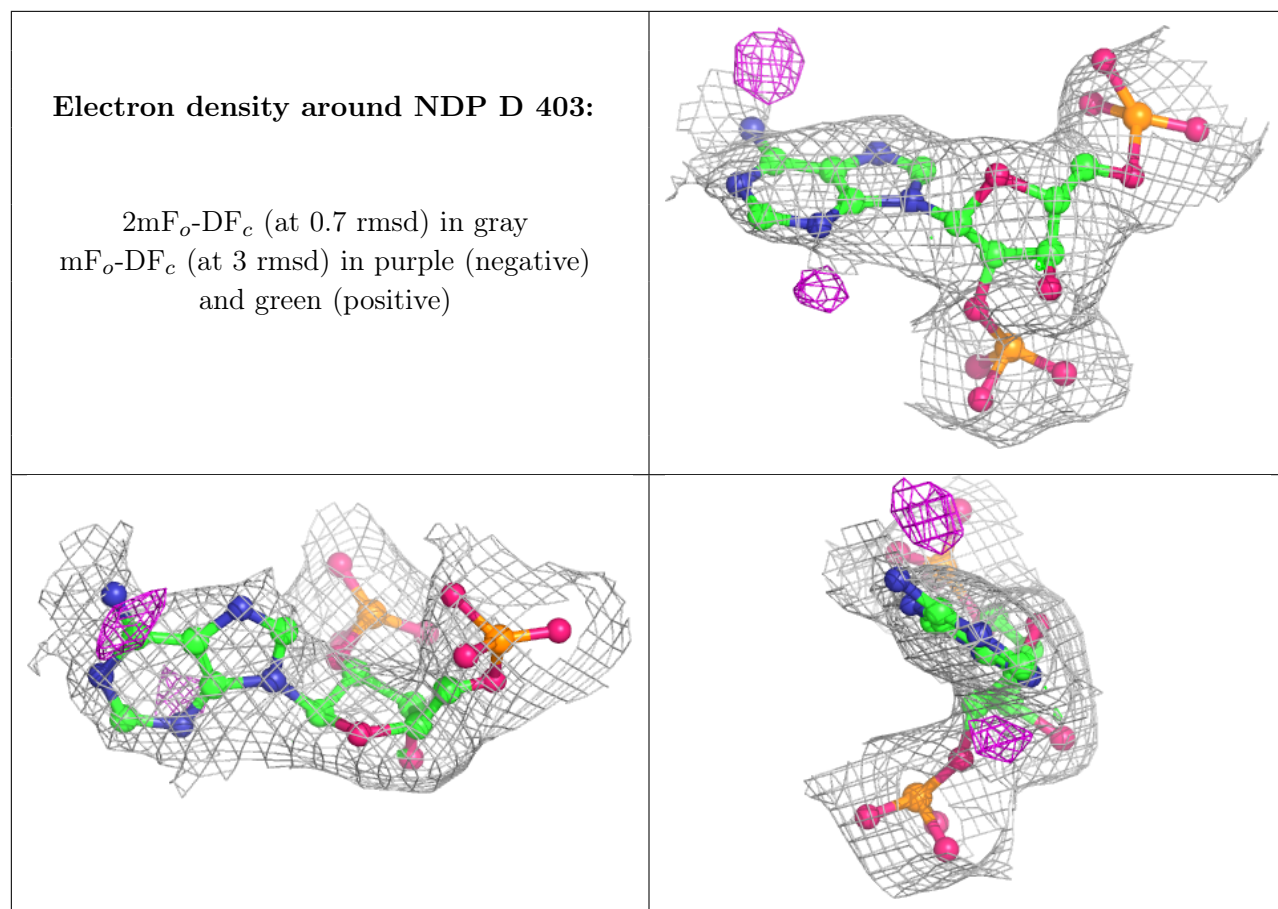and green (positive)
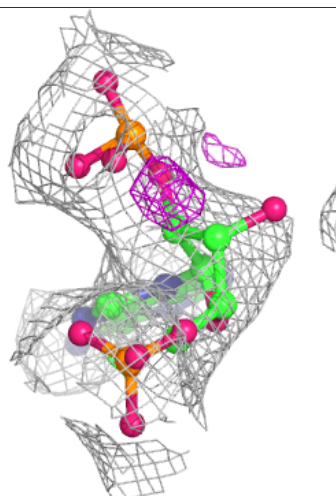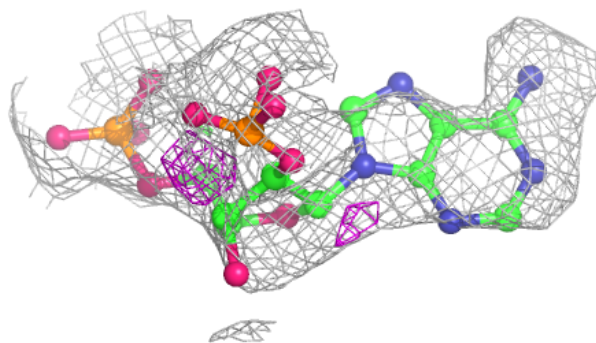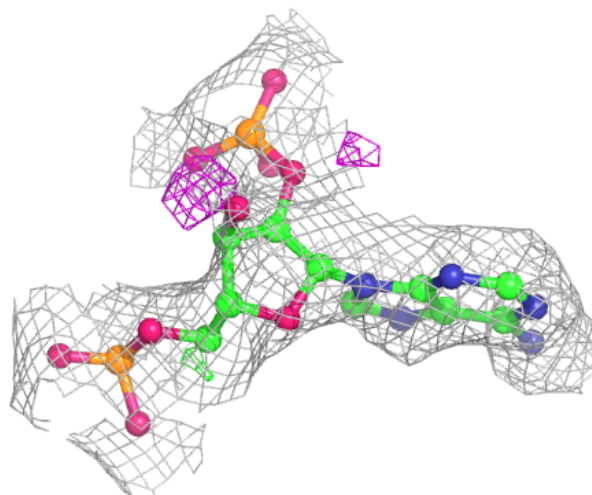
Electron density around NDP B 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
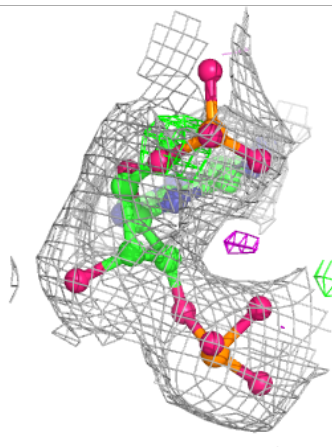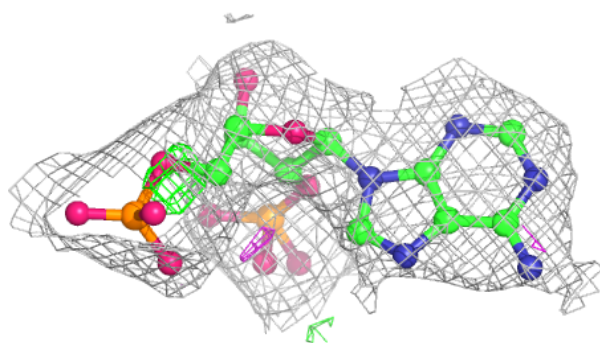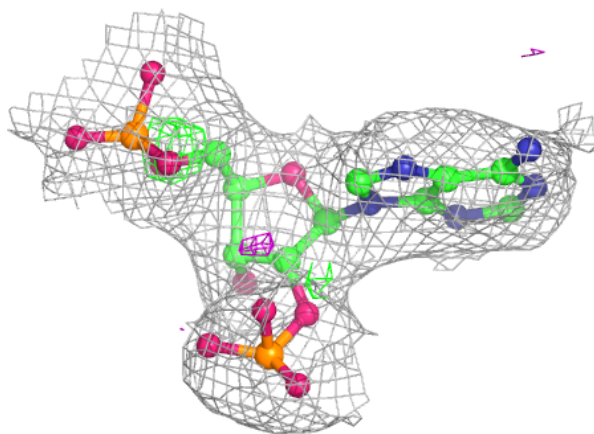
Electron density around NDP C 402:

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

Electron density around NDP D 403:

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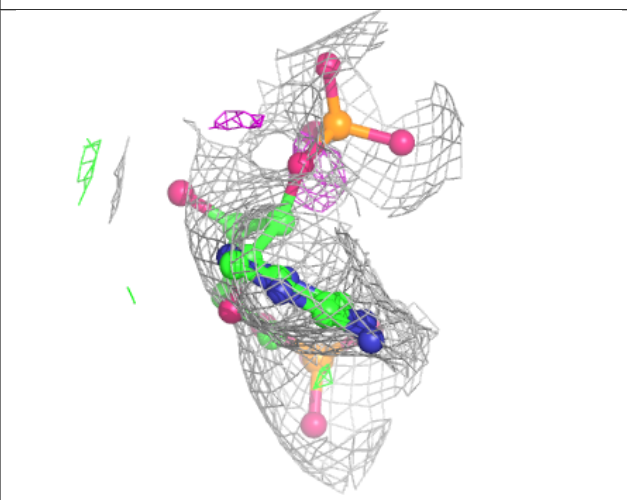
6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.