



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:48 PM UTC

PDB ID : 7CS8 / pdb_00007cs8
Title : IiPLR1 with NADP⁺ and (-)secoisolariciresinol
Authors : Shao, K.; Zhang, P.
Deposited on : 2020-08-14
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

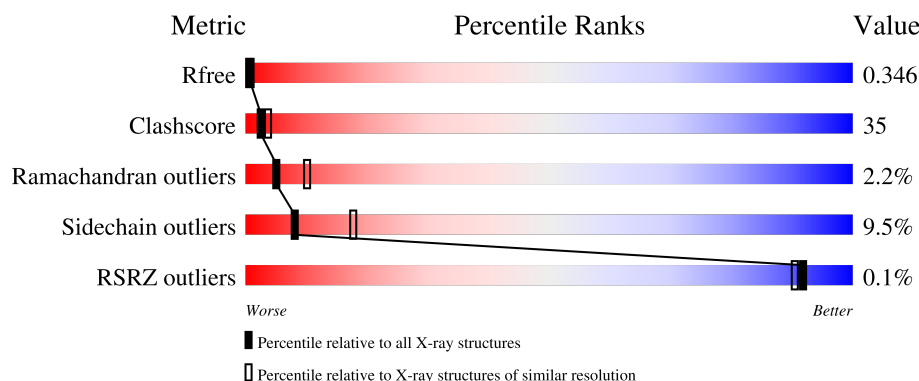
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	317	
1	B	317	
1	C	317	
1	D	317	
1	E	317	

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Mol	Chain	Length	Quality of chain
1	F	317	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (42%), yellow (45%), orange (5%), and grey (7%).

2 Entry composition [i](#)

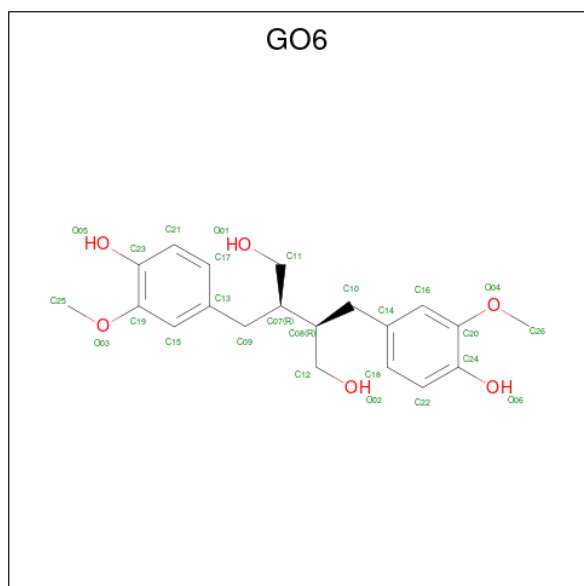
There are 4 unique types of molecules in this entry. The entry contains 14526 atoms, of which 312 are hydrogens and 0 are deuteriums.

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 Pinorensinol-lariciresinol reductase.

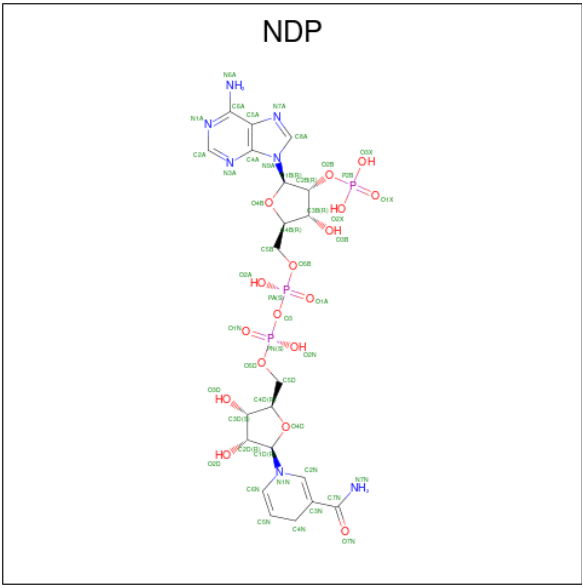
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	0	0
			2281	1449	386	436	10			
1	B	290	Total	C	N	O	S	0	0	0
			2281	1449	386	436	10			
1	C	288	Total	C	N	O	S	0	0	0
			2270	1442	384	434	10			
1	D	286	Total	C	N	O	S	0	0	0
			2256	1434	380	432	10			
1	E	288	Total	C	N	O	S	0	0	0
			2264	1438	382	434	10			
1	F	294	Total	C	N	O	S	0	0	0
			2320	1475	395	440	10			

- Molecule 2 is (2R,3R)-2,3-bis[(3-methoxy-4-oxidanyl-phenyl)methyl]butane-1,4-diol (CCD ID: GO6) (formula: C₂₀H₂₆O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			52	20	26	6		
2	B	1	Total	C	H	O	0	0
			52	20	26	6		
2	C	1	Total	C	H	O	0	0
			52	20	26	6		
2	D	1	Total	C	H	O	0	0
			52	20	26	6		
2	E	1	Total	C	H	O	0	0
			52	20	26	6		
2	F	1	Total	C	H	O	0	0
			52	20	26	6		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			74	21	26	7	17		
3	B	1	Total	C	H	N	O	0	0
			74	21	26	7	17		
3	C	1	Total	C	H	N	O	0	0
			74	21	26	7	17		
3	D	1	Total	C	H	N	O	0	0
			74	21	26	7	17		
3	E	1	Total	C	H	N	O	0	0
			74	21	26	7	17		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	F	1	Total	C	H	N	O	P	0	0
			74	21	26	7	17	3		

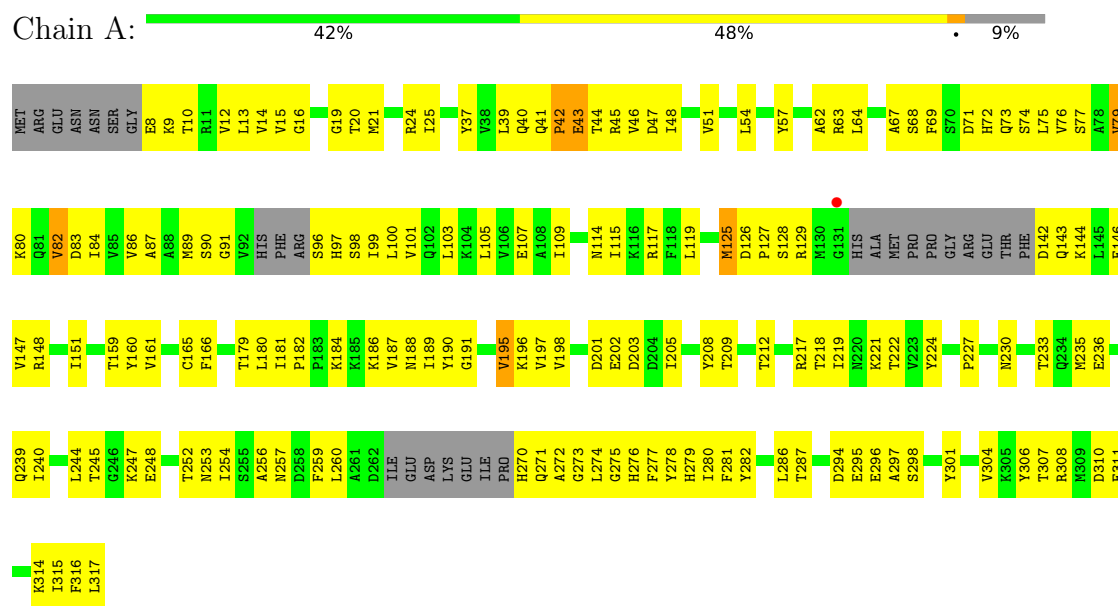
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total	O	0	0
			7	7		
4	B	24	Total	O	0	0
			24	24		
4	C	12	Total	O	0	0
			12	12		
4	D	13	Total	O	0	0
			13	13		
4	E	13	Total	O	0	0
			13	13		
4	F	29	Total	O	0	0
			29	29		

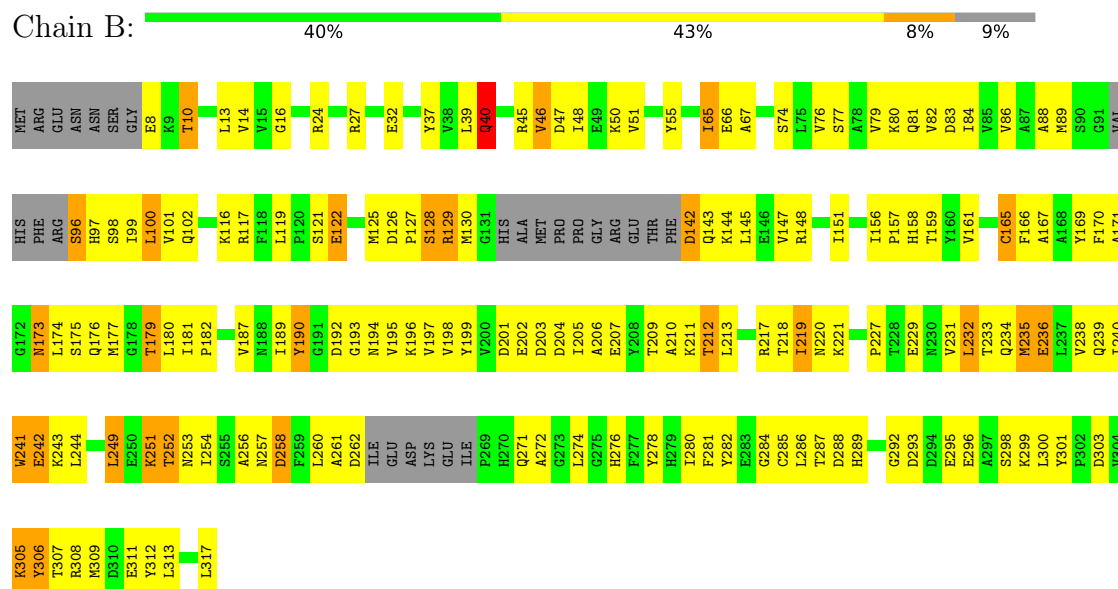
3 Residue-property plots

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.

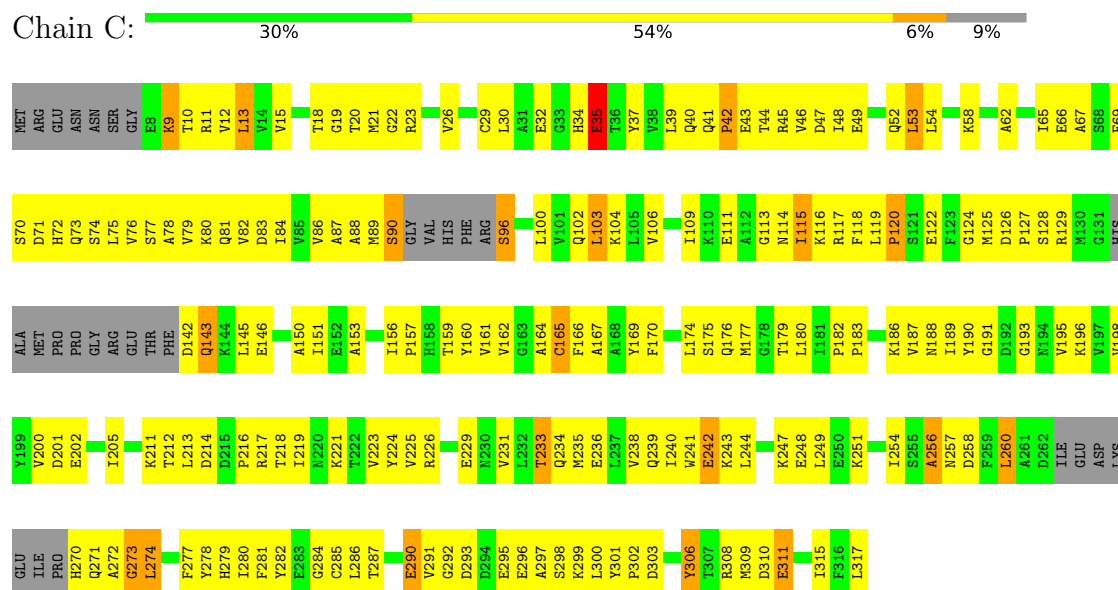
• Molecule 1: Pinoresinol-lariciresinol reductase



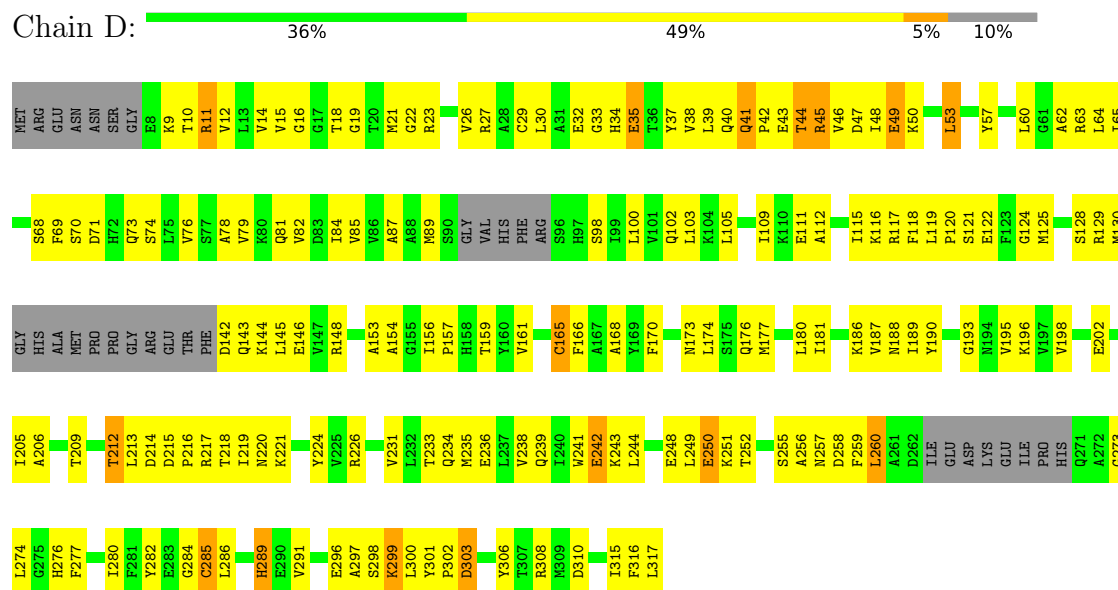
• Molecule 1: Pinoresinol-lariciresinol reductase



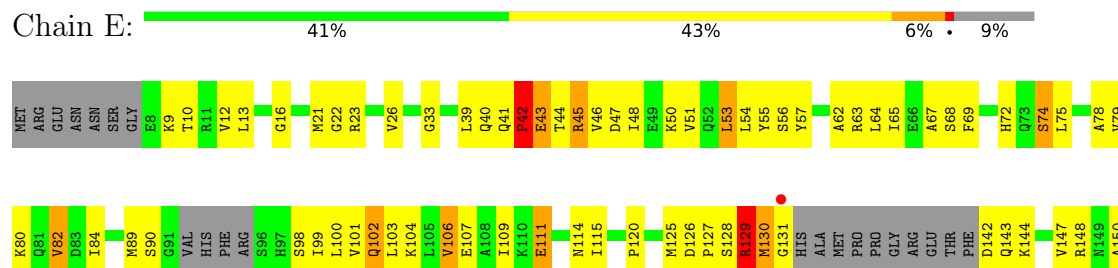
• Molecule 1: Pinoresinol-lariciresinol reductase

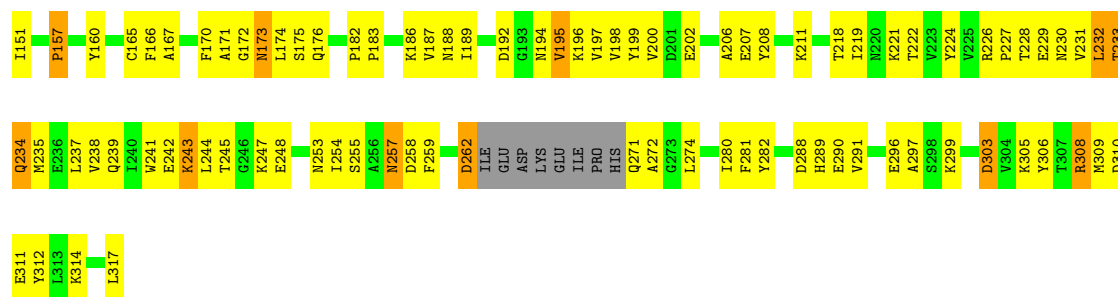


• Molecule 1: Pinoresinol-lariciresinol reductase



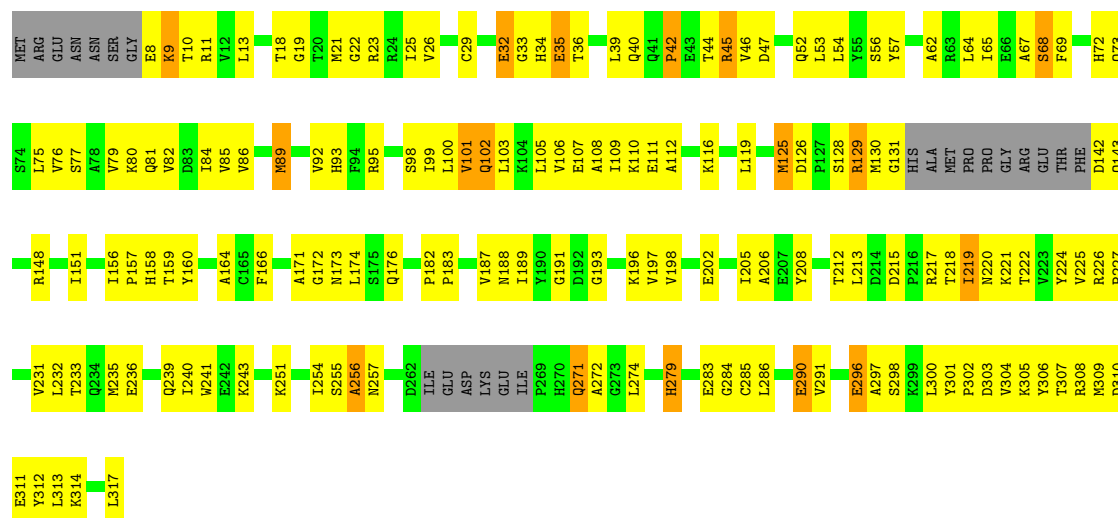
• Molecule 1: Pinoresinol-lariciresinol reductase





• Molecule 1: Pinorensinol-lariciresinol reductase

Chain F: 42% 45% 5% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	244.36Å 244.36Å 76.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.73 – 2.60 40.73 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.73-2.60) 95.6 (40.73-2.60)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.276 , 0.346 0.279 , 0.346	Depositor DCC
R_{free} test set	2000 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 12.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.408 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14526	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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 30.23 % 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 1.3549e-03.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GO6, 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	0.38	0/2319	0.57	0/3132
1	B	0.43	1/2320 (0.0%)	0.60	0/3133
1	C	0.36	0/2308	0.56	0/3117
1	D	0.36	0/2293	0.59	0/3097
1	E	0.40	0/2301	0.61	0/3107
1	F	0.43	0/2362	0.66	0/3191
All	All	0.39	1/13903 (0.0%)	0.60	0/18777

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	40	GLN	C-N	-5.38	1.22	1.33

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	2281	0	2282	134	0
1	B	2281	0	2281	171	0
1	C	2270	0	2270	186	0
1	D	2256	0	2260	186	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2264	0	2266	157	0
1	F	2320	0	2320	151	0
2	A	26	26	0	0	0
2	B	26	26	0	0	0
2	C	26	26	0	2	0
2	D	26	26	0	2	0
2	E	26	26	0	1	0
2	F	26	26	0	1	0
3	A	48	26	24	11	0
3	B	48	26	23	5	0
3	C	48	26	24	9	0
3	D	48	26	23	12	0
3	E	48	26	24	5	0
3	F	48	26	24	8	0
4	A	7	0	0	6	0
4	B	24	0	0	10	0
4	C	12	0	0	9	0
4	D	13	0	0	6	0
4	E	13	0	0	6	0
4	F	29	0	0	12	0
All	All	14214	312	13821	971	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 35.

All (971) 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)
3:A:402:NDP:O4D	3:A:402:NDP:C1D	1.64	1.16
1:A:39:LEU:HD11	1:A:67:ALA:HB3	1.30	1.14
1:B:40:GLN:HG2	1:B:66:GLU:HG2	1.31	1.11
3:A:402:NDP:O4B	3:A:402:NDP:C1B	1.63	1.11
1:F:171:ALA:HB1	1:F:309:MET:HE2	1.35	1.08
1:D:157:PRO:HB3	1:D:219:ILE:HD11	1.38	1.05
1:C:257:ASN:HA	1:C:260:LEU:HD21	1.38	1.04
1:A:54:LEU:HD22	1:A:64:LEU:HD11	1.42	1.01
1:E:41:GLN:NE2	3:E:402:NDP:O2X	1.93	1.01
1:C:15:VAL:HG12	1:C:89:MET:HE1	1.45	0.96
1:C:86:VAL:HG22	1:C:119:LEU:HD13	1.47	0.96
1:C:177:MET:HE2	1:C:274:LEU:HD11	1.46	0.96
1:A:296:GLU:OE1	1:A:298:SER:OG	1.84	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:GLN:NE2	3:C:402:NDP:O2X	2.00	0.93
1:C:39:LEU:HD11	1:C:67:ALA:HB3	1.50	0.93
1:C:142:ASP:O	4:C:501:HOH:O	1.87	0.93
1:E:196:LYS:HG2	1:E:233:THR:HG22	1.49	0.92
1:B:196:LYS:HB3	1:B:287:THR:HG21	1.51	0.92
1:C:72:HIS:NE2	1:C:111:GLU:OE1	2.02	0.92
1:A:235:MET:O	1:A:239:GLN:HG3	1.68	0.92
1:E:45:ARG:O	4:E:501:HOH:O	1.86	0.91
1:D:252:THR:HG21	1:F:271:GLN:HB2	1.53	0.90
1:C:73:GLN:HA	1:C:76:VAL:HB	1.51	0.90
1:C:280:ILE:HG23	1:C:286:LEU:HD12	1.53	0.90
1:A:42:PRO:HG2	1:A:68:SER:HB2	1.52	0.90
1:B:192:ASP:OD1	1:B:194:ASN:ND2	2.05	0.89
1:A:276:HIS:ND1	4:A:501:HOH:O	2.05	0.89
1:B:204:ASP:OD1	4:B:501:HOH:O	1.90	0.89
1:D:30:LEU:HD11	1:D:62:ALA:HB2	1.54	0.89
1:D:111:GLU:OE1	4:D:501:HOH:O	1.92	0.88
1:B:50:LYS:NZ	3:B:402:NDP:O3X	2.06	0.88
1:C:290:GLU:OE1	1:C:291:VAL:N	2.05	0.88
1:D:255:SER:OG	1:D:258:ASP:OD2	1.92	0.87
1:B:260:LEU:O	4:B:503:HOH:O	1.93	0.87
1:B:233:THR:HG23	1:B:236:GLU:H	1.40	0.86
1:E:257:ASN:ND2	4:E:502:HOH:O	2.06	0.86
1:B:241:TRP:O	1:B:244:LEU:N	2.09	0.86
1:B:37:TYR:HD2	1:B:65:ILE:HD11	1.39	0.86
1:A:109:ILE:HG23	1:A:115:ILE:HG13	1.56	0.85
1:C:229:GLU:HG3	1:C:306:TYR:OH	1.76	0.85
1:C:75:LEU:HD12	1:C:104:LYS:HE2	1.57	0.85
1:F:171:ALA:CB	1:F:309:MET:HE2	2.07	0.85
1:F:108:ALA:O	4:F:501:HOH:O	1.94	0.85
1:B:204:ASP:OD2	4:B:504:HOH:O	1.93	0.85
1:A:186:LYS:NZ	1:A:188:ASN:OD1	2.10	0.84
1:C:301:TYR:O	4:C:502:HOH:O	1.93	0.84
1:B:27:ARG:NH2	4:B:505:HOH:O	1.98	0.84
1:C:249:LEU:O	1:C:251:LYS:HG3	1.78	0.84
1:A:217:ARG:O	1:A:221:LYS:NZ	2.12	0.83
1:C:195:VAL:HG21	1:C:281:PHE:O	1.77	0.83
1:C:15:VAL:CG1	1:C:89:MET:HE1	2.07	0.83
1:E:199:TYR:HD2	1:E:232:LEU:HD12	1.43	0.83
1:F:217:ARG:NH2	1:F:300:LEU:O	2.12	0.83
1:A:13:LEU:HB2	1:A:82:VAL:HG21	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ALA:HB1	1:B:309:MET:HE1	1.59	0.82
1:B:89:MET:HE1	1:B:102:GLN:HG3	1.61	0.82
1:C:44:THR:HG23	1:C:45:ARG:HG2	1.62	0.82
1:A:184:LYS:NZ	4:A:503:HOH:O	2.11	0.82
1:C:296:GLU:OE2	1:C:298:SER:OG	1.97	0.81
1:B:40:GLN:HG2	1:B:66:GLU:CG	2.09	0.81
1:C:87:ALA:HB1	1:C:89:MET:HE2	1.61	0.81
1:B:98:SER:O	1:B:101:VAL:HG22	1.81	0.80
1:E:271:GLN:CG	1:E:274:LEU:HD11	2.11	0.80
1:B:179:THR:O	1:B:180:LEU:HD23	1.80	0.80
1:D:252:THR:HG21	1:F:271:GLN:CB	2.11	0.80
1:E:202:GLU:OE2	1:E:202:GLU:N	2.12	0.80
1:A:311:GLU:HA	1:A:314:LYS:HD2	1.63	0.80
1:E:254:ILE:O	1:E:282:TYR:OH	1.98	0.80
1:C:241:TRP:O	1:C:244:LEU:N	2.14	0.80
1:E:195:VAL:HG11	1:E:281:PHE:O	1.82	0.80
1:B:235:MET:O	1:B:239:GLN:HG3	1.82	0.79
1:D:165:CYS:HB2	1:D:198:VAL:O	1.81	0.79
1:C:10:THR:N	4:C:504:HOH:O	2.14	0.79
1:E:199:TYR:O	1:E:230:ASN:ND2	2.16	0.79
1:E:42:PRO:HG2	1:E:68:SER:HB2	1.64	0.79
1:E:271:GLN:HG2	1:E:274:LEU:HD11	1.64	0.79
1:B:204:ASP:OD1	4:B:506:HOH:O	2.01	0.79
1:D:177:MET:HE1	1:D:274:LEU:HD21	1.65	0.79
1:C:187:VAL:HG12	1:C:251:LYS:HA	1.64	0.79
1:E:171:ALA:CB	1:E:309:MET:HE2	2.13	0.79
1:F:218:THR:HA	1:F:221:LYS:HD3	1.65	0.78
1:B:84:ILE:HG21	1:B:213:LEU:HD13	1.64	0.78
1:B:233:THR:HG23	1:B:236:GLU:N	2.00	0.77
1:C:90:SER:HA	3:C:402:NDP:O1A	1.85	0.77
1:C:187:VAL:HG11	1:C:251:LYS:HG2	1.67	0.76
1:D:296:GLU:OE1	1:D:298:SER:OG	2.03	0.76
1:F:307:THR:O	4:F:503:HOH:O	2.03	0.76
1:B:238:VAL:O	1:B:242:GLU:HG3	1.84	0.76
1:F:189:ILE:HD12	1:F:235:MET:HE2	1.66	0.76
1:A:271:GLN:HB3	1:A:274:LEU:HD11	1.67	0.76
1:E:176:GLN:HE22	1:E:188:ASN:HB2	1.51	0.76
1:D:177:MET:SD	1:D:274:LEU:HD21	2.26	0.75
1:E:69:PHE:HA	1:E:75:LEU:HD11	1.67	0.75
1:A:40:GLN:HB2	1:A:64:LEU:HD12	1.69	0.75
1:F:142:ASP:OD1	4:F:504:HOH:O	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HD22	1:B:143:GLN:OE1	1.86	0.75
1:B:296:GLU:OE1	1:B:298:SER:OG	2.03	0.75
1:C:169:TYR:OH	4:C:503:HOH:O	1.96	0.75
1:C:226:ARG:NH1	1:C:290:GLU:HA	2.01	0.75
1:C:143:GLN:HA	4:C:501:HOH:O	1.86	0.74
1:D:142:ASP:OD2	1:D:144:LYS:HB2	1.86	0.74
1:A:15:VAL:CG1	1:A:89:MET:HE3	2.17	0.74
1:D:100:LEU:HD21	1:D:143:GLN:HB3	1.69	0.74
1:D:21:MET:N	3:D:402:NDP:O1N	2.19	0.74
1:C:100:LEU:O	1:C:103:LEU:HD13	1.87	0.74
1:B:37:TYR:CD2	1:B:65:ILE:HD11	2.22	0.74
1:B:258:ASP:O	4:B:503:HOH:O	2.04	0.74
1:C:234:GLN:O	1:C:238:VAL:HG22	1.87	0.74
1:E:274:LEU:H	1:E:274:LEU:HD12	1.53	0.74
1:A:41:GLN:NE2	3:A:402:NDP:O2X	2.19	0.74
1:C:226:ARG:HH12	1:C:290:GLU:HA	1.53	0.73
1:F:18:THR:O	1:F:23:ARG:NH2	2.19	0.73
1:B:196:LYS:CB	1:B:287:THR:HG21	2.18	0.73
1:F:157:PRO:HB3	1:F:219:ILE:HD11	1.70	0.73
1:B:193:GLY:O	1:B:233:THR:OG1	2.06	0.73
1:C:21:MET:HB2	3:C:402:NDP:H51N	1.71	0.73
1:D:306:TYR:CE1	1:D:308:ARG:HD2	2.24	0.73
1:E:99:ILE:HD11	1:E:100:LEU:HD12	1.70	0.73
1:A:103:LEU:O	1:A:107:GLU:HG3	1.88	0.73
1:D:153:ALA:O	4:D:502:HOH:O	2.07	0.72
1:F:197:VAL:HG12	1:F:198:VAL:H	1.53	0.72
1:C:235:MET:O	1:C:239:GLN:HG3	1.89	0.72
1:F:279:HIS:HA	1:F:283:GLU:HB2	1.71	0.72
1:D:9:LYS:HE2	1:D:33:GLY:O	1.88	0.72
1:C:103:LEU:HD12	1:C:103:LEU:H	1.54	0.72
1:E:99:ILE:CD1	1:E:100:LEU:HD12	2.19	0.72
1:A:227:PRO:HB3	1:A:306:TYR:CZ	2.25	0.72
1:C:247:LYS:HG3	1:C:248:GLU:N	2.03	0.72
1:F:235:MET:O	1:F:239:GLN:HG3	1.89	0.72
1:B:88:ALA:O	4:B:507:HOH:O	2.08	0.72
1:A:117:ARG:HD3	1:A:159:THR:OG1	1.89	0.72
1:C:218:THR:HA	1:C:221:LYS:HD3	1.72	0.71
1:E:227:PRO:HB2	1:E:230:ASN:HB2	1.72	0.71
1:D:181:ILE:HG22	1:D:316:PHE:HE1	1.54	0.71
1:D:224:TYR:CD1	1:D:291:VAL:HG11	2.25	0.71
1:B:305:LYS:HD2	1:B:305:LYS:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:HIS:NE2	1:F:111:GLU:OE2	2.20	0.71
1:B:158:HIS:O	1:B:220:ASN:N	2.23	0.70
1:B:96:SER:C	1:B:143:GLN:HE22	1.99	0.70
1:B:252:THR:HG22	1:B:254:ILE:HD11	1.72	0.70
1:D:187:VAL:HG12	1:D:251:LYS:HA	1.72	0.70
1:D:196:LYS:HD2	1:D:231:VAL:HG12	1.74	0.70
1:D:73:GLN:HA	1:D:76:VAL:HG12	1.73	0.70
1:E:199:TYR:CD2	1:E:232:LEU:HD12	2.24	0.70
1:F:22:GLY:O	1:F:26:VAL:HG12	1.90	0.70
1:A:73:GLN:HA	1:A:76:VAL:HG23	1.72	0.70
1:C:156:ILE:HG22	1:C:157:PRO:O	1.91	0.70
1:F:196:LYS:HD2	1:F:231:VAL:HG12	1.74	0.70
1:B:204:ASP:HA	4:B:501:HOH:O	1.91	0.70
1:D:109:ILE:HG23	1:D:115:ILE:HB	1.72	0.70
1:B:77:SER:O	1:B:81:GLN:NE2	2.24	0.70
1:D:21:MET:CE	1:D:206:ALA:HB2	2.22	0.70
1:E:271:GLN:HB3	1:E:274:LEU:CD1	2.22	0.70
1:A:63:ARG:CZ	1:D:11:ARG:HH11	2.05	0.69
1:E:39:LEU:HD11	1:E:67:ALA:HB3	1.74	0.69
1:C:193:GLY:O	1:C:233:THR:OG1	2.09	0.69
1:E:127:PRO:HD2	1:E:148:ARG:HH21	1.56	0.69
1:C:308:ARG:HB2	1:C:310:ASP:OD2	1.93	0.69
1:D:9:LYS:HE2	1:D:33:GLY:C	2.18	0.69
1:A:75:LEU:O	1:A:79:VAL:HG13	1.93	0.69
1:F:174:LEU:O	1:F:176:GLN:NE2	2.26	0.69
1:C:187:VAL:CG1	1:C:251:LYS:HA	2.22	0.69
1:A:98:SER:O	1:A:101:VAL:HG22	1.93	0.68
1:B:122:GLU:HB3	1:B:144:LYS:HD3	1.73	0.68
1:E:90:SER:OG	3:E:402:NDP:O1A	2.10	0.68
1:D:21:MET:HE3	1:D:206:ALA:HB2	1.76	0.68
1:D:177:MET:CE	1:D:274:LEU:HD21	2.23	0.68
1:A:196:LYS:O	1:A:287:THR:OG1	2.07	0.68
1:C:10:THR:HA	1:C:83:ASP:OD2	1.93	0.68
1:D:205:ILE:O	1:D:209:THR:OG1	2.09	0.68
1:D:181:ILE:HG22	1:D:316:PHE:CE1	2.28	0.68
1:D:168:ALA:HB2	4:E:508:HOH:O	1.93	0.68
1:A:308:ARG:HB2	1:A:310:ASP:OD1	1.94	0.67
1:D:166:PHE:H	3:D:402:NDP:H72N	1.42	0.67
1:E:271:GLN:HB3	1:E:274:LEU:HD11	1.76	0.67
1:F:130:MET:HE3	1:F:130:MET:O	1.93	0.67
1:B:241:TRP:O	1:B:243:LYS:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:VAL:C	1:D:233:THR:HG22	2.18	0.67
1:E:290:GLU:OE1	1:E:291:VAL:N	2.21	0.67
1:A:189:ILE:HG13	1:A:235:MET:HE1	1.77	0.67
1:C:18:THR:O	1:C:23:ARG:NH2	2.27	0.67
1:B:189:ILE:HD12	1:B:235:MET:HE2	1.75	0.67
1:C:86:VAL:CG2	1:C:119:LEU:HD13	2.23	0.67
1:B:189:ILE:O	1:B:253:ASN:HA	1.94	0.67
1:D:180:LEU:HD21	1:E:46:VAL:HG13	1.76	0.66
1:F:89:MET:H	1:F:89:MET:HE2	1.61	0.66
1:F:21:MET:HE3	1:F:25:ILE:HG13	1.77	0.66
1:E:21:MET:HE1	1:E:202:GLU:O	1.95	0.66
1:A:19:GLY:HA3	3:A:402:NDP:C5B	2.26	0.66
1:B:252:THR:HG22	1:B:254:ILE:CD1	2.26	0.66
1:F:34:HIS:O	1:F:36:THR:N	2.29	0.66
1:C:257:ASN:HA	1:C:260:LEU:CD2	2.20	0.66
1:F:197:VAL:HG13	1:F:286:LEU:HD12	1.78	0.66
1:B:174:LEU:HD13	1:B:238:VAL:HG22	1.78	0.66
1:B:233:THR:CG2	1:B:236:GLU:HB2	2.26	0.66
1:F:198:VAL:HG21	1:F:226:ARG:HG3	1.77	0.66
1:B:32:GLU:OE2	1:B:211:LYS:NZ	2.29	0.66
1:D:238:VAL:O	1:D:242:GLU:HG3	1.95	0.66
1:D:16:GLY:HA2	3:D:402:NDP:O2B	1.96	0.65
1:A:218:THR:HA	1:A:221:LYS:NZ	2.11	0.65
1:F:86:VAL:HG22	1:F:119:LEU:HD13	1.78	0.65
1:A:212:THR:HA	1:A:301:TYR:OH	1.97	0.65
1:B:122:GLU:HA	1:B:144:LYS:HZ3	1.60	0.65
1:B:190:TYR:HB3	1:B:282:TYR:OH	1.95	0.65
1:D:23:ARG:HG3	1:D:27:ARG:NH2	2.12	0.65
1:D:35:GLU:HG2	1:D:37:TYR:HE1	1.61	0.65
1:C:12:VAL:HA	1:C:84:ILE:O	1.97	0.65
1:C:309:MET:HA	1:C:309:MET:HE2	1.78	0.65
1:F:171:ALA:HB1	1:F:309:MET:CE	2.22	0.65
1:F:271:GLN:HB3	1:F:274:LEU:HD11	1.79	0.65
1:B:205:ILE:O	1:B:209:THR:OG1	2.08	0.65
1:B:169:TYR:OH	4:B:502:HOH:O	1.91	0.64
1:A:99:ILE:CG1	1:A:100:LEU:HD22	2.27	0.64
1:E:109:ILE:HG23	1:E:115:ILE:HG13	1.80	0.64
1:E:43:GLU:OE2	1:E:43:GLU:HA	1.96	0.64
1:E:125:MET:HE2	1:E:280:ILE:HG13	1.80	0.64
1:B:89:MET:HE1	1:B:102:GLN:CG	2.28	0.64
1:F:202:GLU:HA	1:F:205:ILE:HD12	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:O	1:A:37:TYR:HB2	1.98	0.64
1:A:109:ILE:HG23	1:A:115:ILE:CG1	2.27	0.64
1:B:13:LEU:HB2	1:B:82:VAL:HG11	1.80	0.64
1:E:235:MET:O	1:E:239:GLN:HG3	1.97	0.64
3:F:402:NDP:O1X	3:F:402:NDP:O3B	2.16	0.64
1:C:229:GLU:HG3	1:C:306:TYR:HH	1.64	0.63
1:E:271:GLN:CB	1:E:274:LEU:HD11	2.27	0.63
1:D:84:ILE:HG23	1:D:117:ARG:O	1.98	0.63
1:D:177:MET:HE1	1:D:274:LEU:CD2	2.27	0.63
1:C:124:GLY:HA3	2:C:401:GO6:O05	1.98	0.63
1:E:227:PRO:HB3	1:E:306:TYR:CE1	2.34	0.63
1:F:110:LYS:HD3	1:F:111:GLU:N	2.14	0.63
1:B:121:SER:O	1:B:122:GLU:HB3	1.98	0.63
1:B:249:LEU:O	1:B:251:LYS:HG2	1.99	0.63
1:D:100:LEU:HD21	1:D:143:GLN:CB	2.29	0.63
1:A:201:ASP:OD2	1:A:203:ASP:HB2	1.99	0.63
1:D:37:TYR:CD2	1:D:65:ILE:HD11	2.34	0.63
1:F:271:GLN:HB3	1:F:274:LEU:CD1	2.29	0.63
1:D:154:ALA:HB3	1:D:156:ILE:HD12	1.79	0.62
1:A:15:VAL:HG11	1:A:89:MET:HE3	1.80	0.62
1:F:9:LYS:HG2	1:F:33:GLY:O	1.99	0.62
1:A:91:GLY:HA2	1:A:99:ILE:CG2	2.29	0.62
1:C:13:LEU:O	1:C:13:LEU:HG	2.00	0.62
1:E:99:ILE:O	1:E:102:GLN:HB2	1.99	0.62
1:D:105:LEU:HD23	1:D:109:ILE:HD12	1.81	0.62
1:B:201:ASP:OD2	1:B:203:ASP:N	2.33	0.62
1:D:226:ARG:N	1:D:296:GLU:OE2	2.32	0.62
1:A:127:PRO:HD2	1:A:148:ARG:HH21	1.65	0.62
1:D:18:THR:OG1	1:D:50:LYS:NZ	2.30	0.62
1:F:95:ARG:HD3	1:F:143:GLN:NE2	2.14	0.62
1:C:160:TYR:O	1:C:162:VAL:HG13	2.00	0.61
1:E:208:TYR:CD1	1:E:297:ALA:HB1	2.35	0.61
1:A:99:ILE:HG12	1:A:100:LEU:HD22	1.82	0.61
1:C:187:VAL:HG13	1:C:189:ILE:HD11	1.81	0.61
1:A:195:VAL:HG21	1:A:281:PHE:O	2.00	0.61
1:B:233:THR:HG22	1:B:236:GLU:OE1	1.99	0.61
1:C:46:VAL:O	1:C:46:VAL:HG13	2.00	0.61
1:C:9:LYS:HE2	4:C:504:HOH:O	2.00	0.61
1:F:19:GLY:HA3	3:F:402:NDP:C5B	2.30	0.61
1:B:125:MET:HE3	1:B:129:ARG:NH1	2.15	0.61
1:C:165:CYS:HB2	1:C:198:VAL:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:LEU:HD23	1:F:85:VAL:HG22	1.82	0.61
1:C:15:VAL:HG12	1:C:89:MET:CE	2.24	0.61
1:C:103:LEU:HD12	1:C:103:LEU:N	2.15	0.61
1:B:253:ASN:C	1:B:254:ILE:HD12	2.26	0.61
1:D:73:GLN:O	1:D:73:GLN:HG2	1.99	0.60
1:C:216:PRO:O	1:C:219:ILE:HG22	2.01	0.60
1:E:189:ILE:O	1:E:253:ASN:HA	2.00	0.60
1:F:197:VAL:HG12	1:F:198:VAL:N	2.17	0.60
1:C:127:PRO:HB2	1:C:145:LEU:HD13	1.83	0.60
1:B:166:PHE:H	3:B:402:NDP:H72N	1.49	0.60
1:B:190:TYR:HB3	1:B:282:TYR:CZ	2.37	0.60
1:D:15:VAL:CG1	1:D:89:MET:HE1	2.30	0.60
1:D:76:VAL:HA	1:D:79:VAL:HG22	1.84	0.60
1:A:41:GLN:O	1:A:43:GLU:N	2.35	0.60
1:A:304:VAL:HB	4:A:502:HOH:O	2.00	0.60
1:B:217:ARG:O	1:B:221:LYS:HD2	2.01	0.60
1:B:256:ALA:O	1:B:260:LEU:HD12	2.01	0.60
1:C:201:ASP:HB3	4:C:505:HOH:O	2.01	0.60
1:E:241:TRP:CH2	1:E:317:LEU:HD23	2.37	0.60
1:B:202:GLU:H	1:B:202:GLU:CD	2.10	0.59
1:A:15:VAL:HG12	1:A:89:MET:HE3	1.84	0.59
1:F:255:SER:O	1:F:257:ASN:N	2.35	0.59
1:A:54:LEU:CD2	1:A:64:LEU:HD11	2.26	0.59
1:D:11:ARG:HH21	1:D:82:VAL:CA	2.15	0.59
1:F:171:ALA:CB	1:F:309:MET:CE	2.80	0.59
1:B:129:ARG:HD2	1:B:129:ARG:O	2.03	0.59
1:B:231:VAL:HG23	1:B:231:VAL:O	2.02	0.59
1:E:21:MET:HE3	1:E:21:MET:HA	1.83	0.59
1:E:176:GLN:NE2	1:E:188:ASN:HB2	2.18	0.59
1:B:286:LEU:O	4:B:508:HOH:O	2.16	0.59
1:A:105:LEU:HD12	1:A:105:LEU:O	2.03	0.59
1:F:89:MET:HE1	1:F:102:GLN:CD	2.27	0.59
1:C:186:LYS:HG2	1:C:187:VAL:N	2.18	0.59
1:B:122:GLU:CB	1:B:144:LYS:HD3	2.32	0.59
1:D:22:GLY:N	4:D:507:HOH:O	2.30	0.59
1:D:76:VAL:HG23	1:D:112:ALA:HB2	1.83	0.58
1:E:196:LYS:HG2	1:E:233:THR:CG2	2.29	0.58
1:F:103:LEU:O	1:F:107:GLU:HG3	2.02	0.58
1:A:47:ASP:O	1:A:51:VAL:HG23	2.03	0.58
1:C:299:LYS:O	1:C:302:PRO:HD3	2.03	0.58
1:C:65:ILE:HG21	1:C:78:ALA:CB	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LEU:H	1:C:103:LEU:CD1	2.14	0.58
1:D:157:PRO:CB	1:D:219:ILE:HD11	2.24	0.58
1:B:40:GLN:O	1:B:66:GLU:HA	2.02	0.58
1:D:233:THR:OG1	1:D:236:GLU:HG3	2.02	0.58
1:D:37:TYR:HD2	1:D:65:ILE:HD11	1.69	0.58
1:B:207:GLU:O	1:B:211:LYS:HG3	2.04	0.58
1:F:19:GLY:HA3	3:F:402:NDP:H51A	1.84	0.58
1:F:164:ALA:HB2	1:F:225:VAL:HG23	1.86	0.58
1:B:233:THR:HG22	1:B:236:GLU:HB2	1.86	0.58
1:A:69:PHE:HA	1:A:75:LEU:HD11	1.86	0.57
1:D:47:ASP:HB3	1:D:50:LYS:HB3	1.84	0.57
1:A:195:VAL:O	1:A:233:THR:HA	2.05	0.57
1:B:271:GLN:HB3	1:B:274:LEU:HD21	1.86	0.57
1:E:198:VAL:HG11	1:E:226:ARG:HA	1.86	0.57
1:E:207:GLU:O	1:E:211:LYS:HG3	2.05	0.57
1:C:177:MET:CE	1:C:274:LEU:HD11	2.27	0.57
1:D:145:LEU:HD13	1:D:148:ARG:HD2	1.87	0.57
1:F:92:VAL:HG12	4:F:511:HOH:O	2.03	0.57
1:B:241:TRP:CH2	1:B:317:LEU:HD23	2.39	0.57
1:E:57:TYR:C	1:E:62:ALA:HB3	2.29	0.57
1:A:208:TYR:CG	1:A:297:ALA:HB1	2.40	0.57
1:A:63:ARG:NH2	1:D:11:ARG:HD3	2.18	0.57
1:C:233:THR:HG22	1:C:236:GLU:OE1	2.03	0.57
1:F:198:VAL:CG2	1:F:226:ARG:HG3	2.34	0.57
1:B:236:GLU:O	1:B:240:ILE:HG13	2.05	0.57
1:D:188:ASN:O	1:D:234:GLN:NE2	2.30	0.57
1:D:303:ASP:OD1	1:D:303:ASP:N	2.33	0.57
1:B:232:LEU:HB3	1:B:236:GLU:HB3	1.87	0.57
1:D:257:ASN:HA	1:D:260:LEU:HG	1.85	0.57
1:B:171:ALA:CB	1:B:309:MET:HE2	2.35	0.57
1:C:202:GLU:H	1:C:202:GLU:CD	2.10	0.57
1:F:42:PRO:HG2	1:F:68:SER:OG	2.05	0.57
1:C:15:VAL:HB	1:C:87:ALA:HA	1.86	0.56
1:E:45:ARG:NE	1:E:45:ARG:HA	2.19	0.56
1:E:262:ASP:N	1:E:262:ASP:OD1	2.38	0.56
1:B:39:LEU:HD11	1:B:67:ALA:HB3	1.87	0.56
1:C:236:GLU:O	1:C:240:ILE:HG13	2.04	0.56
1:D:284:GLY:O	1:D:286:LEU:N	2.38	0.56
1:C:189:ILE:N	1:C:189:ILE:HD12	2.20	0.56
1:C:235:MET:HA	1:C:238:VAL:CG2	2.35	0.56
1:E:99:ILE:HD11	1:E:143:GLN:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:191:GLY:N	1:F:254:ILE:O	2.37	0.56
1:A:73:GLN:HA	1:A:76:VAL:CG2	2.34	0.56
1:A:126:ASP:OD1	1:A:128:SER:HB3	2.05	0.56
1:A:165:CYS:SG	1:A:280:ILE:HD13	2.45	0.56
1:B:202:GLU:OE1	1:B:202:GLU:N	2.27	0.56
1:D:40:GLN:HG3	1:D:64:LEU:HB3	1.86	0.56
1:D:44:THR:O	1:D:44:THR:OG1	2.22	0.56
1:E:72:HIS:CE1	1:E:107:GLU:HG2	2.41	0.56
1:B:76:VAL:HA	1:B:79:VAL:HG22	1.86	0.56
1:C:102:GLN:O	1:C:106:VAL:HG23	2.06	0.56
1:D:21:MET:HB3	3:D:402:NDP:H51N	1.88	0.56
1:A:257:ASN:O	1:A:260:LEU:N	2.36	0.56
1:C:80:LYS:HA	1:C:114:ASN:OD1	2.05	0.56
1:D:109:ILE:HG12	1:D:115:ILE:HG13	1.86	0.56
1:D:241:TRP:O	1:D:243:LYS:N	2.39	0.56
1:B:65:ILE:HD13	1:B:81:GLN:OE1	2.06	0.56
1:B:16:GLY:HA2	3:B:402:NDP:P2B	2.46	0.56
1:C:122:GLU:HB2	1:C:161:VAL:O	2.06	0.55
1:D:100:LEU:O	1:D:103:LEU:HG	2.06	0.55
1:D:14:VAL:HG11	1:D:26:VAL:HG23	1.89	0.55
1:B:189:ILE:HD12	1:B:235:MET:CE	2.37	0.55
1:A:82:VAL:HG13	1:A:84:ILE:H	1.72	0.55
1:C:79:VAL:C	1:C:81:GLN:H	2.15	0.55
1:D:120:PRO:HD2	1:D:159:THR:O	2.07	0.55
1:E:130:MET:HG3	1:E:131:GLY:O	2.07	0.55
1:E:171:ALA:CB	1:E:309:MET:CE	2.83	0.55
1:B:86:VAL:HG22	1:B:119:LEU:HD13	1.87	0.55
1:F:13:LEU:HB2	1:F:82:VAL:HG11	1.88	0.55
1:F:29:CYS:O	1:F:34:HIS:HB2	2.07	0.55
1:C:225:VAL:HG13	1:C:225:VAL:O	2.04	0.55
1:E:235:MET:O	1:E:235:MET:HG3	2.07	0.55
1:F:40:GLN:OE1	1:F:64:LEU:HD13	2.06	0.55
1:B:239:GLN:HA	1:B:242:GLU:HB2	1.88	0.55
1:C:119:LEU:H	1:C:119:LEU:HD12	1.71	0.55
1:E:171:ALA:HB2	1:E:309:MET:HE2	1.88	0.55
1:A:16:GLY:HA2	3:A:402:NDP:O2B	2.07	0.55
1:A:142:ASP:OD1	1:A:143:GLN:N	2.38	0.55
1:E:274:LEU:HD12	1:E:274:LEU:N	2.20	0.55
1:A:227:PRO:HB3	1:A:306:TYR:CE2	2.41	0.54
1:B:144:LYS:O	1:B:147:VAL:HG12	2.07	0.54
1:C:22:GLY:O	1:C:26:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:VAL:HG22	1:C:119:LEU:CD1	2.29	0.54
1:E:127:PRO:HD2	1:E:148:ARG:NH2	2.22	0.54
1:F:148:ARG:HG2	1:F:160:TYR:CZ	2.42	0.54
1:B:165:CYS:HB2	1:B:198:VAL:O	2.07	0.54
1:C:109:ILE:O	1:C:113:GLY:N	2.30	0.54
1:D:193:GLY:O	1:D:233:THR:HB	2.07	0.54
1:E:229:GLU:HB2	1:E:308:ARG:NH1	2.22	0.54
1:F:84:ILE:HD13	1:F:213:LEU:HD13	1.89	0.54
1:F:225:VAL:HG23	1:F:225:VAL:O	2.07	0.54
1:D:48:ILE:CG2	1:D:49:GLU:HG2	2.37	0.54
1:A:73:GLN:OE1	1:A:73:GLN:O	2.26	0.54
1:B:180:LEU:HD21	1:F:46:VAL:HG13	1.90	0.54
1:C:9:LYS:HB3	4:C:504:HOH:O	2.07	0.54
1:C:125:MET:SD	1:C:280:ILE:HD11	2.48	0.54
1:D:46:VAL:O	1:D:46:VAL:HG12	2.07	0.54
1:E:21:MET:HE2	1:E:206:ALA:HB2	1.89	0.54
1:E:211:LYS:O	4:E:503:HOH:O	2.18	0.54
1:A:144:LYS:O	1:A:147:VAL:N	2.41	0.54
1:C:69:PHE:HE2	3:C:402:NDP:H2A	1.73	0.54
1:F:189:ILE:HD12	1:F:235:MET:CE	2.34	0.54
1:A:143:GLN:O	1:A:146:GLU:HB3	2.08	0.54
1:C:224:TYR:O	1:C:297:ALA:N	2.34	0.54
1:D:119:LEU:HG	1:D:159:THR:HB	1.89	0.54
1:F:119:LEU:CD2	1:F:159:THR:HB	2.38	0.54
1:F:309:MET:HE1	1:F:312:TYR:CD1	2.43	0.54
1:A:245:THR:HG22	1:A:317:LEU:CD2	2.37	0.54
1:B:122:GLU:O	1:B:122:GLU:HG3	2.08	0.54
1:E:208:TYR:CG	1:E:297:ALA:HB1	2.42	0.54
1:E:274:LEU:H	1:E:274:LEU:CD1	2.19	0.54
1:E:227:PRO:HB3	1:E:306:TYR:CZ	2.43	0.54
1:F:13:LEU:O	1:F:13:LEU:HG	2.06	0.54
1:B:218:THR:HA	1:B:221:LYS:HD2	1.90	0.53
1:C:69:PHE:CD1	1:C:75:LEU:HD21	2.43	0.53
1:C:187:VAL:HG13	1:C:189:ILE:CD1	2.38	0.53
1:C:244:LEU:HD22	1:C:317:LEU:HD11	1.88	0.53
1:C:308:ARG:CB	1:C:310:ASP:OD2	2.56	0.53
1:D:11:ARG:HE	1:D:82:VAL:HA	1.72	0.53
1:D:15:VAL:HG11	1:D:89:MET:HE1	1.90	0.53
1:E:157:PRO:HB3	1:E:219:ILE:HD11	1.90	0.53
1:B:233:THR:HG23	1:B:236:GLU:HB2	1.90	0.53
1:C:65:ILE:HG21	1:C:78:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:85:VAL:HG11	1:F:105:LEU:HD21	1.91	0.53
1:F:173:ASN:O	1:F:176:GLN:HG2	2.08	0.53
1:B:296:GLU:O	1:B:300:LEU:HD12	2.09	0.53
1:F:45:ARG:HG3	1:F:46:VAL:N	2.23	0.53
1:F:86:VAL:HG22	1:F:119:LEU:CD1	2.39	0.53
1:F:151:ILE:HG23	1:F:156:ILE:HB	1.91	0.53
3:F:402:NDP:O5D	3:F:402:NDP:H6N	2.08	0.53
1:D:48:ILE:HG23	1:D:49:GLU:HG2	1.90	0.53
1:D:202:GLU:OE1	1:D:202:GLU:N	2.34	0.53
1:A:189:ILE:HG13	1:A:235:MET:CE	2.39	0.53
1:C:15:VAL:O	1:C:88:ALA:N	2.42	0.53
1:A:63:ARG:HH22	1:D:11:ARG:HD3	1.73	0.53
1:B:47:ASP:O	1:B:51:VAL:HG23	2.09	0.53
1:C:127:PRO:HG2	1:C:145:LEU:HD12	1.91	0.53
1:E:42:PRO:CG	1:E:68:SER:HB2	2.38	0.53
1:E:195:VAL:CG1	1:E:281:PHE:O	2.55	0.53
1:F:65:ILE:HD13	1:F:81:GLN:OE1	2.09	0.53
1:F:279:HIS:CA	1:F:283:GLU:HB2	2.39	0.53
1:B:116:LYS:HD3	1:B:116:LYS:N	2.23	0.52
1:E:247:LYS:HD2	1:E:248:GLU:H	1.73	0.52
1:F:23:ARG:HA	1:F:26:VAL:CG1	2.39	0.52
1:C:37:TYR:CD2	1:C:65:ILE:HD11	2.44	0.52
1:D:78:ALA:O	1:D:81:GLN:HB2	2.09	0.52
1:A:82:VAL:CG1	1:A:84:ILE:H	2.22	0.52
1:C:84:ILE:HD13	1:C:213:LEU:O	2.10	0.52
1:C:242:GLU:OE2	1:C:248:GLU:HG3	2.10	0.52
1:E:72:HIS:HE1	1:E:107:GLU:HG2	1.73	0.52
1:A:63:ARG:NH1	1:D:11:ARG:NH1	2.57	0.52
1:D:118:PHE:O	1:D:120:PRO:HD3	2.09	0.52
1:F:208:TYR:CG	1:F:297:ALA:HB1	2.45	0.52
1:A:19:GLY:HA3	3:A:402:NDP:H52A	1.91	0.52
1:F:303:ASP:N	1:F:303:ASP:OD1	2.38	0.52
1:B:119:LEU:N	1:B:119:LEU:HD12	2.25	0.52
1:E:126:ASP:OD1	1:E:128:SER:OG	2.24	0.52
1:F:311:GLU:O	1:F:314:LYS:HB2	2.09	0.52
1:E:13:LEU:HB2	1:E:82:VAL:HG11	1.90	0.52
1:C:77:SER:O	1:C:81:GLN:HG3	2.10	0.52
1:C:170:PHE:HE2	3:C:402:NDP:N7N	2.08	0.52
1:D:145:LEU:CD1	1:D:148:ARG:HD2	2.39	0.52
1:E:187:VAL:HG22	1:E:188:ASN:N	2.24	0.52
1:F:279:HIS:O	1:F:285:CYS:SG	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:HE2	1:A:252:THR:HB	1.91	0.52
1:C:306:TYR:O	1:C:308:ARG:NH1	2.43	0.52
1:A:208:TYR:CD1	1:A:297:ALA:HB1	2.45	0.52
1:B:24:ARG:HH22	1:F:52:GLN:HE22	1.58	0.52
1:B:307:THR:HG21	1:B:312:TYR:HB2	1.91	0.52
1:E:45:ARG:NH2	1:E:46:VAL:HG23	2.25	0.52
1:E:99:ILE:HD11	1:E:100:LEU:CD1	2.40	0.52
1:E:254:ILE:HG22	1:E:259:PHE:HB2	1.92	0.52
1:A:127:PRO:HD2	1:A:148:ARG:NH2	2.24	0.51
1:C:309:MET:HE2	1:C:309:MET:CA	2.40	0.51
1:D:109:ILE:HG23	1:D:115:ILE:CB	2.39	0.51
1:E:218:THR:HA	1:E:221:LYS:HD3	1.92	0.51
1:F:11:ARG:HG2	1:F:35:GLU:HB3	1.92	0.51
1:A:87:ALA:HB1	1:A:89:MET:SD	2.50	0.51
1:C:292:GLY:O	1:C:295:GLU:HG2	2.10	0.51
1:D:177:MET:HE3	1:D:277:PHE:CE1	2.45	0.51
1:B:99:ILE:CG2	1:B:143:GLN:HG3	2.40	0.51
1:B:177:MET:HE1	1:B:274:LEU:HD23	1.91	0.51
1:C:32:GLU:OE2	1:C:211:LYS:HE2	2.09	0.51
1:E:67:ALA:HB1	1:E:74:SER:OG	2.09	0.51
1:A:181:ILE:HD12	4:A:503:HOH:O	2.11	0.51
1:B:128:SER:HB3	1:B:148:ARG:NH1	2.25	0.51
1:C:58:LYS:HA	1:C:62:ALA:O	2.11	0.51
1:E:308:ARG:CD	1:E:308:ARG:N	2.73	0.51
3:F:402:NDP:O3B	3:F:402:NDP:P2B	2.69	0.51
1:B:278:TYR:HA	1:B:282:TYR:HD2	1.75	0.51
1:C:11:ARG:N	1:C:83:ASP:OD2	2.43	0.51
1:D:116:LYS:O	1:D:157:PRO:HB2	2.10	0.51
1:A:202:GLU:OE1	1:A:202:GLU:N	2.33	0.51
1:D:259:PHE:HZ	1:D:274:LEU:HD22	1.75	0.51
1:C:96:SER:N	1:C:143:GLN:HE22	2.09	0.51
1:E:226:ARG:HG2	1:E:231:VAL:CG2	2.40	0.51
1:E:244:LEU:HB3	1:E:317:LEU:HD11	1.92	0.51
1:A:191:GLY:O	1:A:253:ASN:ND2	2.44	0.51
1:B:99:ILE:HG21	1:B:143:GLN:HG3	1.92	0.51
1:D:212:THR:HG22	1:D:213:LEU:N	2.26	0.51
1:E:166:PHE:H	3:E:402:NDP:H72N	1.57	0.51
1:F:69:PHE:CD1	1:F:75:LEU:HD21	2.46	0.51
1:A:63:ARG:CZ	1:D:11:ARG:NH1	2.73	0.51
1:B:10:THR:HA	1:B:83:ASP:OD2	2.11	0.51
1:B:48:ILE:HG21	4:F:502:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:PHE:HE2	3:D:402:NDP:N7N	2.09	0.51
1:D:177:MET:HG3	1:D:190:TYR:OH	2.11	0.51
1:E:303:ASP:OD1	1:E:303:ASP:N	2.31	0.51
1:F:296:GLU:OE1	1:F:297:ALA:N	2.44	0.51
1:F:301:TYR:O	4:F:505:HOH:O	2.19	0.51
1:A:310:ASP:O	1:A:314:LYS:HG3	2.11	0.50
1:D:174:LEU:O	1:D:176:GLN:NE2	2.44	0.50
1:D:217:ARG:NH2	1:D:300:LEU:HD23	2.26	0.50
1:F:42:PRO:HD3	4:F:507:HOH:O	2.11	0.50
1:C:187:VAL:CG1	1:C:251:LYS:HG2	2.38	0.50
1:C:196:LYS:HD2	1:C:231:VAL:HG12	1.94	0.50
2:E:401:GO6:O02	3:E:402:NDP:H5N	2.12	0.50
1:C:280:ILE:CG2	1:C:286:LEU:HD12	2.32	0.50
1:D:19:GLY:CA	3:D:402:NDP:H51A	2.42	0.50
1:E:9:LYS:HD3	1:E:33:GLY:O	2.12	0.50
1:A:294:ASP:OD1	1:A:294:ASP:N	2.43	0.50
1:B:117:ARG:CZ	1:B:219:ILE:HB	2.42	0.50
1:B:189:ILE:CD1	1:B:235:MET:HE2	2.42	0.50
1:B:305:LYS:O	1:B:305:LYS:CD	2.59	0.50
1:D:235:MET:O	1:D:239:GLN:HG3	2.12	0.50
1:E:186:LYS:HD3	1:E:186:LYS:O	2.11	0.50
1:E:308:ARG:N	1:E:308:ARG:HD3	2.26	0.50
1:C:34:HIS:NE2	1:C:213:LEU:HD11	2.26	0.50
1:C:40:GLN:O	1:C:66:GLU:HA	2.11	0.50
1:C:226:ARG:O	1:C:226:ARG:HG3	2.11	0.50
1:E:199:TYR:CZ	1:E:237:LEU:HD22	2.46	0.50
1:F:21:MET:CE	1:F:25:ILE:HG13	2.41	0.50
1:C:13:LEU:HB2	1:C:82:VAL:HG11	1.94	0.50
1:F:110:LYS:HD3	1:F:111:GLU:HA	1.93	0.50
1:B:40:GLN:N	1:B:65:ILE:O	2.38	0.50
1:C:241:TRP:O	1:C:243:LYS:N	2.45	0.50
1:E:188:ASN:ND2	1:E:254:ILE:HD11	2.26	0.50
1:E:195:VAL:O	1:E:233:THR:HA	2.12	0.50
1:E:126:ASP:O	1:E:129:ARG:HG3	2.12	0.49
1:E:172:GLY:O	1:E:182:PRO:HD3	2.12	0.49
1:C:213:LEU:HD12	1:C:214:ASP:N	2.27	0.49
1:A:197:VAL:HG12	1:A:198:VAL:N	2.28	0.49
1:C:170:PHE:HE2	3:C:402:NDP:H71N	1.60	0.49
1:E:82:VAL:O	1:E:114:ASN:ND2	2.45	0.49
1:D:219:ILE:O	1:D:220:ASN:HB2	2.12	0.49
1:E:288:ASP:OD1	1:E:289:HIS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:VAL:HG13	1:F:156:ILE:CD1	2.42	0.49
1:D:129:ARG:O	1:D:130:MET:CB	2.60	0.49
1:F:89:MET:HE1	1:F:102:GLN:HG3	1.95	0.49
1:B:151:ILE:HG23	1:B:156:ILE:HB	1.95	0.49
1:D:15:VAL:HG12	1:D:89:MET:HE1	1.94	0.49
1:E:173:ASN:OD1	1:E:173:ASN:N	2.44	0.49
1:F:187:VAL:O	1:F:251:LYS:HA	2.13	0.49
1:B:167:ALA:CB	1:B:309:MET:HE1	2.36	0.49
1:B:173:ASN:OD1	1:B:173:ASN:N	2.32	0.49
1:A:182:PRO:HG2	1:A:316:PHE:HB3	1.95	0.49
1:C:191:GLY:N	1:C:254:ILE:O	2.30	0.49
1:D:257:ASN:O	1:D:260:LEU:HB2	2.13	0.49
1:E:198:VAL:HG21	1:E:226:ARG:HG3	1.95	0.49
1:C:166:PHE:H	3:C:402:NDP:H72N	1.61	0.48
1:E:271:GLN:HB3	1:E:274:LEU:HD13	1.93	0.48
1:E:296:GLU:OE2	1:E:297:ALA:N	2.46	0.48
1:F:57:TYR:HB3	1:F:62:ALA:HB3	1.95	0.48
1:F:110:LYS:HD3	1:F:111:GLU:CA	2.43	0.48
1:A:96:SER:O	1:A:99:ILE:HG12	2.13	0.48
1:A:99:ILE:HG13	1:A:100:LEU:HD22	1.95	0.48
1:C:167:ALA:N	1:C:200:VAL:O	2.46	0.48
1:B:218:THR:HA	1:B:221:LYS:CD	2.43	0.48
1:D:276:HIS:O	1:D:280:ILE:HG13	2.14	0.48
1:C:179:THR:O	1:C:180:LEU:HD23	2.13	0.48
1:E:125:MET:HE2	1:E:280:ILE:CG1	2.43	0.48
1:A:41:GLN:O	1:A:42:PRO:C	2.56	0.48
1:B:235:MET:O	1:B:239:GLN:CG	2.59	0.48
1:D:89:MET:O	3:D:402:NDP:H3D	2.13	0.48
1:A:166:PHE:H	3:A:402:NDP:H72N	1.62	0.48
1:A:278:TYR:HD2	1:A:282:TYR:CD2	2.31	0.48
1:C:254:ILE:N	1:C:254:ILE:HD12	2.28	0.48
1:E:196:LYS:CG	1:E:233:THR:HG22	2.33	0.48
1:A:9:LYS:H	1:D:63:ARG:NH2	2.12	0.48
1:B:307:THR:CG2	1:B:312:TYR:HB2	2.44	0.48
1:D:32:GLU:O	4:D:504:HOH:O	2.20	0.48
1:F:19:GLY:HA3	3:F:402:NDP:H52A	1.94	0.48
1:D:143:GLN:O	1:D:146:GLU:HB3	2.14	0.48
1:F:174:LEU:HD12	1:F:183:PRO:HD2	1.96	0.48
1:A:39:LEU:HD11	1:A:67:ALA:CB	2.23	0.48
1:A:46:VAL:HG12	1:A:46:VAL:O	2.13	0.48
1:B:76:VAL:O	1:B:80:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:PRO:HB3	1:B:306:TYR:CE2	2.49	0.48
1:D:122:GLU:OE2	4:D:503:HOH:O	2.20	0.48
1:E:40:GLN:HG3	1:E:64:LEU:HB3	1.96	0.48
1:F:227:PRO:HB3	1:F:306:TYR:CZ	2.49	0.48
1:F:302:PRO:C	1:F:304:VAL:H	2.22	0.48
1:F:304:VAL:HG12	1:F:304:VAL:O	2.13	0.48
1:A:218:THR:HA	1:A:221:LYS:HZ3	1.75	0.47
1:C:127:PRO:HG2	1:C:145:LEU:CD1	2.43	0.47
1:D:189:ILE:HA	1:D:234:GLN:OE1	2.14	0.47
1:D:49:GLU:OE1	1:E:23:ARG:NH2	2.46	0.47
1:A:76:VAL:HG12	1:A:80:LYS:HE3	1.96	0.47
1:A:222:THR:HG22	1:A:224:TYR:CE2	2.49	0.47
1:B:156:ILE:HG22	1:B:157:PRO:O	2.14	0.47
1:D:125:MET:SD	1:D:280:ILE:HD11	2.54	0.47
1:B:24:ARG:NH2	1:F:52:GLN:HE22	2.12	0.47
1:C:115:ILE:HD13	1:C:115:ILE:HA	1.70	0.47
1:C:182:PRO:HG2	1:C:241:TRP:CH2	2.50	0.47
1:D:212:THR:HA	1:D:301:TYR:OH	2.14	0.47
1:E:98:SER:O	1:E:101:VAL:HG22	2.15	0.47
1:C:233:THR:O	1:C:234:GLN:C	2.57	0.47
1:F:255:SER:O	1:F:256:ALA:C	2.57	0.47
1:A:14:VAL:N	1:A:37:TYR:O	2.36	0.47
1:A:71:ASP:CG	1:A:74:SER:HB3	2.39	0.47
1:B:171:ALA:CB	1:B:309:MET:CE	2.92	0.47
1:B:235:MET:O	1:B:239:GLN:NE2	2.44	0.47
1:C:170:PHE:HE1	1:C:277:PHE:CE1	2.33	0.47
1:D:19:GLY:HA3	3:D:402:NDP:H51A	1.96	0.47
1:D:87:ALA:HB3	1:D:102:GLN:OE1	2.15	0.47
1:D:299:LYS:O	1:D:302:PRO:HD3	2.15	0.47
1:F:23:ARG:HA	1:F:26:VAL:HG12	1.96	0.47
1:A:179:THR:O	1:A:180:LEU:HD23	2.15	0.47
1:C:116:LYS:O	1:C:157:PRO:HB2	2.14	0.47
1:C:233:THR:O	1:C:236:GLU:N	2.48	0.47
1:D:42:PRO:HG3	1:D:68:SER:HB2	1.95	0.47
1:D:128:SER:HA	1:D:145:LEU:HD22	1.97	0.47
1:A:42:PRO:HD2	1:A:67:ALA:O	2.15	0.47
1:D:15:VAL:HG12	1:D:89:MET:CE	2.44	0.47
1:D:277:PHE:HE1	2:D:401:GO6:C14	2.28	0.47
1:E:65:ILE:HG21	1:E:78:ALA:HA	1.97	0.47
1:A:126:ASP:OD1	1:A:128:SER:N	2.48	0.47
1:C:217:ARG:HH21	1:C:300:LEU:HB3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:GLN:HA	1:D:76:VAL:CG1	2.44	0.47
1:D:187:VAL:CG1	1:D:251:LYS:HA	2.43	0.47
1:D:249:LEU:N	1:D:249:LEU:HD22	2.30	0.47
1:F:112:ALA:CB	4:F:501:HOH:O	2.63	0.47
1:F:308:ARG:HG2	4:F:514:HOH:O	2.14	0.47
1:A:166:PHE:CE1	1:A:205:ILE:HD12	2.50	0.46
1:E:243:LYS:NZ	4:E:507:HOH:O	2.46	0.46
1:F:173:ASN:OD1	1:F:173:ASN:N	2.45	0.46
1:A:86:VAL:HG22	1:A:119:LEU:HB2	1.97	0.46
1:D:85:VAL:HG23	1:D:115:ILE:HD12	1.97	0.46
1:E:271:GLN:HG2	1:E:272:ALA:H	1.79	0.46
1:F:112:ALA:HB2	4:F:501:HOH:O	2.14	0.46
1:F:241:TRP:HB2	1:F:313:LEU:HD13	1.97	0.46
1:B:37:TYR:HD2	1:B:65:ILE:CD1	2.21	0.46
1:E:79:VAL:HB	1:E:115:ILE:HD11	1.96	0.46
1:E:147:VAL:O	1:E:151:ILE:HG13	2.15	0.46
1:A:191:GLY:N	1:A:254:ILE:O	2.29	0.46
1:B:303:ASP:OD1	1:B:303:ASP:N	2.48	0.46
1:D:308:ARG:O	1:D:310:ASP:N	2.48	0.46
1:D:57:TYR:O	1:D:60:LEU:N	2.45	0.46
1:D:69:PHE:CE2	3:D:402:NDP:H2A	2.50	0.46
1:E:127:PRO:HG3	1:E:144:LYS:HB2	1.96	0.46
1:F:271:GLN:HG2	1:F:272:ALA:N	2.30	0.46
1:B:189:ILE:HG21	1:B:235:MET:CE	2.45	0.46
1:C:11:ARG:HG3	1:C:35:GLU:HB3	1.97	0.46
1:C:102:GLN:HE21	1:C:118:PHE:HZ	1.61	0.46
1:F:39:LEU:HD11	1:F:67:ALA:HB3	1.97	0.46
1:F:84:ILE:HG21	1:F:213:LEU:HD13	1.97	0.46
1:F:92:VAL:HG13	1:F:93:HIS:N	2.30	0.46
1:F:125:MET:HG3	2:F:401:GO6:C25	2.45	0.46
1:F:243:LYS:NZ	4:F:506:HOH:O	2.20	0.46
1:A:247:LYS:HD2	1:A:248:GLU:N	2.31	0.46
1:B:117:ARG:HD3	1:B:159:THR:OG1	2.16	0.46
1:C:233:THR:HG23	1:C:236:GLU:H	1.80	0.46
1:E:167:ALA:HB2	1:E:200:VAL:O	2.15	0.46
1:E:257:ASN:OD1	1:E:257:ASN:N	2.48	0.46
1:A:276:HIS:O	1:A:277:PHE:C	2.59	0.46
1:E:100:LEU:O	1:E:103:LEU:HB2	2.16	0.46
1:F:95:ARG:HA	1:F:143:GLN:OE1	2.16	0.46
1:D:38:VAL:HG21	1:D:57:TYR:CD2	2.50	0.46
1:D:57:TYR:HB3	1:D:62:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:245:THR:HG22	1:E:317:LEU:CD2	2.46	0.46
1:B:177:MET:HE1	1:B:274:LEU:CD2	2.46	0.45
1:B:182:PRO:HG2	1:B:241:TRP:CZ2	2.51	0.45
1:B:288:ASP:OD2	1:B:289:HIS:CE1	2.69	0.45
1:C:30:LEU:HD11	1:C:62:ALA:HB2	1.98	0.45
1:C:177:MET:HE2	1:C:274:LEU:CD1	2.32	0.45
1:B:288:ASP:O	1:B:289:HIS:ND1	2.27	0.45
1:D:259:PHE:CZ	1:D:274:LEU:HD22	2.50	0.45
1:E:72:HIS:NE2	1:E:111:GLU:OE2	2.42	0.45
1:E:99:ILE:HD11	1:E:143:GLN:CB	2.47	0.45
1:F:32:GLU:HB3	1:F:34:HIS:CE1	2.51	0.45
1:F:166:PHE:CE1	1:F:205:ILE:HD13	2.51	0.45
1:A:142:ASP:CG	1:A:143:GLN:H	2.23	0.45
1:B:201:ASP:OD2	1:B:203:ASP:HB2	2.17	0.45
1:C:119:LEU:HD12	1:C:119:LEU:N	2.31	0.45
1:C:189:ILE:HA	1:C:234:GLN:OE1	2.17	0.45
1:C:256:ALA:O	1:C:260:LEU:HD23	2.17	0.45
1:F:193:GLY:O	1:F:233:THR:HB	2.17	0.45
1:A:19:GLY:HA3	3:A:402:NDP:H51A	1.99	0.45
1:B:292:GLY:H	1:B:295:GLU:CD	2.22	0.45
1:C:126:ASP:OD1	1:C:128:SER:N	2.42	0.45
1:F:279:HIS:C	1:F:283:GLU:HB2	2.41	0.45
1:B:89:MET:HE3	1:B:89:MET:HB2	1.57	0.45
1:F:54:LEU:HD23	1:F:54:LEU:HA	1.85	0.45
1:A:190:TYR:HB3	1:A:282:TYR:CZ	2.52	0.45
1:B:305:LYS:HB3	1:B:305:LYS:HE3	1.74	0.45
1:C:239:GLN:HA	1:C:242:GLU:HB2	1.99	0.45
1:C:306:TYR:CD2	1:C:308:ARG:NH1	2.85	0.45
1:D:44:THR:O	1:D:45:ARG:HB2	2.16	0.45
1:D:119:LEU:HD12	1:D:119:LEU:H	1.81	0.45
1:A:13:LEU:HA	1:A:37:TYR:O	2.17	0.45
1:D:117:ARG:HD3	1:D:159:THR:OG1	2.17	0.45
1:E:235:MET:O	1:E:239:GLN:CG	2.65	0.45
1:E:299:LYS:HD3	1:E:299:LYS:HA	1.81	0.45
1:F:110:LYS:O	1:F:112:ALA:N	2.50	0.45
1:A:166:PHE:HE1	1:A:205:ILE:HD12	1.80	0.45
1:C:174:LEU:HD12	1:C:183:PRO:HD2	1.98	0.45
1:A:125:MET:HG3	1:A:286:LEU:HD21	1.99	0.45
1:B:171:ALA:HB2	1:B:199:TYR:CD2	2.52	0.45
1:B:241:TRP:HZ3	1:B:313:LEU:O	2.00	0.45
1:C:45:ARG:HG3	1:C:47:ASP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:MET:HE2	1:B:271:GLN:NE2	2.32	0.44
1:D:117:ARG:NH1	1:D:159:THR:OG1	2.51	0.44
1:D:119:LEU:HD12	1:D:119:LEU:N	2.33	0.44
1:D:176:GLN:OE1	1:D:188:ASN:HB2	2.17	0.44
1:E:41:GLN:O	1:E:43:GLU:N	2.50	0.44
1:F:317:LEU:HD23	1:F:317:LEU:HA	1.73	0.44
1:C:125:MET:HG3	2:C:401:GO6:O03	2.16	0.44
1:D:37:TYR:HA	1:D:63:ARG:O	2.16	0.44
1:D:122:GLU:HB2	1:D:161:VAL:O	2.17	0.44
1:F:79:VAL:HG21	1:F:109:ILE:HA	1.98	0.44
1:F:89:MET:HE1	1:F:102:GLN:CG	2.48	0.44
1:F:279:HIS:HA	1:F:283:GLU:CB	2.43	0.44
1:F:284:GLY:O	1:F:286:LEU:N	2.51	0.44
1:B:170:PHE:O	1:B:175:SER:N	2.42	0.44
1:D:256:ALA:O	1:D:260:LEU:N	2.50	0.44
1:D:274:LEU:HD23	1:D:274:LEU:HA	1.69	0.44
1:A:161:VAL:HG21	1:A:209:THR:HG23	2.00	0.44
1:A:280:ILE:HG12	1:A:286:LEU:HG	2.00	0.44
1:B:212:THR:HA	1:B:301:TYR:OH	2.17	0.44
1:B:288:ASP:C	1:B:289:HIS:HD1	2.18	0.44
1:D:105:LEU:HD23	1:D:109:ILE:CD1	2.47	0.44
1:D:196:LYS:HD2	1:D:231:VAL:CG1	2.47	0.44
1:E:198:VAL:HG22	1:E:231:VAL:HG22	1.99	0.44
1:F:188:ASN:ND2	1:F:254:ILE:HD11	2.33	0.44
1:A:82:VAL:CG1	1:A:83:ASP:N	2.81	0.44
1:B:311:GLU:O	1:B:311:GLU:HG2	2.15	0.44
1:C:293:ASP:OD2	1:C:293:ASP:N	2.50	0.44
1:D:37:TYR:HD2	1:D:65:ILE:CD1	2.29	0.44
1:E:99:ILE:HD12	1:E:100:LEU:HD12	1.99	0.44
1:E:196:LYS:HD3	1:E:231:VAL:HG12	1.99	0.44
1:A:222:THR:CG2	1:A:224:TYR:CE2	3.01	0.44
1:B:84:ILE:HD13	1:B:213:LEU:HD12	1.99	0.44
1:B:241:TRP:C	1:B:243:LYS:N	2.76	0.44
1:B:276:HIS:O	1:B:280:ILE:HD12	2.18	0.44
1:F:89:MET:HA	3:F:402:NDP:O4B	2.18	0.44
1:F:116:LYS:N	1:F:116:LYS:HD3	2.32	0.44
1:A:257:ASN:C	1:A:259:PHE:N	2.76	0.44
1:C:75:LEU:CD1	1:C:104:LYS:HG3	2.47	0.44
1:C:164:ALA:HB2	1:C:225:VAL:HG13	2.00	0.44
1:D:122:GLU:CB	1:D:161:VAL:O	2.66	0.44
1:E:244:LEU:HD23	1:E:244:LEU:HA	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ASP:C	1:A:84:ILE:HG13	2.43	0.44
1:A:275:GLY:N	4:A:501:HOH:O	2.50	0.44
1:B:14:VAL:HA	1:B:86:VAL:O	2.18	0.44
1:C:176:GLN:OE1	1:C:188:ASN:HB2	2.17	0.44
1:E:255:SER:OG	1:E:258:ASP:OD2	2.36	0.44
1:C:100:LEU:CD2	1:C:146:GLU:HG2	2.47	0.43
1:C:241:TRP:O	1:C:242:GLU:C	2.61	0.43
1:D:50:LYS:HE2	1:D:50:LYS:HB2	1.86	0.43
1:D:186:LYS:HG2	1:D:250:GLU:OE1	2.18	0.43
1:D:216:PRO:O	1:D:219:ILE:HG22	2.17	0.43
1:D:221:LYS:HE3	1:D:221:LYS:HB3	1.77	0.43
1:E:229:GLU:CG	1:E:308:ARG:HH12	2.31	0.43
1:A:99:ILE:HD11	1:A:143:GLN:HB2	1.99	0.43
1:C:48:ILE:HD11	1:C:52:GLN:NE2	2.33	0.43
1:D:241:TRP:C	1:D:243:LYS:N	2.76	0.43
1:A:148:ARG:HD3	1:A:160:TYR:CE2	2.53	0.43
3:A:402:NDP:H6N	4:A:505:HOH:O	2.18	0.43
1:B:24:ARG:HH22	1:F:52:GLN:NE2	2.16	0.43
1:C:100:LEU:HD22	1:C:103:LEU:HD11	1.99	0.43
1:C:165:CYS:CB	1:C:198:VAL:O	2.64	0.43
1:C:271:GLN:O	1:C:274:LEU:HD13	2.18	0.43
1:D:71:ASP:O	1:D:74:SER:OG	2.35	0.43
1:E:308:ARG:HB2	1:E:310:ASP:OD1	2.18	0.43
1:E:311:GLU:O	1:E:312:TYR:C	2.61	0.43
1:F:53:LEU:O	1:F:54:LEU:C	2.62	0.43
1:B:51:VAL:O	1:B:55:TYR:HD1	2.02	0.43
1:B:174:LEU:HD11	1:B:241:TRP:CD1	2.53	0.43
1:B:187:VAL:O	1:B:251:LYS:HA	2.18	0.43
1:B:201:ASP:HB3	1:B:204:ASP:OD2	2.18	0.43
1:D:15:VAL:HB	1:D:87:ALA:HA	2.00	0.43
1:D:273:GLY:O	1:D:277:PHE:HD1	2.01	0.43
1:C:11:ARG:NH1	1:E:63:ARG:NE	2.65	0.43
1:C:235:MET:O	1:C:238:VAL:HG23	2.19	0.43
1:E:104:LYS:O	1:E:107:GLU:HB3	2.18	0.43
1:F:279:HIS:ND1	1:F:279:HIS:N	2.67	0.43
1:A:20:THR:O	1:A:24:ARG:NH1	2.51	0.43
1:A:227:PRO:HB3	1:A:306:TYR:CE1	2.53	0.43
1:A:230:ASN:ND2	1:A:307:THR:O	2.43	0.43
1:C:102:GLN:NE2	1:C:118:PHE:HZ	2.16	0.43
1:D:284:GLY:C	1:D:286:LEU:H	2.27	0.43
1:B:127:PRO:HG2	1:B:148:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:MET:HB2	1:B:235:MET:HE3	1.77	0.43
1:D:157:PRO:HB3	1:D:219:ILE:CD1	2.29	0.43
1:D:289:HIS:CG	1:D:289:HIS:O	2.72	0.43
1:C:120:PRO:HG3	1:C:160:TYR:CE2	2.53	0.43
1:D:224:TYR:O	1:D:297:ALA:N	2.36	0.43
1:E:238:VAL:O	1:E:242:GLU:HG3	2.18	0.43
1:A:76:VAL:O	1:A:80:LYS:HG3	2.19	0.43
1:B:126:ASP:OD1	1:B:128:SER:N	2.52	0.43
1:E:170:PHE:O	1:E:175:SER:N	2.52	0.43
1:E:247:LYS:HD2	1:E:248:GLU:N	2.33	0.43
1:F:308:ARG:HB2	1:F:310:ASP:OD1	2.19	0.43
1:A:42:PRO:HG2	1:A:68:SER:CB	2.37	0.43
1:A:147:VAL:O	1:A:151:ILE:HG13	2.19	0.43
1:B:128:SER:HB3	1:B:148:ARG:HH12	1.84	0.43
1:D:48:ILE:HA	1:D:48:ILE:HD12	1.77	0.43
1:D:217:ARG:CZ	1:D:300:LEU:HD23	2.49	0.43
1:F:290:GLU:HA	1:F:290:GLU:OE2	2.19	0.43
1:A:100:LEU:HD13	1:A:100:LEU:HA	1.79	0.42
1:B:142:ASP:OD2	1:B:144:LYS:HG3	2.20	0.42
1:C:150:ALA:O	1:C:151:ILE:C	2.61	0.42
1:D:274:LEU:HA	1:D:277:PHE:HB2	2.01	0.42
1:E:51:VAL:O	1:E:55:TYR:HD1	2.02	0.42
1:F:98:SER:O	1:F:101:VAL:HG13	2.19	0.42
1:F:305:LYS:HE3	1:F:305:LYS:HB3	1.83	0.42
1:C:71:ASP:O	1:C:74:SER:OG	2.36	0.42
1:C:100:LEU:C	1:C:103:LEU:HD13	2.43	0.42
1:E:109:ILE:HG23	1:E:115:ILE:CG1	2.46	0.42
1:E:197:VAL:HG12	1:E:198:VAL:N	2.33	0.42
1:A:54:LEU:HD23	1:A:54:LEU:HA	1.69	0.42
1:A:57:TYR:HB3	1:A:62:ALA:HB3	2.02	0.42
1:C:175:SER:O	1:C:190:TYR:OH	2.34	0.42
1:D:215:ASP:HB3	1:D:218:THR:OG1	2.19	0.42
1:D:306:TYR:CD1	1:D:308:ARG:HD2	2.54	0.42
1:E:45:ARG:HA	1:E:45:ARG:HE	1.82	0.42
1:F:236:GLU:O	1:F:240:ILE:HG13	2.19	0.42
1:A:105:LEU:HD12	1:A:109:ILE:HG13	2.01	0.42
1:F:79:VAL:O	1:F:82:VAL:HG22	2.19	0.42
1:B:16:GLY:HA2	3:B:402:NDP:O2B	2.19	0.42
1:B:46:VAL:O	1:B:46:VAL:HG12	2.19	0.42
1:B:89:MET:O	3:B:402:NDP:H52N	2.20	0.42
1:B:179:THR:OG1	1:B:180:LEU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ALA:O	1:B:262:ASP:C	2.62	0.42
1:D:257:ASN:OD1	1:D:257:ASN:N	2.52	0.42
1:E:174:LEU:HD12	1:E:183:PRO:HD2	2.00	0.42
1:B:173:ASN:ND2	1:B:176:GLN:O	2.52	0.42
1:B:285:CYS:HA	1:B:288:ASP:OD1	2.19	0.42
1:B:293:ASP:CG	1:B:299:LYS:HG3	2.45	0.42
1:C:23:ARG:HE	1:C:23:ARG:HB3	1.67	0.42
1:D:12:VAL:HG11	1:D:29:CYS:SG	2.59	0.42
1:D:308:ARG:HB3	1:D:310:ASP:OD1	2.19	0.42
1:E:142:ASP:CG	1:E:144:LYS:HG3	2.45	0.42
1:A:233:THR:OG1	1:A:236:GLU:HG3	2.19	0.42
1:F:202:GLU:OE1	1:F:202:GLU:N	2.39	0.42
1:A:80:LYS:HA	1:A:114:ASN:OD1	2.19	0.42
1:C:12:VAL:HG11	1:C:29:CYS:SG	2.60	0.42
1:E:16:GLY:O	1:E:22:GLY:HA3	2.19	0.42
1:E:171:ALA:HA	1:E:237:LEU:HD21	2.02	0.42
1:E:271:GLN:CG	1:E:272:ALA:H	2.32	0.42
1:B:234:GLN:HB2	1:B:281:PHE:HE1	1.84	0.42
1:B:241:TRP:O	1:B:242:GLU:C	2.63	0.42
1:C:272:ALA:O	1:C:273:GLY:C	2.63	0.42
1:D:173:ASN:O	1:D:174:LEU:HB2	2.20	0.42
1:E:310:ASP:O	1:E:314:LYS:HG3	2.18	0.42
1:F:227:PRO:HB3	1:F:306:TYR:CE2	2.54	0.42
1:A:244:LEU:HD23	1:A:244:LEU:HA	1.88	0.42
1:B:39:LEU:HD12	1:B:39:LEU:HA	1.62	0.42
1:C:117:ARG:HD3	1:C:159:THR:OG1	2.20	0.42
1:D:177:MET:HE3	1:D:277:PHE:CZ	2.55	0.42
1:B:195:VAL:HG21	1:B:281:PHE:HA	2.02	0.41
1:C:13:LEU:HB3	1:C:82:VAL:HG21	2.02	0.41
1:C:18:THR:CG2	1:C:54:LEU:HG	2.50	0.41
1:D:109:ILE:HG23	1:D:115:ILE:CG1	2.49	0.41
1:D:124:GLY:HA3	2:D:401:GO6:O05	2.20	0.41
1:D:186:LYS:HZ3	1:F:274:LEU:HD21	1.83	0.41
1:D:241:TRP:O	1:D:244:LEU:N	2.52	0.41
1:E:47:ASP:OD2	1:E:50:LYS:HE3	2.20	0.41
1:E:235:MET:HB2	1:E:235:MET:HE2	1.69	0.41
1:F:72:HIS:HE2	1:F:111:GLU:CD	2.18	0.41
1:F:89:MET:HB2	1:F:89:MET:HE3	1.55	0.41
1:F:189:ILE:HG13	1:F:235:MET:HE1	2.02	0.41
1:A:21:MET:HE3	1:A:25:ILE:HG13	2.02	0.41
1:A:72:HIS:O	1:A:76:VAL:HG23	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:ALA:HB2	1:B:199:TYR:HD2	1.85	0.41
1:B:284:GLY:O	1:B:286:LEU:N	2.53	0.41
1:D:10:THR:OG1	1:D:34:HIS:CD2	2.73	0.41
1:D:21:MET:HE1	1:D:206:ALA:HB2	1.99	0.41
1:E:106:VAL:HG11	1:E:150:ALA:HB1	2.02	0.41
1:E:222:THR:HG22	1:E:224:TYR:CE2	2.54	0.41
1:F:131:GLY:HA2	4:F:510:HOH:O	2.20	0.41
1:F:224:TYR:CG	1:F:291:VAL:HG11	2.54	0.41
1:C:202:GLU:OE1	1:C:202:GLU:N	2.34	0.41
1:D:166:PHE:HB2	3:D:402:NDP:N7N	2.35	0.41
1:F:84:ILE:HD13	1:F:213:LEU:CD1	2.50	0.41
1:A:218:THR:HA	1:A:221:LYS:HZ2	1.82	0.41
1:B:174:LEU:HD21	1:B:241:TRP:HB2	2.02	0.41
1:C:11:ARG:NH1	1:E:63:ARG:CZ	2.83	0.41
1:C:278:TYR:CD1	1:C:282:TYR:CD2	3.07	0.41
1:E:42:PRO:O	1:E:43:GLU:C	2.63	0.41
1:F:215:ASP:OD1	1:F:217:ARG:NE	2.51	0.41
1:C:129:ARG:NH2	1:C:285:CYS:O	2.54	0.41
1:C:186:LYS:HE3	1:C:186:LYS:HB3	1.91	0.41
1:D:121:SER:OG	3:D:402:NDP:O3D	2.33	0.41
1:E:189:ILE:HA	1:E:234:GLN:OE1	2.20	0.41
1:F:119:LEU:HD21	1:F:159:THR:HB	2.02	0.41
1:A:16:GLY:HA2	3:A:402:NDP:P2B	2.60	0.41
1:B:67:ALA:HA	1:B:74:SER:HB2	2.01	0.41
1:B:201:ASP:O	1:B:204:ASP:HB2	2.21	0.41
1:C:164:ALA:HB2	1:C:225:VAL:CG1	2.49	0.41
1:E:13:LEU:HB3	1:E:82:VAL:HG21	2.03	0.41
1:E:53:LEU:O	1:E:54:LEU:C	2.63	0.41
1:E:57:TYR:O	1:E:62:ALA:HB3	2.20	0.41
1:F:21:MET:HE1	1:F:206:ALA:HB2	2.02	0.41
1:F:172:GLY:O	1:F:182:PRO:HD3	2.20	0.41
1:B:122:GLU:O	1:B:122:GLU:CG	2.68	0.41
1:E:221:LYS:HE3	1:E:221:LYS:HB3	1.76	0.41
1:F:102:GLN:HE21	1:F:102:GLN:HB2	1.76	0.41
1:A:240:ILE:O	1:A:244:LEU:HG	2.21	0.41
1:C:166:PHE:CD2	3:C:402:NDP:H41N	2.56	0.41
1:D:170:PHE:HE1	1:D:277:PHE:CZ	2.39	0.41
1:D:180:LEU:HD13	1:E:48:ILE:CD1	2.50	0.41
1:E:43:GLU:HG3	4:E:513:HOH:O	2.20	0.41
1:F:45:ARG:HG3	1:F:46:VAL:H	1.86	0.41
1:F:89:MET:O	3:F:402:NDP:H52N	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ARG:NH2	1:A:219:ILE:HB	2.36	0.41
1:B:180:LEU:HD11	1:F:46:VAL:HG13	2.03	0.41
1:B:192:ASP:CG	1:B:194:ASN:HD22	2.18	0.41
1:B:206:ALA:O	1:B:210:ALA:N	2.53	0.41
1:C:49:GLU:O	1:C:53:LEU:HB2	2.21	0.41
1:C:143:GLN:O	1:C:146:GLU:HB3	2.20	0.41
1:C:166:PHE:HE1	1:C:205:ILE:HD13	1.86	0.41
1:D:129:ARG:NH2	1:D:285:CYS:O	2.54	0.41
1:D:159:THR:HG21	1:D:212:THR:HG21	2.02	0.41
1:D:190:TYR:HB3	1:D:282:TYR:CZ	2.55	0.41
1:D:212:THR:O	1:D:214:ASP:N	2.54	0.41
1:F:116:LYS:N	1:F:116:LYS:CD	2.84	0.41
1:B:232:LEU:HB3	1:B:236:GLU:CB	2.51	0.41
1:C:284:GLY:O	1:C:286:LEU:N	2.54	0.41
1:D:11:ARG:HH21	1:D:82:VAL:N	2.18	0.41
1:D:49:GLU:O	1:D:53:LEU:HB2	2.21	0.41
1:D:89:MET:HB3	1:D:98:SER:OG	2.21	0.41
1:E:12:VAL:HG22	1:E:84:ILE:HB	2.03	0.41
1:E:308:ARG:HD3	1:E:308:ARG:H	1.86	0.41
1:A:19:GLY:CA	3:A:402:NDP:H52A	2.50	0.40
1:C:19:GLY:HA2	3:C:402:NDP:H51A	2.03	0.40
1:C:120:PRO:HB3	1:C:151:ILE:HD11	2.03	0.40
1:D:73:GLN:CA	1:D:76:VAL:HG12	2.48	0.40
1:D:142:ASP:HA	4:D:510:HOH:O	2.21	0.40
1:E:80:LYS:HZ2	1:E:80:LYS:HB3	1.86	0.40
1:F:79:VAL:HG11	1:F:105:LEU:HD11	2.02	0.40
1:F:126:ASP:OD1	1:F:128:SER:N	2.46	0.40
1:B:306:TYR:CZ	1:B:308:ARG:NH1	2.89	0.40
1:C:34:HIS:CD2	4:C:504:HOH:O	2.73	0.40
1:C:159:THR:CG2	1:C:223:VAL:HG23	2.52	0.40
1:C:271:GLN:O	1:C:272:ALA:C	2.65	0.40
1:C:309:MET:HE2	1:C:309:MET:N	2.36	0.40
1:C:317:LEU:HD23	1:C:317:LEU:HA	1.91	0.40
1:D:105:LEU:HD23	1:D:105:LEU:C	2.47	0.40
1:F:158:HIS:NE2	1:F:160:TYR:CE1	2.89	0.40
1:C:9:LYS:HE2	1:C:9:LYS:HB3	1.79	0.40
1:C:308:ARG:O	1:C:311:GLU:N	2.47	0.40
1:C:309:MET:HA	1:C:309:MET:CE	2.45	0.40
1:D:252:THR:HG21	1:F:271:GLN:CA	2.51	0.40
1:E:41:GLN:O	1:E:42:PRO:C	2.62	0.40
1:E:103:LEU:HD23	1:E:103:LEU:HA	1.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:VAL:O	1:F:80:LYS:HB2	2.22	0.40
1:B:229:GLU:OE1	1:B:308:ARG:HD2	2.21	0.40
1:D:39:LEU:HD12	1:D:39:LEU:HA	1.94	0.40
1:D:41:GLN:NE2	3:D:402:NDP:O2X	2.54	0.40
1:D:317:LEU:HA	1:D:317:LEU:HD23	1.68	0.40
1:E:290:GLU:OE1	1:E:290:GLU:HA	2.22	0.40
1:A:197:VAL:CG1	1:A:198:VAL:N	2.85	0.40
1:C:151:ILE:HG23	1:C:156:ILE:HB	2.02	0.40
1:C:233:THR:HG23	1:C:236:GLU:HB2	2.03	0.40
1:D:186:LYS:NZ	1:F:274:LEU:HD21	2.36	0.40
1:E:89:MET:O	3:E:402:NDP:O5D	2.39	0.40
1:E:120:PRO:HG3	1:E:160:TYR:CE1	2.57	0.40
1:E:198:VAL:CG2	1:E:226:ARG:HG3	2.51	0.40
1:F:99:ILE:O	1:F:102:GLN:HB2	2.22	0.40
1:F:158:HIS:O	1:F:220:ASN:N	2.51	0.40

There are no symmetry-related clashes.

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	282/317 (89%)	246 (87%)	30 (11%)	6 (2%)	5	11
1	B	282/317 (89%)	251 (89%)	26 (9%)	5 (2%)	6	14
1	C	280/317 (88%)	239 (85%)	33 (12%)	8 (3%)	3	6
1	D	278/317 (88%)	237 (85%)	36 (13%)	5 (2%)	6	14
1	E	280/317 (88%)	248 (89%)	26 (9%)	6 (2%)	5	11
1	F	288/317 (91%)	254 (88%)	27 (9%)	7 (2%)	4	9
All	All	1690/1902 (89%)	1475 (87%)	178 (10%)	37 (2%)	5	10

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	PRO
1	A	43	GLU
1	B	122	GLU
1	B	242	GLU
1	D	242	GLU
1	D	285	CYS
1	F	35	GLU
1	F	256	ALA
1	A	272	ALA
1	A	273	GLY
1	B	241	TRP
1	C	242	GLU
1	C	273	GLY
1	C	306	TYR
1	D	35	GLU
1	F	129	ARG
1	F	271	GLN
1	C	35	GLU
1	D	289	HIS
1	E	129	ARG
1	E	130	MET
1	A	295	GLU
1	B	272	ALA
1	B	306	TYR
1	C	153	ALA
1	C	256	ALA
1	E	42	PRO
1	E	228	THR
1	F	45	ARG
1	C	42	PRO
1	D	45	ARG
1	A	256	ALA
1	F	47	ASP
1	F	42	PRO
1	C	120	PRO
1	E	26	VAL
1	E	157	PRO

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	247/271 (91%)	230 (93%)	17 (7%)	14	32
1	B	247/271 (91%)	215 (87%)	32 (13%)	4	8
1	C	246/271 (91%)	220 (89%)	26 (11%)	6	14
1	D	245/271 (90%)	230 (94%)	15 (6%)	17	37
1	E	245/271 (90%)	218 (89%)	27 (11%)	6	13
1	F	251/271 (93%)	228 (91%)	23 (9%)	8	19
All	All	1481/1626 (91%)	1341 (90%)	140 (10%)	8	18

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	10	THR
1	A	44	THR
1	A	45	ARG
1	A	48	ILE
1	A	77	SER
1	A	79	VAL
1	A	82	VAL
1	A	90	SER
1	A	97	HIS
1	A	125	MET
1	A	129	ARG
1	A	187	VAL
1	A	195	VAL
1	A	270	HIS
1	A	279	HIS
1	A	315	ILE
1	B	8	GLU
1	B	10	THR
1	B	40	GLN
1	B	45	ARG
1	B	46	VAL
1	B	65	ILE
1	B	96	SER
1	B	97	HIS
1	B	100	LEU
1	B	128	SER

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Mol	Chain	Res	Type
1	B	129	ARG
1	B	130	MET
1	B	142	ASP
1	B	145	LEU
1	B	161	VAL
1	B	165	CYS
1	B	173	ASN
1	B	179	THR
1	B	181	ILE
1	B	190	TYR
1	B	197	VAL
1	B	212	THR
1	B	219	ILE
1	B	232	LEU
1	B	235	MET
1	B	236	GLU
1	B	249	LEU
1	B	251	LYS
1	B	252	THR
1	B	257	ASN
1	B	258	ASP
1	B	305	LYS
1	C	9	LYS
1	C	13	LEU
1	C	20	THR
1	C	35	GLU
1	C	42	PRO
1	C	43	GLU
1	C	53	LEU
1	C	70	SER
1	C	90	SER
1	C	96	SER
1	C	103	LEU
1	C	115	ILE
1	C	143	GLN
1	C	165	CYS
1	C	212	THR
1	C	233	THR
1	C	258	ASP
1	C	260	LEU
1	C	270	HIS
1	C	274	LEU

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Mol	Chain	Res	Type
1	C	279	HIS
1	C	287	THR
1	C	290	GLU
1	C	303	ASP
1	C	311	GLU
1	C	315	ILE
1	D	11	ARG
1	D	41	GLN
1	D	43	GLU
1	D	44	THR
1	D	49	GLU
1	D	53	LEU
1	D	70	SER
1	D	165	CYS
1	D	212	THR
1	D	248	GLU
1	D	250	GLU
1	D	260	LEU
1	D	299	LYS
1	D	303	ASP
1	D	315	ILE
1	E	10	THR
1	E	42	PRO
1	E	43	GLU
1	E	44	THR
1	E	45	ARG
1	E	53	LEU
1	E	56	SER
1	E	74	SER
1	E	82	VAL
1	E	102	GLN
1	E	106	VAL
1	E	111	GLU
1	E	129	ARG
1	E	165	CYS
1	E	173	ASN
1	E	192	ASP
1	E	194	ASN
1	E	195	VAL
1	E	232	LEU
1	E	233	THR
1	E	234	GLN

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Mol	Chain	Res	Type
1	E	243	LYS
1	E	257	ASN
1	E	262	ASP
1	E	303	ASP
1	E	305	LYS
1	E	308	ARG
1	F	8	GLU
1	F	9	LYS
1	F	10	THR
1	F	32	GLU
1	F	44	THR
1	F	56	SER
1	F	68	SER
1	F	73	GLN
1	F	77	SER
1	F	89	MET
1	F	100	LEU
1	F	101	VAL
1	F	102	GLN
1	F	125	MET
1	F	129	ARG
1	F	212	THR
1	F	219	ILE
1	F	222	THR
1	F	232	LEU
1	F	279	HIS
1	F	290	GLU
1	F	296	GLU
1	F	298	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	253	ASN
1	B	270	HIS
1	C	52	GLN
1	D	34	HIS
1	E	40	GLN
1	E	149	ASN
1	E	188	ASN
1	F	41	GLN
1	F	93	HIS

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Mol	Chain	Res	Type
1	F	239	GLN

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 oligosaccharides 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	NDP	F	402	-	51,52,52	3.60	26 (50%)	71,80,80	2.04	16 (22%)
2	GO6	F	401	-	27,27,27	0.98	2 (7%)	32,36,36	1.42	4 (12%)
2	GO6	D	401	-	27,27,27	1.03	3 (11%)	32,36,36	1.26	3 (9%)
2	GO6	E	401	-	27,27,27	1.08	2 (7%)	32,36,36	1.27	3 (9%)
2	GO6	A	401	-	27,27,27	1.01	2 (7%)	32,36,36	1.36	6 (18%)
3	NDP	D	402	-	51,52,52	3.76	23 (45%)	71,80,80	2.05	18 (25%)
3	NDP	C	402	-	51,52,52	3.83	24 (47%)	71,80,80	2.06	13 (18%)
3	NDP	B	402	-	51,52,52	3.70	25 (49%)	71,80,80	1.97	14 (19%)
2	GO6	C	401	-	27,27,27	1.04	3 (11%)	32,36,36	1.14	4 (12%)
3	NDP	A	402	-	51,52,52	3.90	26 (50%)	71,80,80	2.06	13 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GO6	B	401	-	27,27,27	0.99	2 (7%)	32,36,36	1.13	4 (12%)
3	NDP	E	402	-	51,52,52	3.74	23 (45%)	71,80,80	2.08	18 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	F	402	-	-	8/34/77/77	0/5/5/5
2	GO6	F	401	-	-	10/20/20/20	0/2/2/2
2	GO6	D	401	-	-	8/20/20/20	0/2/2/2
2	GO6	E	401	-	-	10/20/20/20	0/2/2/2
2	GO6	A	401	-	-	11/20/20/20	0/2/2/2
3	NDP	D	402	-	-	12/34/77/77	0/5/5/5
3	NDP	C	402	-	-	9/34/77/77	0/5/5/5
3	NDP	B	402	-	-	12/34/77/77	0/5/5/5
2	GO6	C	401	-	-	15/20/20/20	0/2/2/2
3	NDP	A	402	-	-	13/34/77/77	0/5/5/5
2	GO6	B	401	-	-	9/20/20/20	0/2/2/2
3	NDP	E	402	-	-	13/34/77/77	0/5/5/5

All (161) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	402	NDP	C2B-C1B	-9.64	1.29	1.53
3	A	402	NDP	O4D-C1D	9.50	1.64	1.42
3	A	402	NDP	C2B-C1B	-9.35	1.30	1.53
3	A	402	NDP	O4B-C1B	9.31	1.63	1.42
3	C	402	NDP	C2B-C1B	-9.15	1.30	1.53
3	D	402	NDP	C2B-C1B	-9.10	1.30	1.53
3	E	402	NDP	O4D-C1D	9.03	1.62	1.42
3	B	402	NDP	O4B-C1B	9.01	1.62	1.42
3	F	402	NDP	O4D-C1D	8.95	1.62	1.42
3	C	402	NDP	O4B-C1B	8.93	1.62	1.42
3	C	402	NDP	O4D-C1D	8.76	1.62	1.42
3	E	402	NDP	O4B-C1B	8.64	1.62	1.42
3	B	402	NDP	C2B-C1B	-8.55	1.32	1.53
3	B	402	NDP	O4D-C1D	8.50	1.61	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	NDP	O4D-C1D	8.45	1.61	1.42
3	A	402	NDP	PA-O3	8.43	1.68	1.59
3	C	402	NDP	PA-O3	8.40	1.68	1.59
3	F	402	NDP	O4B-C1B	8.30	1.61	1.42
3	D	402	NDP	O4B-C1B	8.27	1.61	1.42
3	E	402	NDP	PA-O3	7.80	1.67	1.59
3	E	402	NDP	C2D-C1D	-7.58	1.29	1.53
3	D	402	NDP	PN-O3	7.57	1.67	1.59
3	F	402	NDP	C2D-C1D	-7.56	1.29	1.53
3	B	402	NDP	C2D-C1D	-7.53	1.29	1.53
3	E	402	NDP	C6N-C5N	7.32	1.55	1.33
3	B	402	NDP	PA-O3	7.29	1.67	1.59
3	A	402	NDP	C6N-C5N	7.23	1.55	1.33
3	A	402	NDP	C2D-C1D	-7.23	1.30	1.53
3	F	402	NDP	C2B-C1B	-7.21	1.35	1.53
3	C	402	NDP	C2D-C1D	-7.05	1.31	1.53
3	A	402	NDP	PN-O3	7.03	1.67	1.59
3	C	402	NDP	C6N-C5N	6.97	1.54	1.33
3	B	402	NDP	C6N-C5N	6.95	1.54	1.33
3	D	402	NDP	C2D-C1D	-6.95	1.31	1.53
3	F	402	NDP	C6N-C5N	6.93	1.54	1.33
3	D	402	NDP	C6N-C5N	6.88	1.54	1.33
3	D	402	NDP	O4B-C4B	-6.86	1.29	1.45
3	D	402	NDP	PA-O3	6.80	1.66	1.59
3	C	402	NDP	PN-O3	6.74	1.66	1.59
3	B	402	NDP	O4D-C4D	-6.72	1.30	1.45
3	D	402	NDP	O4D-C4D	-6.70	1.30	1.45
3	F	402	NDP	O4D-C4D	-6.65	1.30	1.45
3	C	402	NDP	O4B-C4B	-6.46	1.30	1.45
3	C	402	NDP	O4D-C4D	-6.41	1.30	1.45
3	A	402	NDP	O4B-C4B	-6.36	1.30	1.45
3	C	402	NDP	C2N-C3N	6.32	1.52	1.35
3	E	402	NDP	PN-O3	6.31	1.66	1.59
3	F	402	NDP	O4B-C4B	-6.24	1.31	1.45
3	E	402	NDP	O4D-C4D	-6.21	1.31	1.45
3	B	402	NDP	C2N-C3N	6.17	1.52	1.35
3	B	402	NDP	O4B-C4B	-6.05	1.31	1.45
3	D	402	NDP	C2N-C3N	6.02	1.51	1.35
3	A	402	NDP	O4D-C4D	-5.88	1.31	1.45
3	A	402	NDP	C2N-C3N	5.87	1.51	1.35
3	E	402	NDP	O4B-C4B	-5.86	1.32	1.45
3	F	402	NDP	C2N-C3N	5.66	1.50	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	NDP	C6A-N6A	5.65	1.48	1.34
3	F	402	NDP	PA-O3	5.51	1.65	1.59
3	F	402	NDP	PN-O3	5.44	1.65	1.59
3	E	402	NDP	C2N-C3N	5.44	1.50	1.35
3	B	402	NDP	C6A-N6A	5.33	1.47	1.34
3	E	402	NDP	C6A-N6A	5.31	1.47	1.34
3	F	402	NDP	C6A-N6A	5.21	1.47	1.34
3	C	402	NDP	C6A-N6A	5.20	1.47	1.34
3	B	402	NDP	PN-O3	4.97	1.64	1.59
3	D	402	NDP	C6A-N6A	4.94	1.46	1.34
3	A	402	NDP	C7N-N7N	4.62	1.46	1.33
3	E	402	NDP	C7N-N7N	4.34	1.46	1.33
3	B	402	NDP	C7N-N7N	4.16	1.45	1.33
3	C	402	NDP	C7N-N7N	4.11	1.45	1.33
3	F	402	NDP	P2B-O2B	4.07	1.66	1.59
3	D	402	NDP	C7N-N7N	3.96	1.44	1.33
3	F	402	NDP	C7N-N7N	3.76	1.44	1.33
3	C	402	NDP	C7N-C3N	3.54	1.56	1.48
3	D	402	NDP	C7N-C3N	3.52	1.56	1.48
3	B	402	NDP	C4N-C5N	3.31	1.57	1.49
3	D	402	NDP	C4N-C5N	3.31	1.57	1.49
3	A	402	NDP	C6N-N1N	3.31	1.45	1.37
3	E	402	NDP	C6N-N1N	3.29	1.45	1.37
3	F	402	NDP	O3B-C3B	-3.29	1.34	1.43
3	D	402	NDP	C4N-C3N	3.24	1.56	1.50
3	D	402	NDP	O2D-C2D	3.19	1.50	1.43
3	C	402	NDP	C4N-C5N	3.18	1.57	1.49
3	B	402	NDP	C5A-N7A	-3.16	1.33	1.39
3	F	402	NDP	O3D-C3D	-3.15	1.35	1.43
3	B	402	NDP	C7N-C3N	3.15	1.55	1.48
3	D	402	NDP	P2B-O2B	3.11	1.65	1.59
3	C	402	NDP	P2B-O2B	3.10	1.65	1.59
3	B	402	NDP	O3B-C3B	-3.07	1.35	1.43
3	F	402	NDP	C5A-C4A	-3.06	1.33	1.39
3	A	402	NDP	O2D-C2D	3.06	1.50	1.43
3	B	402	NDP	C5A-C4A	-3.05	1.33	1.39
3	B	402	NDP	O3D-C3D	-3.02	1.35	1.43
3	A	402	NDP	O3B-C3B	-2.99	1.35	1.43
3	C	402	NDP	C4N-C3N	2.99	1.55	1.50
2	D	401	GO6	O04-C20	2.92	1.41	1.37
3	A	402	NDP	O3D-C3D	-2.91	1.35	1.43
3	A	402	NDP	C4N-C5N	2.90	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	NDP	O3B-C3B	-2.89	1.35	1.43
3	A	402	NDP	C7N-C3N	2.89	1.54	1.48
3	F	402	NDP	O2D-C2D	2.85	1.50	1.43
3	F	402	NDP	C4N-C5N	2.85	1.56	1.49
3	A	402	NDP	C5A-C4A	-2.84	1.34	1.39
3	C	402	NDP	O3D-C3D	-2.83	1.35	1.43
3	D	402	NDP	O3D-C3D	-2.82	1.36	1.43
3	C	402	NDP	O3B-C3B	-2.82	1.36	1.43
3	F	402	NDP	C8A-N9A	-2.81	1.32	1.37
3	F	402	NDP	C5A-N7A	-2.81	1.34	1.39
3	C	402	NDP	C6N-N1N	2.80	1.44	1.37
3	E	402	NDP	C4N-C5N	2.76	1.56	1.49
3	A	402	NDP	P2B-O2B	2.75	1.64	1.59
3	D	402	NDP	C6N-N1N	2.75	1.43	1.37
3	D	402	NDP	C5A-N7A	-2.74	1.34	1.39
3	C	402	NDP	C5A-C4A	-2.73	1.34	1.39
3	B	402	NDP	C6N-N1N	2.72	1.43	1.37
2	E	401	GO6	O03-C19	2.71	1.41	1.37
3	B	402	NDP	O2D-C2D	2.70	1.49	1.43
3	C	402	NDP	O2D-C2D	2.68	1.49	1.43
3	C	402	NDP	C5A-N7A	-2.66	1.34	1.39
3	E	402	NDP	O3B-C3B	-2.63	1.36	1.43
3	D	402	NDP	C5A-C4A	-2.63	1.34	1.39
2	F	401	GO6	O05-C23	2.60	1.41	1.36
3	A	402	NDP	C8A-N9A	-2.59	1.33	1.37
3	F	402	NDP	O7N-C7N	-2.57	1.18	1.24
3	E	402	NDP	O3D-C3D	-2.56	1.36	1.43
3	F	402	NDP	C6N-N1N	2.54	1.43	1.37
2	E	401	GO6	O06-C24	2.46	1.41	1.36
2	B	401	GO6	O03-C19	2.45	1.41	1.37
3	E	402	NDP	C5A-C4A	-2.44	1.34	1.39
3	F	402	NDP	C7N-C3N	2.43	1.53	1.48
3	F	402	NDP	C4N-C3N	2.43	1.54	1.50
3	E	402	NDP	C5D-C4D	2.43	1.58	1.51
3	E	402	NDP	O2D-C2D	2.42	1.49	1.43
3	E	402	NDP	O7N-C7N	-2.38	1.18	1.24
2	C	401	GO6	O03-C19	2.34	1.41	1.37
3	B	402	NDP	P2B-O2B	2.34	1.63	1.59
2	A	401	GO6	O03-C19	2.27	1.40	1.37
3	B	402	NDP	C8A-N9A	-2.27	1.33	1.37
3	E	402	NDP	C8A-N9A	-2.26	1.33	1.37
2	D	401	GO6	O06-C24	2.26	1.40	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	402	NDP	C4N-C3N	2.26	1.54	1.50
3	E	402	NDP	PN-O5D	2.26	1.68	1.59
3	E	402	NDP	P2B-O2B	2.24	1.63	1.59
2	A	401	GO6	O05-C23	2.21	1.40	1.36
3	A	402	NDP	C4N-C3N	2.21	1.54	1.50
3	A	402	NDP	C5D-C4D	2.21	1.58	1.51
3	C	402	NDP	O7N-C7N	-2.18	1.19	1.24
3	A	402	NDP	C5A-N7A	-2.17	1.35	1.39
2	C	401	GO6	O05-C23	2.17	1.40	1.36
2	D	401	GO6	O05-C23	2.17	1.40	1.36
3	F	402	NDP	PN-O5D	2.16	1.67	1.59
3	A	402	NDP	O7N-C7N	-2.15	1.19	1.24
3	C	402	NDP	C8A-N9A	-2.14	1.33	1.37
2	B	401	GO6	O05-C23	2.08	1.40	1.36
2	C	401	GO6	O06-C24	2.07	1.40	1.36
2	F	401	GO6	O03-C19	2.05	1.40	1.37
3	D	402	NDP	C8A-N9A	-2.05	1.34	1.37
3	F	402	NDP	O2B-C2B	2.04	1.51	1.44
3	B	402	NDP	O7N-C7N	-2.02	1.19	1.24
3	B	402	NDP	C5D-C4D	2.00	1.57	1.51
3	A	402	NDP	PN-O5D	2.00	1.67	1.59

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	NDP	C4A-N9A-C1B	-6.46	111.52	126.63
3	E	402	NDP	C4A-N9A-C1B	-6.23	112.06	126.63
3	A	402	NDP	C4A-N9A-C1B	-6.21	112.12	126.63
3	C	402	NDP	N6A-C6A-N1A	-6.20	104.57	118.38
3	F	402	NDP	N6A-C6A-N1A	-6.03	104.94	118.38
3	A	402	NDP	N6A-C6A-N1A	-5.92	105.20	118.38
3	F	402	NDP	C4A-N9A-C1B	-5.83	112.99	126.63
3	C	402	NDP	C1B-N9A-C8A	5.80	139.97	127.09
3	D	402	NDP	N6A-C6A-N1A	-5.64	105.81	118.38
3	C	402	NDP	N3A-C2A-N1A	-5.61	120.08	128.58
3	E	402	NDP	N6A-C6A-N1A	-5.60	105.90	118.38
3	E	402	NDP	N3A-C2A-N1A	-5.60	120.11	128.58
3	B	402	NDP	N3A-C2A-N1A	-5.57	120.15	128.58
3	B	402	NDP	C4A-N9A-C1B	-5.51	113.75	126.63
3	B	402	NDP	C5A-C4A-N3A	-5.49	119.16	126.72
3	D	402	NDP	N3A-C2A-N1A	-5.43	120.36	128.58
3	F	402	NDP	N3A-C2A-N1A	-5.42	120.38	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NDP	N3A-C2A-N1A	-5.23	120.67	128.58
3	D	402	NDP	C4A-N9A-C1B	-5.23	114.41	126.63
3	A	402	NDP	C1B-N9A-C8A	5.16	138.54	127.09
3	B	402	NDP	C1B-N9A-C8A	5.12	138.46	127.09
3	E	402	NDP	C1B-N9A-C8A	5.11	138.43	127.09
3	F	402	NDP	C1B-N9A-C8A	5.10	138.42	127.09
3	F	402	NDP	C5A-C4A-N3A	-4.98	119.86	126.72
3	C	402	NDP	C5A-C6A-N6A	4.93	135.49	123.29
3	B	402	NDP	N6A-C6A-N1A	-4.92	107.42	118.38
3	A	402	NDP	C5A-C4A-N3A	-4.77	120.14	126.72
3	A	402	NDP	N9A-C8A-N7A	-4.74	107.21	113.94
3	D	402	NDP	O4B-C1B-N9A	-4.64	99.17	108.09
3	A	402	NDP	C5A-C6A-N6A	4.61	134.70	123.29
3	D	402	NDP	C1B-N9A-C8A	4.51	137.11	127.09
3	F	402	NDP	C5A-C6A-N6A	4.51	134.46	123.29
2	F	401	GO6	C25-O03-C19	4.48	124.09	117.51
3	E	402	NDP	N9A-C8A-N7A	-4.46	107.61	113.94
3	F	402	NDP	N9A-C8A-N7A	-4.40	107.70	113.94
3	D	402	NDP	C5A-C6A-N6A	4.36	134.09	123.29
3	D	402	NDP	C5A-C4A-N3A	-4.35	120.72	126.72
3	C	402	NDP	C5A-C4A-N3A	-4.35	120.73	126.72
3	E	402	NDP	C5A-C6A-N6A	4.34	134.04	123.29
3	E	402	NDP	C5A-C4A-N3A	-4.31	120.78	126.72
3	C	402	NDP	N9A-C8A-N7A	-4.15	108.05	113.94
3	B	402	NDP	N9A-C8A-N7A	-3.91	108.39	113.94
3	B	402	NDP	N3A-C4A-N9A	3.82	133.66	127.17
2	E	401	GO6	C09-C07-C11	-3.65	105.70	110.30
3	D	402	NDP	N9A-C8A-N7A	-3.65	108.76	113.94
3	E	402	NDP	C4A-N9A-C8A	3.58	109.49	105.74
3	B	402	NDP	C5A-C6A-N6A	3.54	132.05	123.29
3	B	402	NDP	C2A-N3A-C4A	3.51	120.41	111.83
3	A	402	NDP	C4A-N9A-C8A	3.40	109.31	105.74
3	A	402	NDP	N3A-C4A-N9A	3.34	132.85	127.17
3	F	402	NDP	C2A-N3A-C4A	3.32	119.94	111.83
2	A	401	GO6	C25-O03-C19	3.30	122.35	117.51
3	E	402	NDP	P2B-O2B-C2B	-3.28	114.67	123.43
3	D	402	NDP	C2B-C1B-N9A	3.23	119.07	113.75
2	F	401	GO6	O03-C19-C23	3.20	119.35	114.55
3	A	402	NDP	C5A-N7A-C8A	3.17	108.44	103.45
3	E	402	NDP	N3A-C4A-N9A	3.17	132.56	127.17
3	F	402	NDP	N3A-C4A-N9A	3.17	132.55	127.17
3	A	402	NDP	C2A-N3A-C4A	3.15	119.53	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	NDP	C2A-N3A-C4A	3.15	119.52	111.83
3	C	402	NDP	C2A-N3A-C4A	3.11	119.43	111.83
3	D	402	NDP	N3A-C4A-N9A	3.11	132.46	127.17
2	D	401	GO6	O04-C20-C24	3.10	119.20	114.55
3	E	402	NDP	C3N-C2N-N1N	-3.03	118.76	123.20
3	D	402	NDP	C2A-N3A-C4A	2.95	119.03	111.83
3	D	402	NDP	C2B-C3B-C4B	2.94	108.31	101.99
3	F	402	NDP	C5A-N7A-C8A	2.92	108.04	103.45
3	C	402	NDP	N3A-C4A-N9A	2.82	131.97	127.17
2	A	401	GO6	C09-C13-C15	-2.72	115.77	120.43
3	F	402	NDP	C4A-N9A-C8A	2.71	108.58	105.74
2	D	401	GO6	O03-C19-C23	2.71	118.61	114.55
2	F	401	GO6	O04-C20-C24	2.69	118.58	114.55
2	B	401	GO6	O03-C19-C23	2.69	118.58	114.55
2	A	401	GO6	C09-C07-C11	-2.67	106.92	110.30
3	B	402	NDP	C5A-N7A-C8A	2.65	107.61	103.45
3	B	402	NDP	C6A-C5A-C4A	2.65	120.79	117.18
3	E	402	NDP	C5A-N7A-C8A	2.63	107.59	103.45
2	C	401	GO6	O03-C19-C23	2.63	118.49	114.55
3	F	402	NDP	P2B-O2B-C2B	2.62	130.42	123.43
3	C	402	NDP	C4A-N9A-C8A	2.61	108.48	105.74
2	B	401	GO6	O04-C20-C24	2.57	118.40	114.55
3	C	402	NDP	C5A-N7A-C8A	2.54	107.44	103.45
3	D	402	NDP	C4A-N9A-C8A	2.52	108.38	105.74
2	E	401	GO6	O04-C20-C24	2.52	118.32	114.55
3	E	402	NDP	O7N-C7N-C3N	-2.50	116.18	120.90
3	B	402	NDP	C2D-C3D-C4D	2.50	107.44	102.61
2	A	401	GO6	O04-C20-C24	2.49	118.29	114.55
2	B	401	GO6	C14-C10-C08	-2.48	109.73	113.61
2	A	401	GO6	C10-C08-C12	-2.39	107.28	110.30
2	E	401	GO6	O03-C19-C23	2.39	118.13	114.55
3	E	402	NDP	C1D-N1N-C2N	-2.38	117.22	121.14
2	D	401	GO6	C26-O04-C20	2.37	120.99	117.51
3	B	402	NDP	O2X-P2B-O2B	2.35	115.00	105.85
2	B	401	GO6	C25-O03-C19	2.29	120.87	117.51
3	A	402	NDP	O4D-C1D-N1N	2.28	112.43	108.08
3	F	402	NDP	C3N-C2N-N1N	-2.26	119.89	123.20
3	F	402	NDP	O4B-C1B-N9A	-2.24	103.79	108.09
2	C	401	GO6	C14-C10-C08	2.24	117.10	113.61
3	E	402	NDP	O2A-PA-O3	2.23	113.31	107.27
2	F	401	GO6	C09-C13-C15	-2.23	116.60	120.43
3	A	402	NDP	C4A-C5A-N7A	-2.23	108.03	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	NDP	C5B-C4B-C3B	-2.22	107.22	115.21
2	C	401	GO6	C10-C14-C16	-2.22	116.62	120.43
3	F	402	NDP	C4A-C5A-N7A	-2.19	108.07	110.58
3	D	402	NDP	O3-PN-O1N	-2.19	104.13	110.70
3	D	402	NDP	O7N-C7N-C3N	2.17	124.98	120.90
3	C	402	NDP	C3D-C2D-C1D	2.14	105.52	101.46
3	E	402	NDP	O4D-C1D-N1N	2.14	112.17	108.08
3	B	402	NDP	O2A-PA-O3	2.12	113.00	107.27
3	D	402	NDP	O2N-PN-O3	2.11	112.98	107.27
3	F	402	NDP	C6A-C5A-C4A	2.11	120.06	117.18
3	C	402	NDP	O7N-C7N-N7N	-2.08	118.22	122.89
3	D	402	NDP	C3D-C2D-C1D	2.06	105.36	101.46
2	A	401	GO6	O03-C19-C23	2.05	117.63	114.55
2	C	401	GO6	O04-C20-C24	2.05	117.63	114.55
3	D	402	NDP	C2D-C3D-C4D	2.05	106.58	102.61

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GO6	C07-C08-C10-C14
2	A	401	GO6	C12-C08-C10-C14
2	A	401	GO6	C09-C07-C08-C10
2	B	401	GO6	C12-C08-C10-C14
2	C	401	GO6	C07-C08-C10-C14
2	C	401	GO6	C12-C08-C10-C14
2	C	401	GO6	C09-C07-C08-C10
2	C	401	GO6	C09-C07-C08-C12
2	C	401	GO6	C11-C07-C08-C10
2	C	401	GO6	C11-C07-C08-C12
2	D	401	GO6	C12-C08-C10-C14
2	E	401	GO6	C09-C07-C08-C10
2	E	401	GO6	C11-C07-C09-C13
2	F	401	GO6	C12-C08-C10-C14
2	F	401	GO6	C09-C07-C08-C10
3	A	402	NDP	C5D-O5D-PN-O3
3	A	402	NDP	C5D-O5D-PN-O1N
3	A	402	NDP	C5D-O5D-PN-O2N
3	A	402	NDP	C2D-C1D-N1N-C6N
3	B	402	NDP	C5B-O5B-PA-O1A
3	B	402	NDP	C5B-O5B-PA-O2A
3	B	402	NDP	C5B-O5B-PA-O3

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Mol	Chain	Res	Type	Atoms
3	C	402	NDP	C5B-O5B-PA-O1A
3	C	402	NDP	C5B-O5B-PA-O3
3	C	402	NDP	PN-O3-PA-O5B
3	C	402	NDP	C5D-O5D-PN-O3
3	C	402	NDP	C5D-O5D-PN-O2N
3	D	402	NDP	C5D-O5D-PN-O3
3	D	402	NDP	C5D-O5D-PN-O1N
3	E	402	NDP	C5B-O5B-PA-O3
3	F	402	NDP	C5B-O5B-PA-O2A
3	F	402	NDP	O4B-C4B-C5B-O5B
2	B	401	GO6	C24-C20-O04-C26
2	A	401	GO6	C07-C09-C13-C15
2	A	401	GO6	C07-C09-C13-C17
2	A	401	GO6	C24-C20-O04-C26
3	F	402	NDP	C3B-C2B-O2B-P2B
2	B	401	GO6	C16-C20-O04-C26
2	D	401	GO6	C07-C09-C13-C17
2	E	401	GO6	C07-C09-C13-C15
2	E	401	GO6	C07-C09-C13-C17
3	A	402	NDP	C2D-C1D-N1N-C2N
2	F	401	GO6	C07-C09-C13-C17
3	A	402	NDP	O4B-C4B-C5B-O5B
2	D	401	GO6	C07-C09-C13-C15
2	A	401	GO6	C16-C20-O04-C26
2	F	401	GO6	C07-C09-C13-C15
3	E	402	NDP	C2D-C1D-N1N-C2N
2	E	401	GO6	C16-C20-O04-C26
3	F	402	NDP	C3B-C4B-C5B-O5B
3	E	402	NDP	C2D-C1D-N1N-C6N
2	C	401	GO6	C07-C09-C13-C17
3	B	402	NDP	C2D-C1D-N1N-C2N
3	B	402	NDP	C3B-C4B-C5B-O5B
3	D	402	NDP	C3B-C4B-C5B-O5B
3	B	402	NDP	C2D-C1D-N1N-C6N
2	E	401	GO6	C24-C20-O04-C26
2	C	401	GO6	C07-C09-C13-C15
3	A	402	NDP	O4D-C4D-C5D-O5D
3	E	402	NDP	O4D-C4D-C5D-O5D
3	C	402	NDP	C2B-O2B-P2B-O1X
3	A	402	NDP	C3D-C4D-C5D-O5D
3	E	402	NDP	C3D-C4D-C5D-O5D
2	C	401	GO6	C24-C20-O04-C26

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Mol	Chain	Res	Type	Atoms
2	D	401	GO6	C24-C20-O04-C26
3	E	402	NDP	C2N-C3N-C7N-N7N
3	D	402	NDP	PA-O3-PN-O5D
2	C	401	GO6	C23-C19-O03-C25
2	B	401	GO6	C07-C09-C13-C17
2	D	401	GO6	C16-C20-O04-C26
3	E	402	NDP	O4D-C1D-N1N-C2N
3	E	402	NDP	O4D-C1D-N1N-C6N
3	E	402	NDP	PA-O3-PN-O1N
2	B	401	GO6	C09-C07-C08-C10
3	B	402	NDP	O4D-C1D-N1N-C2N
2	C	401	GO6	C16-C20-O04-C26
2	C	401	GO6	C07-C08-C12-O02
2	D	401	GO6	C07-C08-C12-O02
3	B	402	NDP	C2B-O2B-P2B-O1X
3	E	402	NDP	C2N-C3N-C7N-O7N
3	B	402	NDP	O4D-C1D-N1N-C6N
2	A	401	GO6	C11-C07-C09-C13
2	B	401	GO6	C07-C08-C10-C14
2	D	401	GO6	C07-C08-C10-C14
2	E	401	GO6	C07-C08-C10-C14
2	E	401	GO6	C12-C08-C10-C14
2	F	401	GO6	C07-C08-C10-C14
3	D	402	NDP	C5D-O5D-PN-O2N
3	F	402	NDP	C5B-O5B-PA-O1A
3	F	402	NDP	C5B-O5B-PA-O3
2	C	401	GO6	C08-C10-C14-C18
2	B	401	GO6	C07-C09-C13-C15
3	A	402	NDP	PN-O3-PA-O2A
3	B	402	NDP	PN-O3-PA-O2A
2	C	401	GO6	C08-C10-C14-C16
3	A	402	NDP	C2B-O2B-P2B-O2X
3	E	402	NDP	C2B-O2B-P2B-O2X
2	C	401	GO6	C15-C19-O03-C25
3	D	402	NDP	O4D-C1D-N1N-C2N
2	E	401	GO6	C23-C19-O03-C25
3	C	402	NDP	O4D-C1D-N1N-C2N
3	D	402	NDP	C1B-C2B-O2B-P2B
3	A	402	NDP	O4D-C1D-N1N-C6N
3	D	402	NDP	O4B-C4B-C5B-O5B
3	F	402	NDP	O4D-C1D-N1N-C2N
3	E	402	NDP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
3	D	402	NDP	PN-O3-PA-O1A
3	D	402	NDP	C3B-C2B-O2B-P2B
3	B	402	NDP	O4B-C4B-C5B-O5B
2	B	401	GO6	C23-C19-O03-C25
3	C	402	NDP	C2D-C1D-N1N-C2N
3	B	402	NDP	PN-O3-PA-O1A
3	F	402	NDP	PN-O3-PA-O2A
2	D	401	GO6	C09-C07-C08-C10
2	E	401	GO6	C15-C19-O03-C25
2	F	401	GO6	C24-C20-O04-C26
2	A	401	GO6	C07-C08-C12-O02
2	F	401	GO6	C07-C08-C12-O02
3	D	402	NDP	C2B-O2B-P2B-O1X
2	A	401	GO6	C09-C07-C08-C12
2	A	401	GO6	C11-C07-C08-C10
2	F	401	GO6	C09-C07-C08-C12
2	F	401	GO6	C11-C07-C08-C10
3	A	402	NDP	C3B-C4B-C5B-O5B
2	B	401	GO6	C15-C19-O03-C25
2	F	401	GO6	C16-C20-O04-C26
3	A	402	NDP	PN-O3-PA-O1A
3	C	402	NDP	PN-O3-PA-O2A
3	D	402	NDP	PN-O3-PA-O2A
3	E	402	NDP	PA-O3-PN-O2N

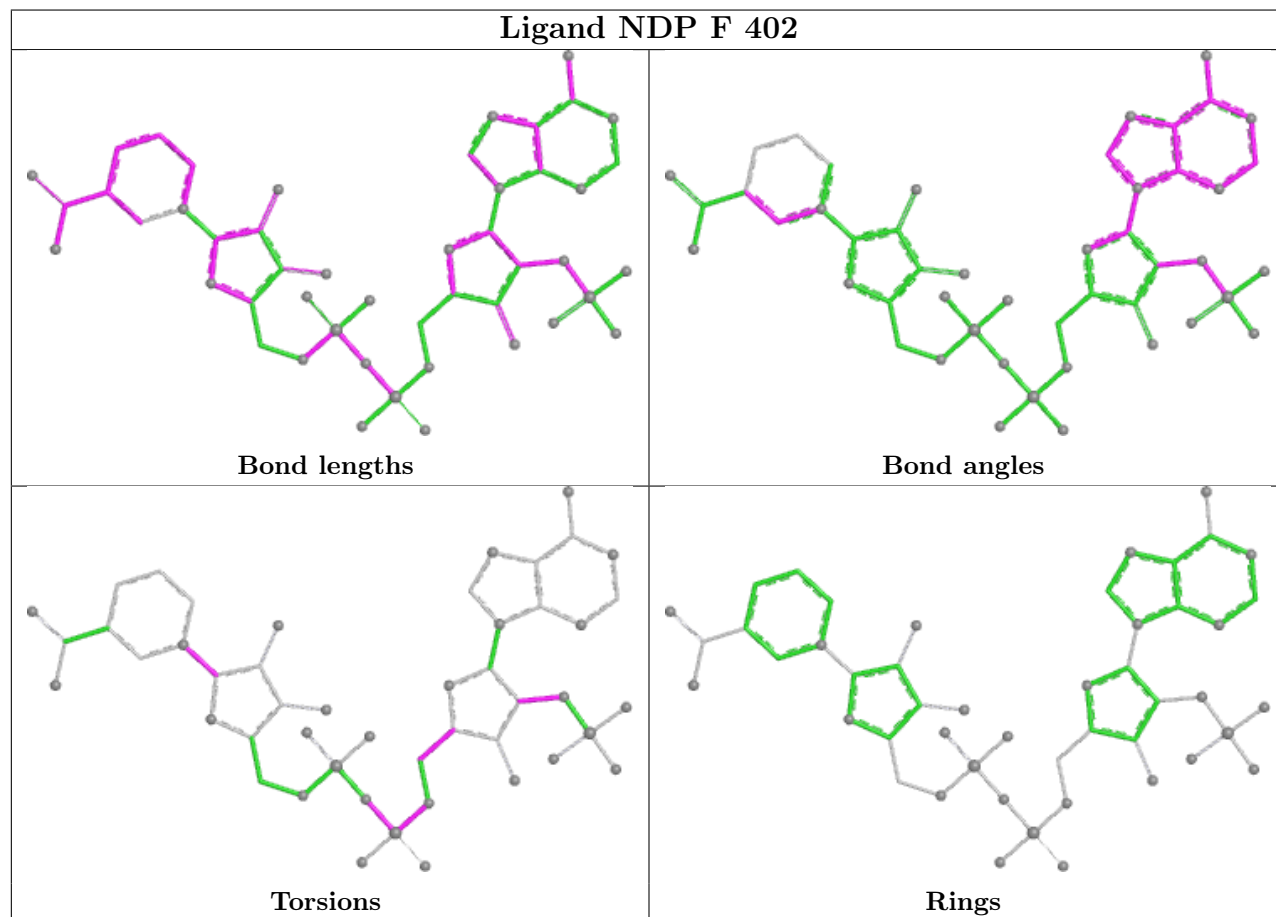
There are no ring outliers.

10 monomers are involved in 55 short contacts:

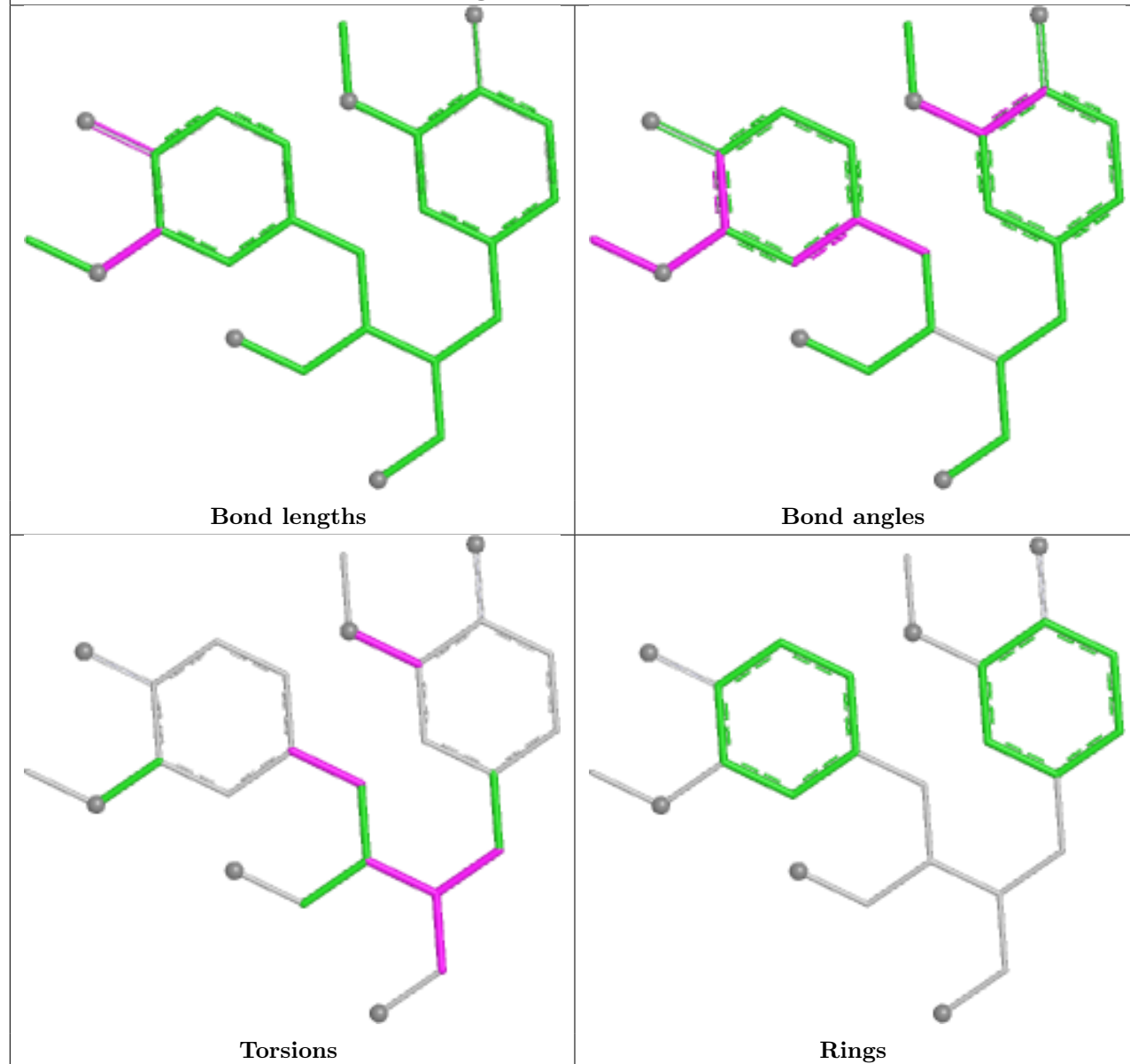
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	402	NDP	8	0
2	F	401	GO6	1	0
2	D	401	GO6	2	0
2	E	401	GO6	1	0
3	D	402	NDP	12	0
3	C	402	NDP	9	0
3	B	402	NDP	5	0
2	C	401	GO6	2	0
3	A	402	NDP	11	0
3	E	402	NDP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

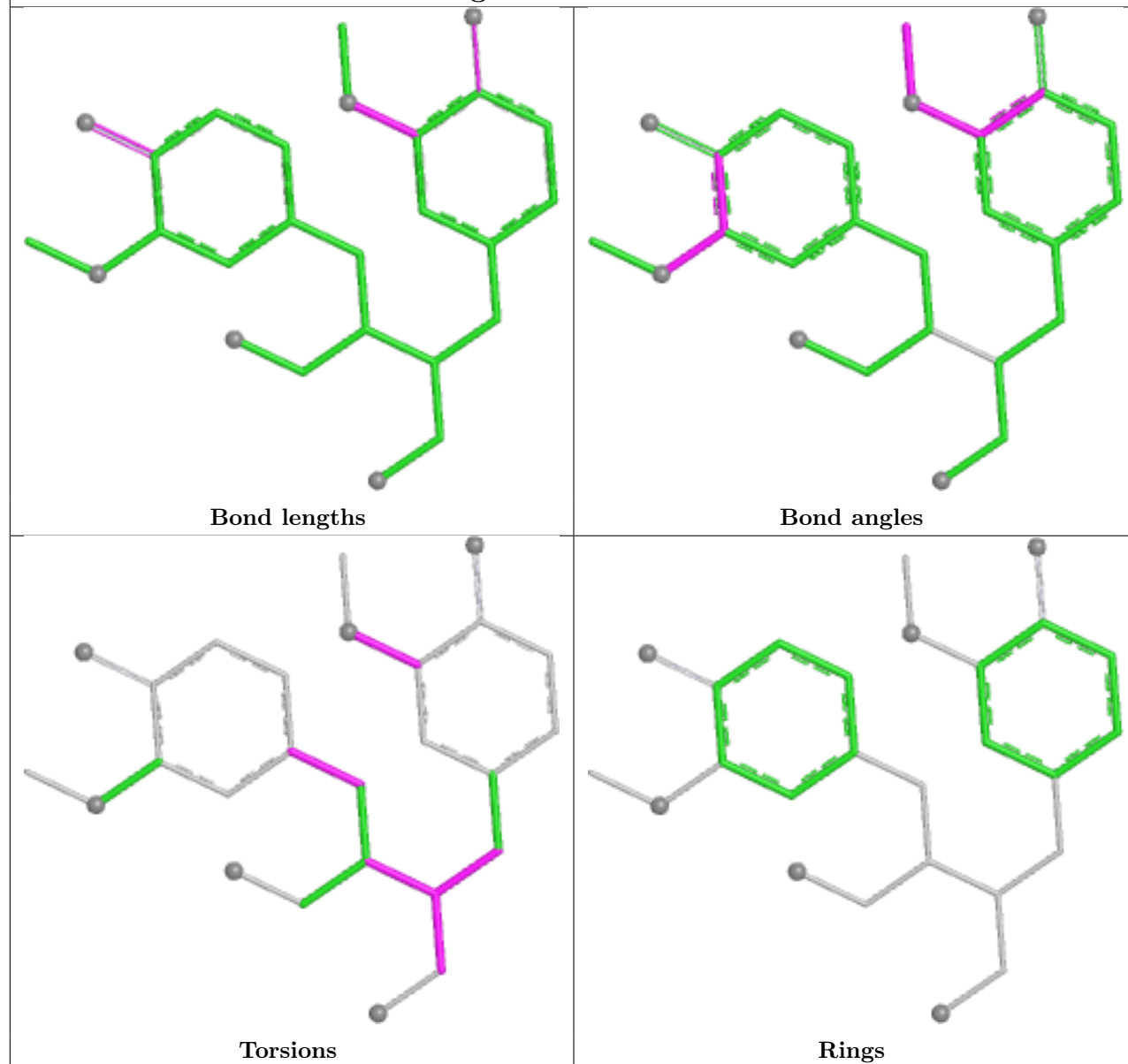
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



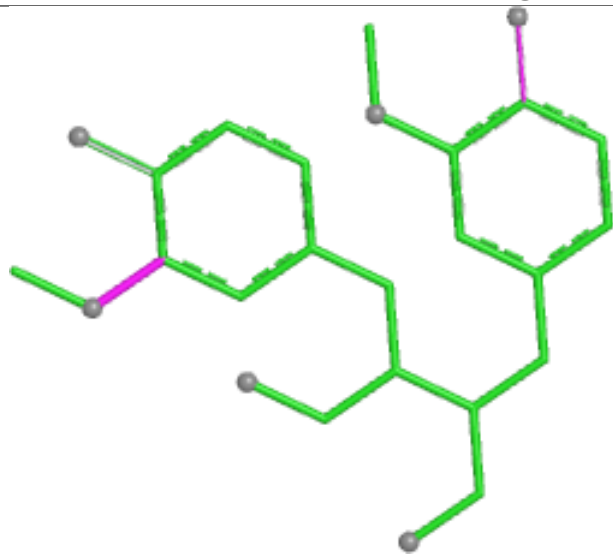
Ligand GO6 F 401



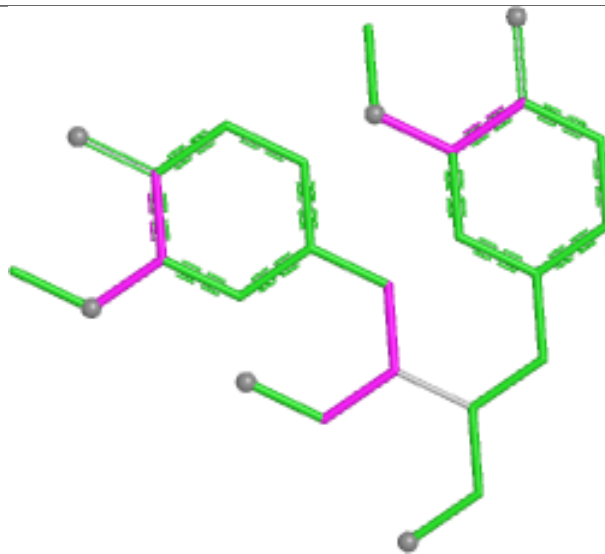
Ligand GO6 D 401



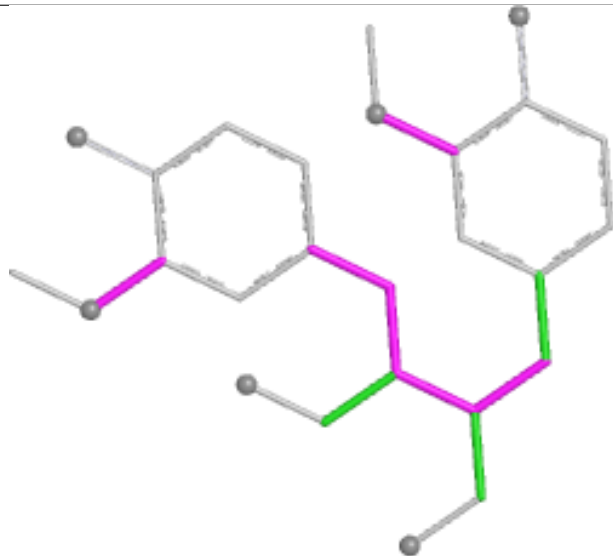
Ligand GO6 E 401



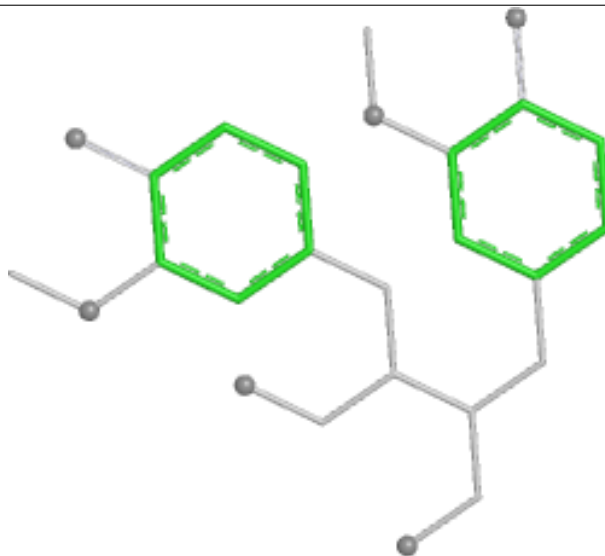
Bond lengths



Bond angles

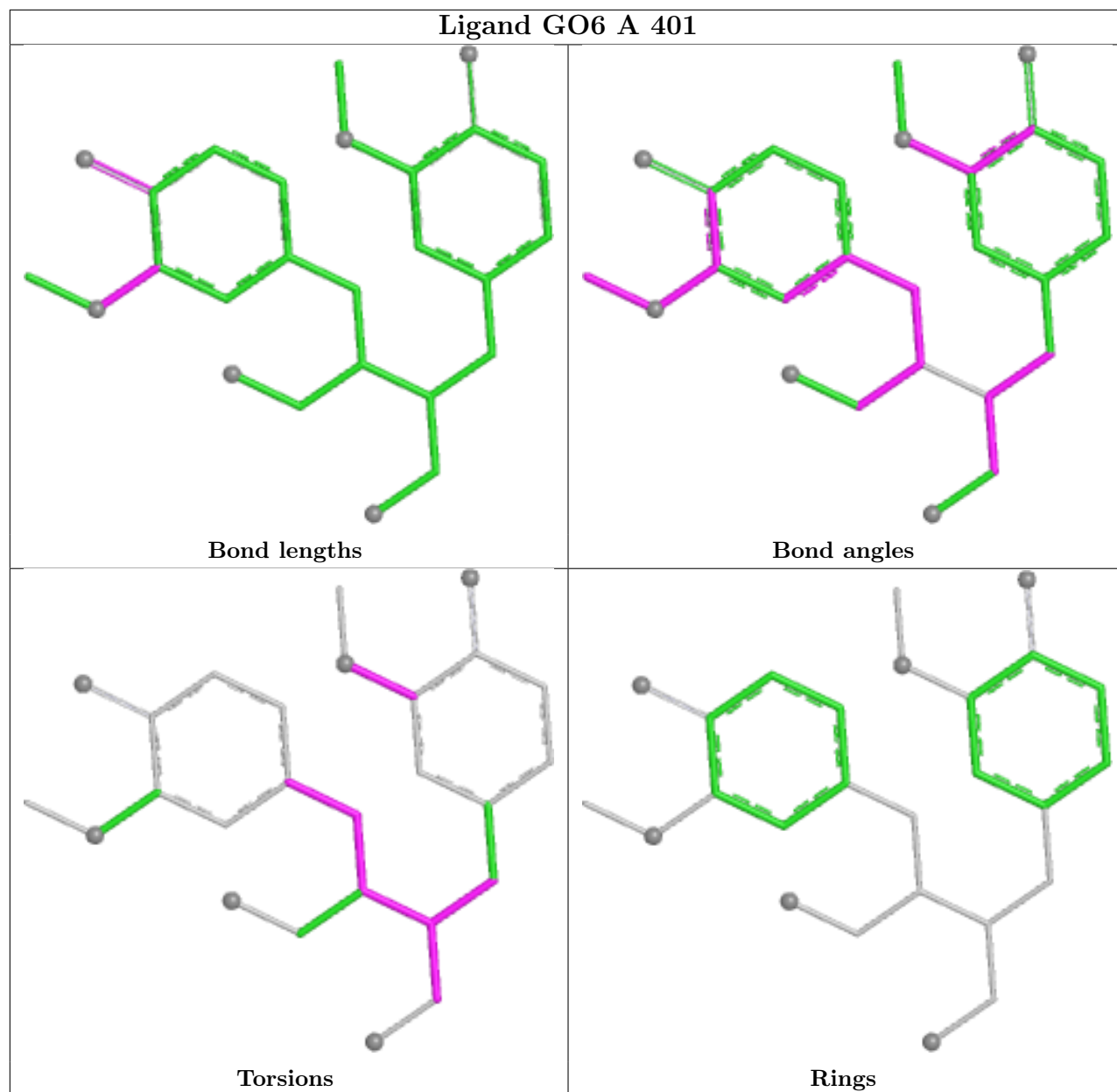


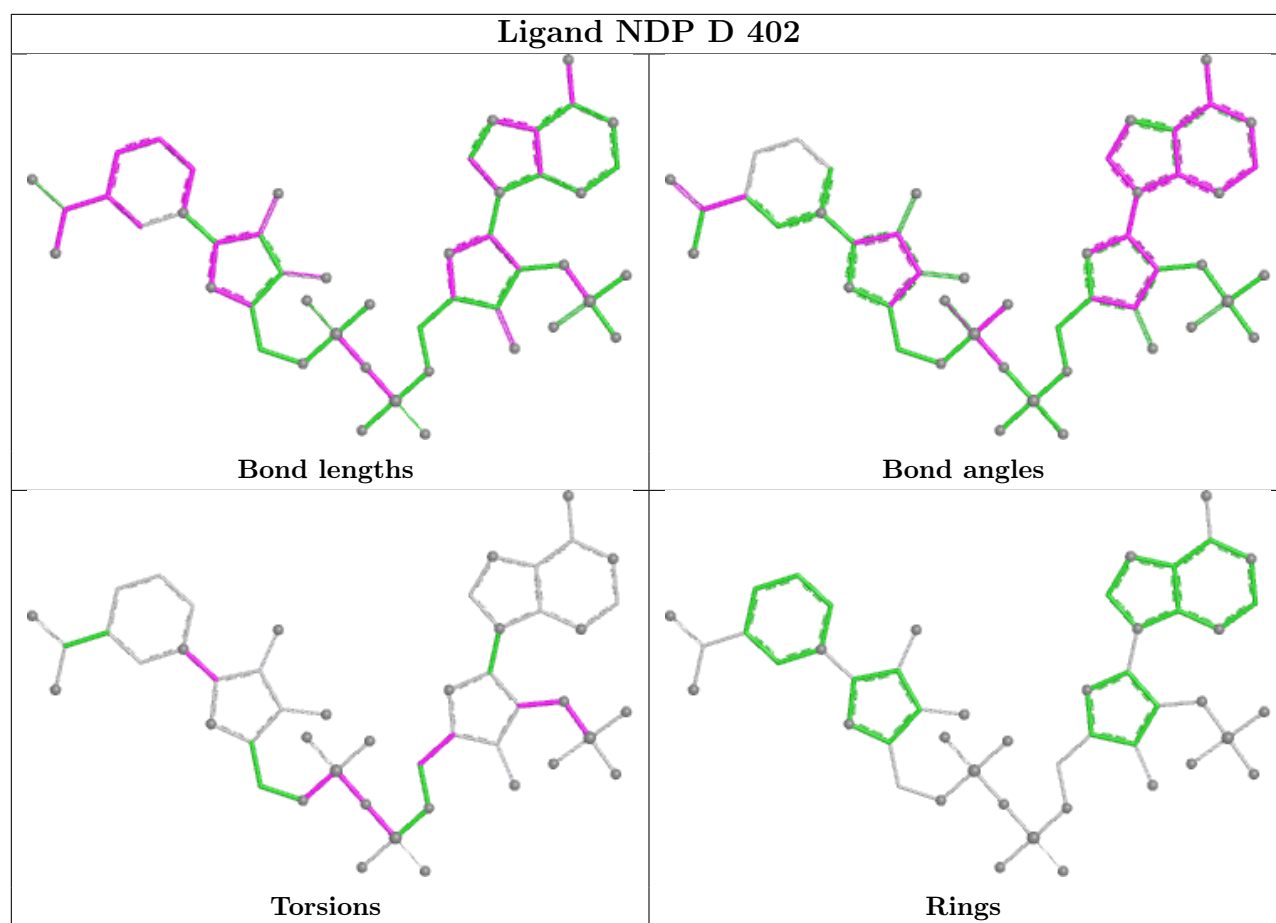
Torsions

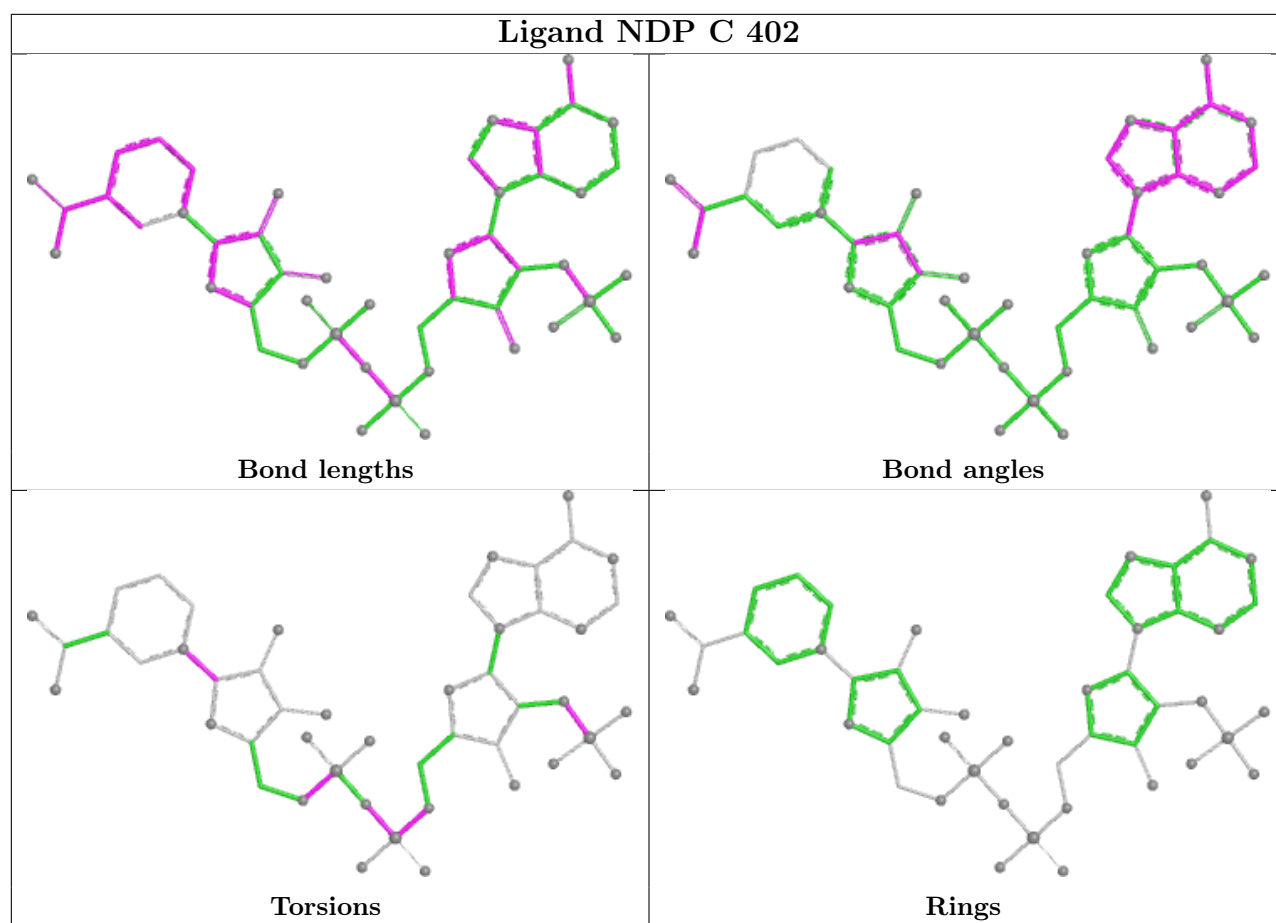


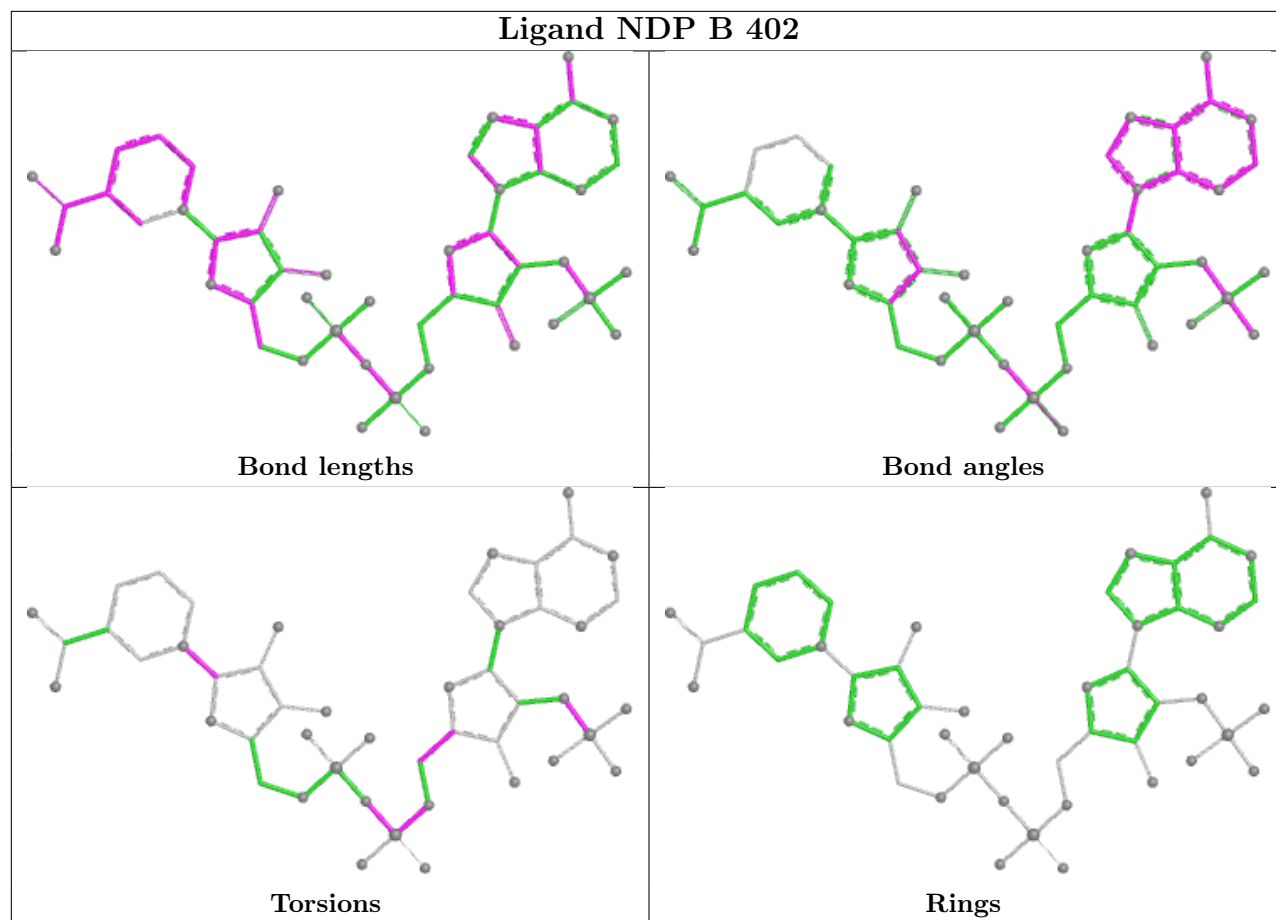
Rings

Ligand GO6 A 401

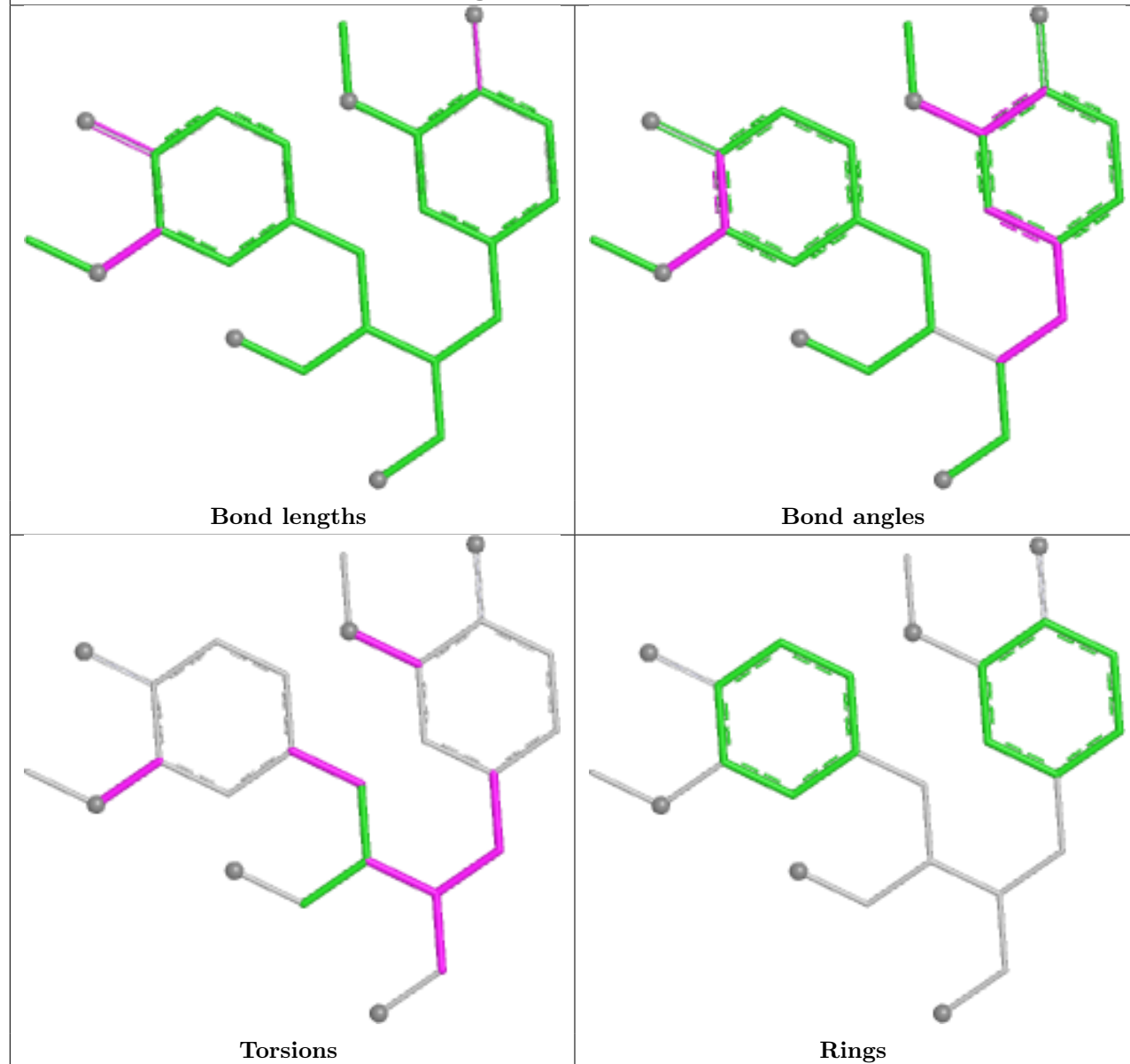


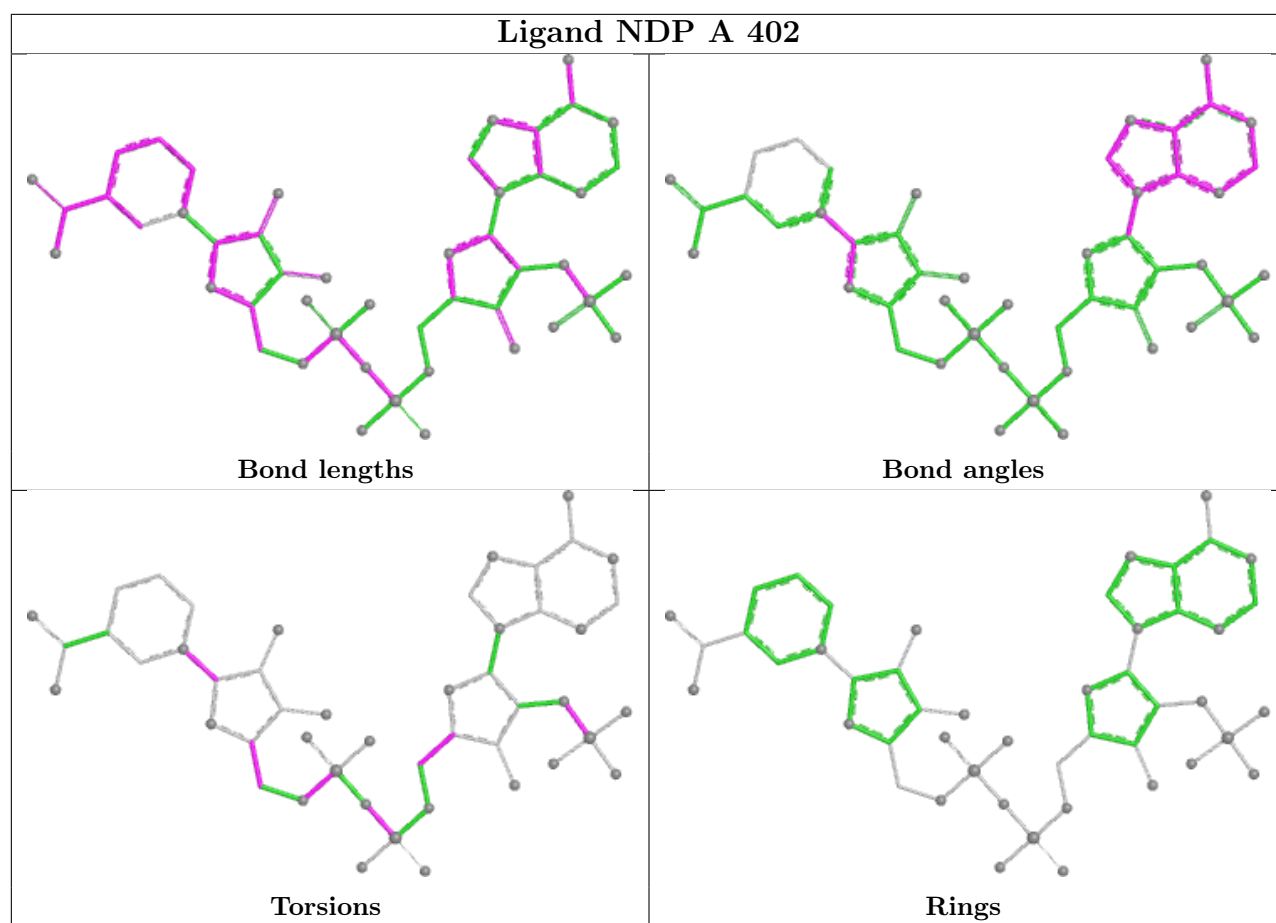




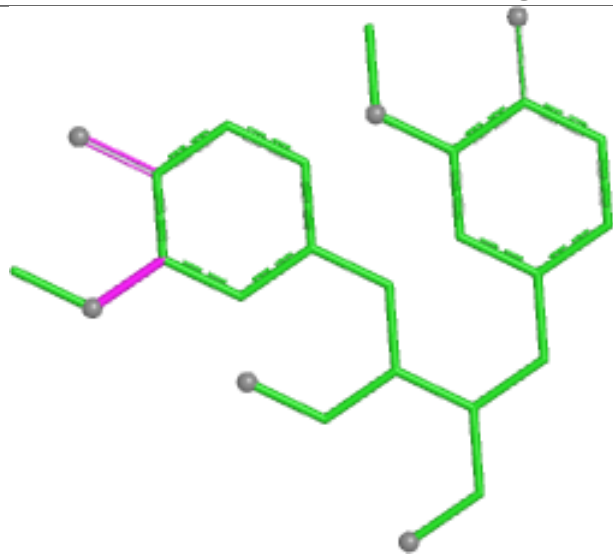


Ligand GO6 C 401

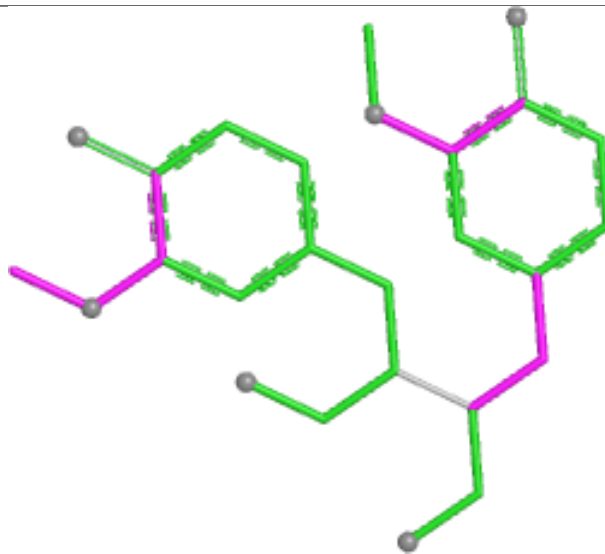




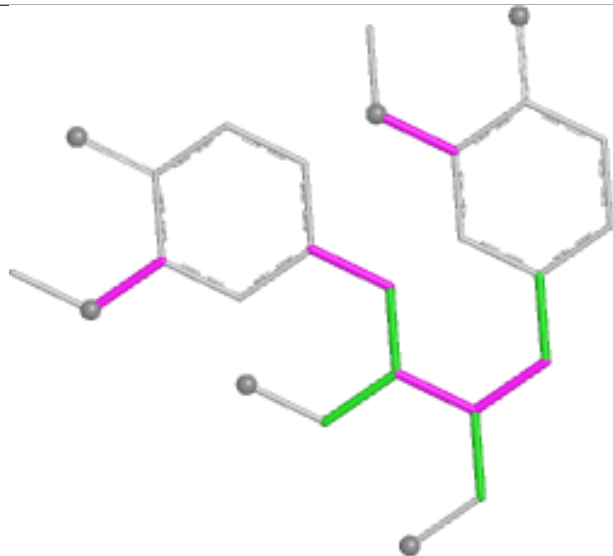
Ligand GO6 B 401



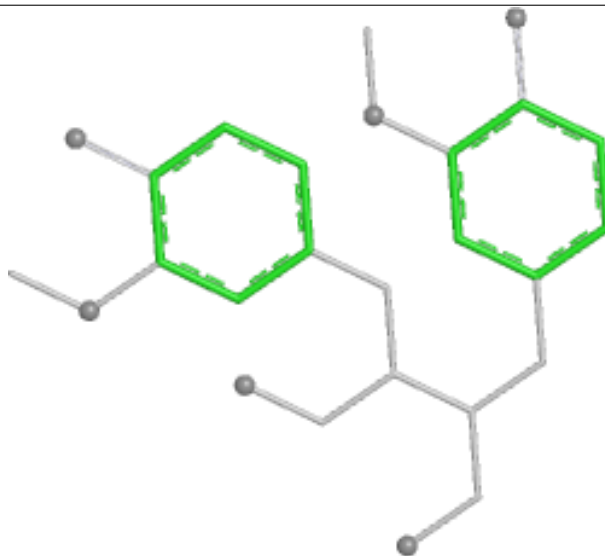
Bond lengths



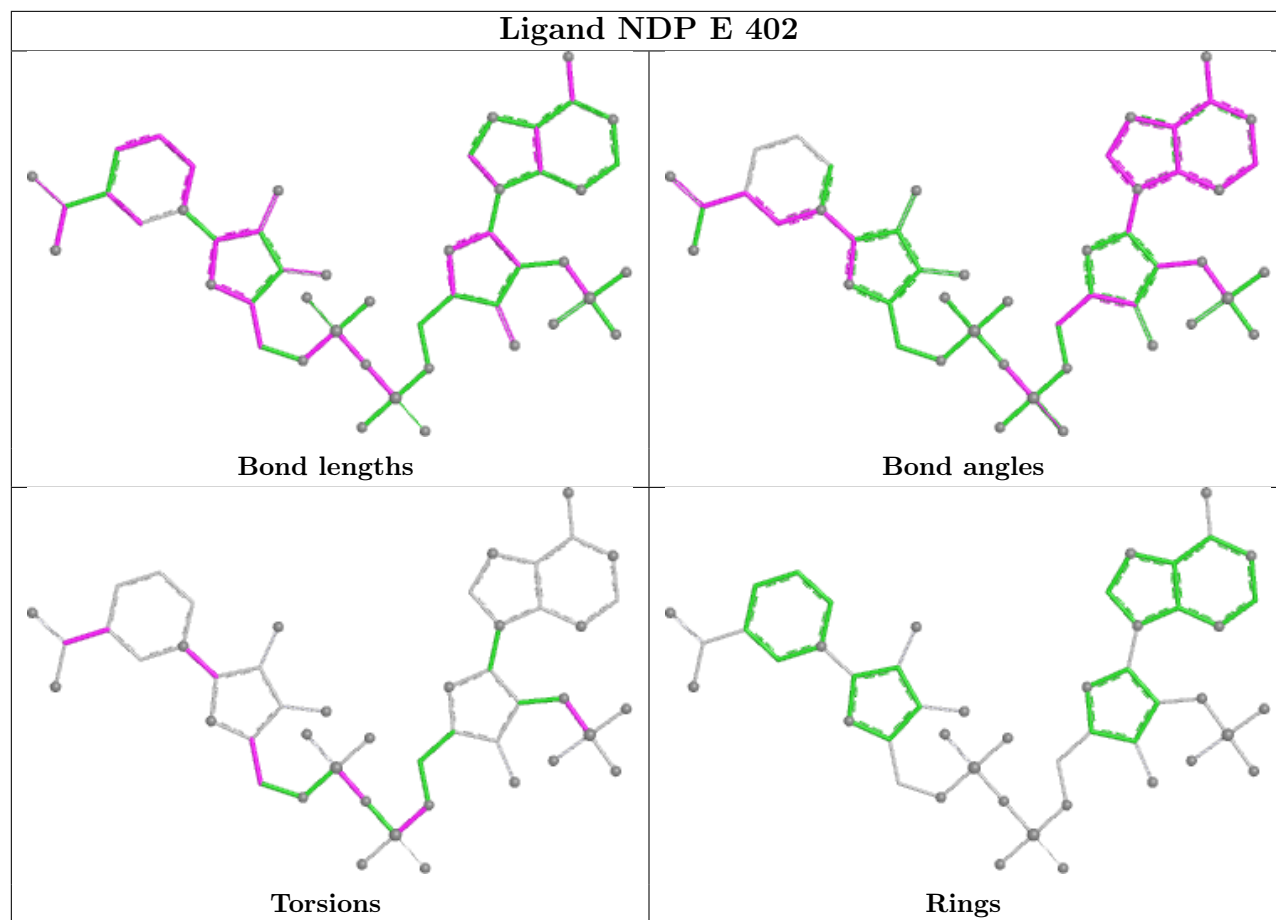
Bond angles



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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	290/317 (91%)	-1.38	1 (0%) 90 88	41, 44, 48, 77	0
1	B	290/317 (91%)	-1.39	0 100 100	31, 35, 55, 79	0
1	C	288/317 (90%)	-1.34	0 100 100	38, 41, 60, 89	0
1	D	286/317 (90%)	-1.38	0 100 100	37, 41, 47, 67	0
1	E	288/317 (90%)	-1.38	1 (0%) 90 88	38, 40, 44, 68	0
1	F	294/317 (92%)	-1.46	0 100 100	31, 34, 37, 54	0
All	All	1736/1902 (91%)	-1.39	2 (0%) 92 90	31, 40, 49, 89	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	131	GLY	2.1
1	A	131	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

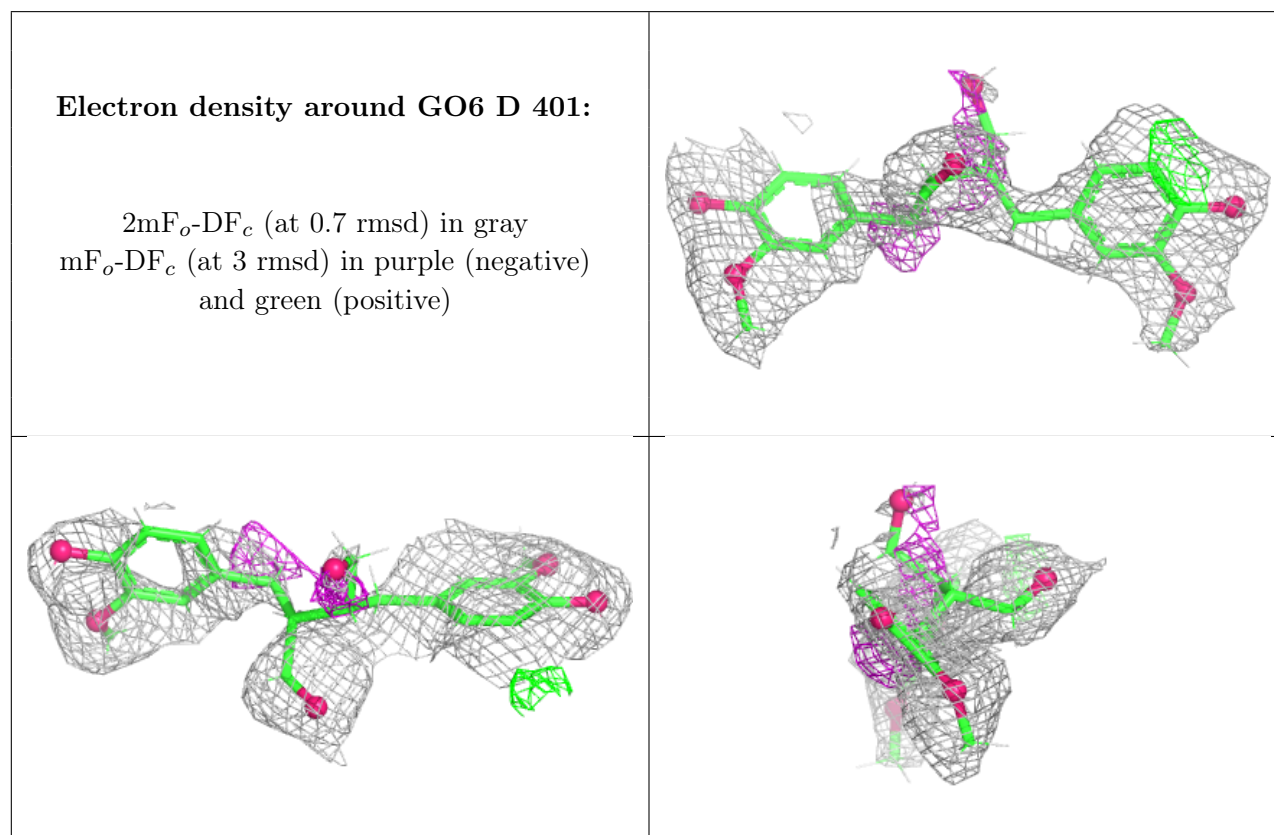
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

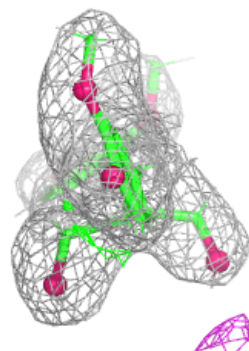
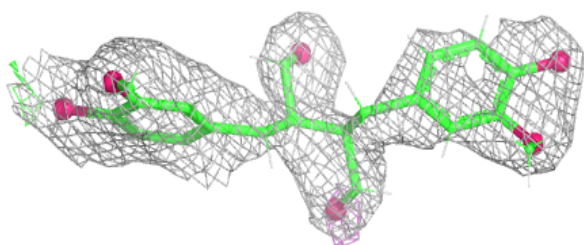
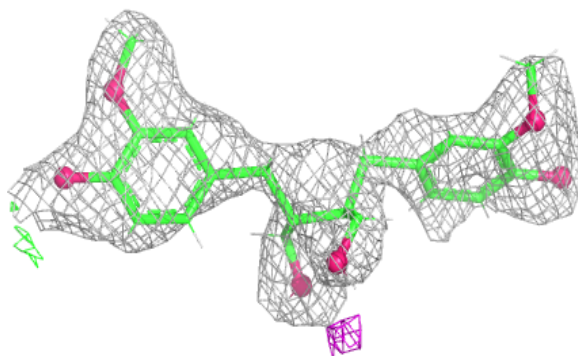
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GO6	D	401	26/26	0.96	0.07	38,41,47,50	0
2	GO6	B	401	26/26	0.98	0.04	35,38,43,46	0
2	GO6	C	401	26/26	0.98	0.04	40,45,50,54	0
2	GO6	A	401	26/26	0.98	0.06	43,52,55,65	0
2	GO6	E	401	26/26	0.98	0.05	39,41,48,49	0
3	NDP	A	402	48/48	0.98	0.05	43,45,55,56	0
3	NDP	C	402	48/48	0.98	0.05	39,40,49,49	0
3	NDP	D	402	48/48	0.98	0.05	39,40,49,62	0
3	NDP	E	402	48/48	0.98	0.05	38,39,48,54	0
3	NDP	B	402	48/48	0.99	0.03	34,35,42,43	0
2	GO6	F	401	26/26	0.99	0.04	34,35,42,42	0
3	NDP	F	402	48/48	1.00	0.03	34,35,46,52	0

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

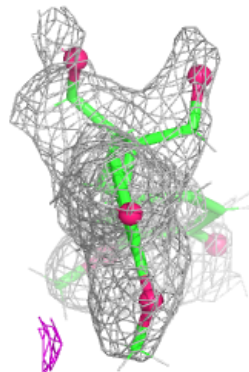
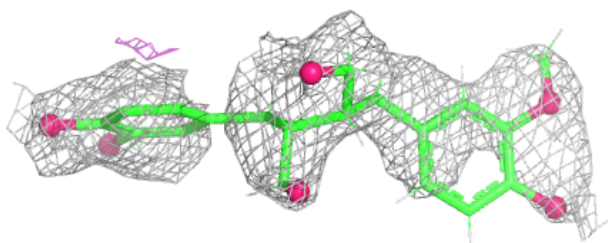
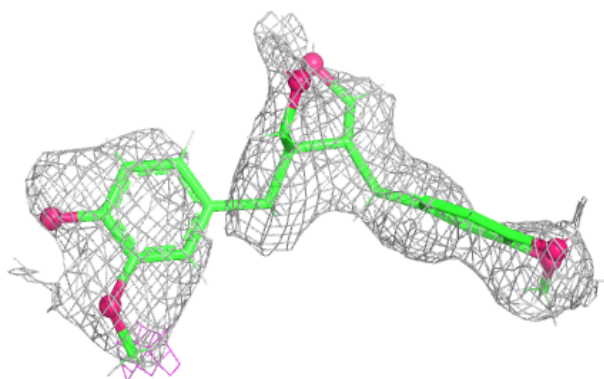


Electron density around GO6 B 401:

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

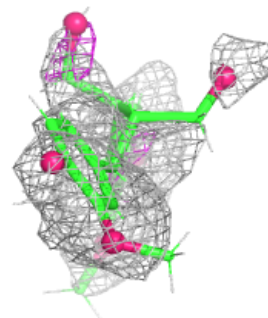
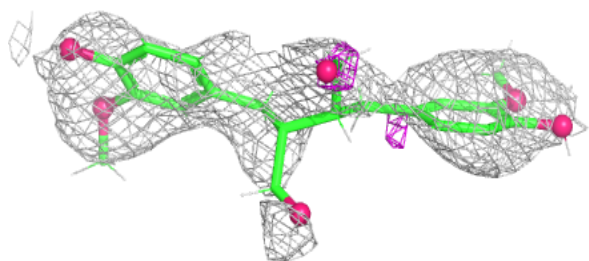
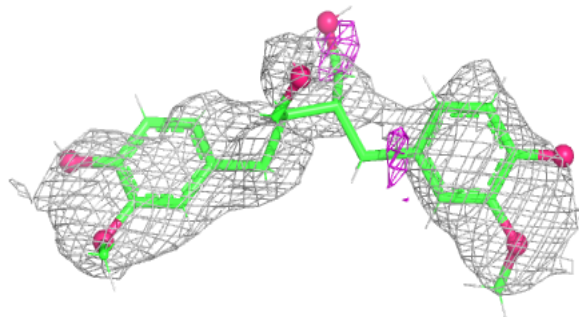
**Electron density around GO6 C 401:**

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

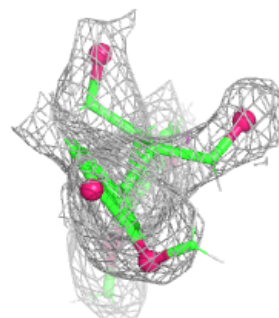
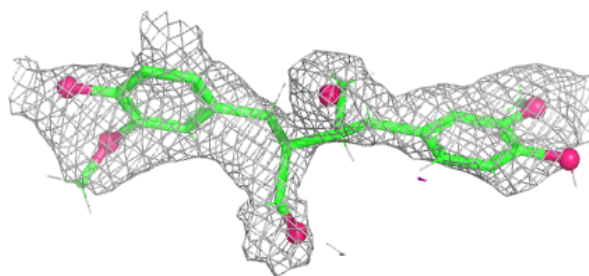
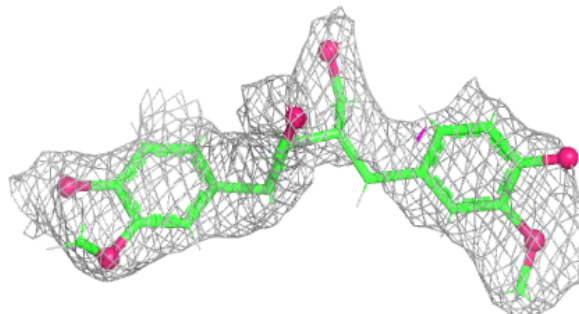


Electron density around GO6 A 401:

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

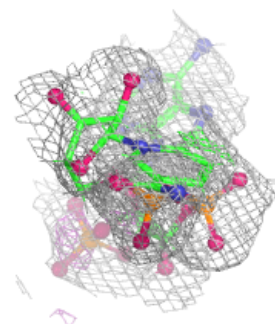
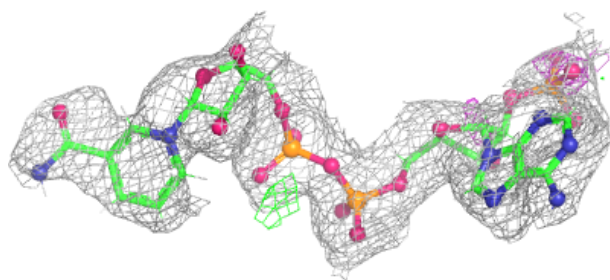
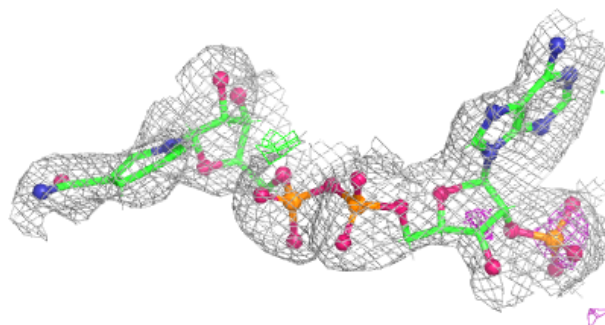
**Electron density around GO6 E 401:**

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

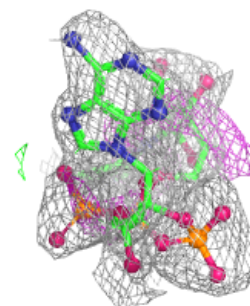
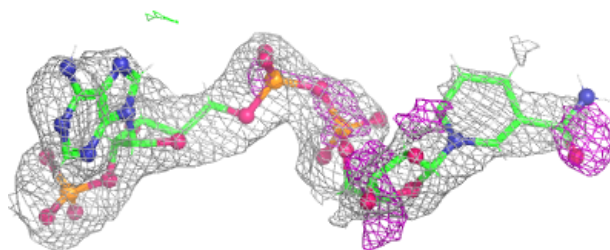
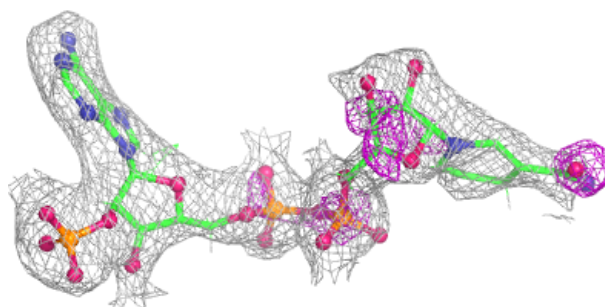


Electron density around NDP A 402:

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

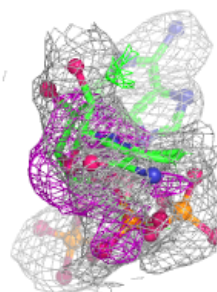
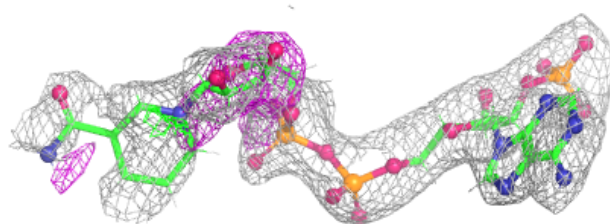
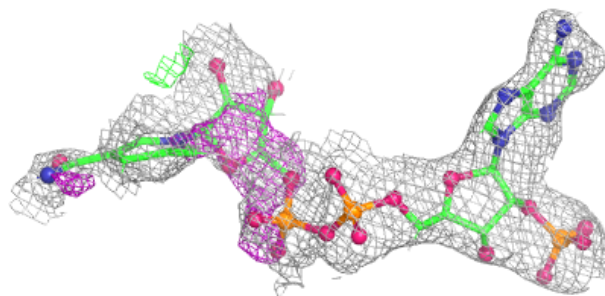
**Electron density around NDP C 402:**

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

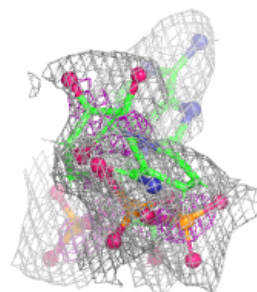
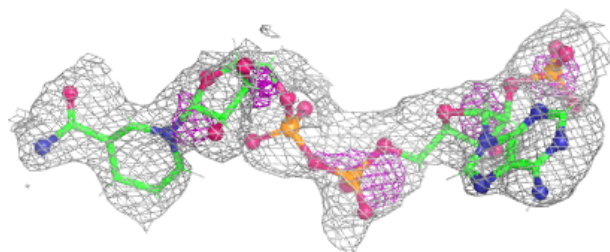
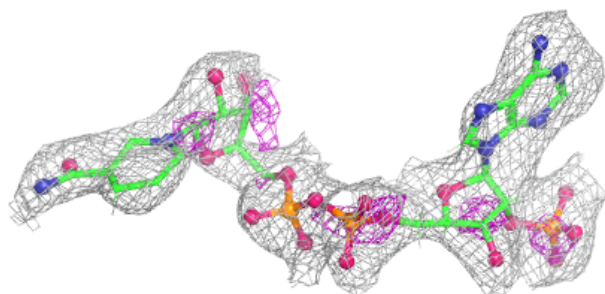


Electron density around NDP D 402:

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

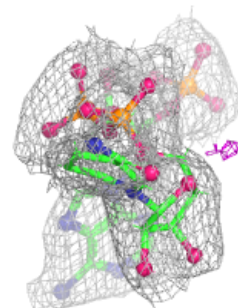
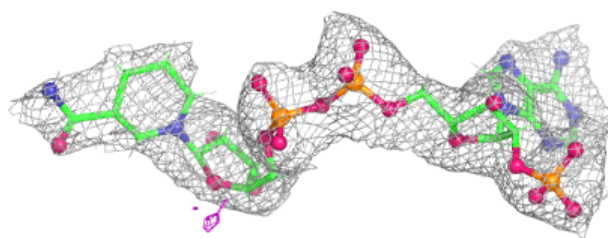
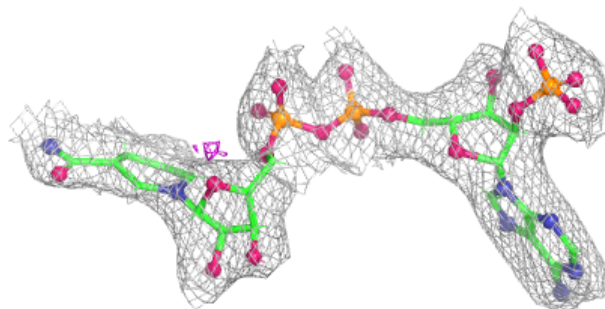
**Electron density around NDP E 402:**

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

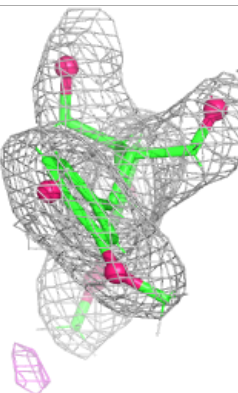
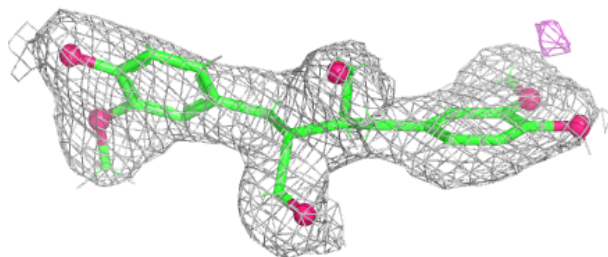
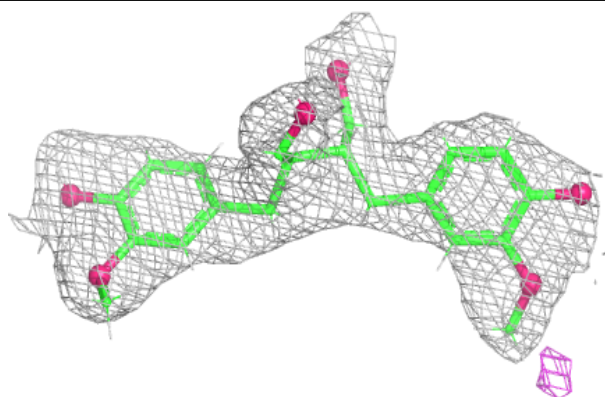


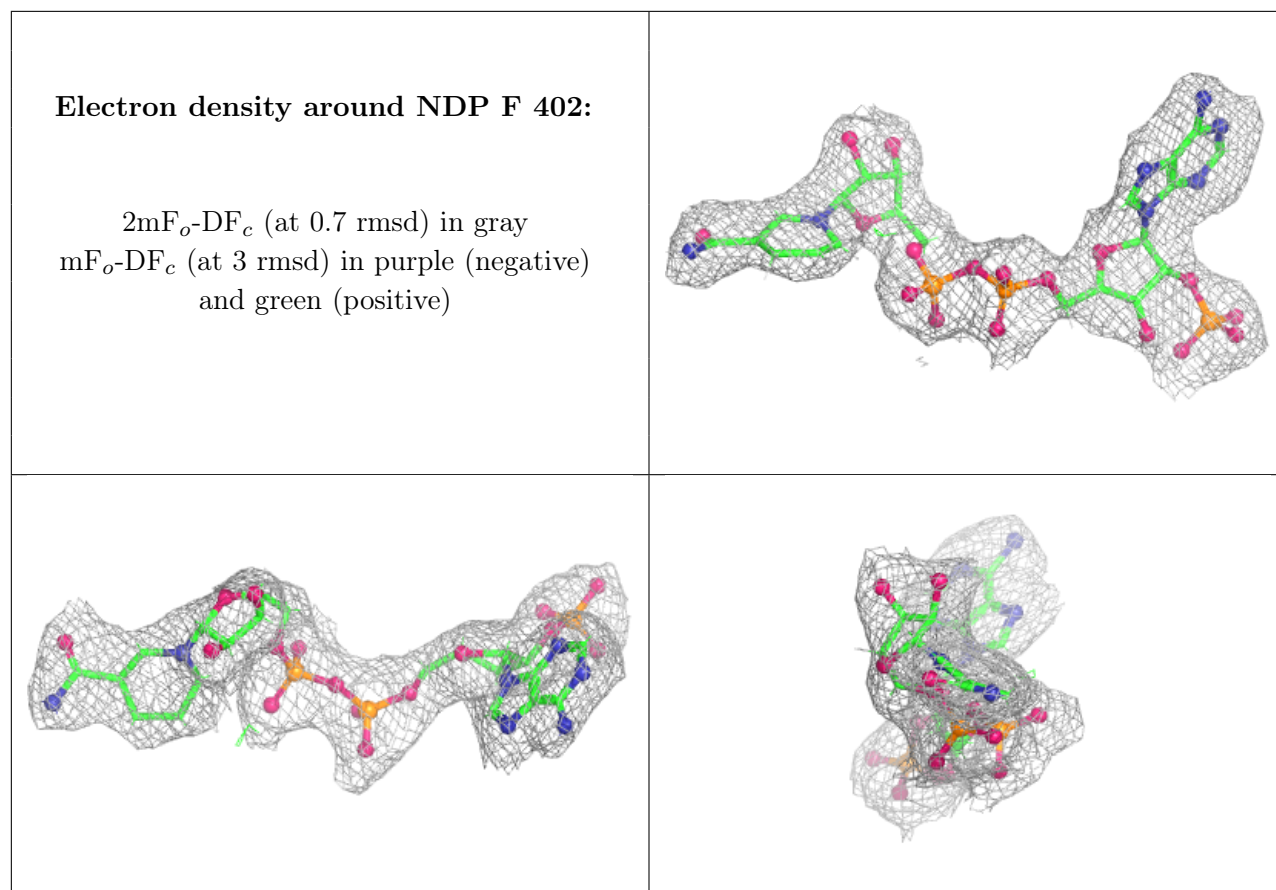
Electron density around NDP B 402:

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

**Electron density around GO6 F 401:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.