



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:59 AM UTC

PDB ID : 3BYZ / pdb_00003byz
Title : 2-Amino-1,3-thiazol-4(5H)-ones as Potent and Selective 11-Hydroxysteroid
Dehydrogenase Type 1 Inhibitors
Authors : Zhang, J.; Jordan, S.R.; Li, V.
Deposited on : 2008-01-16
Resolution : 2.69 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

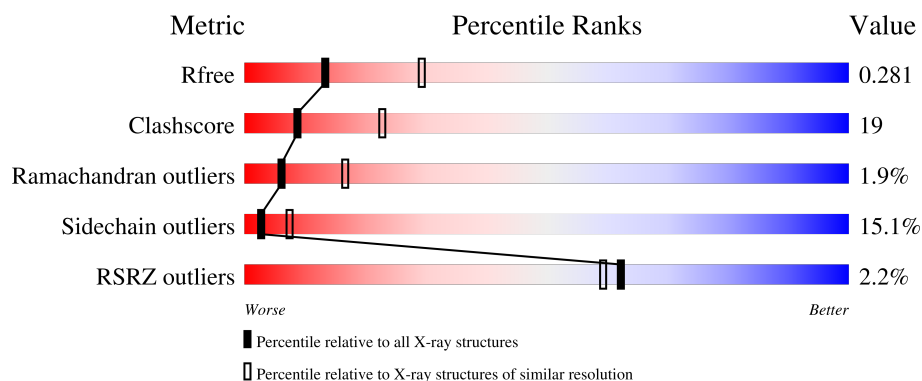
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	275	3% 45% 39% 9% 6%
1	B	275	55% 29% 8% 7%
1	C	275	2% 53% 35% • • 7%
1	D	275	4% 51% 36% 7% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8151 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Corticosteroid 11-beta-dehydrogenase isozyme 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			1976	1261	334	366	15			
1	B	255	Total	C	N	O	S	0	0	0
			1951	1247	331	358	15			
1	C	255	Total	C	N	O	S	0	0	0
			1954	1249	331	359	15			
1	D	261	Total	C	N	O	S	0	0	0
			2002	1277	338	372	15			

There are 32 discrepancies between the modelled and reference sequences:

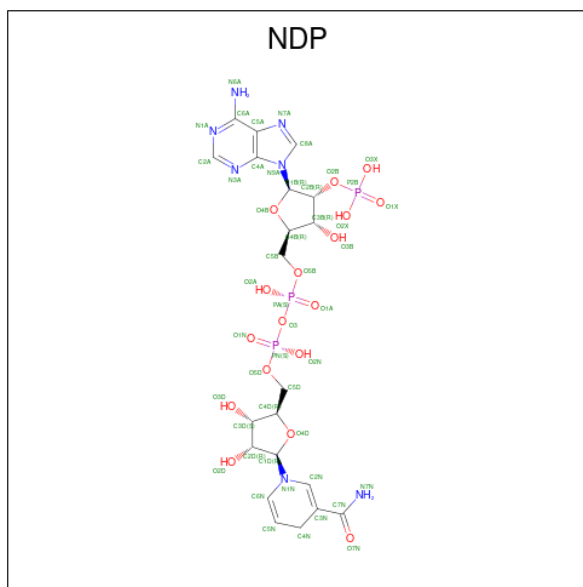
Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	expression tag	UNP P28845
A	19	HIS	-	expression tag	UNP P28845
A	20	HIS	-	expression tag	UNP P28845
A	21	HIS	-	expression tag	UNP P28845
A	22	HIS	-	expression tag	UNP P28845
A	23	HIS	-	expression tag	UNP P28845
A	24	HIS	-	expression tag	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
B	18	MET	-	expression tag	UNP P28845
B	19	HIS	-	expression tag	UNP P28845
B	20	HIS	-	expression tag	UNP P28845
B	21	HIS	-	expression tag	UNP P28845
B	22	HIS	-	expression tag	UNP P28845
B	23	HIS	-	expression tag	UNP P28845
B	24	HIS	-	expression tag	UNP P28845
B	272	SER	CYS	engineered mutation	UNP P28845
C	18	MET	-	expression tag	UNP P28845
C	19	HIS	-	expression tag	UNP P28845
C	20	HIS	-	expression tag	UNP P28845
C	21	HIS	-	expression tag	UNP P28845
C	22	HIS	-	expression tag	UNP P28845

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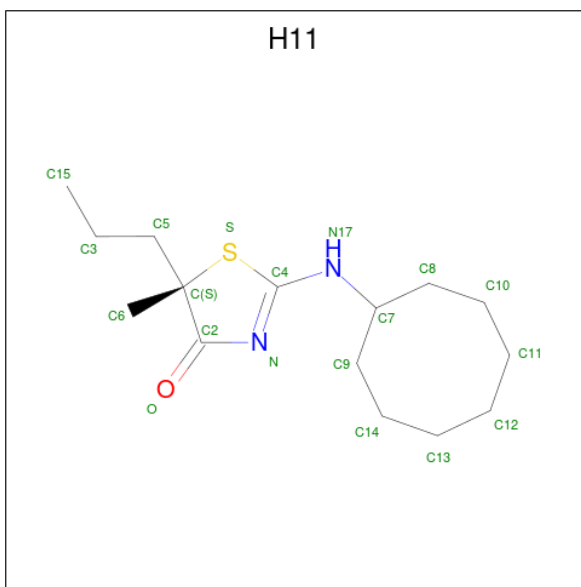
Chain	Residue	Modelled	Actual	Comment	Reference
C	23	HIS	-	expression tag	UNP P28845
C	24	HIS	-	expression tag	UNP P28845
C	272	SER	CYS	engineered mutation	UNP P28845
D	18	MET	-	expression tag	UNP P28845
D	19	HIS	-	expression tag	UNP P28845
D	20	HIS	-	expression tag	UNP P28845
D	21	HIS	-	expression tag	UNP P28845
D	22	HIS	-	expression tag	UNP P28845
D	23	HIS	-	expression tag	UNP P28845
D	24	HIS	-	expression tag	UNP P28845
D	272	SER	CYS	engineered mutation	UNP P28845

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

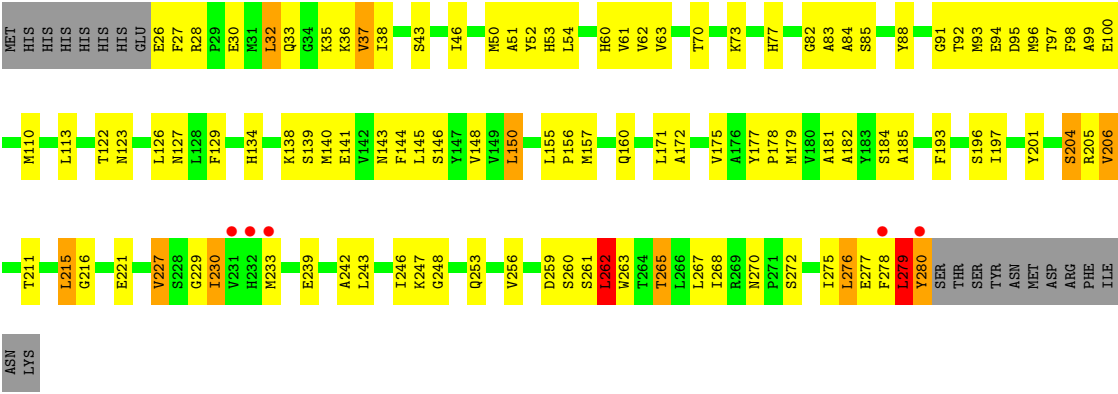


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

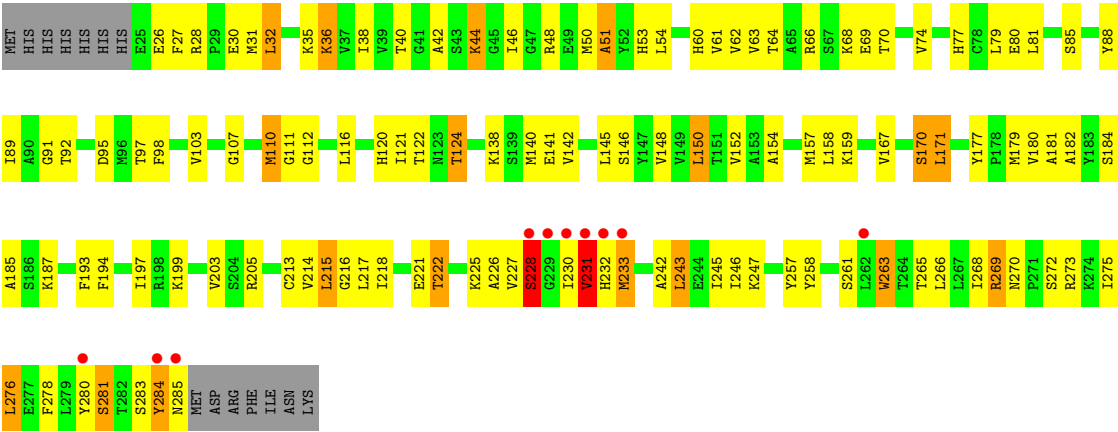
- Molecule 3 is (5S)-2-(cyclooctylamino)-5-methyl-5-propyl-1,3-thiazol-4(5H)-one (CCD ID: H11) (formula: $C_{15}H_{26}N_2OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			19	15	2	1	1		
3	B	1	Total	C	N	O	S	0	0
			19	15	2	1	1		
3	C	1	Total	C	N	O	S	0	0
			19	15	2	1	1		
3	D	1	Total	C	N	O	S	0	0
			19	15	2	1	1		



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.04Å 138.48Å 155.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.69 50.00 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.69) 99.5 (50.00-2.69)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.218 , 0.293 0.211 , 0.281	Depositor DCC
R_{free} test set	1523 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8151	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H11, 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	1.08	1/2009 (0.0%)	1.31	6/2712 (0.2%)
1	B	1.19	3/1984 (0.2%)	1.30	10/2678 (0.4%)
1	C	1.16	1/1987 (0.1%)	1.36	12/2682 (0.4%)
1	D	1.27	3/2036 (0.1%)	1.41	18/2749 (0.7%)
All	All	1.17	8/8016 (0.1%)	1.35	46/10821 (0.4%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	103	VAL	CA-CB	6.60	1.62	1.54
1	D	233	MET	CG-SD	6.50	1.97	1.80
1	D	233	MET	SD-CE	5.62	1.93	1.79
1	B	165	ILE	CA-CB	-5.38	1.48	1.54
1	B	176	ALA	CA-CB	-5.36	1.45	1.53
1	C	99	ALA	CA-CB	-5.31	1.45	1.53
1	A	231	VAL	CA-CB	5.03	1.59	1.53
1	D	231	VAL	CA-CB	5.01	1.61	1.54

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	285	ASN	CA-C-O	24.92	163.16	120.80
1	A	282	THR	CA-C-O	24.55	162.53	120.80
1	C	280	TYR	CA-C-O	-20.91	85.25	120.80
1	C	28	ARG	CA-C-N	8.88	130.93	119.84
1	C	28	ARG	C-N-CA	8.88	130.93	119.84
1	A	152	VAL	N-CA-C	-8.58	102.35	110.42
1	D	138	LYS	N-CA-C	-7.25	103.31	111.14
1	D	233	MET	CB-CG-SD	-6.87	92.10	112.70
1	B	255	GLU	N-CA-C	6.72	119.28	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	196	SER	N-CA-C	-6.69	103.46	111.69
1	A	148	VAL	N-CA-C	-6.49	104.43	110.53
1	B	106	ALA	N-CA-C	-6.48	104.22	111.28
1	D	275	ILE	N-CA-C	6.35	116.52	110.42
1	B	274	LYS	N-CA-C	6.29	118.94	111.33
1	B	51	ALA	N-CA-C	-6.26	103.39	111.02
1	B	61	VAL	N-CA-C	6.25	117.12	108.12
1	D	167	VAL	CB-CA-C	-5.97	101.93	110.83
1	D	177	TYR	CA-C-N	-5.95	114.50	120.21
1	D	177	TYR	C-N-CA	-5.95	114.50	120.21
1	B	174	LYS	N-CA-C	-5.78	108.03	114.62
1	C	270	ASN	CA-C-N	5.72	125.40	119.05
1	C	270	ASN	C-N-CA	5.72	125.40	119.05
1	B	94	GLU	N-CA-C	-5.65	106.34	113.18
1	A	197	ILE	N-CA-C	-5.63	105.01	110.42
1	B	64	THR	N-CA-C	5.49	117.74	109.23
1	D	270	ASN	CA-C-N	5.47	124.99	119.19
1	D	270	ASN	C-N-CA	5.47	124.99	119.19
1	C	134	HIS	N-CA-C	-5.40	105.39	111.28
1	C	262	LEU	N-CA-C	-5.37	106.58	113.23
1	D	27	PHE	N-CA-C	5.31	117.38	109.25
1	D	142	VAL	CB-CA-C	-5.31	105.13	112.24
1	D	51	ALA	N-CA-C	-5.30	104.55	111.02
1	B	119	ASN	N-CA-C	-5.28	108.60	114.62
1	D	38	ILE	CB-CA-C	-5.25	104.40	110.91
1	C	215	LEU	N-CA-C	5.22	118.13	109.46
1	C	206	VAL	CB-CA-C	-5.19	104.66	111.25
1	D	158	LEU	N-CA-C	-5.13	106.17	112.90
1	D	263	TRP	N-CA-C	-5.13	107.09	113.55
1	A	35	LYS	N-CA-C	5.13	117.09	109.25
1	B	72	GLN	N-CA-C	-5.13	105.69	111.28
1	D	272	SER	N-CA-C	-5.13	105.13	111.33
1	C	37	VAL	N-CA-C	5.11	115.26	108.11
1	D	159	LYS	N-CA-C	-5.08	105.75	111.28
1	A	155	LEU	O-C-N	5.05	123.76	120.27
1	D	194	PHE	N-CA-C	5.04	116.77	111.28
1	C	157	MET	N-CA-C	5.03	117.65	111.82

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	1976	0	2026	101	0
1	B	1951	0	2007	66	0
1	C	1954	0	2008	77	0
1	D	2002	0	2046	89	0
2	A	48	0	26	4	0
2	B	48	0	26	4	0
2	C	48	0	26	2	0
2	D	48	0	26	6	0
3	A	19	0	26	1	0
3	B	19	0	26	1	0
3	C	19	0	26	3	0
3	D	19	0	26	3	0
All	All	8151	0	8295	308	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 19.

All (308) 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:32:LEU:HB2	1:B:57:MET:HE2	1.44	0.98
1:D:60:HIS:ND1	1:D:85:SER:HB2	1.86	0.90
1:B:170:SER:HB3	2:B:502:NDP:H5N	1.54	0.88
1:B:32:LEU:HD23	1:B:57:MET:HE1	1.56	0.86
1:A:125:SER:OG	1:A:127:ASN:ND2	2.11	0.83
1:B:216:GLY:HA3	1:B:259:ASP:OD1	1.80	0.81
1:A:227:VAL:HG13	1:A:231:VAL:HB	1.64	0.79
1:B:32:LEU:HB2	1:B:57:MET:CE	2.11	0.79
1:A:50:MET:HE3	1:A:117:ILE:HG21	1.64	0.79
1:B:27:PHE:N	1:B:28:ARG:NH1	2.31	0.78
1:D:60:HIS:ND1	1:D:85:SER:CB	2.46	0.78
1:A:167:VAL:CG2	1:A:212:LEU:HD12	2.14	0.77
1:A:185:ALA:HB2	1:B:193:PHE:HB2	1.66	0.76
1:A:219:ASP:OD2	1:A:237:PRO:HA	1.86	0.76
1:B:28:ARG:O	1:B:31:MET:HB2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:GLY:HA3	1:C:259:ASP:OD1	1.88	0.73
1:D:227:VAL:HG12	1:D:228:SER:N	2.00	0.73
1:A:37:VAL:HG11	1:A:54:LEU:HD22	1.69	0.72
1:A:160:GLN:HE22	1:C:98:PHE:HB2	1.54	0.72
1:D:40:THR:OG1	1:D:120:HIS:HD2	1.73	0.72
1:A:158:LEU:HD22	1:A:163:GLY:HA3	1.72	0.71
1:A:167:VAL:HG23	1:A:212:LEU:HD12	1.71	0.71
1:B:56:LYS:HD2	1:B:81:LEU:HD22	1.72	0.71
1:B:231:VAL:HG12	1:B:233:MET:HB2	1.73	0.70
1:C:60:HIS:CD2	1:C:84:ALA:HB3	2.26	0.70
1:D:242:ALA:O	1:D:246:ILE:HG12	1.91	0.70
1:B:170:SER:HB3	2:B:502:NDP:C5N	2.22	0.69
1:A:60:HIS:CD2	1:A:85:SER:HB3	2.28	0.69
1:D:91:GLY:HA3	1:D:98:PHE:CZ	2.28	0.68
1:C:93:MET:HE2	1:C:98:PHE:HE1	1.58	0.68
1:A:129:PHE:HB3	1:B:197:ILE:HD11	1.76	0.67
1:B:99:ALA:HB1	1:B:150:LEU:HD13	1.77	0.67
1:C:146:SER:O	1:C:150:LEU:HD22	1.95	0.67
1:D:276:LEU:HG	1:D:280:TYR:CE2	2.30	0.67
1:D:243:LEU:HD22	1:D:247:LYS:HE3	1.78	0.65
1:C:60:HIS:CD2	1:C:85:SER:HB2	2.31	0.65
1:C:197:ILE:HD12	1:C:201:TYR:CZ	2.31	0.65
1:D:112:GLY:HA2	1:D:157:MET:HE2	1.77	0.65
1:B:69:GLU:H	1:B:69:GLU:CD	2.05	0.65
1:A:36:LYS:HB3	1:A:110:MET:SD	2.36	0.65
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.79	0.65
1:A:36:LYS:HZ3	1:A:112:GLY:H	1.45	0.64
1:D:230:ILE:HG22	1:D:231:VAL:H	1.63	0.64
1:D:227:VAL:HG12	1:D:228:SER:H	1.63	0.64
1:D:77:HIS:HA	1:D:80:GLU:HG2	1.80	0.64
1:C:175:VAL:HG12	1:D:273:ARG:HG3	1.78	0.64
1:D:28:ARG:O	1:D:31:MET:HB2	1.97	0.64
1:C:50:MET:HG2	1:C:242:ALA:HB1	1.80	0.63
1:D:278:PHE:O	1:D:281:SER:HB3	1.98	0.63
1:C:38:ILE:HD12	1:C:113:LEU:CD1	2.28	0.63
1:C:172:ALA:O	1:C:184:SER:HB2	1.99	0.63
1:A:120:HIS:HE1	1:A:146:SER:OG	1.80	0.63
1:A:140:MET:HE2	1:B:140:MET:CE	2.29	0.62
1:D:61:VAL:N	1:D:110:MET:HE1	2.14	0.62
1:D:32:LEU:HA	1:D:35:LYS:HG3	1.81	0.62
1:C:127:ASN:O	1:C:179:MET:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ALA:O	1:C:246:ILE:HG13	1.98	0.62
1:A:28:ARG:O	1:A:31:MET:HG3	1.99	0.61
1:C:38:ILE:HD12	1:C:113:LEU:HD13	1.81	0.61
1:C:177:TYR:CD1	3:C:604:H11:H15B	2.36	0.61
1:D:227:VAL:CG1	1:D:228:SER:N	2.64	0.61
1:A:140:MET:HE2	1:B:140:MET:HE2	1.84	0.60
1:A:60:HIS:CB	1:A:110:MET:HE2	2.30	0.60
1:A:235:ALA:O	1:A:236:ALA:C	2.45	0.60
1:A:144:PHE:HD1	1:A:190:LEU:HD23	1.67	0.60
1:B:48:ARG:O	1:B:51:ALA:HB3	2.01	0.60
1:D:46:ILE:HG22	1:D:50:MET:HE2	1.83	0.60
1:D:230:ILE:O	1:D:231:VAL:C	2.45	0.59
1:B:272:SER:O	1:B:276:LEU:HB2	2.02	0.59
1:B:46:ILE:HD11	1:B:218:ILE:HG13	1.85	0.59
1:D:60:HIS:HB3	1:D:110:MET:HE2	1.84	0.59
1:D:170:SER:HB3	2:D:504:NDP:H5N	1.85	0.59
1:C:227:VAL:CG1	1:C:227:VAL:O	2.50	0.59
1:B:53:HIS:HE1	1:B:239:GLU:O	1.86	0.59
1:A:160:GLN:OE1	1:C:92:THR:HG22	2.03	0.58
1:C:144:PHE:CE2	1:D:140:MET:HE3	2.38	0.58
1:D:180:VAL:O	1:D:181:ALA:C	2.46	0.58
1:A:229:GLY:O	1:A:230:ILE:HG13	2.03	0.58
1:C:91:GLY:HA3	1:C:98:PHE:CZ	2.39	0.58
1:D:62:VAL:HG23	1:D:110:MET:HE3	1.84	0.58
1:B:32:LEU:CB	1:B:57:MET:HE2	2.27	0.58
1:C:178:PRO:O	1:C:179:MET:HB2	2.03	0.58
1:C:230:ILE:O	1:D:284:TYR:HA	2.04	0.57
1:D:120:HIS:HE1	1:D:146:SER:OG	1.87	0.57
1:D:213:CYS:SG	1:D:245:ILE:HG23	2.44	0.57
1:D:227:VAL:CG1	1:D:228:SER:H	2.16	0.57
1:C:61:VAL:O	1:C:61:VAL:HG13	2.05	0.57
1:A:270:ASN:HD22	1:A:270:ASN:C	2.13	0.57
1:C:62:VAL:HG23	1:C:110:MET:SD	2.45	0.57
1:A:139:SER:O	1:A:143:ASN:HB2	2.05	0.56
1:C:140:MET:HE2	1:D:140:MET:HG2	1.88	0.56
1:A:273:ARG:HG3	1:B:175:VAL:HG22	1.88	0.56
1:B:27:PHE:N	1:B:28:ARG:CZ	2.68	0.56
1:D:32:LEU:HD22	1:D:54:LEU:HD23	1.86	0.56
1:A:44:LYS:HG2	2:A:501:NDP:H3B	1.87	0.55
1:A:247:LYS:HE3	1:A:253:GLN:HE22	1.71	0.55
1:C:227:VAL:O	1:C:227:VAL:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:THR:OG1	1:A:120:HIS:HD2	1.89	0.55
1:D:77:HIS:CE1	1:D:81:LEU:HD11	2.42	0.55
1:A:60:HIS:HB3	1:A:110:MET:HE2	1.89	0.55
1:A:35:LYS:HE3	1:A:114:ASP:OD2	2.08	0.54
1:D:91:GLY:HA3	1:D:98:PHE:CE2	2.42	0.54
1:D:60:HIS:CE1	1:D:85:SER:HB2	2.43	0.54
1:B:67:SER:HB3	2:B:502:NDP:O1X	2.08	0.54
1:C:139:SER:O	1:C:143:ASN:HB2	2.07	0.54
1:A:70:THR:O	1:A:74:VAL:HG23	2.08	0.54
1:B:140:MET:O	1:B:144:PHE:HB3	2.07	0.54
1:C:148:VAL:HG13	1:C:193:PHE:CZ	2.43	0.53
1:A:36:LYS:NZ	1:A:112:GLY:H	2.06	0.53
1:A:167:VAL:CG2	1:A:212:LEU:CD1	2.87	0.53
1:D:88:TYR:O	1:D:89:ILE:HG13	2.09	0.53
1:A:246:ILE:O	1:A:247:LYS:C	2.51	0.53
1:B:35:LYS:O	1:B:60:HIS:N	2.38	0.53
1:B:40:THR:OG1	1:B:120:HIS:HD2	1.92	0.53
1:C:37:VAL:HG11	1:C:54:LEU:HD22	1.90	0.53
1:C:144:PHE:HE2	1:D:140:MET:HE3	1.74	0.53
1:A:276:LEU:HD23	1:B:175:VAL:HG21	1.91	0.53
1:A:278:PHE:O	1:A:281:SER:HB2	2.09	0.53
1:C:60:HIS:HD2	1:C:84:ALA:HB3	1.72	0.53
1:B:178:PRO:O	1:B:179:MET:HB2	2.08	0.52
1:D:48:ARG:O	1:D:51:ALA:HB3	2.08	0.52
1:A:158:LEU:CD2	1:A:163:GLY:HA3	2.38	0.52
1:A:66:ARG:HG2	1:A:92:THR:HB	1.90	0.52
1:A:49:GLU:HG2	1:A:239:GLU:HA	1.92	0.52
1:A:156:PRO:HB3	1:C:95:ASP:HA	1.92	0.52
1:A:223:ALA:O	1:A:227:VAL:HB	2.10	0.52
1:C:46:ILE:O	1:C:50:MET:HG3	2.10	0.52
1:A:120:HIS:CE1	1:A:146:SER:OG	2.62	0.52
1:A:197:ILE:O	1:A:198:ARG:C	2.51	0.52
1:D:61:VAL:C	1:D:110:MET:HE1	2.33	0.52
1:D:269:ARG:CB	1:D:269:ARG:CZ	2.87	0.52
1:D:269:ARG:HB2	1:D:269:ARG:NH2	2.25	0.51
1:D:36:LYS:HG3	1:D:110:MET:HB2	1.93	0.51
1:C:93:MET:CE	1:C:98:PHE:HE1	2.23	0.51
1:B:28:ARG:HH21	1:B:31:MET:HE1	1.76	0.51
1:C:63:VAL:O	1:C:88:TYR:HA	2.11	0.51
1:B:278:PHE:O	1:B:281:SER:HB3	2.11	0.51
1:C:52:TYR:CZ	1:C:77:HIS:HD2	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:VAL:CG2	1:D:150:LEU:HD12	2.40	0.51
1:A:278:PHE:O	1:A:279:LEU:C	2.54	0.51
1:B:92:THR:OG1	1:B:94:GLU:HG2	2.11	0.51
1:D:103:VAL:HG23	1:D:150:LEU:HD12	1.92	0.50
1:A:264:THR:O	1:A:265:THR:C	2.54	0.50
1:C:267:LEU:HB3	1:D:276:LEU:HD22	1.92	0.50
1:C:267:LEU:HD13	1:D:276:LEU:HD13	1.92	0.50
1:A:60:HIS:HB2	1:A:110:MET:HE2	1.93	0.50
1:A:42:ALA:HB3	1:A:63:VAL:HB	1.94	0.49
1:A:133:ILE:HG13	1:A:134:HIS:N	2.26	0.49
1:D:222:THR:HG1	2:D:504:NDP:PA	2.33	0.49
1:A:122:THR:O	1:A:124:THR:HG23	2.12	0.49
1:C:129:PHE:HB3	1:D:197:ILE:CD1	2.42	0.49
1:C:278:PHE:O	1:C:280:TYR:N	2.45	0.49
1:D:60:HIS:ND1	1:D:85:SER:HB3	2.26	0.49
1:C:229:GLY:O	1:C:230:ILE:HG13	2.12	0.49
1:D:276:LEU:HG	1:D:280:TYR:HE2	1.77	0.49
1:A:175:VAL:HG22	1:B:273:ARG:HG3	1.95	0.49
1:A:270:ASN:C	1:A:270:ASN:ND2	2.71	0.49
1:B:170:SER:HA	1:B:215:LEU:H	1.77	0.49
1:C:261:SER:OG	1:C:263:TRP:HB2	2.13	0.48
1:C:267:LEU:CD1	1:D:276:LEU:HD13	2.43	0.48
1:D:179:MET:HB2	1:D:179:MET:HE2	1.67	0.48
1:B:120:HIS:HE1	1:B:146:SER:OG	1.96	0.48
1:B:247:LYS:O	1:B:251:LEU:HG	2.14	0.48
1:C:94:GLU:OE1	1:C:138:LYS:HD2	2.14	0.48
1:D:44:LYS:HE2	1:D:221:GLU:HB2	1.96	0.48
1:A:155:LEU:HB3	1:A:156:PRO:HD3	1.95	0.48
1:D:215:LEU:HD12	1:D:258:TYR:HB3	1.95	0.48
1:D:243:LEU:O	1:D:247:LYS:HG3	2.14	0.48
1:A:66:ARG:NH2	2:A:501:NDP:O2X	2.41	0.48
1:C:211:THR:HG23	1:C:253:GLN:O	2.14	0.48
1:D:116:LEU:HD22	1:D:154:ALA:CB	2.44	0.48
1:D:148:VAL:O	1:D:152:VAL:HG23	2.14	0.48
1:B:92:THR:OG1	1:B:94:GLU:CG	2.62	0.48
1:A:113:LEU:HD11	1:A:115:MET:O	2.13	0.47
1:D:60:HIS:C	1:D:110:MET:HE1	2.39	0.47
1:A:171:LEU:C	1:A:173:GLY:H	2.22	0.47
1:A:220:THR:O	1:A:224:MET:HB2	2.14	0.47
1:A:155:LEU:O	1:A:156:PRO:C	2.55	0.47
1:C:172:ALA:HB1	1:C:184:SER:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:ILE:O	1:C:279:LEU:HB2	2.15	0.47
1:D:61:VAL:CA	1:D:110:MET:HE1	2.45	0.47
1:A:105:GLN:O	1:A:105:GLN:HG3	2.15	0.47
1:B:227:VAL:O	1:B:228:SER:C	2.58	0.47
1:C:82:GLY:O	1:C:83:ALA:C	2.58	0.47
1:C:204:SER:HB2	1:C:206:VAL:HG23	1.95	0.47
1:C:60:HIS:CD2	1:C:85:SER:CB	2.97	0.47
1:D:46:ILE:CD1	1:D:218:ILE:HG21	2.45	0.47
1:D:263:TRP:CD1	1:D:263:TRP:N	2.80	0.47
1:A:155:LEU:O	1:A:158:LEU:N	2.47	0.47
1:A:36:LYS:HZ3	1:A:112:GLY:N	2.11	0.46
1:A:44:LYS:CG	2:A:501:NDP:H3B	2.45	0.46
3:D:603:H11:H14A	3:D:603:H11:H8A	1.67	0.46
1:A:144:PHE:HE2	1:B:140:MET:HG3	1.80	0.46
1:D:107:GLY:O	1:D:111:GLY:N	2.48	0.46
1:A:46:ILE:H	1:A:46:ILE:HG12	1.51	0.46
1:A:92:THR:OG1	1:A:94:GLU:HG3	2.16	0.46
1:A:213:CYS:SG	1:A:256:VAL:CG2	3.03	0.46
1:D:66:ARG:CD	1:D:92:THR:HG22	2.45	0.46
1:B:141:GLU:HA	1:B:145:LEU:HB2	1.98	0.46
1:C:278:PHE:C	1:C:280:TYR:H	2.22	0.46
1:A:66:ARG:HB2	2:A:501:NDP:O3X	2.15	0.46
1:A:148:VAL:O	1:A:152:VAL:HG23	2.16	0.46
1:D:36:LYS:CG	1:D:110:MET:HB2	2.46	0.46
1:A:204:SER:HB2	1:A:206:VAL:HG23	1.98	0.46
1:A:28:ARG:C	1:A:30:GLU:N	2.73	0.45
1:D:217:LEU:HD22	1:D:233:MET:HB3	1.98	0.45
1:D:269:ARG:CZ	1:D:269:ARG:HB2	2.46	0.45
1:C:93:MET:HE2	1:C:98:PHE:CE1	2.46	0.45
1:D:227:VAL:O	1:D:228:SER:HB3	2.15	0.45
1:B:134:HIS:CD2	1:D:95:ASP:HB2	2.51	0.45
1:D:62:VAL:HG23	1:D:110:MET:CE	2.46	0.45
1:D:187:LYS:HE3	2:D:504:NDP:O2D	2.17	0.45
1:A:171:LEU:C	1:A:173:GLY:N	2.75	0.45
1:D:216:GLY:O	2:D:504:NDP:H42N	2.16	0.45
1:B:155:LEU:HG	1:B:159:LYS:HE3	1.99	0.45
3:C:604:H11:H14A	3:C:604:H11:H11A	1.63	0.45
1:D:107:GLY:CA	1:D:157:MET:HE1	2.46	0.45
1:C:171:LEU:HB2	3:C:604:H11:O	2.16	0.45
1:A:63:VAL:O	1:A:88:TYR:HA	2.17	0.45
1:B:43:SER:O	1:B:48:ARG:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ALA:HB1	1:D:193:PHE:CD2	2.52	0.45
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.98	0.45
1:B:219:ASP:HB2	1:B:238:LYS:H	1.82	0.45
1:D:112:GLY:CA	1:D:157:MET:HE2	2.46	0.45
1:B:38:ILE:HG13	1:B:113:LEU:HD13	1.98	0.44
3:B:602:H11:H14A	3:B:602:H11:H8A	1.49	0.44
1:C:122:THR:HG22	1:C:143:ASN:OD1	2.17	0.44
1:D:181:ALA:O	1:D:182:ALA:C	2.61	0.44
1:A:94:GLU:OE1	1:A:138:LYS:NZ	2.50	0.44
1:C:178:PRO:O	1:C:179:MET:CB	2.65	0.44
1:A:108:LYS:HE2	1:C:100:GLU:OE1	2.18	0.44
1:C:30:GLU:HA	1:C:33:GLN:HG2	1.99	0.44
1:A:171:LEU:HD13	1:B:280:TYR:CZ	2.53	0.44
1:A:197:ILE:HG22	1:A:210:ILE:CD1	2.47	0.44
1:C:172:ALA:O	1:C:184:SER:CB	2.66	0.44
1:B:92:THR:O	1:B:92:THR:HG23	2.16	0.44
1:C:155:LEU:O	1:C:156:PRO:C	2.61	0.44
1:C:38:ILE:HD12	1:C:113:LEU:HD11	2.00	0.43
1:C:52:TYR:CE1	1:C:77:HIS:HD2	2.36	0.43
1:C:93:MET:HG2	2:C:503:NDP:H2A	1.99	0.43
1:B:279:LEU:O	1:B:280:TYR:C	2.62	0.43
1:D:199:LYS:O	1:D:203:VAL:HG23	2.18	0.43
1:A:113:LEU:HD23	1:A:154:ALA:HB1	2.00	0.43
1:A:196:SER:O	1:A:200:GLU:HG3	2.18	0.43
1:B:191:ASP:O	1:B:195:SER:HB2	2.18	0.43
1:A:280:TYR:C	1:A:282:THR:H	2.27	0.43
1:D:122:THR:O	1:D:124:THR:HG22	2.18	0.43
1:C:27:PHE:CG	1:C:247:LYS:HG2	2.54	0.43
1:C:32:LEU:HA	1:C:35:LYS:HG3	2.01	0.43
1:A:36:LYS:HD3	1:A:112:GLY:H	1.84	0.43
1:B:37:VAL:HG11	1:B:54:LEU:CD1	2.49	0.43
1:A:263:TRP:N	1:A:263:TRP:CE3	2.87	0.43
1:C:216:GLY:O	2:C:503:NDP:H42N	2.19	0.43
1:B:56:LYS:C	1:B:58:GLY:H	2.27	0.42
1:C:50:MET:CG	1:C:242:ALA:HB1	2.48	0.42
1:A:101:GLN:O	1:A:102:PHE:C	2.62	0.42
1:A:140:MET:HE2	1:B:140:MET:HE1	2.00	0.42
1:A:224:MET:HE3	1:A:224:MET:HA	1.99	0.42
1:C:262:LEU:HA	1:C:265:THR:OG1	2.19	0.42
1:A:176:ALA:HB3	1:B:199:LYS:HE2	2.01	0.42
1:B:64:THR:HB	1:B:102:PHE:CE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:PHE:HB2	1:D:185:ALA:HB2	2.01	0.42
1:D:42:ALA:HB3	1:D:63:VAL:HB	2.02	0.42
1:D:121:ILE:HG12	2:D:504:NDP:H3D	2.01	0.42
1:D:226:ALA:CB	3:D:603:H11:H12	2.49	0.42
1:B:38:ILE:HG13	1:B:113:LEU:CD1	2.50	0.42
1:C:277:GLU:O	1:C:278:PHE:C	2.61	0.42
1:D:171:LEU:HD13	1:D:214:VAL:HG12	2.02	0.42
1:A:167:VAL:HG23	1:A:167:VAL:O	2.18	0.42
1:D:66:ARG:HG2	1:D:92:THR:HG22	2.02	0.42
1:D:216:GLY:O	1:D:218:ILE:HG12	2.20	0.42
1:A:174:LYS:NZ	1:A:191:ASP:OD2	2.30	0.42
1:B:228:SER:O	1:B:230:ILE:HG13	2.20	0.42
1:B:278:PHE:O	1:B:279:LEU:C	2.63	0.42
1:C:182:ALA:O	1:C:185:ALA:HB3	2.20	0.42
1:C:276:LEU:HD12	1:C:276:LEU:HA	1.79	0.42
1:A:40:THR:O	1:A:119:ASN:ND2	2.53	0.42
1:A:169:SER:HA	1:A:187:LYS:HD2	2.01	0.42
1:C:53:HIS:HE1	1:C:239:GLU:O	2.03	0.42
1:A:64:THR:HG21	1:A:93:MET:HE2	2.01	0.42
1:A:227:VAL:CG1	1:A:231:VAL:HB	2.42	0.42
1:B:35:LYS:HD3	1:B:35:LYS:HA	1.91	0.42
1:B:79:LEU:HA	1:B:79:LEU:HD13	1.74	0.42
1:A:106:ALA:O	1:A:110:MET:HG3	2.20	0.42
1:C:278:PHE:C	1:C:280:TYR:N	2.76	0.42
3:D:603:H11:H14A	3:D:603:H11:H11A	1.75	0.41
1:C:50:MET:O	1:C:51:ALA:C	2.61	0.41
1:A:36:LYS:NZ	1:A:112:GLY:N	2.68	0.41
1:B:73:LYS:HE2	1:B:73:LYS:HB3	1.92	0.41
1:D:145:LEU:O	1:D:146:SER:C	2.63	0.41
1:A:64:THR:HB	1:A:102:PHE:CE1	2.56	0.41
1:D:257:TYR:CD1	1:D:268:ILE:HG21	2.56	0.41
1:A:213:CYS:SG	1:A:245:ILE:HG23	2.60	0.41
1:B:36:LYS:HB2	1:B:113:LEU:HA	2.02	0.41
1:C:96:MET:HE3	1:C:141:GLU:HG3	2.03	0.41
1:A:231:VAL:HG21	3:A:601:H11:H15A	2.02	0.41
1:A:247:LYS:HG3	1:A:248:GLY:N	2.36	0.41
1:B:161:SER:O	1:B:162:ASN:C	2.63	0.41
1:D:40:THR:HA	1:D:64:THR:HG22	2.04	0.41
1:D:187:LYS:CE	2:D:504:NDP:O2D	2.69	0.40
1:A:219:ASP:OD1	1:A:238:LYS:N	2.51	0.40
1:B:197:ILE:HD13	1:B:197:ILE:HA	1.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:THR:O	1:B:265:THR:C	2.64	0.40
1:A:114:ASP:OD1	1:A:114:ASP:C	2.64	0.40
1:A:126:LEU:HG	1:A:179:MET:HB3	2.04	0.40
1:B:216:GLY:O	2:B:502:NDP:H42N	2.21	0.40
1:C:185:ALA:HB2	1:D:193:PHE:HB2	2.03	0.40
1:D:120:HIS:CE1	1:D:146:SER:OG	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	256/275 (93%)	222 (87%)	26 (10%)	8 (3%)	3	8
1	B	253/275 (92%)	221 (87%)	27 (11%)	5 (2%)	6	16
1	C	253/275 (92%)	227 (90%)	24 (10%)	2 (1%)	16	37
1	D	259/275 (94%)	234 (90%)	21 (8%)	4 (2%)	8	22
All	All	1021/1100 (93%)	904 (88%)	98 (10%)	19 (2%)	6	17

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ALA
1	B	228	SER
1	D	231	VAL
1	D	283	SER
1	B	33	GLN
1	B	219	ASP
1	C	230	ILE
1	C	279	LEU
1	A	80	GLU

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Mol	Chain	Res	Type
1	A	93	MET
1	A	205	ARG
1	A	264	THR
1	B	131	ASP
1	B	280	TYR
1	D	30	GLU
1	D	228	SER
1	A	230	ILE
1	A	106	ALA
1	A	236	ALA

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	215/232 (93%)	181 (84%)	34 (16%)	2	7
1	B	212/232 (91%)	175 (82%)	37 (18%)	2	5
1	C	212/232 (91%)	186 (88%)	26 (12%)	4	12
1	D	218/232 (94%)	186 (85%)	32 (15%)	3	8
All	All	857/928 (92%)	728 (85%)	129 (15%)	3	7

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	32	LEU
1	A	37	VAL
1	A	46	ILE
1	A	49	GLU
1	A	50	MET
1	A	56	LYS
1	A	79	LEU
1	A	85	SER
1	A	103	VAL
1	A	109	LEU

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Mol	Chain	Res	Type
1	A	114	ASP
1	A	126	LEU
1	A	141	GLU
1	A	145	LEU
1	A	151	THR
1	A	159	LYS
1	A	167	VAL
1	A	170	SER
1	A	175	VAL
1	A	197	ILE
1	A	203	VAL
1	A	221	GLU
1	A	224	MET
1	A	225	LYS
1	A	228	SER
1	A	234	GLN
1	A	239	GLU
1	A	247	LYS
1	A	261	SER
1	A	263	TRP
1	A	268	ILE
1	A	269	ARG
1	A	281	SER
1	B	28	ARG
1	B	30	GLU
1	B	32	LEU
1	B	33	GLN
1	B	36	LYS
1	B	50	MET
1	B	56	LYS
1	B	69	GLU
1	B	74	VAL
1	B	76	SER
1	B	79	LEU
1	B	94	GLU
1	B	97	THR
1	B	103	VAL
1	B	108	LYS
1	B	116	LEU
1	B	124	THR
1	B	128	LEU
1	B	141	GLU

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Mol	Chain	Res	Type
1	B	150	LEU
1	B	160	GLN
1	B	165	ILE
1	B	167	VAL
1	B	170	SER
1	B	175	VAL
1	B	197	ILE
1	B	203	VAL
1	B	205	ARG
1	B	215	LEU
1	B	222	THR
1	B	225	LYS
1	B	233	MET
1	B	234	GLN
1	B	243	LEU
1	B	255	GLU
1	B	262	LEU
1	B	281	SER
1	C	26	GLU
1	C	32	LEU
1	C	36	LYS
1	C	43	SER
1	C	70	THR
1	C	73	LYS
1	C	97	THR
1	C	123	ASN
1	C	126	LEU
1	C	145	LEU
1	C	150	LEU
1	C	160	GLN
1	C	204	SER
1	C	205	ARG
1	C	215	LEU
1	C	221	GLU
1	C	227	VAL
1	C	233	MET
1	C	243	LEU
1	C	260	SER
1	C	262	LEU
1	C	265	THR
1	C	268	ILE
1	C	272	SER

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Mol	Chain	Res	Type
1	C	276	LEU
1	C	279	LEU
1	D	26	GLU
1	D	32	LEU
1	D	36	LYS
1	D	44	LYS
1	D	53	HIS
1	D	68	LYS
1	D	69	GLU
1	D	70	THR
1	D	74	VAL
1	D	79	LEU
1	D	97	THR
1	D	110	MET
1	D	124	THR
1	D	141	GLU
1	D	150	LEU
1	D	170	SER
1	D	171	LEU
1	D	184	SER
1	D	205	ARG
1	D	215	LEU
1	D	222	THR
1	D	225	LYS
1	D	228	SER
1	D	232	HIS
1	D	243	LEU
1	D	261	SER
1	D	265	THR
1	D	266	LEU
1	D	269	ARG
1	D	276	LEU
1	D	281	SER
1	D	284	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	101	GLN
1	A	105	GLN
1	A	119	ASN

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Mol	Chain	Res	Type
1	A	120	HIS
1	A	127	ASN
1	A	135	HIS
1	A	162	ASN
1	A	207	ASN
1	A	253	GLN
1	A	270	ASN
1	B	33	GLN
1	B	53	HIS
1	B	77	HIS
1	B	101	GLN
1	B	120	HIS
1	B	134	HIS
1	B	160	GLN
1	B	234	GLN
1	B	270	ASN
1	C	33	GLN
1	C	53	HIS
1	C	60	HIS
1	C	77	HIS
1	C	123	ASN
1	C	162	ASN
1	C	207	ASN
1	D	53	HIS
1	D	72	GLN
1	D	120	HIS
1	D	123	ASN
1	D	134	HIS
1	D	234	GLN
1	D	253	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	H11	B	602	-	20,20,20	1.71	4 (20%)	18,27,27	2.90	6 (33%)
2	NDP	B	502	-	51,52,52	1.83	12 (23%)	71,80,80	1.68	15 (21%)
2	NDP	A	501	-	51,52,52	2.07	14 (27%)	71,80,80	1.89	16 (22%)
2	NDP	C	503	-	51,52,52	1.62	12 (23%)	71,80,80	2.00	17 (23%)
3	H11	D	603	-	20,20,20	1.56	5 (25%)	18,27,27	3.15	7 (38%)
2	NDP	D	504	-	51,52,52	2.08	17 (33%)	71,80,80	2.13	22 (30%)
3	H11	A	601	-	20,20,20	1.25	2 (10%)	18,27,27	2.62	8 (44%)
3	H11	C	604	-	20,20,20	1.18	3 (15%)	18,27,27	1.71	4 (22%)

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	H11	B	602	-	-	1/8/33/33	0/2/2/2
2	NDP	B	502	-	-	7/34/77/77	0/5/5/5
2	NDP	A	501	-	-	11/34/77/77	0/5/5/5
2	NDP	C	503	-	-	6/34/77/77	0/5/5/5
3	H11	D	603	-	-	1/8/33/33	0/2/2/2
2	NDP	D	504	-	-	8/34/77/77	0/5/5/5
3	H11	A	601	-	-	3/8/33/33	0/2/2/2
3	H11	C	604	-	-	5/8/33/33	0/2/2/2

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NDP	PN-O3	6.52	1.66	1.59
2	D	504	NDP	C4N-C3N	-5.96	1.38	1.50
2	A	501	NDP	PA-O3	5.79	1.65	1.59
2	B	502	NDP	C4N-C3N	-5.31	1.40	1.50
2	A	501	NDP	C4N-C3N	-4.92	1.40	1.50
2	D	504	NDP	P2B-O1X	4.85	1.65	1.50
2	C	503	NDP	C4N-C3N	-4.81	1.40	1.50
2	D	504	NDP	P2B-O2X	4.65	1.72	1.54
3	B	602	H11	C4-S	-4.52	1.70	1.75
2	B	502	NDP	P2B-O1X	4.34	1.64	1.50
3	A	601	H11	C-S	-3.85	1.80	1.85
2	D	504	NDP	C4N-C5N	-3.51	1.39	1.49
2	B	502	NDP	C5A-N7A	-3.50	1.32	1.39
2	C	503	NDP	C5A-N7A	-3.48	1.32	1.39
3	B	602	H11	C-C2	3.41	1.58	1.54
2	B	502	NDP	C4N-C5N	-3.40	1.40	1.49
2	A	501	NDP	C4N-C5N	-3.37	1.40	1.49
3	B	602	H11	C-S	-3.37	1.80	1.85
3	D	603	H11	C8-C7	3.36	1.57	1.52
2	B	502	NDP	PA-O3	-3.34	1.55	1.59
2	C	503	NDP	C4N-C5N	-3.20	1.40	1.49
2	D	504	NDP	C4A-N9A	-3.19	1.31	1.37
2	A	501	NDP	C5A-N7A	-3.09	1.33	1.39
2	B	502	NDP	PN-O3	-3.06	1.56	1.59
2	B	502	NDP	C8A-N9A	-3.05	1.32	1.37
2	D	504	NDP	PA-O3	3.05	1.62	1.59
3	D	603	H11	C4-S	-2.98	1.72	1.75
2	D	504	NDP	C5D-C4D	2.88	1.60	1.51
2	C	503	NDP	C6N-N1N	2.83	1.44	1.37
2	A	501	NDP	C7N-C3N	2.82	1.54	1.48
2	D	504	NDP	PN-O3	2.78	1.62	1.59
3	A	601	H11	C2-N	-2.72	1.33	1.38
2	C	503	NDP	P2B-O1X	2.72	1.58	1.50
2	B	502	NDP	O4B-C4B	2.71	1.51	1.45
2	D	504	NDP	C6N-N1N	2.70	1.43	1.37
2	D	504	NDP	O4B-C1B	2.63	1.48	1.42
2	A	501	NDP	P2B-O2X	2.62	1.64	1.54
2	C	503	NDP	C8A-N9A	-2.62	1.33	1.37
2	C	503	NDP	C7N-C3N	2.60	1.54	1.48
2	D	504	NDP	C5A-N7A	-2.57	1.34	1.39
2	D	504	NDP	O5D-C5D	2.56	1.54	1.44
2	D	504	NDP	C6N-C5N	2.55	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	NDP	C4A-N9A	-2.51	1.32	1.37
2	C	503	NDP	O4D-C4D	-2.50	1.39	1.45
2	A	501	NDP	P2B-O3X	-2.50	1.45	1.54
2	A	501	NDP	C6N-N1N	2.49	1.43	1.37
2	A	501	NDP	P2B-O1X	2.49	1.58	1.50
2	D	504	NDP	O3D-C3D	2.49	1.49	1.43
3	C	604	H11	C-S	-2.49	1.82	1.85
2	A	501	NDP	C5D-C4D	2.47	1.59	1.51
2	A	501	NDP	C8A-N9A	-2.45	1.33	1.37
2	B	502	NDP	O4B-C1B	2.41	1.47	1.42
3	D	603	H11	C4-N17	-2.38	1.31	1.34
2	C	503	NDP	C6N-C5N	2.34	1.40	1.33
3	C	604	H11	C5-C	-2.29	1.50	1.55
3	C	604	H11	C6-C	-2.27	1.50	1.53
3	D	603	H11	C6-C	2.24	1.55	1.53
2	D	504	NDP	C2N-C3N	2.23	1.41	1.35
2	C	503	NDP	P2B-O3X	-2.23	1.46	1.54
2	D	504	NDP	O4B-C4B	-2.22	1.40	1.45
2	A	501	NDP	P2B-O2B	2.21	1.63	1.59
2	D	504	NDP	C8A-N9A	-2.21	1.33	1.37
2	B	502	NDP	C6N-C5N	2.17	1.39	1.33
3	D	603	H11	C-C2	2.11	1.57	1.54
2	A	501	NDP	C2N-C3N	2.11	1.41	1.35
2	C	503	NDP	PN-O2N	-2.08	1.45	1.55
3	B	602	H11	C2-N	-2.06	1.35	1.38
2	B	502	NDP	C6N-N1N	2.05	1.42	1.37
2	C	503	NDP	C2N-C3N	2.02	1.40	1.35

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	603	H11	C2-C-S	-10.29	98.89	104.16
3	B	602	H11	C2-C-S	-8.54	99.78	104.16
3	A	601	H11	C2-C-S	-7.46	100.34	104.16
2	C	503	NDP	C5A-C4A-N3A	-7.07	116.99	126.72
2	A	501	NDP	C5A-C4A-N3A	-5.78	118.76	126.72
2	D	504	NDP	C4A-N9A-C8A	5.59	111.60	105.74
2	D	504	NDP	C3N-C2N-N1N	-5.25	115.50	123.20
2	D	504	NDP	N9A-C8A-N7A	-5.12	106.67	113.94
2	D	504	NDP	C6N-N1N-C2N	5.09	124.77	119.32
2	B	502	NDP	C5A-C4A-N3A	-5.01	119.81	126.72
2	A	501	NDP	N3A-C2A-N1A	-4.88	121.19	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	NDP	O4B-C1B-C2B	-4.68	98.53	106.59
2	C	503	NDP	N3A-C4A-N9A	4.62	135.02	127.17
2	A	501	NDP	N9A-C8A-N7A	-4.51	107.53	113.94
3	B	602	H11	O-C2-N	-4.40	118.27	125.08
2	D	504	NDP	C2B-C1B-N9A	4.34	120.90	113.75
2	A	501	NDP	C2A-N3A-C4A	4.24	122.19	111.83
3	B	602	H11	O-C2-C	4.23	125.60	120.83
3	C	604	H11	C2-C-S	-4.10	102.06	104.16
2	B	502	NDP	O4B-C1B-N9A	4.10	115.96	108.09
3	D	603	H11	C7-N17-C4	-4.10	117.29	124.48
2	D	504	NDP	O3B-C3B-C4B	-4.09	99.33	111.08
2	D	504	NDP	N3A-C2A-N1A	-4.03	122.49	128.58
2	A	501	NDP	N3A-C4A-N9A	3.87	133.75	127.17
2	C	503	NDP	C2D-C1D-N1N	-3.85	103.84	113.31
2	C	503	NDP	O4B-C1B-N9A	-3.85	100.70	108.09
3	D	603	H11	C6-C-S	3.84	113.64	108.46
2	C	503	NDP	C2A-N3A-C4A	3.81	121.14	111.83
3	A	601	H11	O-C2-N	-3.80	119.20	125.08
2	D	504	NDP	N6A-C6A-N1A	3.63	126.46	118.38
3	D	603	H11	O-C2-N	-3.47	119.71	125.08
2	B	502	NDP	N3A-C2A-N1A	-3.45	123.36	128.58
2	C	503	NDP	N3A-C2A-N1A	-3.43	123.39	128.58
2	A	501	NDP	O2B-P2B-O1X	-3.42	97.14	109.33
3	A	601	H11	C-C2-N	3.26	118.21	115.42
2	C	503	NDP	C2B-C1B-N9A	-3.26	108.39	113.75
2	A	501	NDP	C5A-N7A-C8A	3.22	108.50	103.45
2	C	503	NDP	C3N-C2N-N1N	-3.19	118.51	123.20
2	A	501	NDP	C3N-C2N-N1N	-3.17	118.54	123.20
2	B	502	NDP	C2A-N3A-C4A	3.17	119.57	111.83
2	C	503	NDP	C4A-C5A-N7A	-3.08	107.06	110.58
2	D	504	NDP	C5A-C4A-N3A	-3.05	122.52	126.72
2	B	502	NDP	C3N-C2N-N1N	-3.02	118.76	123.20
3	B	602	H11	C6-C-S	3.02	112.53	108.46
2	B	502	NDP	N3A-C4A-N9A	3.01	132.28	127.17
3	C	604	H11	C7-N17-C4	-2.99	119.23	124.48
3	A	601	H11	C7-N17-C4	-2.98	119.25	124.48
2	A	501	NDP	C4A-N9A-C8A	2.96	108.84	105.74
2	D	504	NDP	C5A-N7A-C8A	2.95	108.09	103.45
2	B	502	NDP	N9A-C8A-N7A	-2.93	109.79	113.94
2	A	501	NDP	O3-PN-O1N	-2.92	101.93	110.70
2	B	502	NDP	C4A-C5A-N7A	-2.86	107.32	110.58
2	C	503	NDP	O2A-PA-O3	2.85	114.97	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	504	NDP	C5A-C6A-N6A	-2.77	116.43	123.29
2	A	501	NDP	O3X-P2B-O1X	2.75	121.56	110.83
2	A	501	NDP	O2N-PN-O3	2.74	114.69	107.27
2	A	501	NDP	O4B-C4B-C5B	-2.74	100.56	109.33
2	D	504	NDP	N3A-C4A-N9A	2.71	131.78	127.17
2	A	501	NDP	P2B-O2B-C2B	-2.71	116.21	123.43
2	C	503	NDP	O2N-PN-O3	2.67	114.50	107.27
2	C	503	NDP	O3-PN-O1N	-2.59	102.91	110.70
2	A	501	NDP	C4A-C5A-N7A	-2.56	107.65	110.58
2	C	503	NDP	C5A-N7A-C8A	2.53	107.43	103.45
3	D	603	H11	O-C2-C	2.53	123.68	120.83
3	D	603	H11	C8-C7-N17	-2.49	100.36	109.50
2	D	504	NDP	C2B-C3B-C4B	2.48	107.32	101.99
2	D	504	NDP	O4B-C1B-C2B	-2.46	102.36	106.59
3	A	601	H11	N17-C4-N	-2.46	121.43	124.26
2	B	502	NDP	O4D-C4D-C5D	-2.41	101.61	109.33
3	B	602	H11	C6-C-C2	2.41	112.17	108.76
2	C	503	NDP	C6A-C5A-C4A	2.41	120.46	117.18
2	C	503	NDP	C2D-C3D-C4D	2.40	107.25	102.61
3	A	601	H11	C11-C10-C8	-2.39	107.24	117.37
3	B	602	H11	C7-N17-C4	-2.38	120.30	124.48
2	B	502	NDP	C5A-N7A-C8A	2.38	107.19	103.45
2	C	503	NDP	N9A-C8A-N7A	-2.35	110.60	113.94
2	D	504	NDP	C4A-C5A-N7A	-2.33	107.92	110.58
3	C	604	H11	C11-C10-C8	-2.32	107.53	117.37
2	A	501	NDP	O3X-P2B-O2B	2.31	114.86	105.85
2	B	502	NDP	C4A-N9A-C1B	-2.28	121.31	126.63
2	D	504	NDP	O4D-C1D-N1N	2.26	112.40	108.08
3	A	601	H11	C6-C-C2	2.25	111.95	108.76
2	B	502	NDP	O3B-C3B-C4B	-2.24	104.66	111.08
2	D	504	NDP	C1D-N1N-C6N	-2.18	116.15	120.77
2	B	502	NDP	O4B-C4B-C5B	2.16	116.24	109.33
3	A	601	H11	C8-C7-N17	-2.14	101.63	109.50
2	D	504	NDP	C2A-N3A-C4A	2.13	117.05	111.83
2	D	504	NDP	O4D-C1D-C2D	-2.10	102.13	106.62
3	D	603	H11	C9-C7-N17	2.08	117.14	109.50
2	D	504	NDP	C5D-C4D-C3D	-2.06	107.80	115.21
2	B	502	NDP	O4D-C1D-C2D	-2.04	102.25	106.62
3	C	604	H11	O-C2-N	-2.03	121.94	125.08
2	B	502	NDP	O4D-C1D-N1N	-2.02	104.24	108.08
2	D	504	NDP	O7N-C7N-C3N	-2.01	117.12	120.90
2	D	504	NDP	O2A-PA-O3	2.01	112.70	107.27

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NDP	C5B-O5B-PA-O1A
2	A	501	NDP	C5B-O5B-PA-O2A
2	A	501	NDP	C5B-O5B-PA-O3
2	A	501	NDP	C5D-O5D-PN-O3
2	A	501	NDP	C5D-O5D-PN-O2N
2	A	501	NDP	O4D-C1D-N1N-C6N
2	B	502	NDP	C5B-O5B-PA-O2A
2	B	502	NDP	C5D-O5D-PN-O2N
2	B	502	NDP	O4D-C1D-N1N-C6N
2	C	503	NDP	O4D-C1D-N1N-C6N
2	D	504	NDP	O4D-C1D-N1N-C6N
3	A	601	H11	C6-C-C5-C3
3	A	601	H11	S-C-C5-C3
3	A	601	H11	C2-C-C5-C3
3	C	604	H11	S-C-C5-C3
3	C	604	H11	C2-C-C5-C3
2	D	504	NDP	C1B-C2B-O2B-P2B
2	A	501	NDP	C3B-C4B-C5B-O5B
2	C	503	NDP	O4D-C4D-C5D-O5D
2	D	504	NDP	O4D-C4D-C5D-O5D
2	A	501	NDP	O4B-C4B-C5B-O5B
2	B	502	NDP	O4B-C4B-C5B-O5B
3	C	604	H11	C15-C3-C5-C
2	B	502	NDP	C3B-C4B-C5B-O5B
3	B	602	H11	C8-C7-N17-C4
3	C	604	H11	C8-C7-N17-C4
3	D	603	H11	C8-C7-N17-C4
2	C	503	NDP	PN-O3-PA-O1A
2	A	501	NDP	C2B-O2B-P2B-O1X
2	A	501	NDP	C5D-O5D-PN-O1N
3	C	604	H11	C6-C-C5-C3
2	D	504	NDP	C3B-C2B-O2B-P2B
2	D	504	NDP	O4B-C4B-C5B-O5B
2	B	502	NDP	C2N-C3N-C7N-N7N
2	C	503	NDP	C2N-C3N-C7N-N7N
2	B	502	NDP	C2B-O2B-P2B-O1X
2	D	504	NDP	PN-O3-PA-O1A
2	A	501	NDP	PA-O3-PN-O1N
2	C	503	NDP	PN-O3-PA-O2A
2	D	504	NDP	PN-O3-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	D	504	NDP	C3D-C4D-C5D-O5D
2	C	503	NDP	C3D-C4D-C5D-O5D

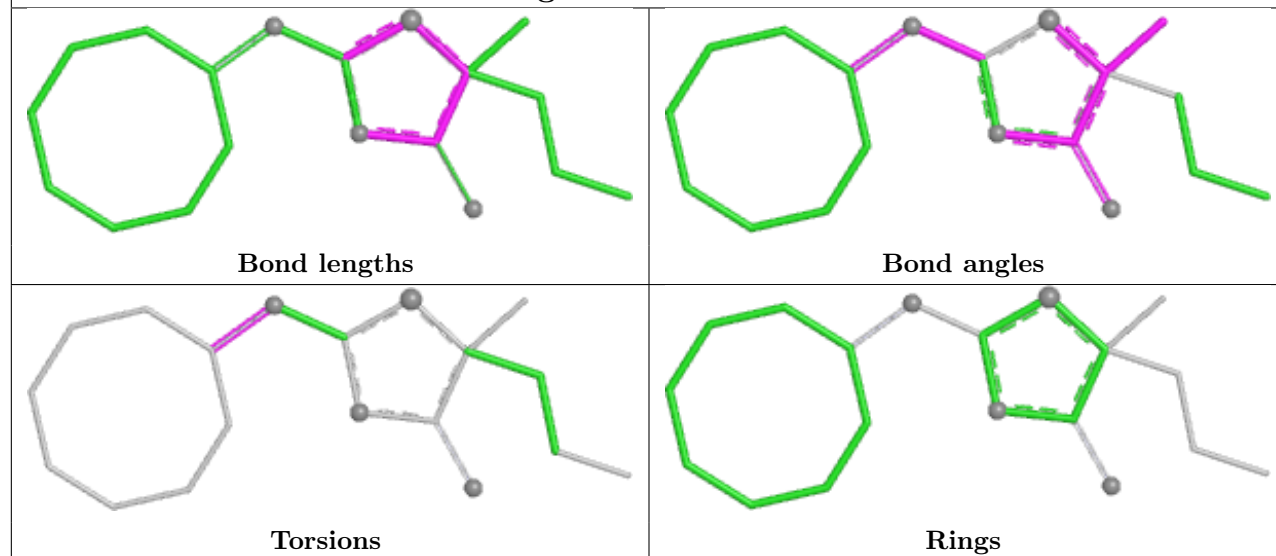
There are no ring outliers.

8 monomers are involved in 24 short contacts:

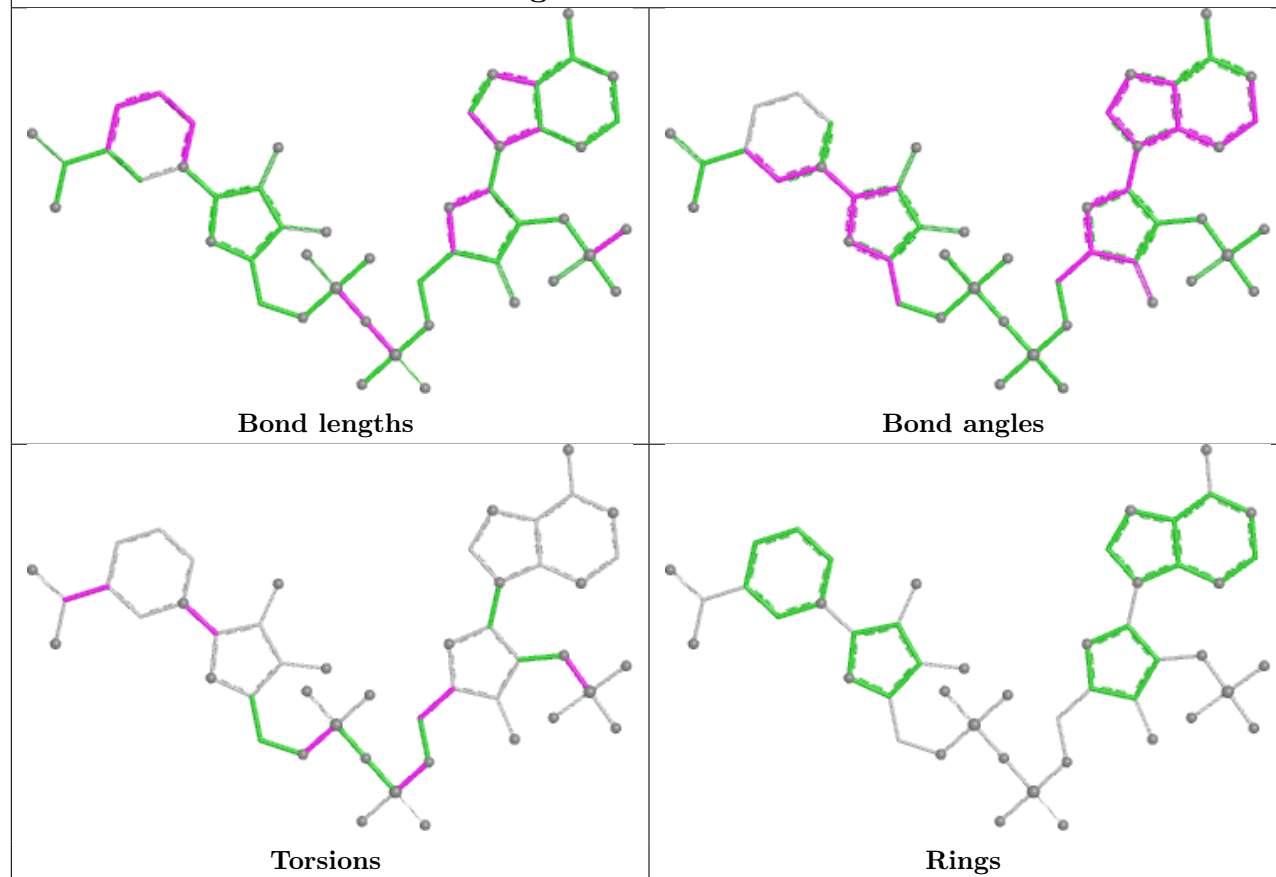
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	H11	1	0
2	B	502	NDP	4	0
2	A	501	NDP	4	0
2	C	503	NDP	2	0
3	D	603	H11	3	0
2	D	504	NDP	6	0
3	A	601	H11	1	0
3	C	604	H11	3	0

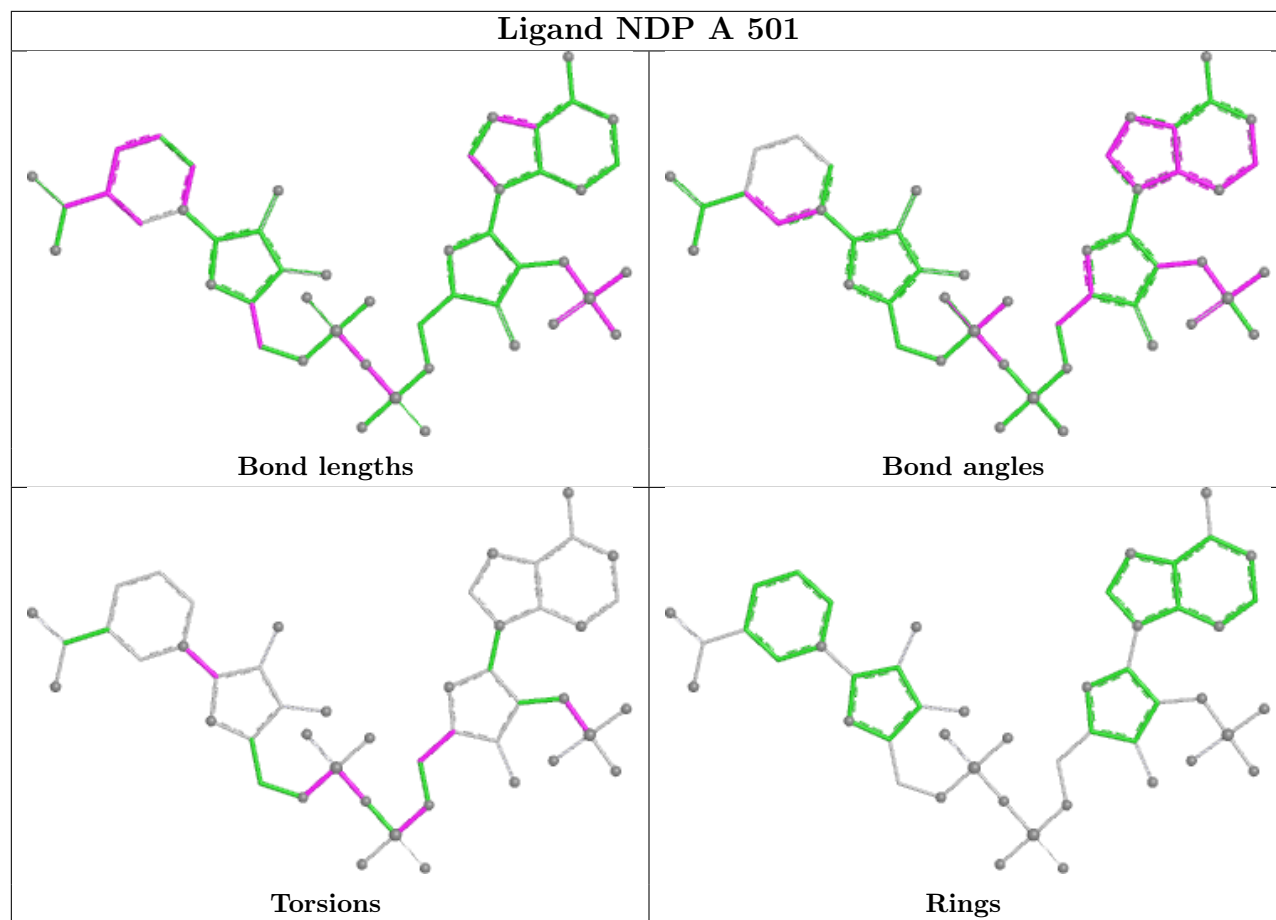
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

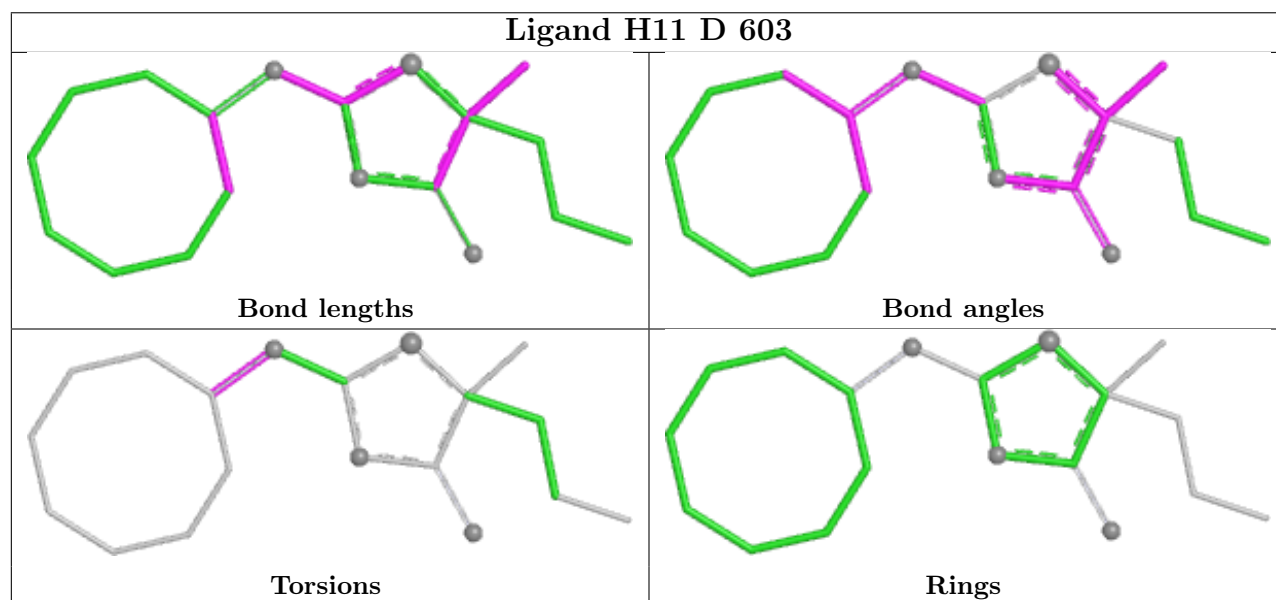
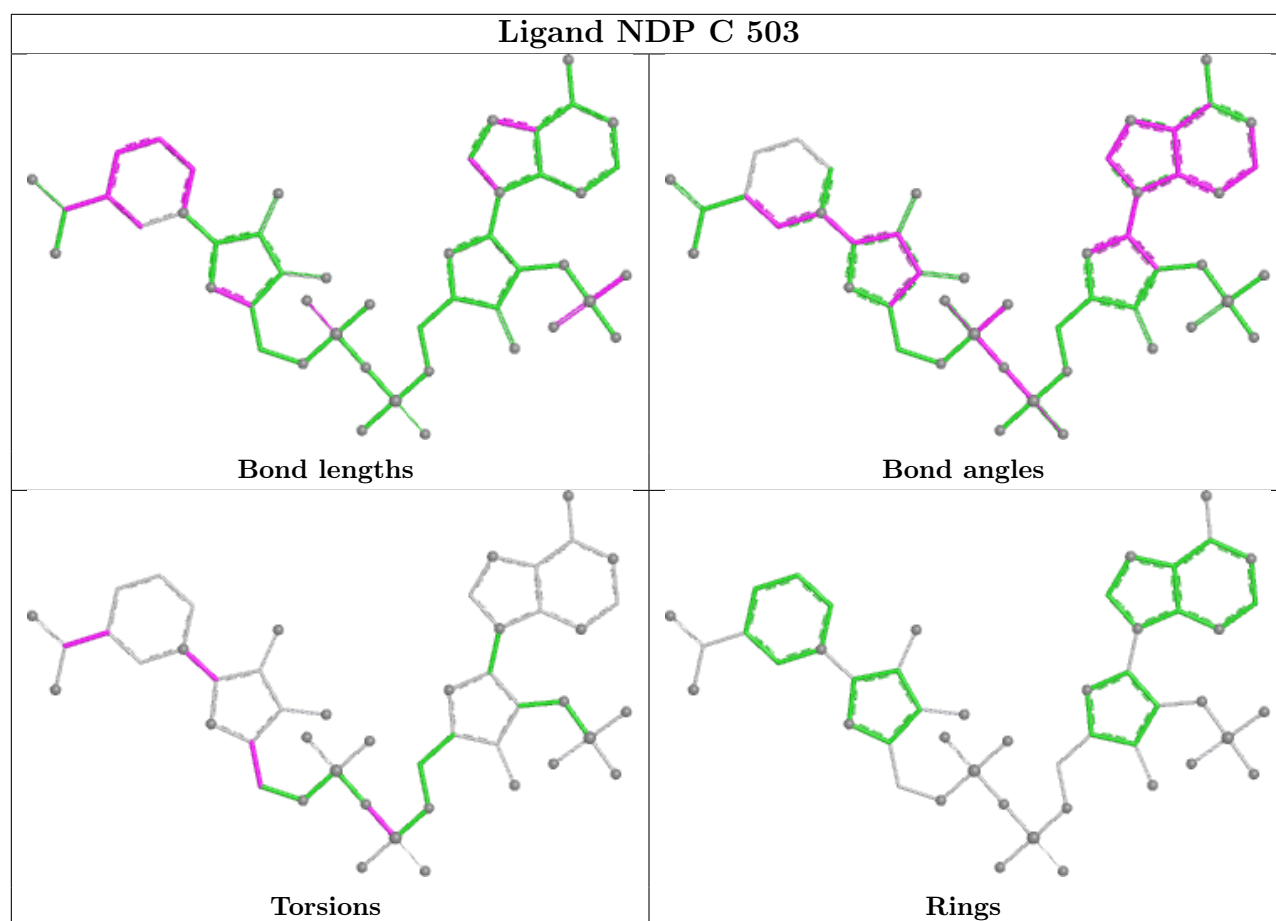
Ligand H11 B 602

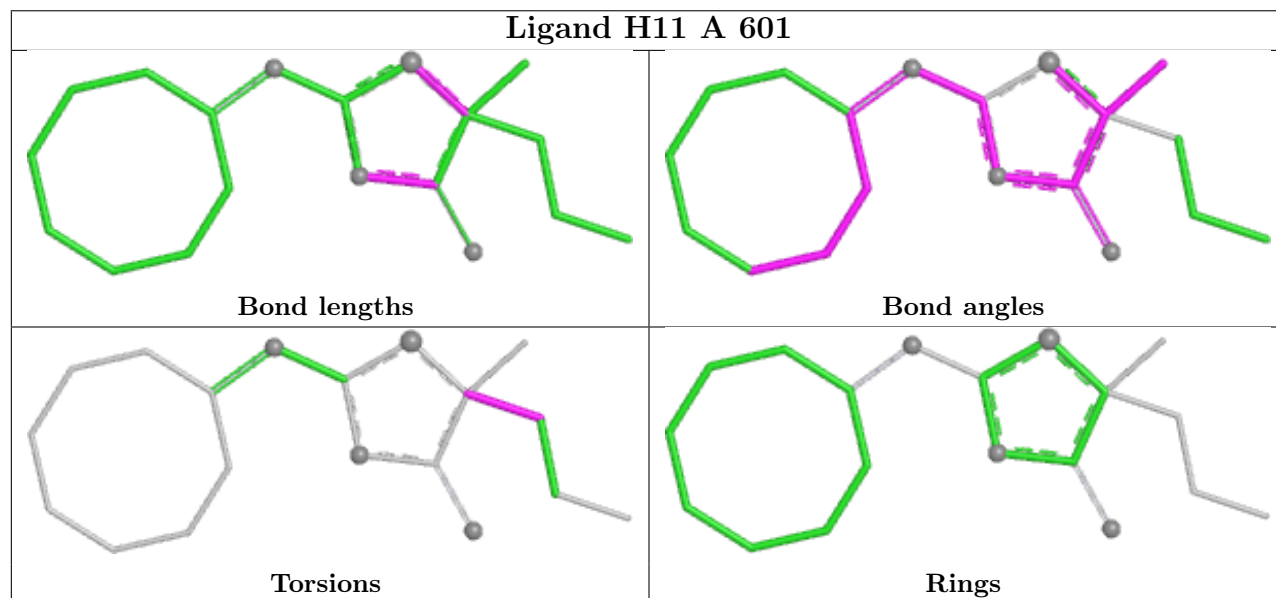
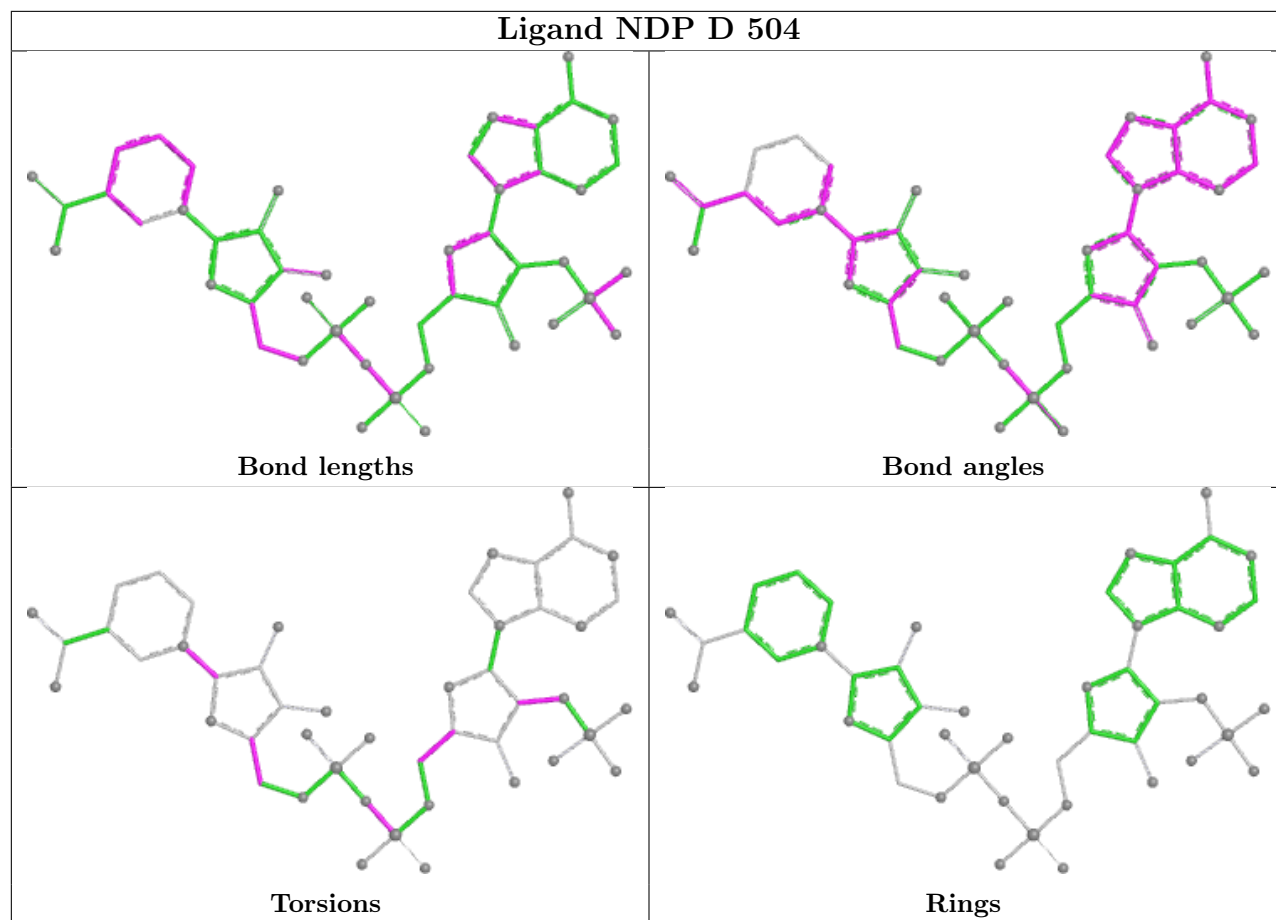


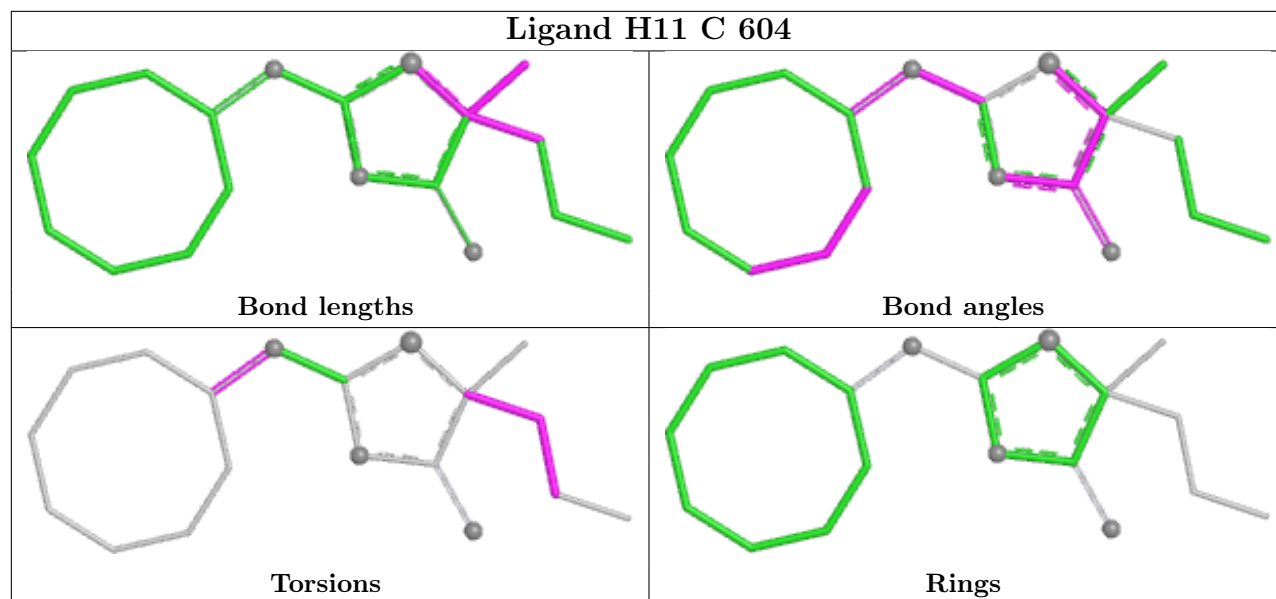
Ligand NDP B 502











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	258/275 (93%)	0.19	7 (2%) 56 53	18, 46, 69, 91	0
1	B	255/275 (92%)	-0.18	1 (0%) 88 87	22, 35, 55, 70	0
1	C	255/275 (92%)	-0.35	5 (1%) 65 62	14, 32, 56, 71	0
1	D	261/275 (94%)	-0.21	10 (3%) 44 40	18, 33, 61, 81	0
All	All	1029/1100 (93%)	-0.14	23 (2%) 62 59	14, 35, 63, 91	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	231	VAL	5.7
1	D	230	ILE	4.6
1	D	229	GLY	4.4
1	D	232	HIS	4.0
1	C	280	TYR	3.8
1	A	282	THR	3.5
1	A	262	LEU	3.3
1	D	233	MET	3.2
1	D	280	TYR	3.1
1	A	280	TYR	3.0
1	A	231	VAL	2.8
1	A	263	TRP	2.6
1	C	233	MET	2.5
1	D	285	ASN	2.4
1	C	232	HIS	2.4
1	A	29	PRO	2.4
1	C	278	PHE	2.3
1	D	284	TYR	2.3
1	D	228	SER	2.1
1	B	239	GLU	2.1
1	A	79	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	262	LEU	2.1
1	C	231	VAL	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](#)

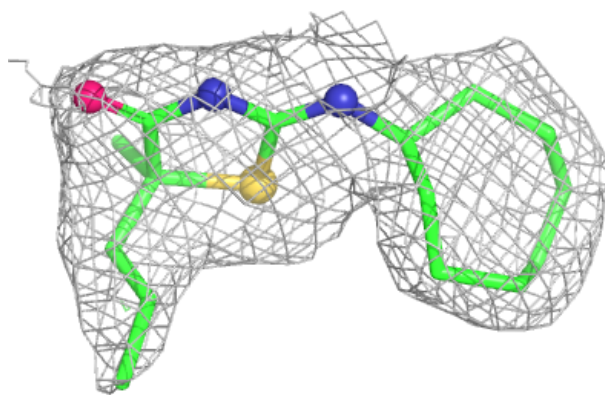
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	H11	D	603	19/19	0.93	0.09	27,32,32,33	0
3	H11	B	602	19/19	0.94	0.10	37,38,40,41	0
3	H11	C	604	19/19	0.96	0.08	25,26,32,34	0
3	H11	A	601	19/19	0.96	0.07	30,32,34,35	0
2	NDP	B	502	48/48	0.97	0.06	18,29,32,34	0
2	NDP	D	504	48/48	0.97	0.06	17,23,28,29	0
2	NDP	A	501	48/48	0.97	0.06	25,31,34,35	0
2	NDP	C	503	48/48	0.98	0.05	15,26,30,32	0

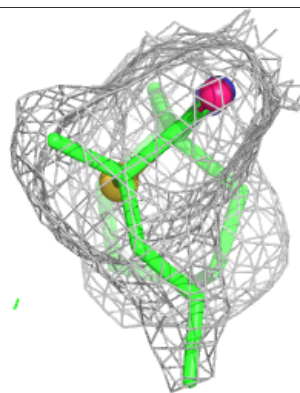
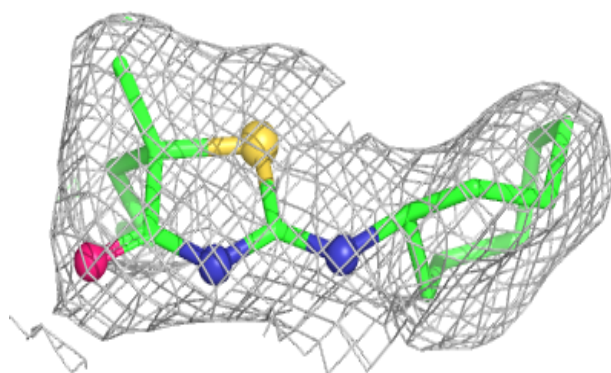
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around H11 D 603:

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



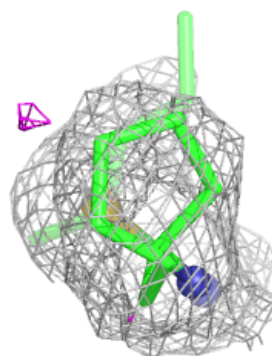
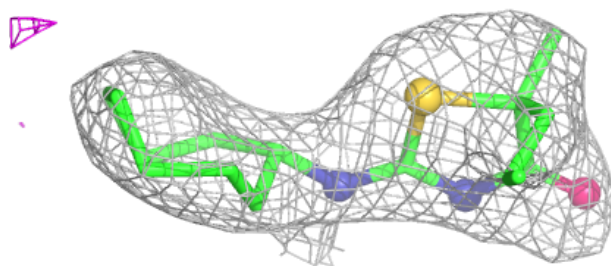
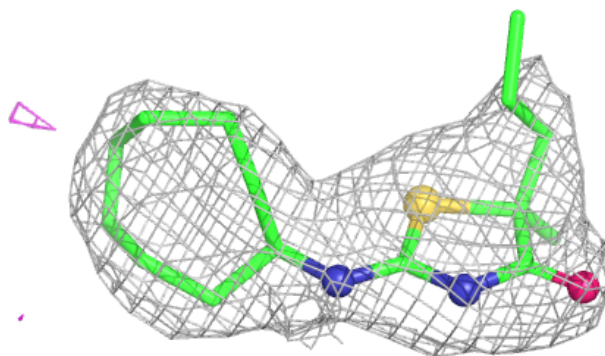
A



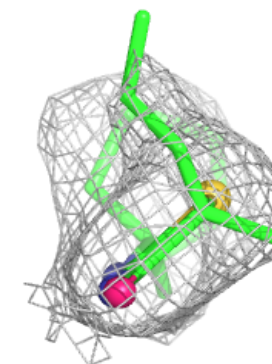
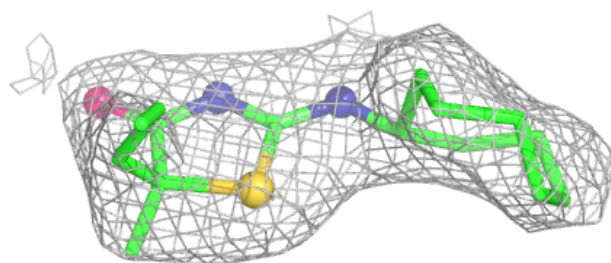
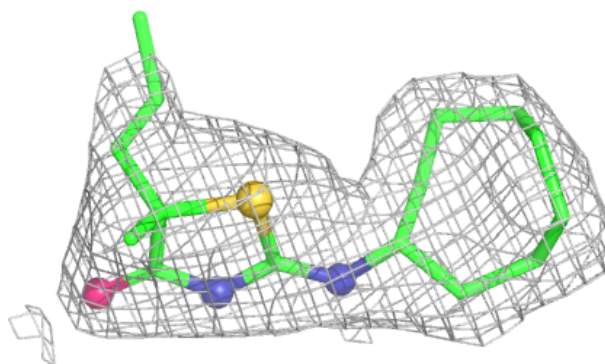
B

Electron density around H11 B 602:

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

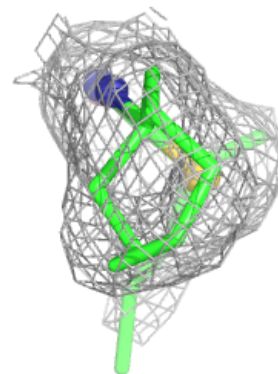
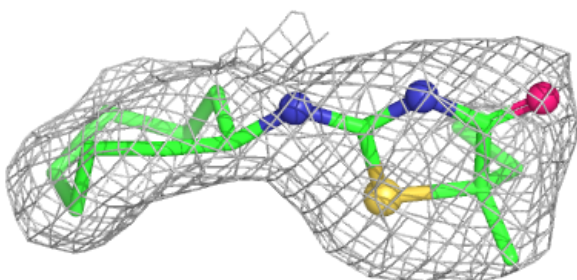
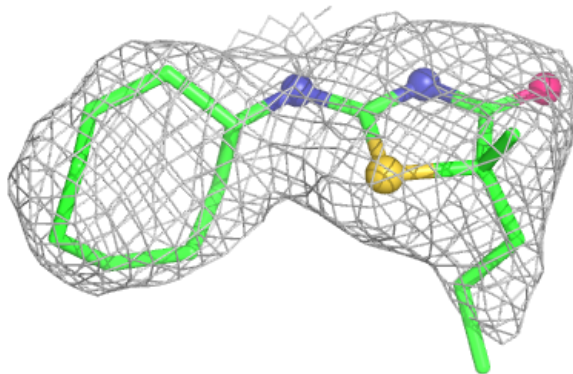
**Electron density around H11 C 604:**

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

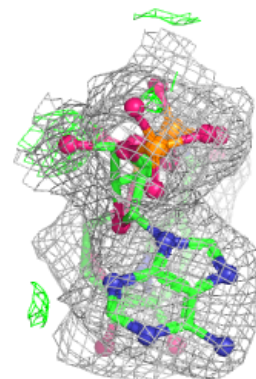
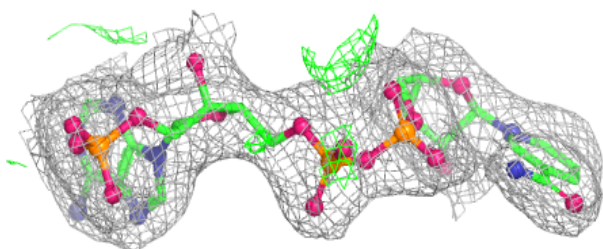
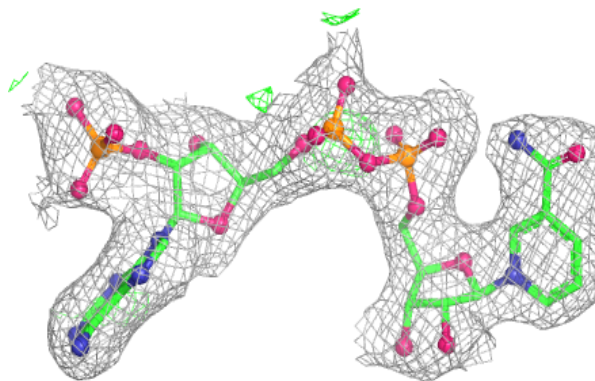


Electron density around H11 A 601:

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

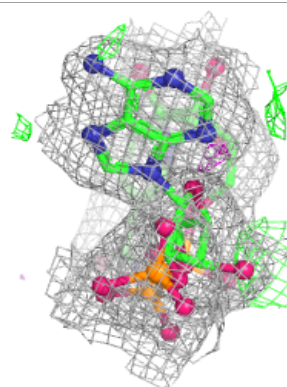
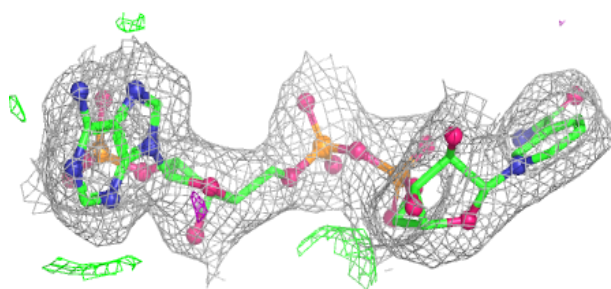
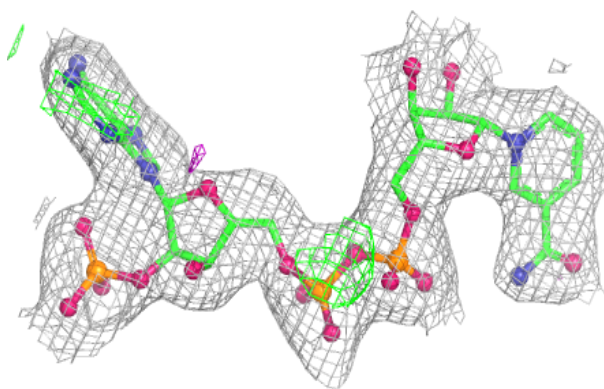
**Electron density around NDP B 502:**

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

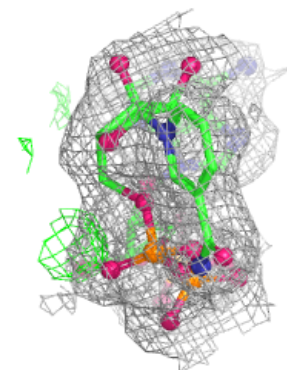
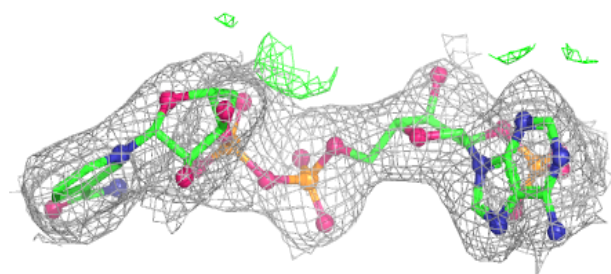
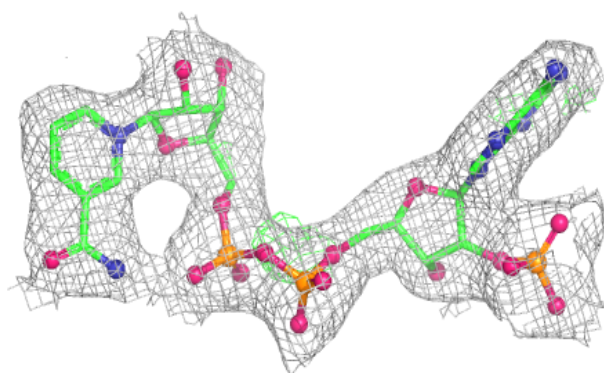


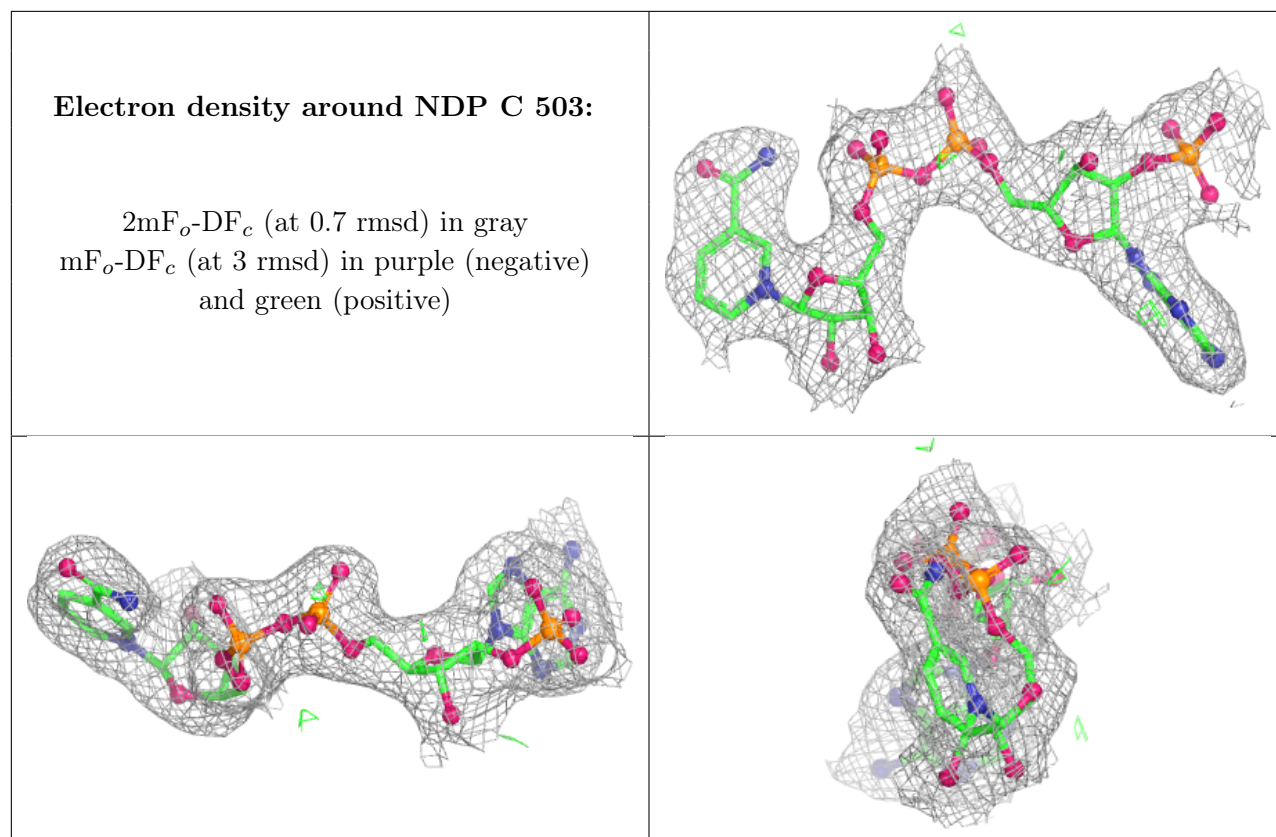
Electron density around NDP D 504:

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

**Electron density around NDP A 501:**

$2mF_o-DF_c$ (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.