



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:47 AM UTC

PDB ID : 4E5Y / pdb_00004e5y
Title : Structure of human FX protein, the key enzyme in the biosynthesis of GDP-L-fucose
Authors : Zhou, H.; He, J.H.
Deposited on : 2012-03-15
Resolution : 2.37 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

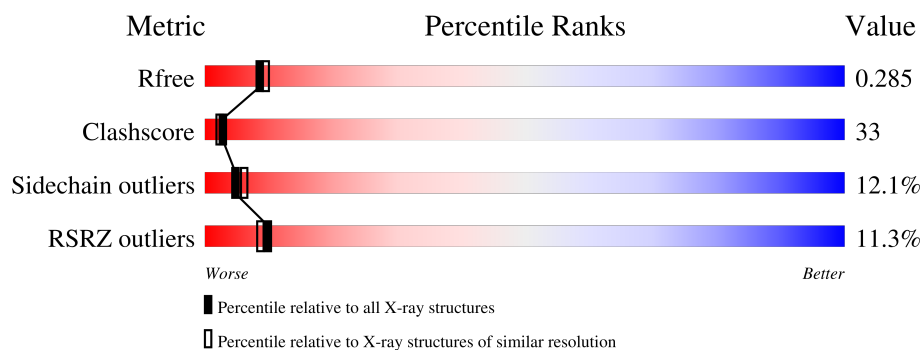
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	321	7% 58% 28% 8% . .
1	B	321	10% 56% 33% 7% .
1	C	321	18% 48% 32% 9% . 10%
1	D	321	8% 61% 32% 5% ..

2 Entry composition ⓘ

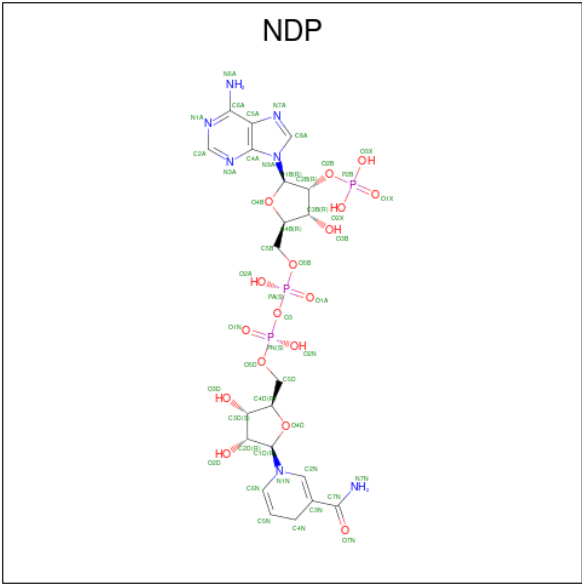
There are 3 unique types of molecules in this entry. The entry contains 9903 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GDP-L-fucose synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2433	1555	418	450	10			
1	B	309	Total	C	N	O	S	0	0	0
			2452	1566	421	455	10			
1	C	290	Total	C	N	O	S	0	0	0
			2295	1462	392	431	10			
1	D	318	Total	C	N	O	S	0	0	0
			2509	1601	431	467	10			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

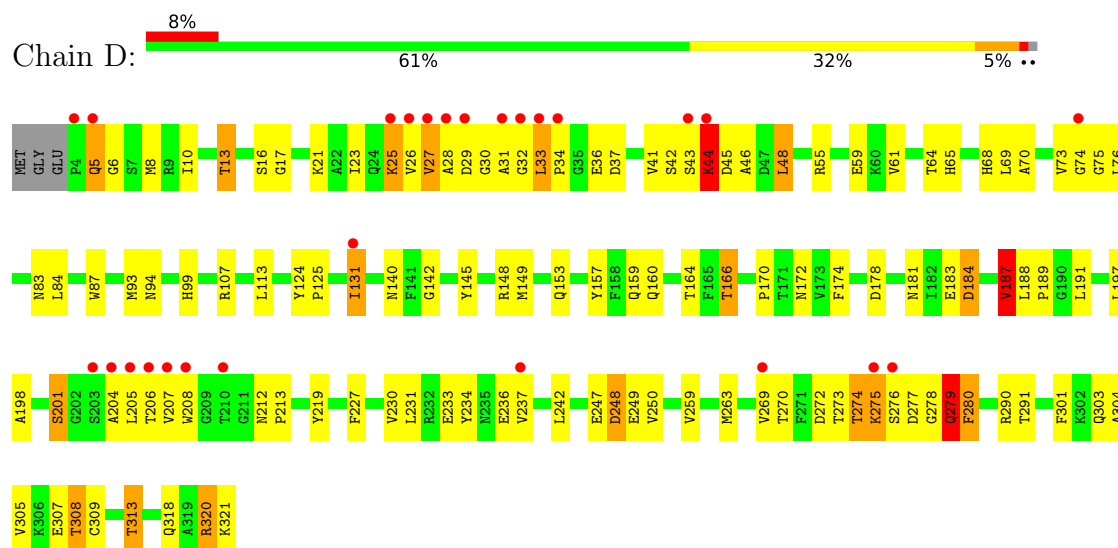


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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		
3	B	5	Total	O	0	0
			5	5		
3	C	6	Total	O	0	0
			6	6		
3	D	8	Total	O	0	0
			8	8		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.77Å 136.44Å 139.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.27 – 2.37 39.27 – 2.37	Depositor EDS
% Data completeness (in resolution range)	93.6 (39.27-2.37) 92.6 (39.27-2.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.232 , 0.291 (Not available) , 0.285	Depositor DCC
R_{free} test set	2000 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.569	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -h,l,k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9903	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	0.60	0/2493	0.96	4/3379 (0.1%)
1	B	0.53	0/2510	0.84	0/3399
1	C	0.60	0/2348	0.99	7/3182 (0.2%)
1	D	0.60	0/2573	0.93	7/3491 (0.2%)
All	All	0.58	0/9924	0.93	18/13451 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	3
1	D	0	1
All	All	0	7

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	GLY	N-CA-C	-11.82	99.56	114.92
1	C	274	THR	N-CA-C	11.09	125.86	108.67
1	D	75	GLY	N-CA-C	-10.69	101.85	115.42
1	D	248	ASP	N-CA-C	-7.50	101.18	110.41
1	D	187	VAL	N-CA-C	7.43	117.51	110.53
1	C	135	PRO	CA-C-N	7.18	127.14	120.03
1	C	135	PRO	C-N-CA	7.18	127.14	120.03
1	C	273	THR	N-CA-C	6.50	124.64	110.80
1	D	279	GLN	N-CA-C	6.48	121.39	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	SER	N-CA-C	6.33	117.48	108.74
1	D	30	GLY	N-CA-C	-6.14	105.10	113.27
1	D	184	ASP	N-CA-C	-6.05	101.46	110.23
1	A	61	VAL	N-CA-C	-5.75	102.16	109.80
1	C	29	ASP	N-CA-C	5.57	118.53	109.24
1	C	247	GLU	N-CA-C	-5.52	108.33	114.62
1	C	122	THR	N-CA-C	5.45	122.42	110.80
1	A	64	THR	N-CA-C	-5.04	107.30	113.50
1	D	166	THR	CB-CA-C	-5.03	101.85	114.11

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	ASP	Peptide
1	A	42	SER	Peptide
1	A	44	LYS	Peptide
1	C	209	GLY	Peptide
1	C	273	THR	Peptide
1	C	43	SER	Peptide
1	D	44	LYS	Peptide

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	2433	0	2364	144	0
1	B	2452	0	2384	162	0
1	C	2295	0	2228	217	0
1	D	2509	0	2442	146	0
2	A	48	0	26	2	0
2	B	48	0	26	5	0
2	C	48	0	26	3	0
2	D	48	0	26	1	0
3	A	3	0	0	0	0
3	B	5	0	0	0	0
3	C	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	8	0	0	0	0
All	All	9903	0	9522	640	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 33.

All (640) 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:B:42:SER:HA	1:B:43:SER:O	1.39	1.20
1:A:64:THR:HG23	1:A:65:HIS:HD2	1.00	1.14
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.13	1.13
1:A:64:THR:HG23	1:A:65:HIS:CD2	1.85	1.11
1:C:64:THR:HG23	1:C:65:HIS:HD2	1.05	1.09
1:D:33:LEU:HG	1:D:34:PRO:HA	1.28	1.08
1:B:181:ASN:HD21	1:B:183:GLU:HG2	0.94	1.08
1:A:27:VAL:HA	1:A:28:ALA:C	1.82	1.04
1:D:13:THR:HG21	1:D:68:HIS:HD2	1.18	1.03
1:C:64:THR:HG23	1:C:65:HIS:CD2	1.94	1.02
1:B:181:ASN:ND2	1:B:183:GLU:HG2	1.75	1.01
1:D:33:LEU:CG	1:D:34:PRO:HA	1.90	1.01
1:B:279:GLN:N	1:B:280:PHE:HA	1.74	1.00
1:B:26:VAL:HG12	1:B:27:VAL:HG22	1.44	1.00
1:A:121:LYS:HZ3	1:A:121:LYS:H	1.08	0.99
1:C:43:SER:HB2	1:C:45:ASP:HB2	1.41	0.99
1:C:13:THR:HG21	1:C:68:HIS:CD2	2.00	0.96
1:D:32:GLY:HA3	1:D:33:LEU:HD13	1.48	0.96
1:C:191:LEU:HB3	1:C:192:ILE:HG13	1.46	0.95
1:D:205:LEU:HA	1:D:206:THR:OG1	1.67	0.93
1:C:13:THR:HG21	1:C:68:HIS:HD2	1.29	0.93
1:C:249:GLU:O	1:C:250:VAL:HG22	1.69	0.93
1:A:121:LYS:CG	1:A:122:THR:H	1.80	0.93
1:C:187:VAL:O	1:C:188:LEU:HD13	1.67	0.93
1:A:64:THR:CG2	1:A:65:HIS:HD2	1.80	0.92
1:D:13:THR:HG21	1:D:68:HIS:CD2	2.04	0.92
1:C:9:ARG:H	1:C:64:THR:HG22	1.32	0.92
1:D:269:VAL:HG13	1:D:270:THR:H	1.35	0.91
1:D:181:ASN:HD21	1:D:183:GLU:HG2	1.33	0.91
1:C:13:THR:HG22	1:C:69:LEU:H	1.34	0.91
1:D:33:LEU:HD11	1:D:36:GLU:H	1.31	0.91
1:C:214:ARG:HG2	1:C:214:ARG:NH1	1.83	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:VAL:HG22	1:B:208:TRP:H	1.36	0.90
1:D:27:VAL:N	1:D:28:ALA:HB3	1.87	0.90
1:C:214:ARG:HA	1:C:215:ARG:CB	1.99	0.90
1:C:43:SER:CB	1:C:45:ASP:HB2	2.02	0.90
1:D:27:VAL:H	1:D:28:ALA:HB3	1.37	0.89
1:A:61:VAL:HG22	1:A:63:PRO:HD3	1.56	0.88
1:B:158:PHE:HZ	1:C:273:THR:HG23	1.39	0.88
1:C:246:GLU:H	1:C:246:GLU:CD	1.79	0.88
1:B:27:VAL:HA	1:B:28:ALA:O	1.74	0.87
1:B:166:THR:HG22	1:B:167:ALA:H	1.39	0.86
1:D:83:ASN:HD22	1:D:142:GLY:H	1.24	0.86
1:B:181:ASN:HD22	1:B:184:ASP:H	1.24	0.86
1:B:42:SER:HA	1:B:43:SER:C	1.99	0.86
1:B:237:VAL:H	1:C:274:THR:HG21	1.39	0.85
1:C:212:ASN:N	1:C:213:PRO:HD3	1.90	0.85
1:C:249:GLU:HG3	1:C:250:VAL:HG13	1.58	0.84
1:A:166:THR:HG21	1:A:234:TYR:HE2	1.42	0.84
1:B:181:ASN:HD21	1:B:183:GLU:CG	1.87	0.83
1:C:208:TRP:HD1	1:C:277:ASP:HA	1.42	0.83
1:C:116:CYS:HB2	1:C:282:LYS:NZ	1.94	0.83
1:D:31:ALA:C	1:D:33:LEU:HB2	2.03	0.83
1:A:194:LYS:HZ3	1:A:207:VAL:HG23	1.44	0.82
1:D:205:LEU:HB3	1:D:206:THR:O	1.80	0.82
1:C:27:VAL:HA	1:C:28:ALA:O	1.79	0.81
1:C:213:PRO:HA	1:C:214:ARG:HB3	1.61	0.81
1:D:43:SER:OG	1:D:44:LYS:HA	1.80	0.81
1:A:121:LYS:HG3	1:A:122:THR:H	1.44	0.81
1:B:269:VAL:HG13	1:B:270:THR:H	1.43	0.81
1:C:260:VAL:HG12	1:C:261:GLU:H	1.45	0.81
1:C:64:THR:CG2	1:C:65:HIS:HD2	1.93	0.80
1:B:158:PHE:CZ	1:C:273:THR:HG23	2.15	0.80
1:C:116:CYS:HB2	1:C:282:LYS:HZ3	1.46	0.80
1:C:44:LYS:HA	1:C:46:ALA:N	1.96	0.80
1:C:259:VAL:HA	1:C:260:VAL:C	2.07	0.80
1:D:26:VAL:O	1:D:27:VAL:HG22	1.83	0.79
1:D:83:ASN:ND2	1:D:142:GLY:H	1.79	0.79
1:A:121:LYS:HE3	1:A:135:PRO:HD2	1.64	0.79
1:B:276:SER:O	1:B:277:ASP:HB2	1.84	0.78
1:D:181:ASN:ND2	1:D:184:ASP:H	1.81	0.78
1:A:121:LYS:H	1:A:121:LYS:NZ	1.82	0.77
1:B:27:VAL:HA	1:B:28:ALA:C	2.09	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ASP:O	1:D:249:GLU:HB2	1.83	0.77
1:C:83:ASN:HB2	1:D:159:GLN:NE2	2.00	0.76
1:A:8:MET:HB2	1:A:64:THR:HG21	1.66	0.76
1:C:273:THR:OG1	1:C:274:THR:HG22	1.85	0.76
1:D:206:THR:HB	1:D:207:VAL:HA	1.68	0.76
1:B:237:VAL:HG22	1:C:274:THR:HG23	1.66	0.75
1:A:119:PRO:HB3	1:A:121:LYS:HE2	1.68	0.75
1:D:13:THR:HG22	1:D:70:ALA:H	1.51	0.75
1:A:43:SER:HB3	1:A:44:LYS:C	2.12	0.74
1:A:121:LYS:CG	1:A:122:THR:N	2.50	0.74
1:B:24:GLN:C	1:B:25:LYS:HG3	2.11	0.74
1:C:257:GLU:C	1:C:259:VAL:H	1.93	0.74
1:D:73:VAL:HG22	1:D:74:GLY:H	1.53	0.74
1:C:131:ILE:HD12	1:C:148:ARG:HG2	1.70	0.74
1:D:32:GLY:CA	1:D:33:LEU:HD13	2.18	0.74
1:C:208:TRP:CD1	1:C:277:ASP:HA	2.23	0.73
1:C:83:ASN:H	1:D:159:GLN:HE22	1.35	0.73
1:A:55:ARG:O	1:A:59:GLU:HG2	1.88	0.73
1:C:191:LEU:HB3	1:C:192:ILE:CG1	2.18	0.73
1:C:214:ARG:HA	1:C:215:ARG:HB2	1.68	0.73
1:B:279:GLN:N	1:B:280:PHE:CA	2.52	0.73
1:A:155:ARG:HH21	1:B:138:ASN:HD21	1.37	0.73
1:A:43:SER:HB3	1:A:46:ALA:H	1.53	0.73
1:C:44:LYS:HA	1:C:46:ALA:H	1.54	0.73
1:D:33:LEU:CD1	1:D:36:GLU:H	2.02	0.73
1:C:13:THR:CG2	1:C:70:ALA:H	2.02	0.72
1:B:24:GLN:O	1:B:25:LYS:HG3	1.90	0.72
1:D:181:ASN:HD22	1:D:184:ASP:H	1.35	0.72
1:B:25:LYS:HA	1:B:27:VAL:H	1.52	0.72
1:C:13:THR:HG22	1:C:69:LEU:N	2.05	0.72
1:D:33:LEU:CD1	1:D:36:GLU:HB2	2.19	0.72
1:D:13:THR:CG2	1:D:70:ALA:H	2.02	0.72
1:B:207:VAL:HG22	1:B:208:TRP:N	2.03	0.71
1:B:248:ASP:O	1:B:249:GLU:HB3	1.91	0.71
1:A:166:THR:HG23	1:A:236:GLU:O	1.91	0.70
1:B:269:VAL:HG13	1:B:270:THR:N	2.06	0.70
1:B:273:THR:O	1:B:274:THR:HB	1.89	0.70
1:C:42:SER:H	1:C:43:SER:HB3	1.55	0.70
1:C:42:SER:N	1:C:43:SER:HB3	2.06	0.70
1:C:212:ASN:O	1:C:212:ASN:ND2	2.25	0.70
1:C:260:VAL:HG12	1:C:261:GLU:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:ARG:HB2	1:C:281:LYS:HA	1.73	0.70
1:B:43:SER:HA	2:B:401:NDP:O2X	1.92	0.70
1:A:138:ASN:HD21	1:B:155:ARG:HH21	1.38	0.70
1:D:73:VAL:HG23	1:D:76:LEU:HD22	1.73	0.70
1:D:32:GLY:HA3	1:D:33:LEU:CD1	2.22	0.70
1:D:304:ALA:O	1:D:308:THR:HG23	1.91	0.69
1:A:215:ARG:HD3	1:A:279:GLN:HE22	1.57	0.69
1:A:27:VAL:HA	1:A:28:ALA:O	1.91	0.69
1:D:74:GLY:C	1:D:76:LEU:H	2.00	0.69
1:B:237:VAL:H	1:C:274:THR:CG2	2.05	0.69
1:D:33:LEU:HD11	1:D:36:GLU:HB2	1.74	0.69
1:C:83:ASN:ND2	1:C:142:GLY:H	1.91	0.69
1:C:245:GLY:C	1:C:247:GLU:H	2.00	0.69
1:C:42:SER:CA	1:C:43:SER:HB3	2.22	0.69
1:C:128:GLU:HG2	1:C:239:PRO:O	1.93	0.69
1:D:33:LEU:HD11	1:D:36:GLU:N	2.06	0.68
1:C:250:VAL:HB	1:C:251:SER:CB	2.23	0.68
1:C:9:ARG:H	1:C:64:THR:CG2	2.06	0.68
1:C:278:GLY:HA2	1:C:279:GLN:C	2.19	0.68
1:C:309:CYS:O	1:C:313:THR:HG23	1.94	0.68
1:B:181:ASN:ND2	1:B:184:ASP:H	1.90	0.68
1:A:204:ALA:O	1:A:205:LEU:HB2	1.94	0.68
1:A:23:ILE:O	1:A:26:VAL:HB	1.94	0.68
1:D:206:THR:CB	1:D:207:VAL:HA	2.24	0.68
1:D:269:VAL:HG13	1:D:270:THR:N	2.08	0.68
1:B:248:ASP:O	1:B:249:GLU:CB	2.41	0.68
1:C:61:VAL:O	1:C:63:PRO:HD3	1.94	0.68
1:D:279:GLN:N	1:D:280:PHE:HA	2.09	0.67
1:C:191:LEU:HB3	1:C:192:ILE:HA	1.75	0.67
1:C:203:SER:HB3	1:C:204:ALA:HB3	1.76	0.67
1:C:70:ALA:HB1	1:C:93:MET:CE	2.24	0.67
1:C:203:SER:HA	1:C:204:ALA:HB3	1.75	0.67
1:C:212:ASN:O	1:C:212:ASN:CG	2.38	0.67
1:D:8:MET:O	1:D:36:GLU:O	2.12	0.67
1:B:29:ASP:OD2	1:B:31:ALA:HB2	1.95	0.67
1:A:178:ASP:O	1:A:320:ARG:HG3	1.95	0.67
1:B:9:ARG:HB2	1:B:9:ARG:NH1	2.10	0.67
1:B:178:ASP:O	1:B:320:ARG:HG3	1.94	0.66
1:C:166:THR:HG21	1:C:234:TYR:HE2	1.59	0.66
1:D:33:LEU:HD12	1:D:34:PRO:C	2.21	0.66
1:D:248:ASP:O	1:D:249:GLU:CB	2.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ARG:HB2	1:B:9:ARG:CZ	2.25	0.66
1:A:194:LYS:HE2	1:A:206:THR:O	1.96	0.66
1:B:187:VAL:HG13	1:B:188:LEU:N	2.11	0.66
1:C:25:LYS:HA	1:C:26:VAL:C	2.21	0.66
1:C:213:PRO:HB2	1:C:251:SER:HA	1.78	0.66
1:A:23:ILE:C	1:A:25:LYS:H	2.04	0.65
1:A:178:ASP:OD2	1:A:189:PRO:HG3	1.96	0.65
1:C:250:VAL:HB	1:C:251:SER:HB3	1.78	0.65
1:C:214:ARG:HD2	1:C:279:GLN:O	1.96	0.65
1:B:274:THR:HG22	1:B:275:LYS:HG2	1.77	0.65
1:A:279:GLN:HB2	1:A:281:LYS:N	2.11	0.65
1:A:194:LYS:NZ	1:A:207:VAL:HA	2.12	0.65
1:D:36:GLU:O	1:D:37:ASP:HB3	1.96	0.65
1:C:182:ILE:HD11	1:C:190:GLY:HA2	1.79	0.65
1:A:43:SER:HA	1:A:44:LYS:O	1.97	0.65
1:C:118:PHE:CE2	1:C:131:ILE:HG22	2.32	0.65
1:C:208:TRP:HA	1:C:276:SER:O	1.97	0.64
1:C:68:HIS:HE1	1:C:94:ASN:OD1	1.79	0.64
1:C:261:GLU:O	1:C:262:ALA:CB	2.46	0.64
1:C:181:ASN:ND2	1:C:321:LYS:HD3	2.12	0.64
1:D:17:GLY:O	1:D:21:LYS:HG2	1.97	0.64
1:B:215:ARG:HH22	1:B:279:GLN:N	1.96	0.64
1:C:203:SER:CA	1:C:204:ALA:HB3	2.28	0.64
1:D:197:LEU:O	1:D:201:SER:HB3	1.98	0.64
1:A:25:LYS:HA	1:A:26:VAL:HG12	1.80	0.64
1:A:23:ILE:O	1:A:25:LYS:N	2.31	0.64
1:D:70:ALA:C	1:D:93:MET:HE1	2.23	0.64
1:D:73:VAL:HG23	1:D:76:LEU:CD2	2.28	0.64
1:B:206:THR:CB	1:B:207:VAL:HA	2.28	0.63
1:D:13:THR:HG22	1:D:69:LEU:H	1.63	0.63
1:C:188:LEU:HD12	1:C:189:PRO:HD3	1.80	0.63
1:A:83:ASN:ND2	1:A:142:GLY:H	1.96	0.63
1:C:252:ILE:C	1:C:254:GLU:H	2.04	0.63
1:D:205:LEU:HA	1:D:206:THR:CB	2.27	0.63
1:A:84:LEU:HD22	1:A:88:ARG:HG3	1.79	0.63
1:A:194:LYS:HZ1	1:A:207:VAL:HA	1.62	0.63
1:D:73:VAL:HG22	1:D:74:GLY:N	2.13	0.63
1:C:42:SER:HB2	1:C:43:SER:HA	1.79	0.63
1:A:67:ILE:HD11	1:A:231:LEU:HD22	1.79	0.62
1:C:304:ALA:O	1:C:308:THR:HG22	2.00	0.62
1:D:43:SER:HA	1:D:44:LYS:C	2.22	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:LYS:C	1:B:201:SER:H	2.07	0.62
1:C:83:ASN:HB2	1:D:159:GLN:HE21	1.61	0.62
1:C:48:LEU:HD22	2:C:401:NDP:H2A	1.81	0.62
1:D:272:ASP:OD1	1:D:274:THR:HB	1.99	0.62
1:B:237:VAL:N	1:C:274:THR:HG21	2.13	0.62
1:C:67:ILE:HD11	1:C:231:LEU:HD22	1.81	0.62
1:C:191:LEU:HB3	1:C:192:ILE:CA	2.29	0.62
1:D:206:THR:O	1:D:270:THR:O	2.17	0.62
1:A:8:MET:CB	1:A:64:THR:HG21	2.29	0.62
1:B:253:LYS:HE3	1:B:257:GLU:OE2	2.00	0.61
1:C:42:SER:OG	1:C:43:SER:HB3	1.99	0.61
1:A:166:THR:HG21	1:A:234:TYR:CE2	2.31	0.61
1:B:212:ASN:N	1:B:213:PRO:HD2	2.15	0.61
1:C:208:TRP:HD1	1:C:277:ASP:CA	2.13	0.61
1:D:28:ALA:O	1:D:29:ASP:HB2	1.99	0.61
1:B:83:ASN:HD21	1:B:140:ASN:HA	1.65	0.61
1:A:215:ARG:HD3	1:A:279:GLN:NE2	2.15	0.61
1:B:207:VAL:CG2	1:B:208:TRP:H	2.10	0.61
1:C:273:THR:OG1	1:C:274:THR:N	2.31	0.61
1:A:73:VAL:HG23	1:A:76:LEU:HD22	1.81	0.61
1:A:159:GLN:NE2	1:B:83:ASN:H	1.98	0.61
1:D:13:THR:HG23	1:D:70:ALA:CB	2.31	0.61
1:A:159:GLN:HE22	1:B:83:ASN:H	1.46	0.60
1:A:279:GLN:H	1:A:280:PHE:HA	1.66	0.60
1:B:131:ILE:HD11	1:B:132:HIS:CE1	2.36	0.60
1:B:25:LYS:HA	1:B:27:VAL:N	2.15	0.60
1:C:277:ASP:O	1:C:278:GLY:O	2.18	0.60
1:A:48:LEU:HD22	2:A:401:NDP:H2A	1.83	0.60
1:C:203:SER:HA	1:C:204:ALA:CB	2.32	0.60
1:D:13:THR:HG23	1:D:70:ALA:HB2	1.82	0.60
1:A:26:VAL:HG13	1:A:26:VAL:O	2.02	0.60
1:B:25:LYS:N	1:B:26:VAL:HB	2.16	0.60
1:B:155:ARG:HD2	1:C:275:LYS:HE3	1.84	0.60
1:C:26:VAL:O	1:C:27:VAL:HG13	2.01	0.60
1:C:212:ASN:N	1:C:213:PRO:CD	2.64	0.60
1:C:13:THR:HG23	1:C:70:ALA:HB2	1.84	0.59
1:A:27:VAL:CA	1:A:28:ALA:C	2.66	0.59
1:C:116:CYS:CB	1:C:282:LYS:HZ2	2.15	0.59
1:B:47:ASP:OD1	1:B:49:THR:HB	2.02	0.59
1:D:26:VAL:C	1:D:27:VAL:HG22	2.28	0.59
1:D:27:VAL:HA	1:D:28:ALA:C	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:SER:HB3	1:A:45:ASP:HB3	1.83	0.59
1:A:138:ASN:ND2	1:B:155:ARG:HH21	2.00	0.59
1:A:246:GLU:CD	1:A:246:GLU:H	2.11	0.59
1:D:178:ASP:OD2	1:D:189:PRO:HG3	2.02	0.59
1:A:43:SER:CB	1:A:45:ASP:HB3	2.32	0.58
1:B:207:VAL:O	1:B:271:PHE:O	2.19	0.58
1:A:194:LYS:NZ	1:A:207:VAL:HG23	2.18	0.58
1:B:194:LYS:HD2	1:B:206:THR:OG1	2.02	0.58
1:C:116:CYS:CB	1:C:282:LYS:NZ	2.64	0.58
1:C:214:ARG:HA	1:C:215:ARG:CG	2.32	0.58
1:C:252:ILE:C	1:C:254:GLU:N	2.60	0.58
1:A:83:ASN:HD22	1:A:142:GLY:H	1.50	0.58
1:A:87:TRP:HZ3	1:B:153:GLN:NE2	2.01	0.58
1:B:45:ASP:C	1:B:45:ASP:OD1	2.45	0.58
1:C:70:ALA:HB1	1:C:93:MET:HE2	1.86	0.58
1:B:206:THR:O	1:B:270:THR:O	2.22	0.58
1:C:257:GLU:CD	1:C:257:GLU:H	2.12	0.58
1:D:26:VAL:O	1:D:26:VAL:HG12	2.03	0.57
1:C:42:SER:CA	1:C:43:SER:CB	2.80	0.57
1:D:68:HIS:HE1	1:D:94:ASN:OD1	1.87	0.57
1:A:215:ARG:HD3	1:A:279:GLN:OE1	2.04	0.57
1:D:64:THR:OG1	1:D:65:HIS:HD2	1.87	0.57
1:D:43:SER:HA	1:D:45:ASP:N	2.20	0.57
1:B:202:GLY:O	1:B:203:SER:C	2.47	0.57
1:C:13:THR:HG23	1:C:70:ALA:CB	2.35	0.57
1:D:23:ILE:C	1:D:25:LYS:H	2.12	0.57
1:A:279:GLN:HG3	1:A:280:PHE:C	2.30	0.57
1:A:304:ALA:O	1:A:308:THR:HG23	2.05	0.57
1:A:72:MET:HE3	1:A:86:PHE:CE1	2.39	0.56
1:C:189:PRO:O	1:C:190:GLY:C	2.47	0.56
1:B:208:TRP:CE3	1:B:275:LYS:HG3	2.40	0.56
1:D:70:ALA:O	1:D:93:MET:HE1	2.05	0.56
1:A:87:TRP:HZ3	1:B:153:GLN:HE21	1.51	0.56
1:B:301:PHE:O	1:B:305:VAL:HG23	2.05	0.56
1:C:187:VAL:C	1:C:188:LEU:HD13	2.29	0.56
1:A:26:VAL:C	1:A:27:VAL:HG22	2.29	0.56
1:C:203:SER:CB	1:C:204:ALA:HB3	2.35	0.56
1:B:304:ALA:O	1:B:308:THR:HG23	2.06	0.56
1:A:47:ASP:OD1	1:A:49:THR:HB	2.07	0.55
1:C:245:GLY:C	1:C:247:GLU:N	2.64	0.55
1:C:191:LEU:HB3	1:C:192:ILE:CB	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:HIS:HE1	1:A:94:ASN:OD1	1.89	0.55
1:B:131:ILE:HD12	1:B:148:ARG:HG2	1.89	0.55
1:C:99:HIS:HD2	1:C:157:TYR:OH	1.89	0.55
1:C:166:THR:HG21	1:C:234:TYR:CE2	2.41	0.55
1:A:43:SER:HB3	1:A:46:ALA:N	2.20	0.55
1:D:230:VAL:O	1:D:233:GLU:O	2.23	0.55
1:B:166:THR:HG22	1:B:167:ALA:N	2.16	0.55
1:D:99:HIS:HD2	1:D:157:TYR:OH	1.89	0.55
1:B:36:GLU:O	1:B:37:ASP:CB	2.54	0.55
1:D:301:PHE:O	1:D:305:VAL:HG23	2.07	0.55
1:B:27:VAL:CA	1:B:28:ALA:C	2.77	0.55
1:D:83:ASN:HD22	1:D:142:GLY:N	2.00	0.55
1:C:13:THR:HG23	1:C:70:ALA:H	1.69	0.55
1:C:42:SER:CB	1:C:43:SER:HB3	2.37	0.55
1:C:116:CYS:HA	1:C:282:LYS:HD3	1.88	0.55
1:D:33:LEU:HD13	1:D:36:GLU:HB2	1.89	0.54
1:B:230:VAL:O	1:B:233:GLU:O	2.25	0.54
1:B:191:LEU:HD21	1:B:207:VAL:HB	1.89	0.54
1:B:269:VAL:CG1	1:B:270:THR:H	2.17	0.54
1:D:23:ILE:O	1:D:25:LYS:N	2.41	0.54
1:B:43:SER:C	1:B:45:ASP:H	2.16	0.54
1:B:15:GLY:N	1:B:42:SER:O	2.41	0.54
1:B:23:ILE:C	1:B:25:LYS:H	2.15	0.54
1:A:10:ILE:HG12	1:A:231:LEU:HD21	1.88	0.54
1:C:251:SER:O	1:C:253:LYS:N	2.41	0.54
1:D:269:VAL:CG1	1:D:270:THR:H	2.16	0.54
1:C:254:GLU:CA	1:C:254:GLU:OE1	2.56	0.54
1:A:15:GLY:N	1:A:42:SER:OG	2.41	0.54
1:C:214:ARG:HB2	1:C:280:PHE:O	2.08	0.54
1:A:58:PHE:O	1:A:61:VAL:O	2.26	0.53
1:B:112:CYS:SG	1:B:227:PHE:HZ	2.30	0.53
1:B:128:GLU:HG2	1:B:239:PRO:O	2.08	0.53
1:B:273:THR:O	1:B:274:THR:CB	2.57	0.53
1:C:303:GLN:O	1:C:307:GLU:HG3	2.08	0.53
1:A:48:LEU:HD22	2:A:401:NDP:C2A	2.37	0.53
1:C:8:MET:HB2	1:C:64:THR:HG21	1.89	0.53
1:C:181:ASN:HD22	1:C:321:LYS:HD3	1.72	0.53
1:D:74:GLY:C	1:D:76:LEU:N	2.66	0.53
1:D:204:ALA:O	1:D:205:LEU:HB2	2.08	0.53
1:A:159:GLN:HE21	1:B:83:ASN:HB2	1.73	0.53
1:B:48:LEU:HD22	2:B:401:NDP:C2A	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:GLU:O	1:C:250:VAL:CG2	2.52	0.53
1:B:131:ILE:CD1	1:B:148:ARG:HG2	2.39	0.53
1:C:10:ILE:HD12	1:C:10:ILE:N	2.24	0.53
1:D:26:VAL:O	1:D:26:VAL:CG1	2.56	0.53
1:A:99:HIS:HD2	1:A:157:TYR:OH	1.91	0.52
1:B:206:THR:HB	1:B:207:VAL:HA	1.91	0.52
1:C:164:THR:HG22	1:C:164:THR:O	2.09	0.52
1:A:16:SER:N	1:A:42:SER:OG	2.41	0.52
1:A:304:ALA:O	1:A:308:THR:CG2	2.58	0.52
1:D:33:LEU:CD1	1:D:34:PRO:HA	2.38	0.52
1:A:209:GLY:H	1:A:272:ASP:C	2.17	0.52
1:A:116:CYS:HB3	1:A:282:LYS:NZ	2.24	0.52
1:A:230:VAL:O	1:A:233:GLU:O	2.27	0.52
1:A:113:LEU:O	1:A:170:PRO:HD2	2.10	0.52
1:C:276:SER:O	1:C:277:ASP:HB3	2.10	0.52
1:D:198:ALA:HB2	1:D:204:ALA:HB3	1.92	0.52
1:D:303:GLN:O	1:D:307:GLU:HG3	2.11	0.51
1:C:254:GLU:OE1	1:C:254:GLU:HA	2.09	0.51
1:C:261:GLU:O	1:C:262:ALA:HB3	2.10	0.51
1:D:32:GLY:N	1:D:33:LEU:HB2	2.24	0.51
1:D:32:GLY:HA2	1:D:36:GLU:CD	2.35	0.51
1:C:42:SER:CB	1:C:43:SER:CA	2.88	0.51
1:C:257:GLU:C	1:C:259:VAL:N	2.62	0.51
1:A:131:ILE:CD1	1:A:148:ARG:HG2	2.40	0.51
1:A:205:LEU:CB	1:A:206:THR:HA	2.39	0.51
1:C:213:PRO:HB3	1:C:252:ILE:HG12	1.92	0.51
1:D:206:THR:HG22	1:D:208:TRP:CH2	2.45	0.51
1:A:42:SER:C	1:A:43:SER:OG	2.53	0.51
1:A:172:ASN:HD22	1:A:172:ASN:C	2.19	0.51
1:C:27:VAL:HA	1:C:28:ALA:C	2.36	0.51
1:A:121:LYS:HG2	1:A:122:THR:N	2.26	0.51
1:A:8:MET:HB2	1:A:64:THR:CG2	2.40	0.50
1:C:131:ILE:HD11	1:C:132:HIS:CE1	2.46	0.50
1:C:276:SER:OG	1:C:277:ASP:N	2.42	0.50
1:D:31:ALA:O	1:D:33:LEU:HB2	2.10	0.50
1:A:84:LEU:HA	1:B:156:ALA:HB1	1.93	0.50
1:B:26:VAL:O	1:B:29:ASP:HA	2.10	0.50
1:B:83:ASN:ND2	1:B:142:GLY:H	2.10	0.50
1:B:195:VAL:O	1:B:198:ALA:HB3	2.12	0.50
1:C:257:GLU:CD	1:C:257:GLU:N	2.69	0.50
1:B:57:LEU:O	1:B:57:LEU:HD12	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:VAL:C	1:A:208:TRP:CG	2.90	0.50
1:A:204:ALA:O	1:A:205:LEU:HD13	2.11	0.50
1:C:203:SER:CA	1:C:204:ALA:CB	2.90	0.50
1:D:43:SER:HA	1:D:45:ASP:H	1.76	0.50
1:D:32:GLY:N	1:D:33:LEU:HD13	2.27	0.49
1:A:188:LEU:HB3	1:A:189:PRO:HD3	1.93	0.49
1:A:214:ARG:HG2	1:A:214:ARG:HH11	1.77	0.49
1:C:68:HIS:CD2	1:C:97:VAL:HG11	2.48	0.49
1:C:171:THR:HB	1:C:216:GLN:O	2.11	0.49
1:D:273:THR:O	1:D:273:THR:HG22	2.12	0.49
1:A:16:SER:OG	1:A:42:SER:HB3	2.11	0.49
1:D:10:ILE:HG12	1:D:231:LEU:HD21	1.94	0.49
1:A:203:SER:O	1:A:204:ALA:HB3	2.11	0.49
1:B:194:LYS:HD2	1:B:206:THR:HG1	1.77	0.49
1:B:205:LEU:HB3	1:B:269:VAL:O	2.13	0.49
1:C:42:SER:HB2	1:C:43:SER:CA	2.42	0.49
1:B:173:VAL:HG23	2:B:401:NDP:H42N	1.94	0.49
1:B:23:ILE:HG22	1:B:40:PHE:HZ	1.78	0.49
1:C:99:HIS:CD2	1:C:157:TYR:OH	2.65	0.49
1:C:216:GLN:HG3	1:C:249:GLU:CB	2.43	0.49
1:A:279:GLN:N	1:A:280:PHE:HA	2.27	0.49
1:C:207:VAL:O	1:C:208:TRP:HB2	2.12	0.49
1:D:145:TYR:O	1:D:149:MET:HG2	2.12	0.49
1:C:65:HIS:HB3	1:C:231:LEU:HD11	1.95	0.49
1:B:65:HIS:HB3	1:B:231:LEU:HD11	1.95	0.49
1:C:193:HIS:N	1:C:193:HIS:ND1	2.59	0.49
1:C:214:ARG:HA	1:C:215:ARG:HG3	1.95	0.49
1:D:25:LYS:HA	1:D:26:VAL:C	2.37	0.49
1:A:77:PHE:HB2	1:A:184:ASP:O	2.13	0.49
1:A:245:GLY:C	1:A:247:GLU:H	2.21	0.49
1:B:199:LYS:O	1:B:201:SER:N	2.46	0.48
1:D:113:LEU:O	1:D:170:PRO:HD2	2.12	0.48
1:A:233:GLU:O	1:A:234:TYR:HB3	2.13	0.48
1:C:246:GLU:CD	1:C:246:GLU:N	2.58	0.48
1:A:212:ASN:N	1:A:213:PRO:CD	2.76	0.48
1:B:23:ILE:O	1:B:25:LYS:N	2.42	0.48
1:B:41:VAL:HG13	1:B:42:SER:HB2	1.95	0.48
1:A:23:ILE:C	1:A:25:LYS:N	2.64	0.48
1:A:9:ARG:O	1:A:64:THR:HG22	2.13	0.48
1:B:23:ILE:HG22	1:B:40:PHE:CZ	2.49	0.48
1:B:209:GLY:O	1:B:271:PHE:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:GLN:OE1	1:B:279:GLN:HA	2.13	0.48
1:B:305:VAL:HG12	1:B:309:CYS:SG	2.54	0.48
1:C:215:ARG:HD3	1:C:282:LYS:C	2.38	0.48
1:B:205:LEU:HA	1:B:206:THR:C	2.38	0.48
1:C:207:VAL:O	1:C:208:TRP:CE3	2.66	0.48
1:A:215:ARG:HD3	1:A:279:GLN:CD	2.38	0.48
1:B:25:LYS:CA	1:B:27:VAL:H	2.25	0.48
1:C:215:ARG:HD2	1:C:216:GLN:OE1	2.14	0.48
1:C:259:VAL:HA	1:C:260:VAL:O	2.11	0.48
1:D:204:ALA:O	1:D:205:LEU:HD12	2.14	0.48
1:B:315:ASN:O	1:B:316:TYR:C	2.57	0.48
1:A:207:VAL:O	1:A:208:TRP:CD1	2.67	0.47
1:B:41:VAL:HG22	1:B:42:SER:N	2.29	0.47
1:C:48:LEU:HD22	2:C:401:NDP:C2A	2.43	0.47
1:C:252:ILE:O	1:C:254:GLU:N	2.47	0.47
1:B:26:VAL:O	1:B:27:VAL:HG13	2.15	0.47
1:D:73:VAL:CG2	1:D:74:GLY:H	2.24	0.47
1:B:67:ILE:HD11	1:B:231:LEU:HD22	1.96	0.47
1:B:187:VAL:CG1	1:B:188:LEU:N	2.77	0.47
1:B:320:ARG:H	1:B:320:ARG:HG2	1.54	0.47
1:A:43:SER:HB2	1:A:46:ALA:O	2.14	0.47
1:C:44:LYS:HE3	1:C:44:LYS:HB3	1.70	0.47
1:C:244:VAL:HG22	1:C:245:GLY:H	1.79	0.47
1:A:280:PHE:C	1:A:280:PHE:CD2	2.92	0.47
1:D:99:HIS:CD2	1:D:157:TYR:OH	2.67	0.47
1:D:178:ASP:O	1:D:320:ARG:HG3	2.14	0.47
1:B:166:THR:HG21	1:B:234:TYR:HE2	1.80	0.47
1:B:205:LEU:HA	1:B:206:THR:OG1	2.15	0.47
1:B:304:ALA:O	1:B:308:THR:CG2	2.62	0.47
1:C:214:ARG:HH11	1:C:214:ARG:CG	2.00	0.47
1:D:23:ILE:C	1:D:25:LYS:N	2.71	0.47
1:A:9:ARG:HD3	1:A:37:ASP:OD2	2.15	0.47
1:C:191:LEU:CB	1:C:192:ILE:HA	2.44	0.47
1:D:205:LEU:CB	1:D:206:THR:O	2.58	0.47
1:A:121:LYS:HZ3	1:A:121:LYS:N	1.92	0.47
1:B:64:THR:OG1	1:B:65:HIS:HD2	1.97	0.47
1:B:212:ASN:HB2	1:D:291:THR:OG1	2.15	0.47
1:C:81:LYS:C	1:C:82:TYR:HD2	2.23	0.47
1:B:319:ALA:O	1:B:321:LYS:HG3	2.15	0.47
1:C:83:ASN:H	1:D:159:GLN:NE2	2.10	0.47
1:C:81:LYS:C	1:C:82:TYR:CD2	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:TYR:CZ	1:B:221:LEU:HD23	2.50	0.46
1:C:156:ALA:HB1	1:D:84:LEU:CA	2.45	0.46
1:D:36:GLU:O	1:D:37:ASP:CB	2.58	0.46
1:C:8:MET:HB2	1:C:64:THR:CG2	2.45	0.46
1:D:31:ALA:O	1:D:32:GLY:C	2.58	0.46
1:D:275:LYS:CG	1:D:276:SER:H	2.28	0.46
1:A:28:ALA:O	1:A:29:ASP:HB2	2.15	0.46
1:B:206:THR:CB	1:B:207:VAL:CA	2.93	0.46
1:C:18:LEU:HD22	1:C:178:ASP:CG	2.40	0.46
1:D:259:VAL:O	1:D:263:MET:HG3	2.15	0.46
1:D:33:LEU:HD12	1:D:33:LEU:HA	1.47	0.46
1:C:181:ASN:HA	1:C:321:LYS:HG2	1.97	0.46
1:C:215:ARG:HB3	1:C:216:GLN:H	1.33	0.46
1:A:9:ARG:H	1:A:64:THR:HG22	1.81	0.46
1:A:29:ASP:OD2	1:A:31:ALA:HB2	2.16	0.46
1:A:207:VAL:O	1:A:208:TRP:CG	2.68	0.46
1:C:207:VAL:O	1:C:208:TRP:CB	2.62	0.46
1:B:61:VAL:HG22	1:B:63:PRO:HD3	1.97	0.46
1:C:292:TYR:O	1:C:293:LEU:HD23	2.16	0.46
1:B:199:LYS:C	1:B:201:SER:N	2.74	0.46
1:D:8:MET:HG3	1:D:65:HIS:CD2	2.50	0.46
1:A:99:HIS:CD2	1:A:157:TYR:OH	2.68	0.45
1:C:182:ILE:HD11	1:C:190:GLY:CA	2.45	0.45
1:D:8:MET:HE3	1:D:8:MET:HB2	1.70	0.45
1:D:55:ARG:O	1:D:59:GLU:HG2	2.16	0.45
1:D:275:LYS:O	1:D:276:SER:HB3	2.16	0.45
1:B:280:PHE:CD2	1:B:280:PHE:C	2.94	0.45
1:C:214:ARG:NH1	1:C:214:ARG:CG	2.62	0.45
1:B:206:THR:OG1	1:B:207:VAL:HA	2.17	0.45
1:A:26:VAL:O	1:A:27:VAL:HG22	2.16	0.45
1:C:210:THR:HG22	1:C:253:LYS:HG3	1.99	0.45
1:C:221:LEU:HD13	1:C:221:LEU:HA	1.71	0.45
1:D:206:THR:CB	1:D:207:VAL:CA	2.94	0.45
1:D:174:PHE:CG	1:D:188:LEU:HD23	2.52	0.45
1:D:205:LEU:HB3	1:D:206:THR:C	2.41	0.45
1:A:320:ARG:H	1:A:320:ARG:HG2	1.56	0.45
1:B:236:GLU:HA	1:C:274:THR:HG21	1.98	0.45
1:C:26:VAL:C	1:C:27:VAL:HG22	2.42	0.45
1:D:48:LEU:HB3	1:D:93:MET:HG2	1.97	0.45
1:C:118:PHE:CG	1:C:126:ILE:HD12	2.52	0.45
1:D:8:MET:HG2	1:D:10:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LYS:HD3	1:B:206:THR:HG21	1.99	0.45
1:B:205:LEU:N	1:B:205:LEU:HD23	2.32	0.45
1:C:131:ILE:O	1:C:132:HIS:HB2	2.17	0.45
1:C:164:THR:O	1:C:165:PHE:HD1	2.00	0.45
1:A:9:ARG:H	1:A:64:THR:CG2	2.30	0.44
1:D:83:ASN:HD21	1:D:140:ASN:HA	1.83	0.44
1:D:181:ASN:HA	1:D:321:LYS:C	2.41	0.44
1:D:212:ASN:N	1:D:213:PRO:CD	2.80	0.44
1:A:43:SER:CB	1:A:44:LYS:C	2.87	0.44
1:A:155:ARG:HH21	1:B:138:ASN:ND2	2.10	0.44
1:B:290:ARG:HD3	1:B:290:ARG:HA	1.74	0.44
1:D:5:GLN:HA	1:D:6:GLY:HA3	1.80	0.44
1:D:33:LEU:CB	1:D:34:PRO:HA	2.42	0.44
1:D:290:ARG:HD3	1:D:290:ARG:HA	1.73	0.44
1:C:27:VAL:CA	1:C:28:ALA:O	2.59	0.44
1:D:198:ALA:HB2	1:D:204:ALA:CB	2.46	0.44
1:B:131:ILE:HG13	1:B:132:HIS:CD2	2.53	0.44
1:C:87:TRP:CE2	1:C:91:VAL:HG21	2.53	0.44
1:A:174:PHE:CE1	1:A:217:PHE:HB3	2.53	0.44
1:A:205:LEU:HB3	1:A:206:THR:HA	1.99	0.44
1:B:212:ASN:N	1:B:213:PRO:CD	2.81	0.44
1:C:173:VAL:HG23	2:C:401:NDP:H42N	1.99	0.44
1:C:211:GLY:C	1:C:213:PRO:HD3	2.40	0.44
1:C:213:PRO:HA	1:C:214:ARG:CB	2.30	0.44
1:A:204:ALA:O	1:A:205:LEU:CB	2.63	0.44
1:B:9:ARG:CZ	1:B:9:ARG:CB	2.95	0.44
1:C:84:LEU:C	1:C:84:LEU:HD13	2.42	0.44
1:C:275:LYS:HA	1:C:276:SER:HA	1.63	0.44
1:D:204:ALA:O	1:D:205:LEU:CB	2.66	0.44
1:B:54:THR:HG21	1:B:96:ASN:HB3	1.99	0.44
1:B:108:LYS:HG2	1:B:109:VAL:N	2.32	0.44
1:D:13:THR:HG22	1:D:69:LEU:N	2.31	0.44
1:D:33:LEU:HD11	1:D:36:GLU:CB	2.44	0.44
1:B:38:TRP:HB3	1:B:40:PHE:CE1	2.52	0.44
1:B:48:LEU:HD22	2:B:401:NDP:H2A	1.98	0.44
1:C:70:ALA:CB	1:C:93:MET:HE2	2.48	0.43
1:C:115:THR:OG1	1:C:215:ARG:NH1	2.51	0.43
1:C:121:LYS:O	1:C:122:THR:O	2.36	0.43
1:B:131:ILE:HG13	1:B:132:HIS:N	2.31	0.43
1:C:173:VAL:HG12	1:C:174:PHE:N	2.34	0.43
1:A:84:LEU:HD11	1:B:157:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:HG3	1:A:241:ILE:HG13	2.00	0.43
1:B:173:VAL:H	2:B:401:NDP:H71N	1.66	0.43
1:C:43:SER:OG	1:C:45:ASP:HB2	2.19	0.43
1:C:188:LEU:HD12	1:C:189:PRO:CD	2.46	0.43
1:C:223:LEU:O	1:C:227:PHE:HB2	2.18	0.43
1:A:116:CYS:CB	1:A:282:LYS:NZ	2.82	0.43
1:A:87:TRP:CZ3	1:B:153:GLN:HG2	2.53	0.43
1:C:8:MET:HE2	1:C:8:MET:HB3	1.68	0.43
1:C:26:VAL:O	1:C:26:VAL:HG12	2.18	0.43
1:B:78:ARG:HH11	1:B:183:GLU:HB2	1.84	0.43
1:C:26:VAL:O	1:C:27:VAL:HG22	2.19	0.43
1:C:117:ILE:HG22	1:C:144:SER:HA	1.99	0.43
1:C:215:ARG:HD3	1:C:282:LYS:HG3	2.01	0.43
1:D:277:ASP:HB3	1:D:278:GLY:H	1.68	0.43
1:C:260:VAL:CG1	1:C:261:GLU:N	2.77	0.43
1:D:124:TYR:HA	1:D:125:PRO:C	2.43	0.43
1:B:17:GLY:O	1:B:21:LYS:HG2	2.19	0.43
1:C:43:SER:OG	1:C:45:ASP:CB	2.67	0.43
1:D:164:THR:O	1:D:164:THR:HG22	2.18	0.43
1:D:207:VAL:HG22	1:D:208:TRP:N	2.34	0.43
1:B:182:ILE:HD12	1:B:194:LYS:HG3	2.01	0.42
1:B:233:GLU:HB3	1:B:234:TYR:H	1.74	0.42
1:C:191:LEU:CB	1:C:192:ILE:CA	2.97	0.42
1:C:30:GLY:HA2	1:C:232:ARG:HH22	1.83	0.42
1:C:41:VAL:HG13	1:C:45:ASP:HB3	2.02	0.42
1:A:74:GLY:H	1:A:76:LEU:HB2	1.84	0.42
1:B:24:GLN:HG2	1:B:40:PHE:CE2	2.54	0.42
1:B:206:THR:HA	1:B:207:VAL:O	2.20	0.42
1:C:188:LEU:HB3	1:C:189:PRO:HD2	2.00	0.42
1:B:281:LYS:O	1:B:281:LYS:HG2	2.18	0.42
1:C:238:GLU:HG3	1:C:239:PRO:HD2	2.02	0.42
1:D:275:LYS:O	1:D:276:SER:CB	2.68	0.42
1:C:178:ASP:O	1:C:320:ARG:HG3	2.19	0.42
1:D:191:LEU:HD21	1:D:207:VAL:CG2	2.50	0.42
1:B:13:THR:HG1	1:B:69:LEU:H	1.68	0.42
1:B:41:VAL:HG22	1:B:42:SER:H	1.82	0.42
1:C:82:TYR:CD2	1:C:82:TYR:N	2.86	0.42
1:A:9:ARG:N	1:A:64:THR:HG22	2.35	0.42
1:B:44:LYS:HB3	1:B:44:LYS:HE2	1.90	0.42
1:B:57:LEU:HD12	1:B:57:LEU:C	2.45	0.42
1:C:27:VAL:CA	1:C:28:ALA:C	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLU:HG2	1:A:239:PRO:O	2.20	0.42
1:C:10:ILE:HD12	1:C:10:ILE:H	1.83	0.42
1:C:131:ILE:HG13	1:C:132:HIS:CG	2.55	0.42
1:C:84:LEU:HB3	1:D:160:GLN:OE1	2.19	0.42
1:D:269:VAL:CG1	1:D:270:THR:N	2.79	0.42
1:A:121:LYS:O	1:A:122:THR:HG22	2.18	0.42
1:C:9:ARG:N	1:C:64:THR:HG22	2.16	0.42
1:D:28:ALA:O	1:D:29:ASP:CB	2.68	0.42
1:D:234:TYR:CZ	1:D:236:GLU:HB2	2.55	0.42
1:A:8:MET:CA	1:A:64:THR:HG21	2.49	0.41
1:A:87:TRP:CZ3	1:B:153:GLN:CG	3.04	0.41
1:C:18:LEU:HD22	1:C:178:ASP:OD1	2.19	0.41
1:C:164:THR:C	1:C:165:PHE:HD1	2.28	0.41
1:C:187:VAL:O	1:C:187:VAL:HG22	2.19	0.41
1:D:131:ILE:HD12	1:D:148:ARG:HG2	2.00	0.41
1:B:13:THR:OG1	1:B:68:HIS:HD2	2.04	0.41
1:B:87:TRP:HD1	1:B:142:GLY:O	2.03	0.41
1:B:180:PHE:HB2	1:B:320:ARG:O	2.20	0.41
1:B:276:SER:OG	1:B:277:ASP:N	2.53	0.41
1:C:153:GLN:HG2	1:D:87:TRP:CZ3	2.54	0.41
1:A:45:ASP:OD1	1:A:45:ASP:C	2.63	0.41
1:A:57:LEU:O	1:A:61:VAL:HG13	2.20	0.41
1:A:74:GLY:C	1:A:76:LEU:H	2.20	0.41
1:B:43:SER:C	1:B:45:ASP:N	2.78	0.41
1:D:32:GLY:CA	1:D:36:GLU:CD	2.93	0.41
1:A:198:ALA:CB	1:A:204:ALA:HB3	2.50	0.41
1:C:301:PHE:O	1:C:305:VAL:HG23	2.21	0.41
1:D:43:SER:OG	1:D:46:ALA:C	2.64	0.41
1:A:181:ASN:HB2	1:A:321:LYS:HB3	2.01	0.41
1:A:195:VAL:HG21	1:A:259:VAL:HG12	2.01	0.41
1:B:205:LEU:CD1	1:B:269:VAL:HA	2.51	0.41
1:C:260:VAL:CG1	1:C:261:GLU:H	2.20	0.41
1:D:187:VAL:O	1:D:191:LEU:HG	2.20	0.41
1:D:247:GLU:H	1:D:247:GLU:CD	2.28	0.41
1:B:188:LEU:HB3	1:B:189:PRO:HD3	2.03	0.41
1:C:131:ILE:HG13	1:C:132:HIS:CD2	2.56	0.41
1:A:9:ARG:HH21	1:A:62:GLN:HB2	1.85	0.41
1:A:13:THR:HG1	1:A:70:ALA:H	1.68	0.41
1:B:41:VAL:O	1:B:42:SER:O	2.38	0.41
1:B:275:LYS:O	1:B:276:SER:C	2.63	0.41
1:B:11:LEU:HD11	1:B:41:VAL:CG1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:GLN:HG3	1:C:249:GLU:HB3	2.03	0.41
1:A:45:ASP:O	1:A:46:ALA:HB2	2.21	0.41
1:B:198:ALA:HA	1:B:203:SER:O	2.21	0.41
1:D:170:PRO:HA	1:D:242:LEU:O	2.20	0.41
1:D:206:THR:HG22	1:D:208:TRP:CZ3	2.55	0.41
1:D:280:PHE:CD2	1:D:280:PHE:C	2.99	0.41
1:A:203:SER:O	1:A:204:ALA:CB	2.69	0.41
1:A:259:VAL:O	1:A:263:MET:HG3	2.21	0.41
1:C:25:LYS:N	1:C:25:LYS:CD	2.84	0.41
1:D:309:CYS:O	1:D:313:THR:HG23	2.20	0.41
1:A:44:LYS:HA	1:A:46:ALA:H	1.86	0.40
1:C:8:MET:CB	1:C:64:THR:HG21	2.51	0.40
1:C:258:ALA:C	1:C:259:VAL:HG22	2.46	0.40
1:A:30:GLY:O	1:A:31:ALA:HB3	2.21	0.40
1:A:214:ARG:HG2	1:A:214:ARG:NH1	2.36	0.40
1:B:13:THR:O	1:B:69:LEU:HB2	2.21	0.40
1:B:166:THR:CG2	1:B:167:ALA:H	2.19	0.40
1:C:42:SER:N	1:C:43:SER:CB	2.80	0.40
1:C:42:SER:CB	1:C:43:SER:HA	2.46	0.40
1:C:159:GLN:HE21	1:C:159:GLN:HB3	1.70	0.40
1:C:254:GLU:N	1:C:254:GLU:OE1	2.54	0.40
1:D:16:SER:OG	2:D:401:NDP:O3B	2.28	0.40
1:D:25:LYS:HA	1:D:27:VAL:N	2.37	0.40
1:A:262:ALA:O	1:A:306:LYS:HE3	2.21	0.40
1:B:228:ILE:HG22	1:B:229:TRP:N	2.35	0.40
1:A:12:VAL:HG21	1:A:40:PHE:CE2	2.56	0.40
1:B:24:GLN:O	1:B:25:LYS:CG	2.63	0.40
1:B:78:ARG:NH1	1:B:183:GLU:HB2	2.37	0.40
1:D:219:TYR:HE1	1:D:308:THR:HG22	1.86	0.40
1:A:67:ILE:HG23	1:A:227:PHE:CE1	2.56	0.40
1:A:166:THR:CG2	1:A:236:GLU:O	2.66	0.40
1:A:268:GLU:OE1	1:A:270:THR:HG22	2.21	0.40
1:C:297:ARG:HA	1:C:297:ARG:HD3	1.62	0.40
1:D:321:LYS:HE3	1:D:321:LYS:HB2	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

There are no protein backbone outliers to report in this entry.

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	261/273 (96%)	227 (87%)	34 (13%)	4	5
1	B	265/273 (97%)	236 (89%)	29 (11%)	6	8
1	C	248/273 (91%)	213 (86%)	35 (14%)	3	4
1	D	270/273 (99%)	242 (90%)	28 (10%)	7	9
All	All	1044/1092 (96%)	918 (88%)	126 (12%)	5	6

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	26	VAL
1	A	27	VAL
1	A	41	VAL
1	A	43	SER
1	A	44	LYS
1	A	45	ASP
1	A	48	LEU
1	A	61	VAL
1	A	84	LEU
1	A	113	LEU
1	A	121	LYS
1	A	131	ILE
1	A	166	THR
1	A	172	ASN
1	A	188	LEU
1	A	194	LYS
1	A	206	THR

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Mol	Chain	Res	Type
1	A	237	VAL
1	A	246	GLU
1	A	249	GLU
1	A	250	VAL
1	A	253	LYS
1	A	261	GLU
1	A	264	ASP
1	A	268	GLU
1	A	270	THR
1	A	279	GLN
1	A	280	PHE
1	A	281	LYS
1	A	282	LYS
1	A	306	LYS
1	A	308	THR
1	A	320	ARG
1	B	26	VAL
1	B	27	VAL
1	B	29	ASP
1	B	45	ASP
1	B	48	LEU
1	B	49	THR
1	B	57	LEU
1	B	61	VAL
1	B	72	MET
1	B	121	LYS
1	B	131	ILE
1	B	172	ASN
1	B	183	GLU
1	B	188	LEU
1	B	194	LYS
1	B	197	LEU
1	B	206	THR
1	B	227	PHE
1	B	246	GLU
1	B	260	VAL
1	B	261	GLU
1	B	274	THR
1	B	277	ASP
1	B	279	GLN
1	B	280	PHE
1	B	281	LYS

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Mol	Chain	Res	Type
1	B	308	THR
1	B	318	GLN
1	B	320	ARG
1	C	13	THR
1	C	25	LYS
1	C	27	VAL
1	C	42	SER
1	C	44	LYS
1	C	48	LEU
1	C	49	THR
1	C	61	VAL
1	C	73	VAL
1	C	81	LYS
1	C	116	CYS
1	C	131	ILE
1	C	164	THR
1	C	166	THR
1	C	187	VAL
1	C	188	LEU
1	C	192	ILE
1	C	193	HIS
1	C	214	ARG
1	C	215	ARG
1	C	221	LEU
1	C	233	GLU
1	C	237	VAL
1	C	246	GLU
1	C	249	GLU
1	C	251	SER
1	C	254	GLU
1	C	257	GLU
1	C	259	VAL
1	C	261	GLU
1	C	274	THR
1	C	290	ARG
1	C	291	THR
1	C	297	ARG
1	C	302	LYS
1	D	5	GLN
1	D	13	THR
1	D	25	LYS
1	D	27	VAL

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Mol	Chain	Res	Type
1	D	33	LEU
1	D	41	VAL
1	D	42	SER
1	D	44	LYS
1	D	48	LEU
1	D	61	VAL
1	D	107	ARG
1	D	131	ILE
1	D	153	GLN
1	D	166	THR
1	D	172	ASN
1	D	187	VAL
1	D	201	SER
1	D	227	PHE
1	D	237	VAL
1	D	250	VAL
1	D	274	THR
1	D	275	LYS
1	D	279	GLN
1	D	280	PHE
1	D	308	THR
1	D	313	THR
1	D	318	GLN
1	D	320	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	68	HIS
1	A	83	ASN
1	A	99	HIS
1	A	138	ASN
1	A	159	GLN
1	A	172	ASN
1	B	24	GLN
1	B	65	HIS
1	B	68	HIS
1	B	79	ASN
1	B	83	ASN
1	B	99	HIS
1	B	138	ASN

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Mol	Chain	Res	Type
1	B	153	GLN
1	B	172	ASN
1	B	181	ASN
1	B	193	HIS
1	C	24	GLN
1	C	65	HIS
1	C	68	HIS
1	C	83	ASN
1	C	99	HIS
1	C	133	ASN
1	C	138	ASN
1	C	140	ASN
1	C	153	GLN
1	C	159	GLN
1	C	177	HIS
1	C	212	ASN
1	D	24	GLN
1	D	65	HIS
1	D	68	HIS
1	D	79	ASN
1	D	83	ASN
1	D	99	HIS
1	D	159	GLN
1	D	181	ASN
1	D	186	HIS
1	D	196	HIS
1	D	225	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

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	A	401	-	51,52,52	1.99	18 (35%)	71,80,80	1.59	12 (16%)
2	NDP	D	401	-	51,52,52	1.83	15 (29%)	71,80,80	1.71	11 (15%)
2	NDP	C	401	-	51,52,52	1.95	17 (33%)	71,80,80	1.86	15 (21%)
2	NDP	B	401	-	51,52,52	1.81	12 (23%)	71,80,80	1.65	14 (19%)

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	A	401	-	-	7/34/77/77	0/5/5/5
2	NDP	D	401	-	-	7/34/77/77	0/5/5/5
2	NDP	C	401	-	-	5/34/77/77	0/5/5/5
2	NDP	B	401	-	-	12/34/77/77	0/5/5/5

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	NDP	C5A-N7A	-4.98	1.30	1.39
2	B	401	NDP	PA-O3	-4.44	1.54	1.59
2	C	401	NDP	C4A-N9A	-4.33	1.28	1.37
2	A	401	NDP	PN-O3	-4.24	1.54	1.59
2	D	401	NDP	C5A-N7A	-4.17	1.31	1.39
2	A	401	NDP	C5A-N7A	-4.14	1.31	1.39
2	C	401	NDP	C8A-N9A	-4.13	1.30	1.37
2	A	401	NDP	C4A-N9A	-4.11	1.29	1.37
2	B	401	NDP	PN-O3	-4.08	1.55	1.59
2	D	401	NDP	C4A-N9A	-3.82	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NDP	C4A-N9A	-3.76	1.29	1.37
2	D	401	NDP	C8A-N9A	-3.70	1.31	1.37
2	A	401	NDP	C8A-N9A	-3.53	1.31	1.37
2	D	401	NDP	P2B-O2X	-3.50	1.41	1.54
2	B	401	NDP	C5A-N7A	-3.31	1.33	1.39
2	A	401	NDP	PN-O2N	-3.19	1.40	1.55
2	B	401	NDP	C8A-N9A	-3.15	1.32	1.37
2	C	401	NDP	P2B-O2X	-3.14	1.43	1.54
2	A	401	NDP	C5A-C4A	3.07	1.44	1.39
2	C	401	NDP	PA-O3	-3.07	1.56	1.59
2	A	401	NDP	PA-O3	-2.99	1.56	1.59
2	C	401	NDP	P2B-O3X	-2.98	1.43	1.54
2	A	401	NDP	P2B-O2X	-2.94	1.43	1.54
2	C	401	NDP	O7N-C7N	-2.93	1.17	1.24
2	B	401	NDP	C5A-C4A	2.88	1.44	1.39
2	A	401	NDP	P2B-O3X	-2.81	1.44	1.54
2	A	401	NDP	PA-O2A	-2.73	1.42	1.55
2	D	401	NDP	P2B-O3X	-2.67	1.44	1.54
2	D	401	NDP	P2B-O2B	-2.66	1.54	1.59
2	D	401	NDP	PA-O2A	-2.63	1.43	1.55
2	B	401	NDP	P2B-O3X	-2.61	1.45	1.54
2	C	401	NDP	C6N-N1N	-2.55	1.31	1.37
2	B	401	NDP	P2B-O2X	-2.54	1.45	1.54
2	D	401	NDP	P2B-O1X	-2.52	1.42	1.50
2	C	401	NDP	PA-O2A	-2.52	1.43	1.55
2	A	401	NDP	C6N-N1N	-2.51	1.31	1.37
2	A	401	NDP	O7N-C7N	-2.49	1.18	1.24
2	A	401	NDP	O4D-C4D	-2.46	1.39	1.45
2	A	401	NDP	PA-O1A	-2.46	1.42	1.50
2	B	401	NDP	PA-O2A	-2.40	1.44	1.55
2	A	401	NDP	PN-O1N	-2.40	1.42	1.50
2	C	401	NDP	PA-O1A	-2.36	1.42	1.50
2	A	401	NDP	P2B-O2B	-2.34	1.55	1.59
2	A	401	NDP	C5A-C6A	2.31	1.47	1.41
2	B	401	NDP	C6N-N1N	-2.29	1.31	1.37
2	C	401	NDP	PN-O2N	-2.28	1.44	1.55
2	D	401	NDP	C5A-C4A	2.28	1.43	1.39
2	D	401	NDP	PN-O2N	-2.25	1.44	1.55
2	C	401	NDP	P2B-O1X	-2.22	1.43	1.50
2	C	401	NDP	PN-O1N	-2.15	1.43	1.50
2	D	401	NDP	C3B-C2B	-2.14	1.48	1.53
2	D	401	NDP	O7N-C7N	-2.13	1.19	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	NDP	PN-O2N	-2.11	1.45	1.55
2	C	401	NDP	P2B-O2B	-2.11	1.55	1.59
2	A	401	NDP	P2B-O1X	-2.10	1.43	1.50
2	C	401	NDP	O4D-C4D	-2.06	1.40	1.45
2	C	401	NDP	O4B-C4B	-2.05	1.40	1.45
2	D	401	NDP	C2A-N1A	-2.05	1.30	1.33
2	D	401	NDP	C6N-N1N	-2.03	1.32	1.37
2	B	401	NDP	C3B-C2B	-2.03	1.48	1.53
2	D	401	NDP	C2A-N3A	-2.02	1.30	1.33
2	C	401	NDP	C2D-C3D	-2.01	1.47	1.53

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NDP	C5A-C4A-N3A	-6.00	118.46	126.72
2	C	401	NDP	C5A-C4A-N3A	-5.36	119.33	126.72
2	A	401	NDP	C5A-C4A-N3A	-5.29	119.43	126.72
2	C	401	NDP	N3A-C4A-N9A	5.21	136.03	127.17
2	C	401	NDP	C4A-N9A-C8A	4.76	110.74	105.74
2	B	401	NDP	C5A-C4A-N3A	-4.67	120.29	126.72
2	D	401	NDP	N3A-C4A-N9A	4.63	135.04	127.17
2	D	401	NDP	C2A-N3A-C4A	4.21	122.12	111.83
2	B	401	NDP	N3A-C2A-N1A	-4.17	122.27	128.58
2	B	401	NDP	N3A-C4A-N9A	4.04	134.04	127.17
2	A	401	NDP	C4A-C5A-N7A	-3.98	106.03	110.58
2	D	401	NDP	C4A-C5A-N7A	-3.91	106.11	110.58
2	B	401	NDP	C2A-N3A-C4A	3.74	120.96	111.83
2	A	401	NDP	C2A-N3A-C4A	3.60	120.61	111.83
2	B	401	NDP	C4A-N9A-C8A	3.56	109.48	105.74
2	D	401	NDP	N3A-C2A-N1A	-3.44	123.38	128.58
2	C	401	NDP	N9A-C8A-N7A	-3.43	109.06	113.94
2	C	401	NDP	C2A-N3A-C4A	3.41	120.17	111.83
2	C	401	NDP	O4D-C1D-N1N	3.26	114.30	108.08
2	C	401	NDP	C5A-N7A-C8A	3.24	108.54	103.45
2	A	401	NDP	N3A-C4A-N9A	3.22	132.64	127.17
2	D	401	NDP	C2B-C1B-N9A	-3.18	108.51	113.75
2	C	401	NDP	C4A-C5A-N7A	-3.13	107.01	110.58
2	C	401	NDP	N3A-C2A-N1A	-3.12	123.85	128.58
2	D	401	NDP	C4A-N9A-C8A	3.11	109.00	105.74
2	C	401	NDP	C3N-C7N-N7N	3.09	123.15	117.67
2	B	401	NDP	C6N-N1N-C2N	3.08	122.62	119.32
2	A	401	NDP	O4B-C1B-N9A	3.07	113.98	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	NDP	C5A-N7A-C8A	2.90	108.01	103.45
2	B	401	NDP	C6A-C5A-N7A	2.89	137.66	132.09
2	B	401	NDP	C4A-C5A-N7A	-2.86	107.32	110.58
2	A	401	NDP	N3A-C2A-N1A	-2.85	124.27	128.58
2	A	401	NDP	O4B-C1B-C2B	-2.75	101.85	106.59
2	C	401	NDP	C1D-N1N-C6N	-2.69	115.08	120.77
2	D	401	NDP	C6A-C5A-N7A	2.67	137.25	132.09
2	B	401	NDP	C2A-N1A-C6A	2.62	123.04	118.73
2	A	401	NDP	C6A-C5A-N7A	2.60	137.11	132.09
2	A	401	NDP	O7N-C7N-N7N	-2.50	117.28	122.89
2	D	401	NDP	N9A-C8A-N7A	-2.50	110.38	113.94
2	B	401	NDP	C2B-C1B-N9A	-2.45	109.72	113.75
2	A	401	NDP	O3X-P2B-O2X	2.41	116.84	107.80
2	C	401	NDP	C2B-C1B-N9A	-2.38	109.83	113.75
2	C	401	NDP	O7N-C7N-N7N	-2.27	117.79	122.89
2	A	401	NDP	O2X-P2B-O2B	-2.27	97.01	105.85
2	C	401	NDP	O2N-PN-O1N	2.18	122.59	112.44
2	B	401	NDP	O2N-PN-O1N	2.13	122.34	112.44
2	A	401	NDP	C2A-N1A-C6A	2.11	122.19	118.73
2	C	401	NDP	O3D-C3D-C2D	-2.06	105.21	111.82
2	B	401	NDP	O3D-C3D-C4D	-2.06	105.16	111.08
2	D	401	NDP	O7N-C7N-N7N	-2.06	118.28	122.89
2	B	401	NDP	O3B-C3B-C2B	-2.05	105.45	111.19
2	B	401	NDP	N9A-C8A-N7A	-2.00	111.09	113.94

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NDP	C5D-O5D-PN-O3
2	A	401	NDP	C5D-O5D-PN-O1N
2	B	401	NDP	C5B-O5B-PA-O1A
2	B	401	NDP	C5B-O5B-PA-O3
2	B	401	NDP	C5D-O5D-PN-O3
2	B	401	NDP	C5D-O5D-PN-O2N
2	C	401	NDP	C5D-O5D-PN-O3
2	C	401	NDP	C5D-O5D-PN-O1N
2	D	401	NDP	C5D-O5D-PN-O1N
2	B	401	NDP	O4D-C4D-C5D-O5D
2	B	401	NDP	C3D-C4D-C5D-O5D
2	B	401	NDP	C3B-C4B-C5B-O5B
2	B	401	NDP	O4B-C4B-C5B-O5B

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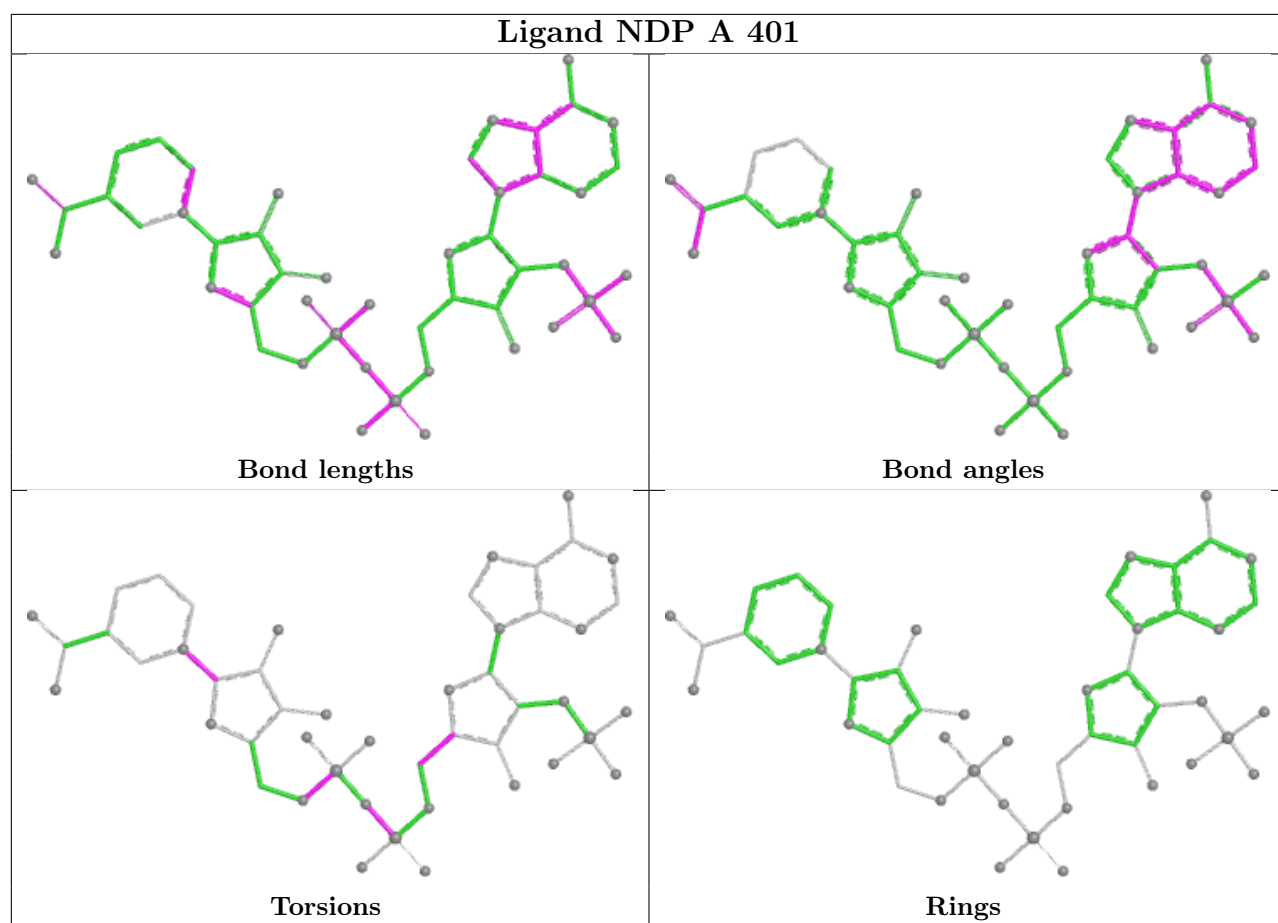
Mol	Chain	Res	Type	Atoms
2	C	401	NDP	O4D-C1D-N1N-C6N
2	D	401	NDP	PN-O3-PA-O2A
2	A	401	NDP	C5D-O5D-PN-O2N
2	B	401	NDP	C5B-O5B-PA-O2A
2	C	401	NDP	C5D-O5D-PN-O2N
2	D	401	NDP	C5D-O5D-PN-O3
2	D	401	NDP	C5D-O5D-PN-O2N
2	A	401	NDP	O4D-C1D-N1N-C6N
2	B	401	NDP	O4D-C1D-N1N-C6N
2	D	401	NDP	O4D-C1D-N1N-C6N
2	C	401	NDP	C2B-O2B-P2B-O1X
2	B	401	NDP	C2D-C1D-N1N-C6N
2	D	401	NDP	C2D-C1D-N1N-C6N
2	A	401	NDP	C2D-C1D-N1N-C6N
2	D	401	NDP	PN-O3-PA-O1A
2	A	401	NDP	O4B-C4B-C5B-O5B
2	B	401	NDP	C2B-O2B-P2B-O2X
2	A	401	NDP	PN-O3-PA-O2A

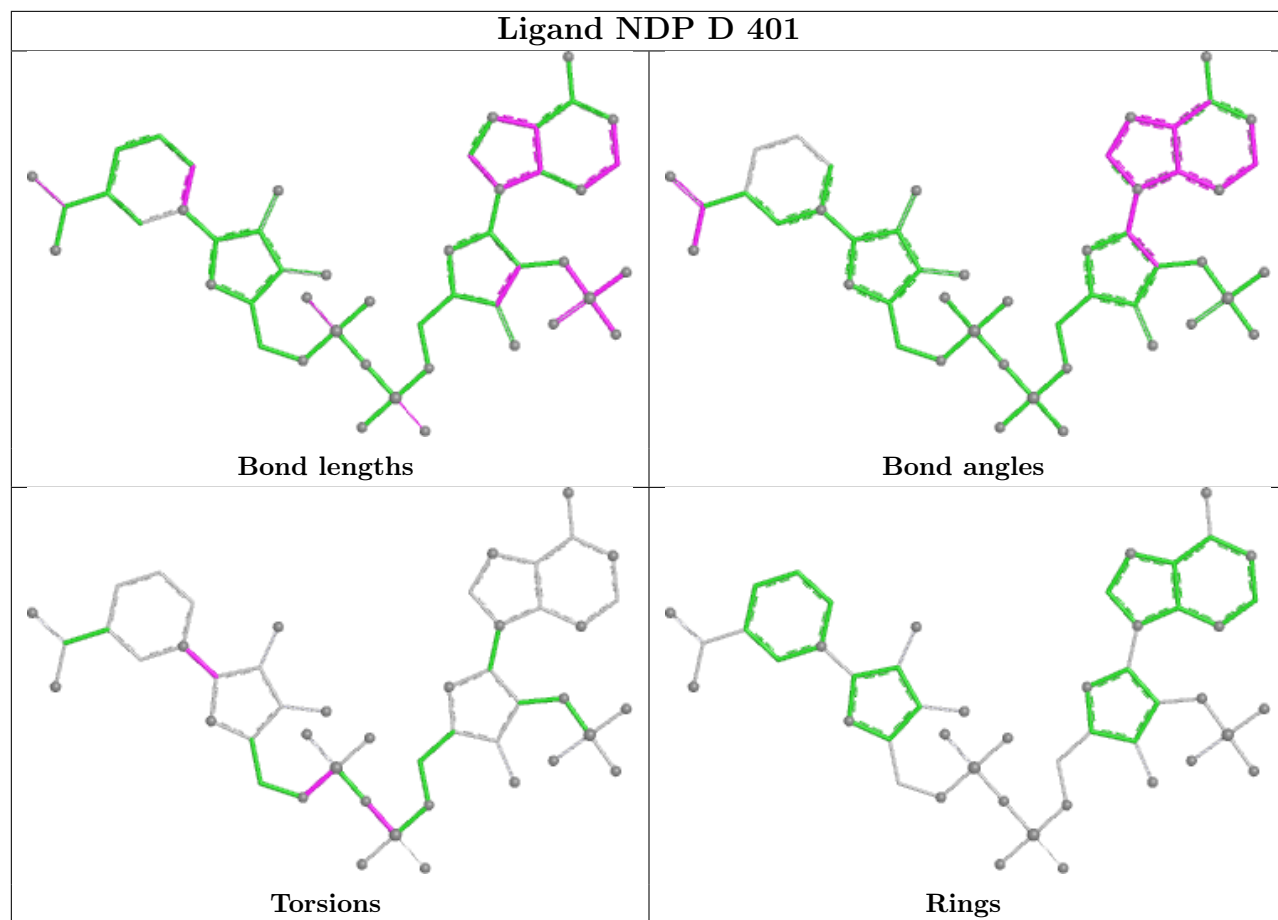
There are no ring outliers.

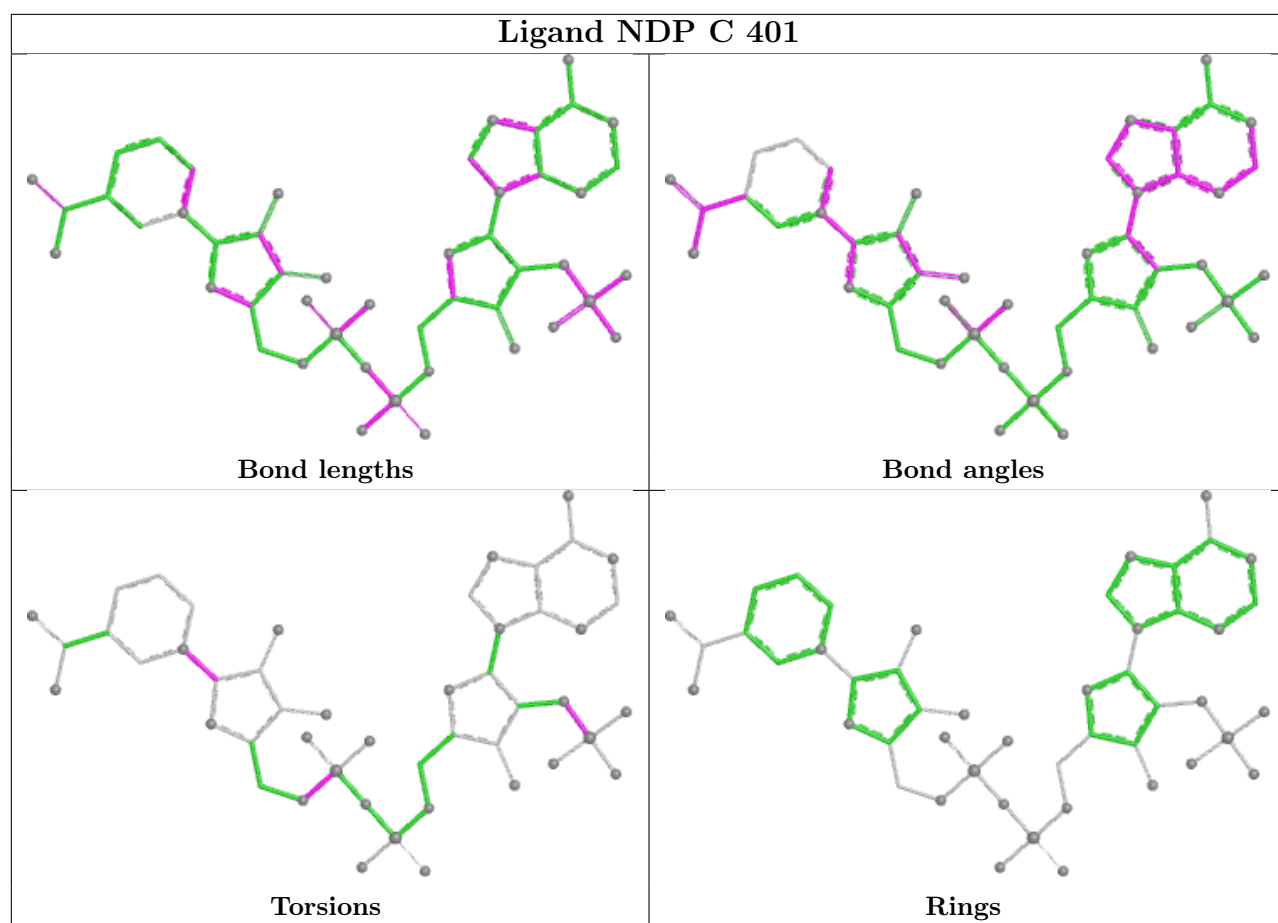
4 monomers are involved in 11 short contacts:

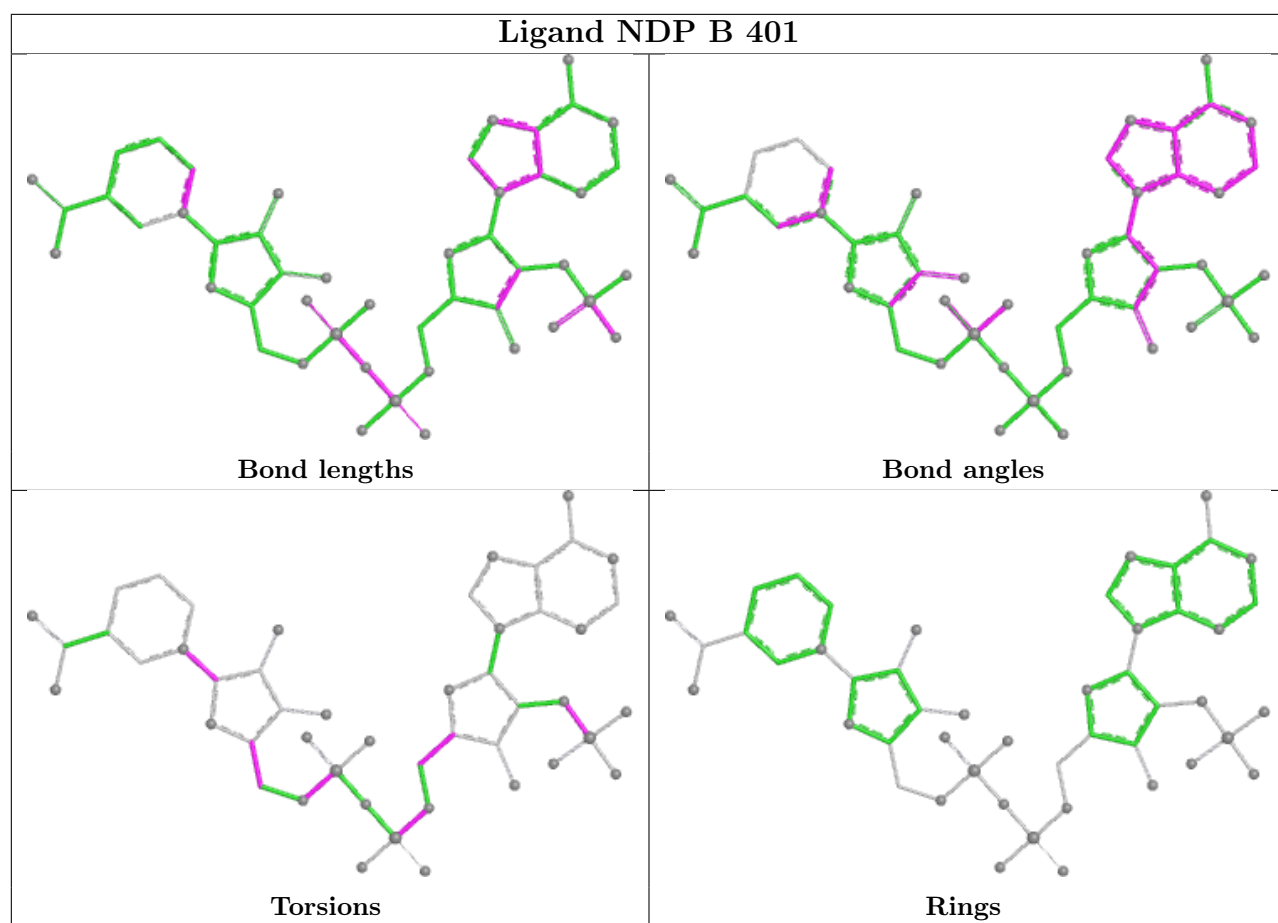
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	NDP	2	0
2	D	401	NDP	1	0
2	C	401	NDP	3	0
2	B	401	NDP	5	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	307/321 (95%)	0.40	24 (7%) 19 17	23, 34, 58, 79	0
1	B	309/321 (96%)	0.81	31 (10%) 12 11	24, 44, 66, 81	0
1	C	290/321 (90%)	1.01	57 (19%) 3 2	24, 39, 69, 84	0
1	D	318/321 (99%)	0.50	26 (8%) 17 16	23, 35, 59, 73	0
All	All	1224/1284 (95%)	0.67	138 (11%) 10 9	23, 38, 64, 84	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	VAL	8.6
1	C	250	VAL	7.4
1	C	260	VAL	6.9
1	D	204	ALA	6.8
1	B	42	SER	6.7
1	C	208	TRP	6.6
1	C	191	LEU	6.3
1	C	189	PRO	5.6
1	C	273	THR	5.6
1	A	278	GLY	5.6
1	C	188	LEU	5.4
1	C	210	THR	5.4
1	A	208	TRP	5.4
1	C	192	ILE	5.2
1	C	190	GLY	5.1
1	D	28	ALA	4.9
1	C	32	GLY	4.8
1	B	206	THR	4.7
1	D	205	LEU	4.7
1	C	251	SER	4.7
1	C	215	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	273	THR	4.6
1	B	207	VAL	4.6
1	A	32	GLY	4.6
1	C	276	SER	4.6
1	B	205	LEU	4.5
1	C	213	PRO	4.5
1	D	206	THR	4.4
1	C	255	ALA	4.4
1	D	34	PRO	4.4
1	B	203	SER	4.3
1	C	193	HIS	4.2
1	C	44	LYS	4.2
1	A	206	THR	4.2
1	C	214	ARG	4.1
1	A	30	GLY	3.9
1	C	42	SER	3.7
1	A	27	VAL	3.7
1	C	209	GLY	3.6
1	B	269	VAL	3.6
1	D	4	PRO	3.6
1	C	246	GLU	3.6
1	C	205	LEU	3.6
1	C	204	ALA	3.6
1	D	275	LYS	3.5
1	B	26	VAL	3.5
1	B	32	GLY	3.5
1	C	211	GLY	3.5
1	B	277	ASP	3.5
1	B	279	GLN	3.5
1	A	42	SER	3.5
1	C	207	VAL	3.4
1	A	26	VAL	3.4
1	D	27	VAL	3.4
1	D	207	VAL	3.4
1	C	187	VAL	3.3
1	C	259	VAL	3.3
1	B	43	SER	3.3
1	A	272	ASP	3.3
1	A	203	SER	3.3
1	C	262	ALA	3.2
1	D	210	THR	3.2
1	C	278	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	205	LEU	3.2
1	B	28	ALA	3.1
1	B	183	GLU	3.1
1	D	74	GLY	3.1
1	C	274	THR	3.0
1	A	269	VAL	3.0
1	D	208	TRP	3.0
1	D	276	SER	3.0
1	C	277	ASP	3.0
1	D	269	VAL	3.0
1	C	212	ASN	3.0
1	C	257	GLU	2.9
1	D	33	LEU	2.9
1	B	30	GLY	2.8
1	A	210	THR	2.8
1	C	261	GLU	2.8
1	B	75	GLY	2.8
1	C	203	SER	2.8
1	B	45	ASP	2.8
1	C	202	GLY	2.8
1	D	31	ALA	2.8
1	C	258	ALA	2.7
1	A	28	ALA	2.7
1	C	61	VAL	2.7
1	D	29	ASP	2.7
1	C	275	LYS	2.7
1	D	203	SER	2.7
1	D	43	SER	2.7
1	B	60	LYS	2.6
1	B	27	VAL	2.6
1	C	263	MET	2.6
1	C	254	GLU	2.6
1	C	252	ILE	2.6
1	C	310	ALA	2.6
1	B	107	ARG	2.6
1	D	131	ILE	2.6
1	A	87	TRP	2.6
1	C	295	ASP	2.5
1	A	74	GLY	2.5
1	A	44	LYS	2.5
1	C	81	LYS	2.5
1	C	131	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	305	VAL	2.4
1	B	87	TRP	2.4
1	C	253	LYS	2.4
1	D	44	LYS	2.4
1	B	276	SER	2.4
1	C	184	ASP	2.3
1	B	41	VAL	2.3
1	B	180	PHE	2.3
1	D	5	GLN	2.3
1	D	26	VAL	2.3
1	B	29	ASP	2.3
1	C	140	ASN	2.3
1	C	116	CYS	2.3
1	C	27	VAL	2.3
1	A	29	ASP	2.2
1	D	32	GLY	2.2
1	A	279	GLN	2.2
1	B	318	GLN	2.2
1	A	204	ALA	2.2
1	C	248	ASP	2.2
1	D	237	VAL	2.2
1	C	29	ASP	2.1
1	A	202	GLY	2.1
1	C	313	THR	2.1
1	B	44	LYS	2.1
1	D	25	LYS	2.1
1	B	7	SER	2.1
1	B	8	MET	2.1
1	A	246	GLU	2.1
1	B	57	LEU	2.1
1	B	235	ASN	2.1
1	C	272	ASP	2.1
1	A	280	PHE	2.1

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

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

6.3 Carbohydrates ⓘ

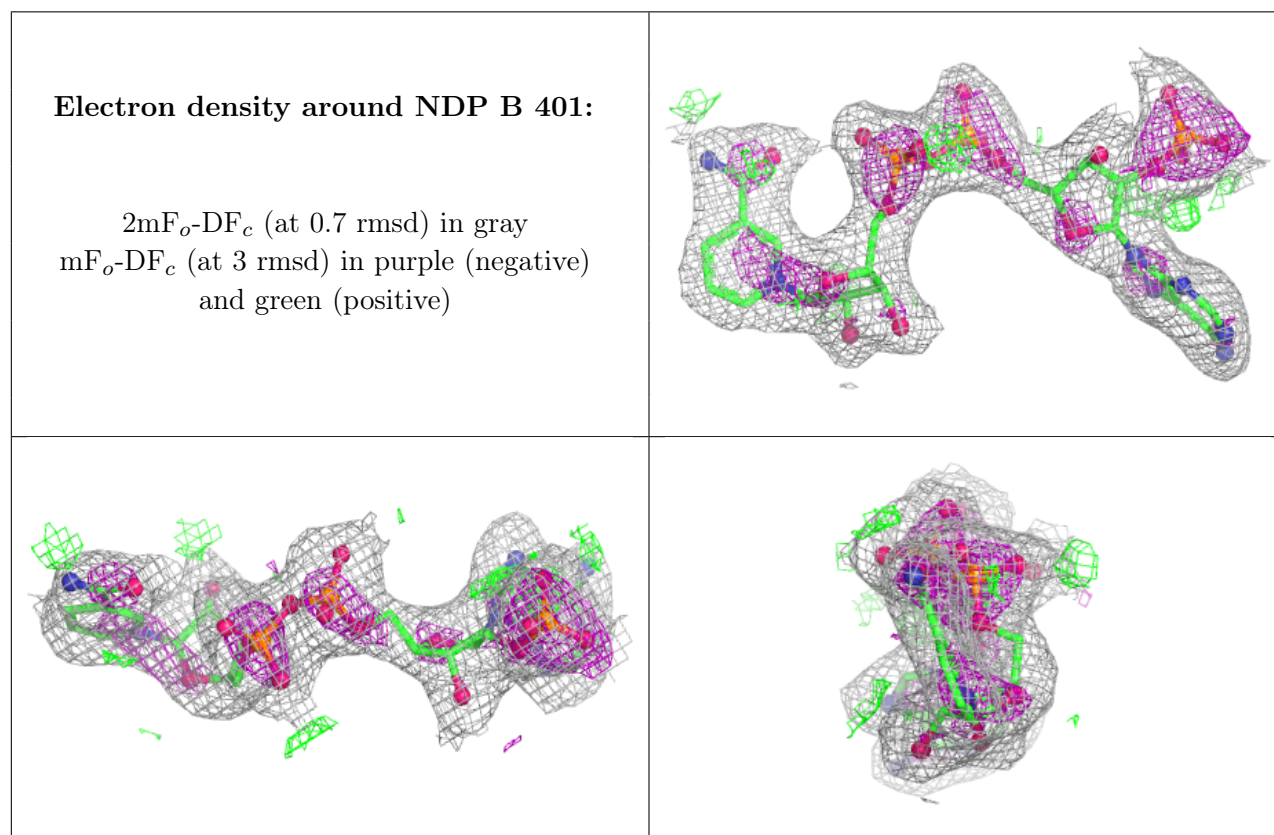
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

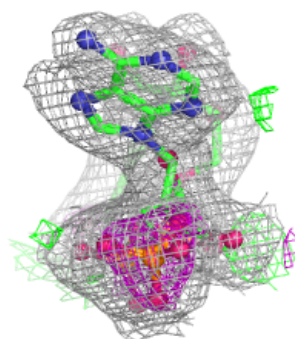
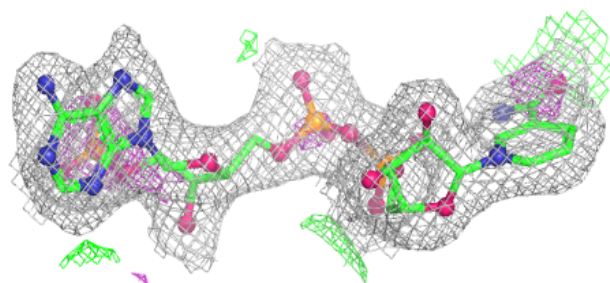
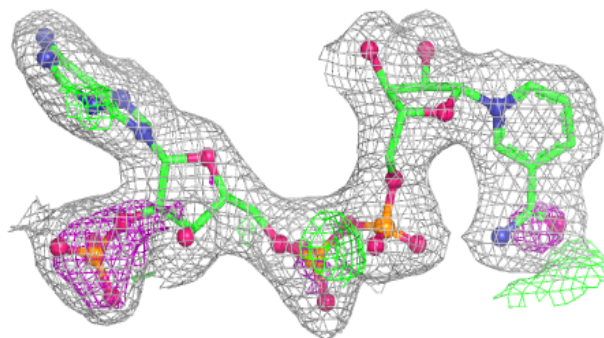
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NDP	B	401	48/48	0.92	0.10	20,20,20,20	0
2	NDP	A	401	48/48	0.95	0.08	20,20,20,20	0
2	NDP	D	401	48/48	0.95	0.08	20,20,20,20	0
2	NDP	C	401	48/48	0.96	0.08	20,20,20,20	0

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.

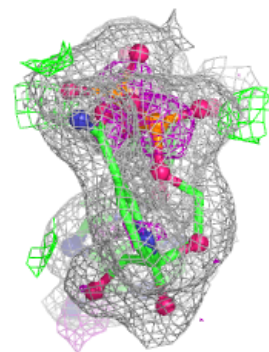
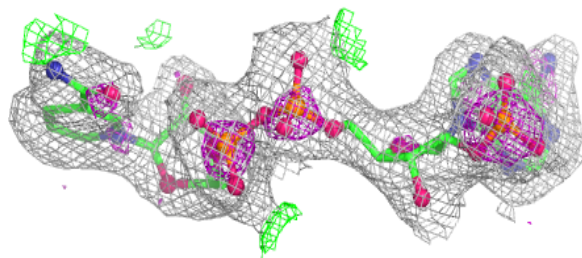
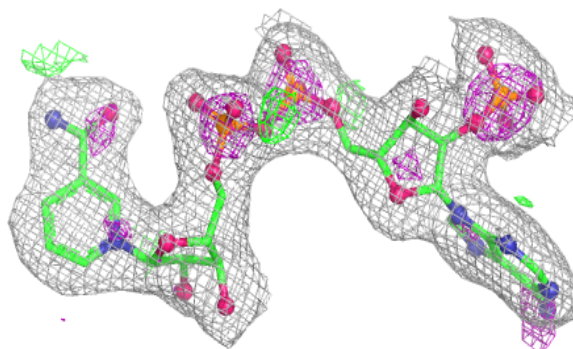


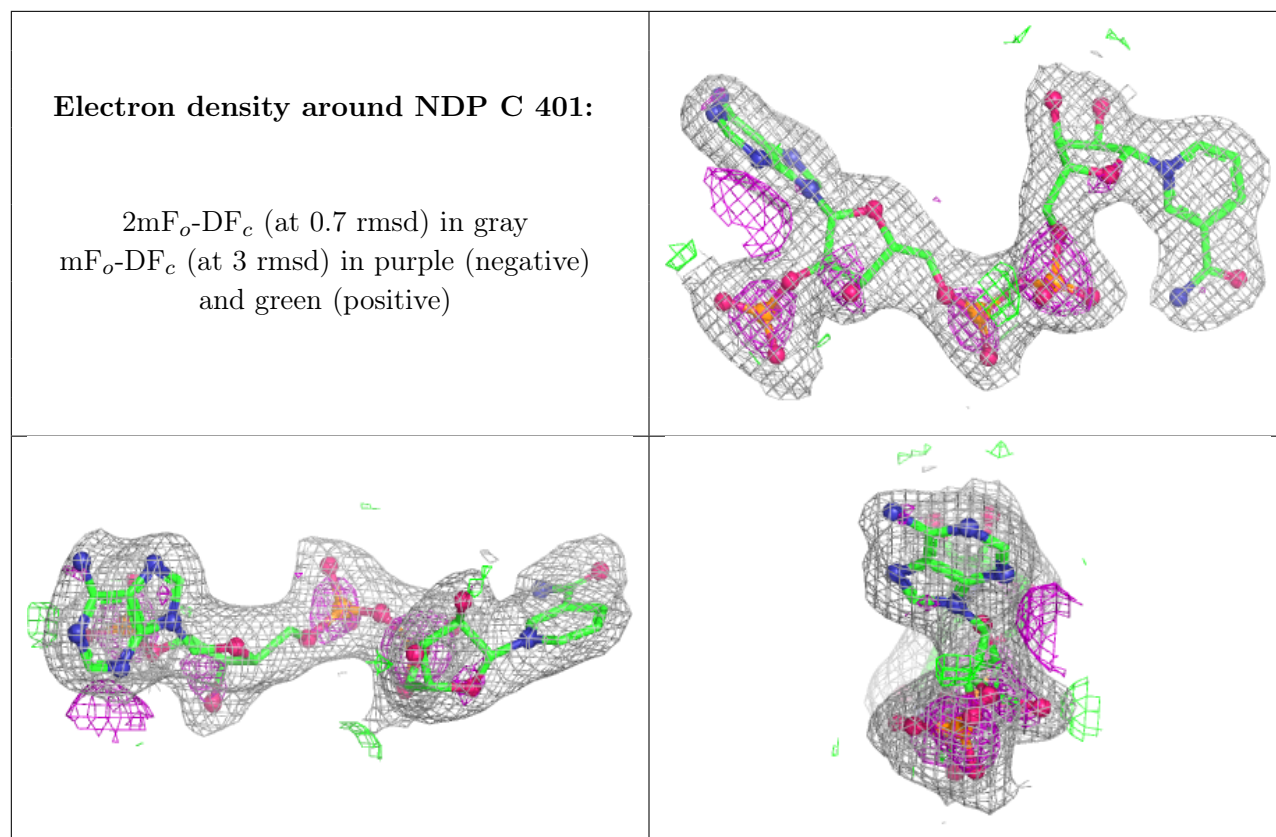
Electron density around NDP A 401:

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

**Electron density around NDP D 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 [i](#)

There are no such residues in this entry.