Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 07:20 PM EST

PDB ID	:	3QQP
Title	:	Crystal Structure of 11beta-Hydroxysteroid Dehydrogenase 1 (11b-HSD1) in Complex with Urea Inhibitor
Authors	:	Loenze, P.; Schimanski-Breves, S.; Engel, C.K.
Deposited on	:	2011-02-16
Resolution	:	2.72 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

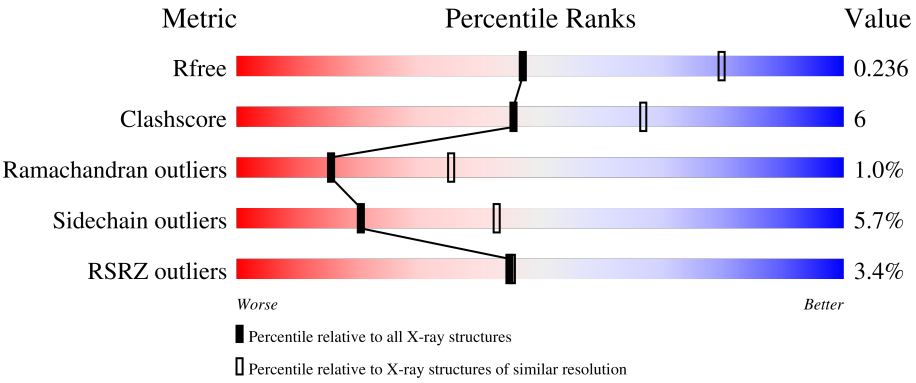
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.72 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}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	286	5% 81% 14% 6%
1	B	286	4% 78% 13% • 7%
1	C	286	2% 78% 12% • 8%
1	D	286	2% 77% 13% 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8650 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	270	Total	C	N	O	S	0	5	0
			2092	1332	353	391	16			
1	B	266	Total	C	N	O	S	0	7	0
			2074	1322	350	386	16			
1	C	262	Total	C	N	O	S	0	3	0
			2020	1288	343	374	15			
1	D	258	Total	C	N	O	S	0	5	0
			1985	1261	338	371	15			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	expression tag	UNP P28845
A	8	LYS	-	expression tag	UNP P28845
A	9	HIS	-	expression tag	UNP P28845
A	10	GLN	-	expression tag	UNP P28845
A	11	HIS	-	expression tag	UNP P28845
A	12	GLN	-	expression tag	UNP P28845
A	13	HIS	-	expression tag	UNP P28845
A	14	GLN	-	expression tag	UNP P28845
A	15	HIS	-	expression tag	UNP P28845
A	16	GLN	-	expression tag	UNP P28845
A	17	HIS	-	expression tag	UNP P28845
A	18	GLN	-	expression tag	UNP P28845
A	19	HIS	-	expression tag	UNP P28845
A	20	GLN	-	expression tag	UNP P28845
A	21	GLN	-	expression tag	UNP P28845
A	22	PRO	-	expression tag	UNP P28845
A	23	LEU	-	expression tag	UNP P28845
A	272	SER	CYS	engineered mutation	UNP P28845
B	7	MET	-	expression tag	UNP P28845
B	8	LYS	-	expression tag	UNP P28845
B	9	HIS	-	expression tag	UNP P28845

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Chain	Residue	Modelled	Actual	Comment	Reference
B	10	GLN	-	expression tag	UNP P28845
B	11	HIS	-	expression tag	UNP P28845
B	12	GLN	-	expression tag	UNP P28845
B	13	HIS	-	expression tag	UNP P28845
B	14	GLN	-	expression tag	UNP P28845
B	15	HIS	-	expression tag	UNP P28845
B	16	GLN	-	expression tag	UNP P28845
B	17	HIS	-	expression tag	UNP P28845
B	18	GLN	-	expression tag	UNP P28845
B	19	HIS	-	expression tag	UNP P28845
B	20	GLN	-	expression tag	UNP P28845
B	21	GLN	-	expression tag	UNP P28845
B	22	PRO	-	expression tag	UNP P28845
B	23	LEU	-	expression tag	UNP P28845
B	272	SER	CYS	engineered mutation	UNP P28845
C	7	MET	-	expression tag	UNP P28845
C	8	LYS	-	expression tag	UNP P28845
C	9	HIS	-	expression tag	UNP P28845
C	10	GLN	-	expression tag	UNP P28845
C	11	HIS	-	expression tag	UNP P28845
C	12	GLN	-	expression tag	UNP P28845
C	13	HIS	-	expression tag	UNP P28845
C	14	GLN	-	expression tag	UNP P28845
C	15	HIS	-	expression tag	UNP P28845
C	16	GLN	-	expression tag	UNP P28845
C	17	HIS	-	expression tag	UNP P28845
C	18	GLN	-	expression tag	UNP P28845
C	19	HIS	-	expression tag	UNP P28845
C	20	GLN	-	expression tag	UNP P28845
C	21	GLN	-	expression tag	UNP P28845
C	22	PRO	-	expression tag	UNP P28845
C	23	LEU	-	expression tag	UNP P28845
C	272	SER	CYS	engineered mutation	UNP P28845
D	7	MET	-	expression tag	UNP P28845
D	8	LYS	-	expression tag	UNP P28845
D	9	HIS	-	expression tag	UNP P28845
D	10	GLN	-	expression tag	UNP P28845
D	11	HIS	-	expression tag	UNP P28845
D	12	GLN	-	expression tag	UNP P28845
D	13	HIS	-	expression tag	UNP P28845
D	14	GLN	-	expression tag	UNP P28845
D	15	HIS	-	expression tag	UNP P28845

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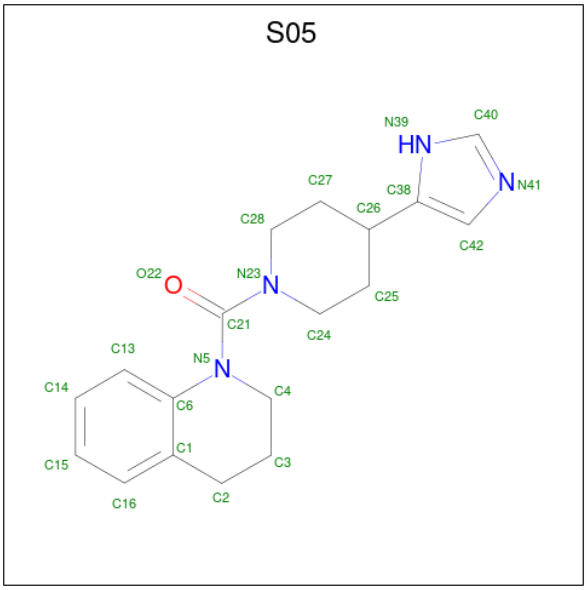
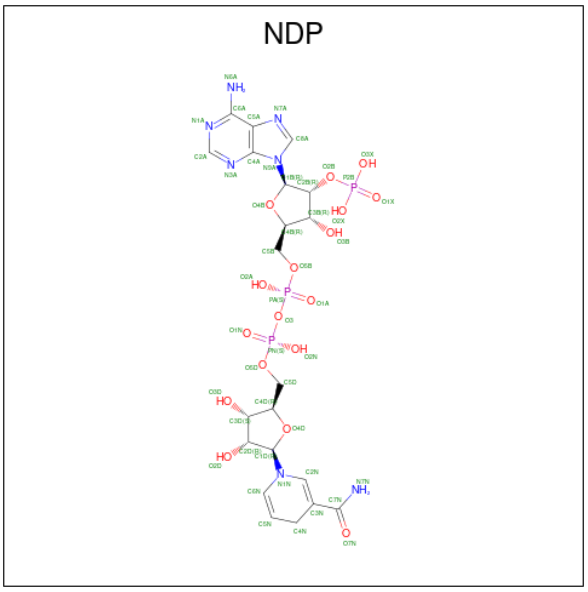
Chain	Residue	Modelled	Actual	Comment	Reference
D	16	GLN	-	expression tag	UNP P28845
D	17	HIS	-	expression tag	UNP P28845
D	18	GLN	-	expression tag	UNP P28845
D	19	HIS	-	expression tag	UNP P28845
D	20	GLN	-	expression tag	UNP P28845
D	21	GLN	-	expression tag	UNP P28845
D	22	PRO	-	expression tag	UNP P28845
D	23	LEU	-	expression tag	UNP P28845
D	272	SER	CYS	engineered mutation	UNP P28845

- Molecule 2 is 3,4-dihydroquinolin-1(2H)-yl[4-(1H-imidazol-5-yl)piperidin-1-yl]methanone (three-letter code: S05) (formula: $C_{18}H_{22}N_4O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 23 18 4 1	0	0
2	B	1	Total C N O 23 18 4 1	0	0
2	C	1	Total C N O 23 18 4 1	0	0
2	D	1	Total C N O 23 18 4 1	0	0

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 4 is water.

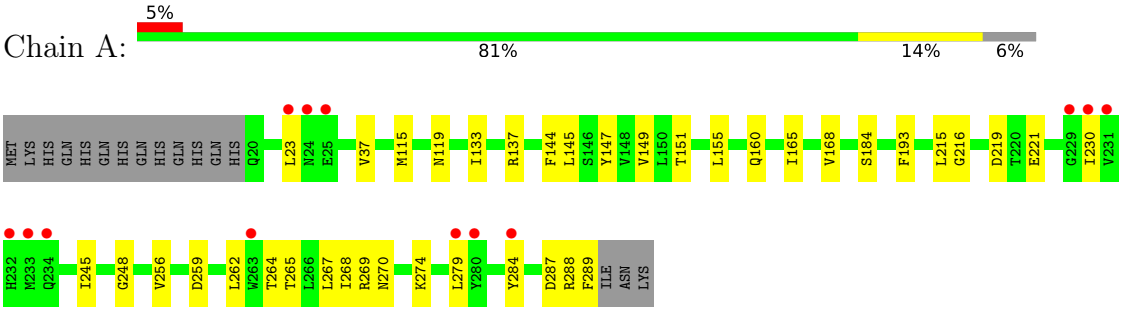
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		
4	B	37	Total	O	0	0
			37	37		
4	C	57	Total	O	0	0
			57	57		
4	D	38	Total	O	0	0
			38	38		

3 Residue-property plots (i)

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

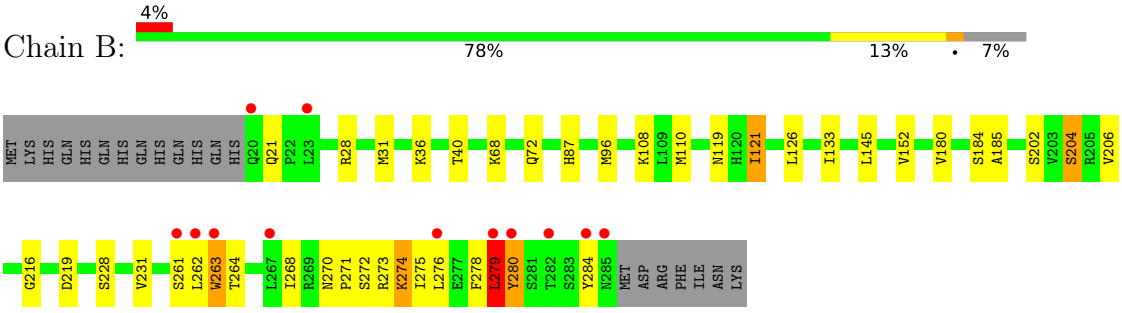
• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain A:



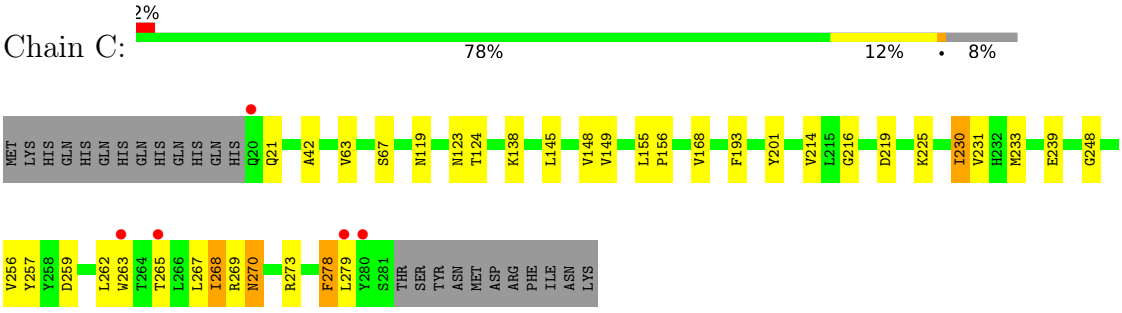
• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

Chain B:



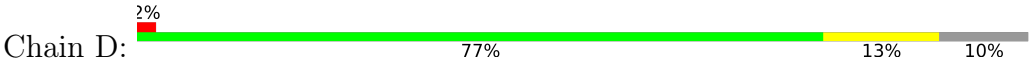
• Molecule 1: Corticosteroid 11-beta-dehydrogenase isozyme 1

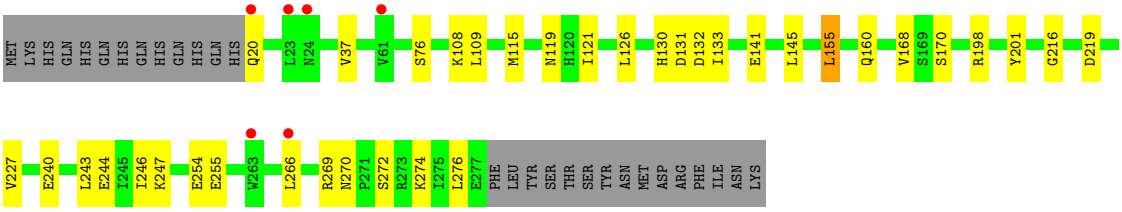
Chain C:



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

Chain D:




MET LYS HIS GLN HIS GLN HIS GLN HIS GLN HIS GLN HIS
Q20
L23 N24
V37
V61
S76
K108 L109
M115
N119 H120 I121
L126
H130 D131 D132 I133
E141
L145
L155
Q160
V168 S169 S170
R198
Y201
G216
D219
V227
E240
L243 E244 I245 I246 K247
E254 E255
W263
L266
R269 N270 P271 S272 R273 K274 I275 L276 E277
PHE LEU TYR SER THR SER TYR ASN MET ASP ARG PHE ILE ASN LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.93Å 153.38Å 74.18Å 90.00° 93.46° 90.00°	Depositor
Resolution (Å)	36.71 – 2.72 74.04 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.71-2.72) 99.8 (74.04-2.72)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.08 (at 2.73Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.7, BUSTER 2.9.7	Depositor
R, R_{free}	0.164 , 0.234 0.170 , 0.236	Depositor DCC
R_{free} test set	1684 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.616	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8650	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, S05

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	0.50	0/2148	0.70	0/2900
1	B	0.49	0/2134	0.70	0/2882
1	C	0.49	0/2067	0.70	0/2791
1	D	0.48	0/2037	0.70	0/2750
All	All	0.49	0/8386	0.70	0/11323

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2092	0	2128	17	0
1	B	2074	0	2110	51	0
1	C	2020	0	2064	26	0
1	D	1985	0	2031	29	0
2	A	23	0	22	0	0
2	B	23	0	22	0	0
2	C	23	0	22	1	0
2	D	23	0	22	0	0
3	A	48	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	26	3	0
3	C	48	0	26	2	0
3	D	48	0	26	9	0
4	A	63	0	0	1	0
4	B	37	0	0	1	0
4	C	57	0	0	0	0
4	D	38	0	0	0	0
All	All	8650	0	8525	108	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 6.

All (108) 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:274:LYS:HD2	1:D:266:LEU:HD13	1.21	1.15
1:B:278:PHE:CD2	1:B:279:LEU:CD2	2.30	1.14
1:C:265:THR:O	1:C:268:ILE:HG22	1.64	0.98
1:B:278:PHE:CD2	1:B:279:LEU:HD22	1.97	0.97
1:B:274:LYS:HE3	1:D:266:LEU:HD22	1.53	0.90
1:B:279:LEU:HD23	1:B:279:LEU:H	1.39	0.88
1:C:265:THR:O	1:C:268:ILE:CG2	2.22	0.88
1:B:274:LYS:HD2	1:D:266:LEU:CD1	2.02	0.87
1:B:275:ILE:HG23	1:B:279:LEU:HG	1.61	0.81
1:B:279:LEU:O	1:B:280:TYR:CD2	2.33	0.81
1:C:214:VAL:HG11	1:C:268:ILE:CD1	2.11	0.81
1:B:121:ILE:HG12	3:B:293:NDP:H3D	1.64	0.79
1:B:278:PHE:CD2	1:B:279:LEU:HD21	2.15	0.79
1:B:263:TRP:H	1:B:263:TRP:HD1	1.25	0.79
1:B:271:PRO:HA	1:B:274:LYS:HG2	1.65	0.78
1:B:263:TRP:CD1	1:B:263:TRP:N	2.51	0.77
1:B:279:LEU:HD23	1:B:279:LEU:N	2.00	0.76
1:C:257:TYR:CE2	1:C:268:ILE:HG12	2.20	0.76
1:B:261:SER:O	1:B:262:LEU:HD23	1.85	0.75
1:B:274:LYS:CE	1:D:266:LEU:HD22	2.18	0.74
1:B:279:LEU:CD2	1:B:279:LEU:N	2.50	0.73
1:C:214:VAL:HG11	1:C:268:ILE:HD11	1.74	0.70
1:B:278:PHE:CE2	1:B:279:LEU:HD22	2.29	0.68
1:D:155:LEU:HD21	1:D:201:TYR:OH	1.94	0.68
1:C:257:TYR:CD2	1:C:268:ILE:HG12	2.30	0.67
1:C:265:THR:C	1:C:268:ILE:HG22	2.16	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:LEU:HD21	1:C:201:TYR:OH	1.97	0.64
1:B:278:PHE:O	1:B:280:TYR:N	2.30	0.62
1:A:151:THR:HG23	1:A:165:ILE:HD13	1.85	0.58
1:C:248:GLY:HA3	1:C:256:VAL:HG21	1.85	0.58
1:B:204:SER:HB2	1:B:206:VAL:HG23	1.86	0.58
1:B:271:PRO:O	1:B:274:LYS:HG3	2.05	0.56
1:D:170:SER:CB	3:D:293:NDP:H5N	2.35	0.56
1:B:279:LEU:CD2	1:B:279:LEU:H	2.11	0.56
1:A:265:THR:O	1:A:268:ILE:HG22	2.06	0.55
1:C:149:VAL:HG22	1:D:133:ILE:HD12	1.87	0.55
1:B:278:PHE:C	1:B:280:TYR:H	2.09	0.55
1:B:68:LYS:O	1:B:72[B]:GLN:HB3	2.07	0.54
1:B:278:PHE:CE2	1:B:279:LEU:CD2	2.87	0.54
1:B:261:SER:C	1:B:262:LEU:HD23	2.27	0.53
1:B:216:GLY:O	3:B:293:NDP:H42N	2.09	0.53
1:A:193:PHE:HB2	1:B:185:ALA:HB2	1.90	0.53
1:D:126:LEU:HD11	1:D:227:VAL:HG12	1.92	0.52
1:B:278:PHE:HD2	1:B:279:LEU:HD21	1.69	0.52
1:A:149:VAL:HG22	1:B:133:ILE:HD13	1.91	0.52
1:D:170:SER:HB3	3:D:293:NDP:C5N	2.41	0.51
1:B:278:PHE:HD2	1:B:279:LEU:CD2	2.12	0.51
1:D:170:SER:HB3	3:D:293:NDP:H5N	1.93	0.50
1:D:119:ASN:HD22	1:D:168:VAL:HG21	1.76	0.50
1:D:243:LEU:HG	1:D:247:LYS:HE3	1.92	0.49
1:A:248:GLY:HA3	1:A:256:VAL:HG21	1.95	0.49
1:C:216:GLY:O	3:C:293:NDP:H42N	2.12	0.49
1:D:119:ASN:ND2	3:D:293:NDP:H4D	2.28	0.49
1:D:240:GLU:O	1:D:244:GLU:HG2	2.13	0.49
1:C:278:PHE:HD2	1:C:278:PHE:C	2.16	0.49
1:B:278:PHE:C	1:B:278:PHE:CD1	2.86	0.48
1:B:278:PHE:CG	1:B:279:LEU:CD2	2.93	0.48
1:D:121:ILE:HG12	3:D:293:NDP:H3D	1.95	0.48
1:C:278:PHE:C	1:C:278:PHE:CD2	2.87	0.48
1:B:40:THR:O	1:B:119:ASN:HB3	2.15	0.47
1:A:267:LEU:O	1:B:272:SER:HB3	2.15	0.47
1:A:279:LEU:HD22	1:C:263:TRP:CD1	2.50	0.47
1:B:275:ILE:HD11	1:D:266:LEU:HB2	1.95	0.47
1:C:214:VAL:HG11	1:C:268:ILE:HD13	1.94	0.47
1:A:264:THR:HG23	1:B:276:LEU:HD11	1.97	0.46
1:B:278:PHE:CG	1:B:279:LEU:HD22	2.49	0.46
1:C:216:GLY:HA3	1:C:259:ASP:OD2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:LEU:O	1:D:272:SER:HB3	2.16	0.46
1:B:279:LEU:O	1:B:280:TYR:CG	2.69	0.46
1:C:270:ASN:C	1:C:270:ASN:HD22	2.20	0.46
1:C:278:PHE:HD2	1:C:278:PHE:O	1.99	0.46
1:D:37:VAL:HG13	1:D:115:MET:HB3	1.98	0.46
1:D:170:SER:HB3	3:D:293:NDP:C6N	2.45	0.46
1:C:119:ASN:HD22	1:C:168:VAL:HG21	1.80	0.45
1:D:141:GLU:HA	1:D:145:LEU:HB2	1.97	0.45
1:B:263:TRP:HD1	1:B:263:TRP:N	1.97	0.45
1:B:126:LEU:HD23	1:B:180:VAL:HG13	1.98	0.45
2:C:3:S05:H4A	3:C:293:NDP:H41N	1.99	0.45
1:C:42:ALA:HB3	1:C:63:VAL:HB	1.98	0.44
1:B:119:ASN:ND2	3:B:293:NDP:H4D	2.32	0.44
1:B:36:LYS:HG2	1:B:110:MET:HB3	2.00	0.44
1:B:278:PHE:C	1:B:280:TYR:N	2.71	0.43
1:C:270:ASN:ND2	1:C:273:ARG:H	2.16	0.43
1:C:230:ILE:HD12	1:C:231:VAL:O	2.18	0.43
1:A:284:TYR:HB3	1:B:231:VAL:HG22	2.01	0.43
1:A:144:PHE:O	1:A:147:TYR:HB2	2.19	0.42
1:B:274:LYS:CD	1:D:266:LEU:HD13	2.15	0.42
1:A:119:ASN:HD22	1:A:168:VAL:HG21	1.84	0.42
1:C:148:VAL:HG13	1:C:193:PHE:CZ	2.54	0.42
1:D:130:HIS:O	1:D:131:ASP:HB2	2.19	0.42
1:D:216:GLY:O	3:D:293:NDP:H42N	2.19	0.42
1:D:170:SER:HB3	3:D:293:NDP:H6N	2.02	0.41
1:A:133:ILE:HD11	1:B:152:VAL:HG21	2.02	0.41
1:A:155:LEU:HD12	1:A:155:LEU:HA	1.88	0.41
1:B:28:ARG:HG2	1:B:31:MET:HG3	2.02	0.41
1:D:243:LEU:HA	1:D:246:ILE:HD12	2.01	0.41
1:A:37:VAL:HG22	1:A:115:MET:HB3	2.03	0.41
1:A:215:LEU:HD11	1:A:245:ILE:HD11	2.03	0.41
1:D:20:GLN:HG2	1:D:254:GLU:HG2	2.02	0.41
1:D:131:ASP:O	1:D:133:ILE:N	2.54	0.41
1:A:216:GLY:HA3	1:A:259:ASP:OD2	2.20	0.41
4:A:337:HOH:O	1:B:273:ARG:NH1	2.53	0.41
1:C:155:LEU:N	1:C:156:PRO:CD	2.84	0.41
1:D:170:SER:HB2	3:D:293:NDP:H5N	2.02	0.41
1:B:87:HIS:HD2	4:B:299:HOH:O	2.04	0.40
1:D:198:ARG:NH2	1:D:254:GLU:O	2.55	0.40
1:C:123:ASN:ND2	1:C:123:ASN:H	2.19	0.40
1:A:137:ARG:HH22	1:B:96:MET:HG3	1.87	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	273/286 (96%)	261 (96%)	10 (4%)	2 (1%)	22	45
1	B	271/286 (95%)	247 (91%)	20 (7%)	4 (2%)	10	24
1	C	263/286 (92%)	251 (95%)	10 (4%)	2 (1%)	19	41
1	D	261/286 (91%)	247 (95%)	12 (5%)	2 (1%)	19	41
All	All	1068/1144 (93%)	1006 (94%)	52 (5%)	10 (1%)	15	38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	TYR
1	B	279	LEU
1	D	132	ASP
1	D	219	ASP
1	A	287	ASP
1	A	219	ASP
1	C	67	SER
1	B	219	ASP
1	B	264	THR
1	C	219	ASP

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	232/243 (96%)	220 (95%)	12 (5%)	23	47
1	B	230/243 (95%)	216 (94%)	14 (6%)	18	39
1	C	222/243 (91%)	208 (94%)	14 (6%)	18	38
1	D	220/243 (90%)	209 (95%)	11 (5%)	24	49
All	All	904/972 (93%)	853 (94%)	51 (6%)	20	43

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	145	LEU
1	A	160	GLN
1	A	184	SER
1	A	221	GLU
1	A	230	ILE
1	A	262	LEU
1	A	269	ARG
1	A	270	ASN
1	A	274	LYS
1	A	288	ARG
1	A	289	PHE
1	B	21	GLN
1	B	108	LYS
1	B	121	ILE
1	B	145	LEU
1	B	184	SER
1	B	202	SER
1	B	204	SER
1	B	228	SER
1	B	263	TRP
1	B	268	ILE
1	B	270	ASN
1	B	274	LYS
1	B	279	LEU
1	B	284	TYR
1	C	21	GLN
1	C	124	THR
1	C	138	LYS
1	C	145	LEU
1	C	225	LYS
1	C	230	ILE
1	C	233	MET

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Mol	Chain	Res	Type
1	C	239	GLU
1	C	262	LEU
1	C	268	ILE
1	C	269	ARG
1	C	270	ASN
1	C	278	PHE
1	C	279	LEU
1	D	76[A]	SER
1	D	76[B]	SER
1	D	108	LYS
1	D	109	LEU
1	D	155	LEU
1	D	160	GLN
1	D	255	GLU
1	D	269	ARG
1	D	270	ASN
1	D	274	LYS
1	D	276	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	87	HIS
1	A	119	ASN
1	A	127	ASN
1	A	234	GLN
1	B	87	HIS
1	B	119	ASN
1	B	127	ASN
1	B	270	ASN
1	C	119	ASN
1	C	123	ASN
1	C	135	HIS
1	C	270	ASN
1	D	105	GLN
1	D	119	ASN
1	D	160	GLN
1	D	270	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	$\#\|Z\| > 2$
2	S05	A	1	-	22,26,26	1.23	3 (13%)	31,36,36	1.68	6 (19%)
2	S05	D	4	-	22,26,26	1.23	3 (13%)	31,36,36	1.55	6 (19%)
3	NDP	A	293	-	45,52,52	1.30	5 (11%)	53,80,80	1.39	9 (16%)
3	NDP	B	293	-	45,52,52	1.24	4 (8%)	53,80,80	1.21	4 (7%)
3	NDP	D	293	-	45,52,52	1.09	2 (4%)	53,80,80	1.28	5 (9%)
2	S05	B	2	-	22,26,26	1.08	2 (9%)	31,36,36	1.48	5 (16%)
3	NDP	C	293	-	45,52,52	1.34	4 (8%)	53,80,80	1.20	3 (5%)
2	S05	C	3	-	22,26,26	1.26	4 (18%)	31,36,36	1.55	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	S05	A	1	-	-	7/10/32/32	0/4/4/4
2	S05	D	4	-	-	5/10/32/32	0/4/4/4
3	NDP	A	293	-	-	4/30/77/77	0/5/5/5
3	NDP	B	293	-	-	6/30/77/77	0/5/5/5
3	NDP	D	293	-	-	7/30/77/77	0/5/5/5
2	S05	B	2	-	-	5/10/32/32	1/4/4/4
3	NDP	C	293	-	-	7/30/77/77	0/5/5/5
2	S05	C	3	-	-	4/10/32/32	1/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	293	NDP	O4B-C1B	4.80	1.47	1.41
3	A	293	NDP	C2A-N3A	4.60	1.39	1.32
3	D	293	NDP	C2A-N3A	4.10	1.38	1.32
3	A	293	NDP	O4B-C1B	4.07	1.46	1.41
3	C	293	NDP	C2A-N3A	3.76	1.38	1.32
3	C	293	NDP	P2B-O2B	3.58	1.66	1.59
3	B	293	NDP	C2A-N3A	3.47	1.37	1.32
2	A	1	S05	C24-N23	3.00	1.52	1.47
2	C	3	S05	C6-N5	2.91	1.46	1.41
2	A	1	S05	C4-N5	2.51	1.51	1.47
3	D	293	NDP	P2B-O2B	2.47	1.64	1.59
2	D	4	S05	C2-C1	2.43	1.55	1.51
2	C	3	S05	C4-N5	2.32	1.51	1.47
2	D	4	S05	C24-N23	2.26	1.51	1.47
3	C	293	NDP	C7N-N7N	2.23	1.39	1.33
3	B	293	NDP	O4B-C1B	2.20	1.44	1.41
2	C	3	S05	C2-C1	2.20	1.55	1.51
3	B	293	NDP	C8A-N7A	-2.19	1.30	1.34
3	A	293	NDP	C2A-N1A	2.17	1.37	1.33
2	C	3	S05	C28-N23	2.10	1.50	1.47
3	B	293	NDP	P2B-O2B	2.09	1.63	1.59
2	D	4	S05	C4-N5	2.07	1.51	1.47
2	A	1	S05	C28-N23	2.07	1.50	1.47
3	A	293	NDP	C3B-C2B	2.03	1.57	1.52
3	A	293	NDP	O4B-C4B	2.01	1.49	1.45
2	B	2	S05	C24-N23	2.01	1.50	1.47
2	B	2	S05	C28-N23	2.00	1.50	1.47

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1	S05	C28-N23-C24	4.95	122.15	112.62
2	D	4	S05	C28-N23-C24	4.18	120.68	112.62
3	D	293	NDP	O4D-C1D-N1N	3.85	115.59	108.06
3	B	293	NDP	O2B-P2B-O1X	-3.83	94.61	109.39
2	B	2	S05	C28-N23-C24	3.69	119.72	112.62
3	A	293	NDP	C4A-C5A-N7A	3.67	113.22	109.40
2	C	3	S05	C28-N23-C24	3.50	119.36	112.62
3	A	293	NDP	O3B-C3B-C4B	-3.37	101.30	111.05
2	B	2	S05	O22-C21-N23	-3.35	116.45	123.80
2	A	1	S05	C25-C24-N23	3.33	115.89	110.82
2	A	1	S05	O22-C21-N23	-3.24	116.68	123.80
3	B	293	NDP	O3X-P2B-O2X	3.12	119.57	107.64
2	D	4	S05	C24-C25-C26	3.12	114.72	111.04
2	C	3	S05	C24-C25-C26	2.98	114.56	111.04
2	D	4	S05	C28-C27-C26	2.97	114.55	111.04
3	A	293	NDP	O4D-C1D-N1N	2.93	113.78	108.06
2	B	2	S05	C24-C25-C26	2.92	114.50	111.04
2	A	1	S05	C24-C25-C26	2.91	114.48	111.04
3	C	293	NDP	O4D-C1D-N1N	2.83	113.58	108.06
2	D	4	S05	O22-C21-N23	-2.76	117.73	123.80
2	C	3	S05	O22-C21-N23	-2.75	117.75	123.80
2	C	3	S05	C27-C26-C25	2.69	115.17	109.56
2	C	3	S05	C28-C27-C26	2.56	114.07	111.04
3	B	293	NDP	O3X-P2B-O1X	2.47	120.37	110.68
3	A	293	NDP	O2N-PN-O1N	2.45	124.36	112.24
3	D	293	NDP	O2N-PN-O1N	2.41	124.16	112.24
3	D	293	NDP	O7N-C7N-C3N	-2.30	116.57	120.90
3	A	293	NDP	C4D-O4D-C1D	-2.29	104.41	109.47
3	C	293	NDP	C5A-C6A-N6A	2.29	123.83	120.35
3	D	293	NDP	C4A-C5A-N7A	2.29	111.78	109.40
3	A	293	NDP	O3D-C3D-C4D	2.28	117.64	111.05
2	D	4	S05	C42-C38-C26	-2.24	126.18	129.26
2	C	3	S05	C42-N41-C40	2.23	109.27	105.78
3	A	293	NDP	C2D-C3D-C4D	-2.21	98.34	102.64
3	A	293	NDP	C2D-C1D-N1N	-2.20	107.78	113.30
2	A	1	S05	C27-C26-C25	2.20	114.14	109.56
2	C	3	S05	C2-C1-C6	2.17	123.82	119.16
3	D	293	NDP	O2B-P2B-O1X	-2.17	101.03	109.39
2	A	1	S05	C42-C38-C26	-2.15	126.29	129.26
3	B	293	NDP	O7N-C7N-N7N	-2.15	117.85	122.88
3	C	293	NDP	O5B-C5B-C4B	-2.15	101.60	108.99
3	A	293	NDP	O2A-PA-O1A	2.14	122.83	112.24
2	D	4	S05	C27-C26-C25	2.13	113.99	109.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2	S05	C28-C27-C26	2.10	113.53	111.04
2	B	2	S05	C27-C26-C25	2.06	113.85	109.56
2	C	3	S05	C14-C13-C6	2.00	122.46	118.26

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	S05	O22-C21-N5-C4
2	A	1	S05	N23-C21-N5-C4
2	A	1	S05	N5-C21-N23-C24
2	A	1	S05	N5-C21-N23-C28
2	A	1	S05	O22-C21-N23-C24
2	A	1	S05	O22-C21-N23-C28
2	B	2	S05	N23-C21-N5-C6
2	B	2	S05	N5-C21-N23-C24
2	B	2	S05	N5-C21-N23-C28
2	B	2	S05	O22-C21-N23-C24
2	B	2	S05	O22-C21-N23-C28
2	C	3	S05	N5-C21-N23-C24
2	C	3	S05	N5-C21-N23-C28
2	C	3	S05	O22-C21-N23-C24
2	C	3	S05	O22-C21-N23-C28
2	D	4	S05	N23-C21-N5-C6
2	D	4	S05	N5-C21-N23-C24
2	D	4	S05	N5-C21-N23-C28
2	D	4	S05	O22-C21-N23-C24
2	D	4	S05	O22-C21-N23-C28
3	B	293	NDP	C2B-O2B-P2B-O2X
3	D	293	NDP	C5D-O5D-PN-O1N
3	C	293	NDP	O4D-C1D-N1N-C6N
3	C	293	NDP	O4D-C4D-C5D-O5D
3	C	293	NDP	C3D-C4D-C5D-O5D
3	A	293	NDP	O4D-C1D-N1N-C6N
3	B	293	NDP	O4D-C1D-N1N-C6N
3	D	293	NDP	O4D-C1D-N1N-C6N
3	D	293	NDP	C3B-C2B-O2B-P2B
3	D	293	NDP	C1B-C2B-O2B-P2B
3	C	293	NDP	C1B-C2B-O2B-P2B
3	A	293	NDP	PN-O3-PA-O1A
3	B	293	NDP	PN-O3-PA-O1A
3	C	293	NDP	C3B-C2B-O2B-P2B

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Mol	Chain	Res	Type	Atoms
3	C	293	NDP	O4B-C4B-C5B-O5B
3	D	293	NDP	O4B-C4B-C5B-O5B
3	D	293	NDP	C5D-O5D-PN-O3
3	A	293	NDP	O4B-C4B-C5B-O5B
3	B	293	NDP	O4B-C4B-C5B-O5B
3	B	293	NDP	PN-O3-PA-O2A
2	A	1	S05	C27-C26-C38-C42
3	A	293	NDP	C2N-C3N-C7N-N7N
3	B	293	NDP	C2N-C3N-C7N-N7N
3	C	293	NDP	C2N-C3N-C7N-N7N
3	D	293	NDP	C2N-C3N-C7N-N7N

All (2) ring outliers are listed below:

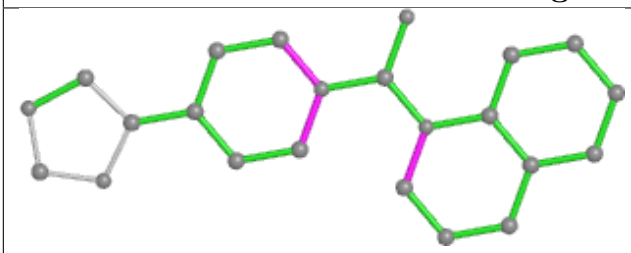
Mol	Chain	Res	Type	Atoms
2	C	3	S05	C24-C25-C26-C27-C28-N23
2	B	2	S05	C24-C25-C26-C27-C28-N23

4 monomers are involved in 14 short contacts:

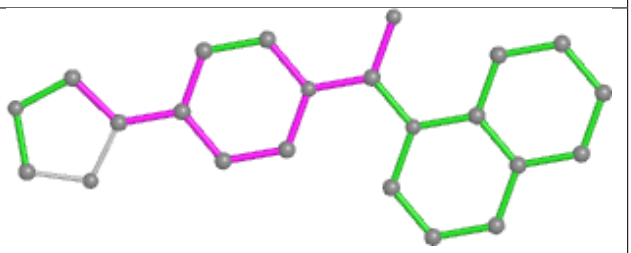
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	293	NDP	3	0
3	D	293	NDP	9	0
3	C	293	NDP	2	0
2	C	3	S05	1	0

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

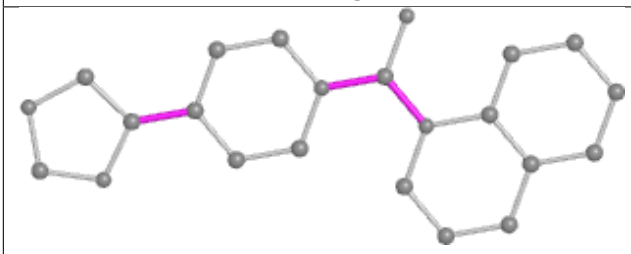
Ligand S05 A 1



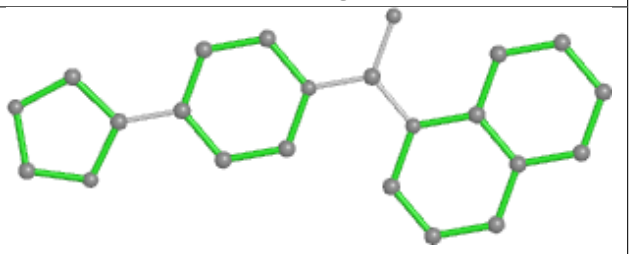
Bond lengths



Bond angles

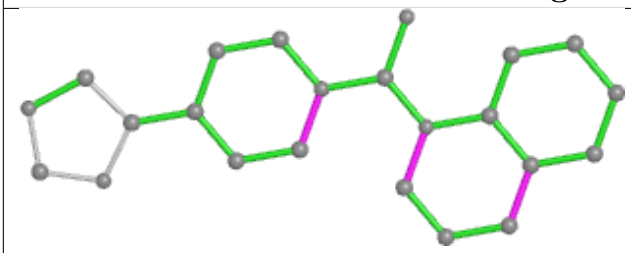


Torsions

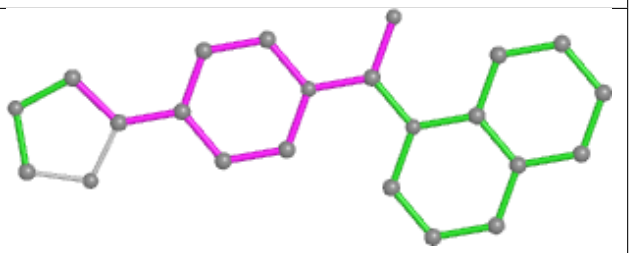


Rings

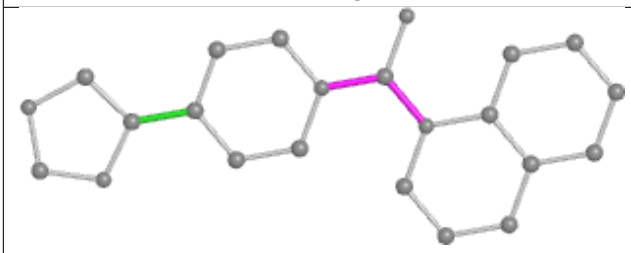
Ligand S05 D 4



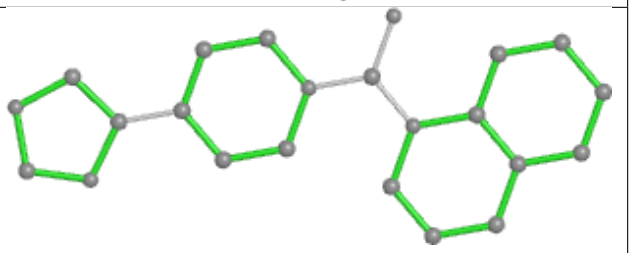
Bond lengths



Bond angles

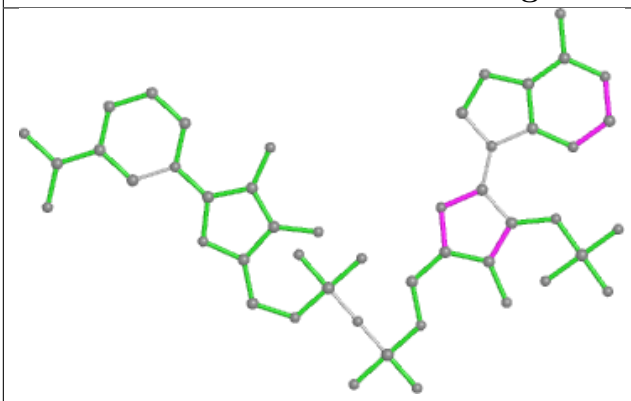


Torsions

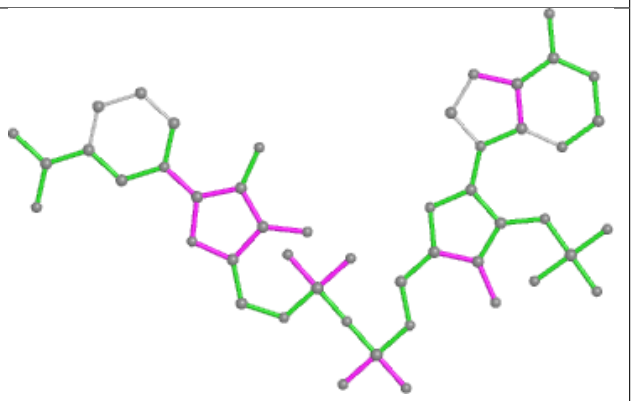


Rings

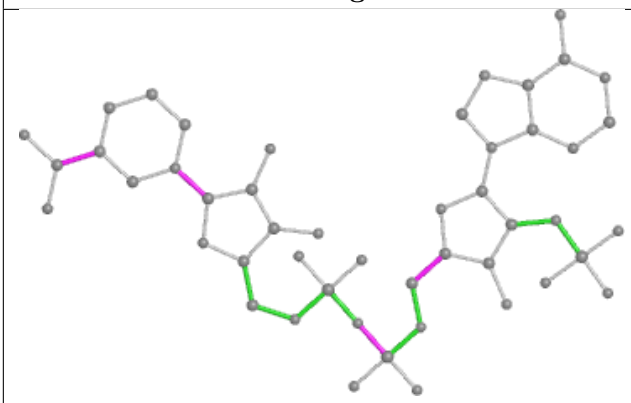
Ligand NDP A 293



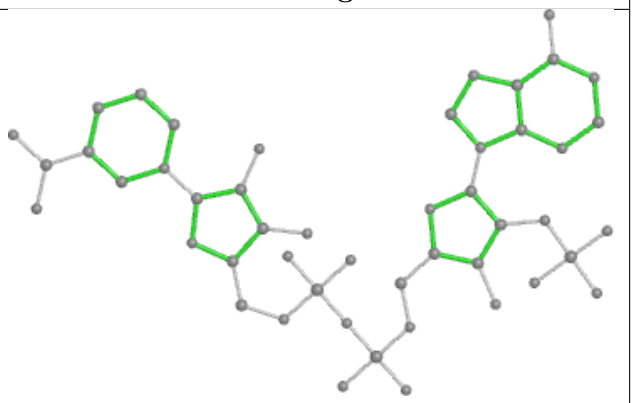
Bond lengths



Bond angles

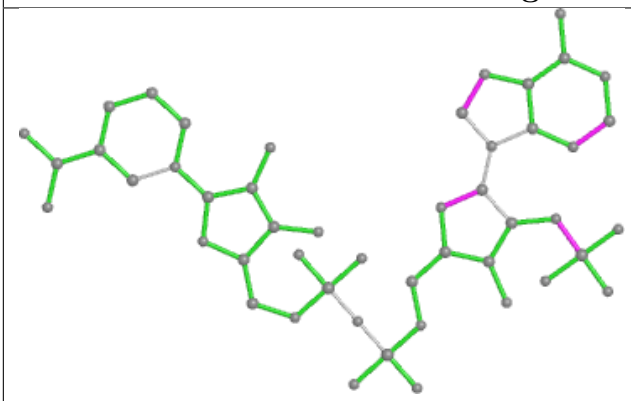


Torsions

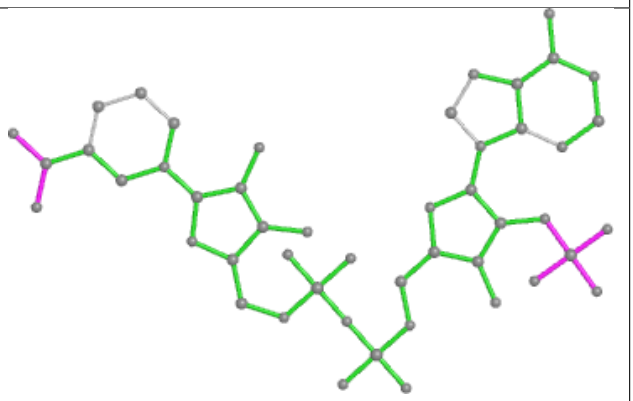


Rings

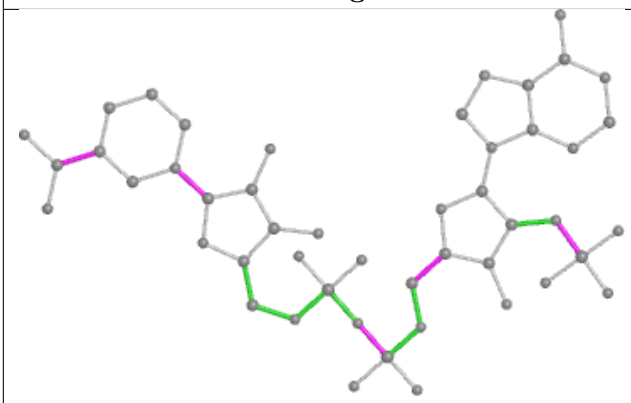
Ligand NDP B 293



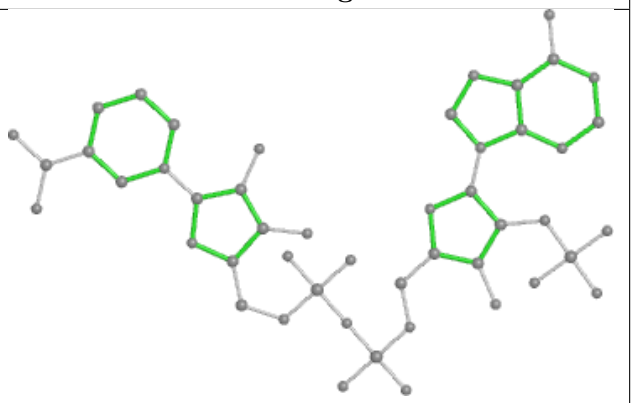
Bond lengths



Bond angles

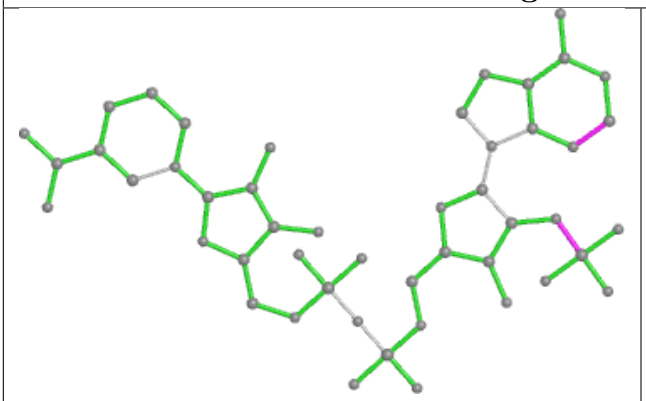


Torsions

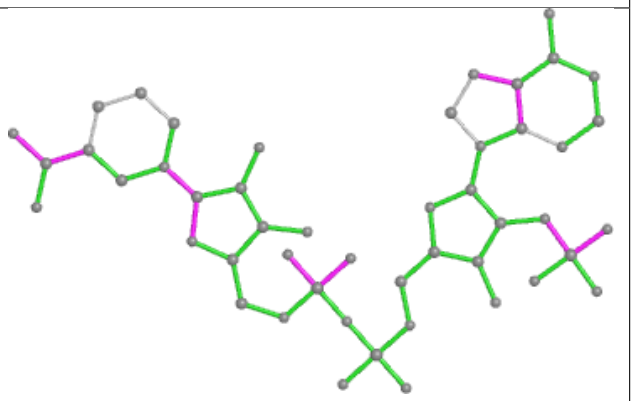


Rings

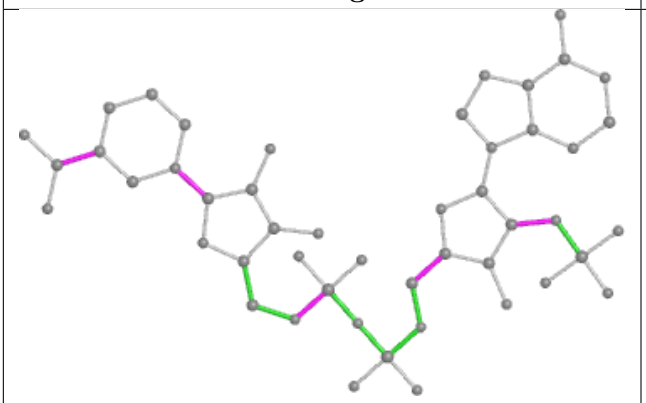
Ligand NDP D 293



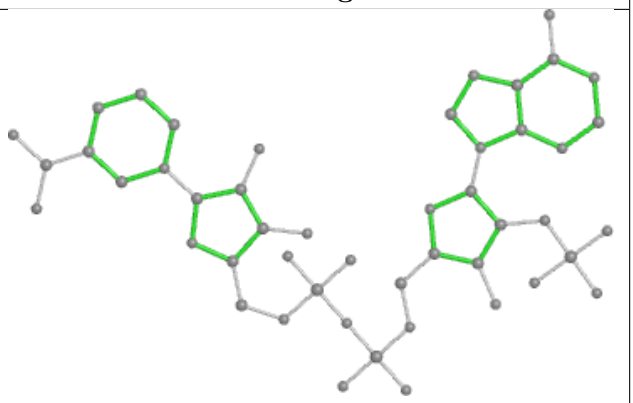
Bond lengths



Bond angles

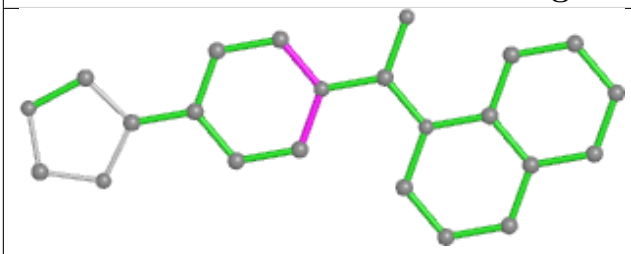


Torsions

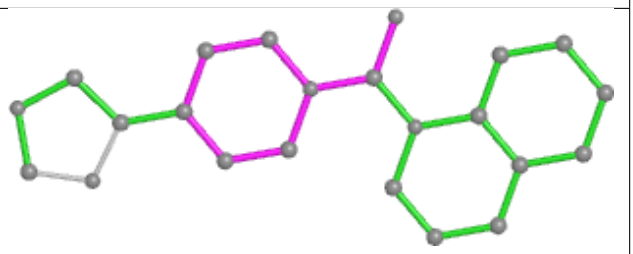


Rings

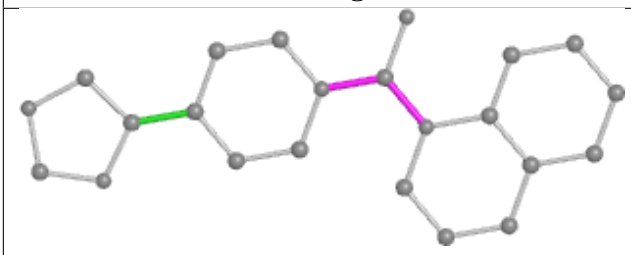
Ligand S05 B 2



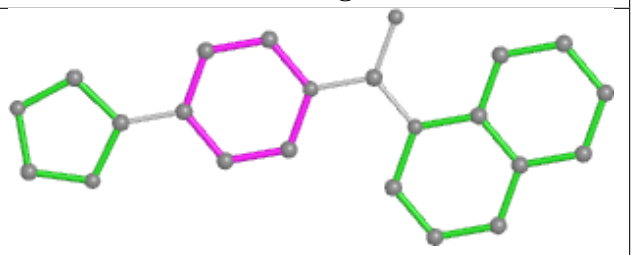
Bond lengths



Bond angles

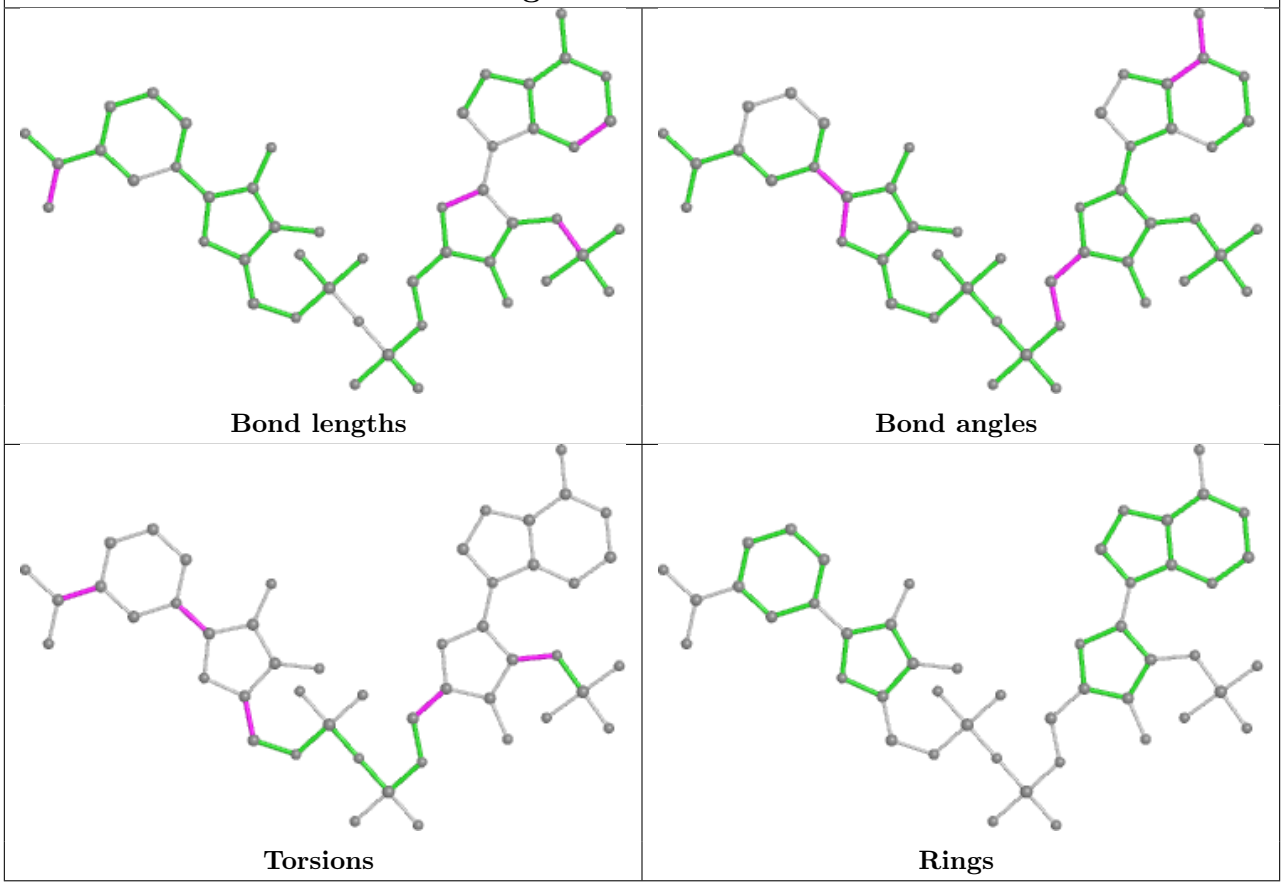


Torsions

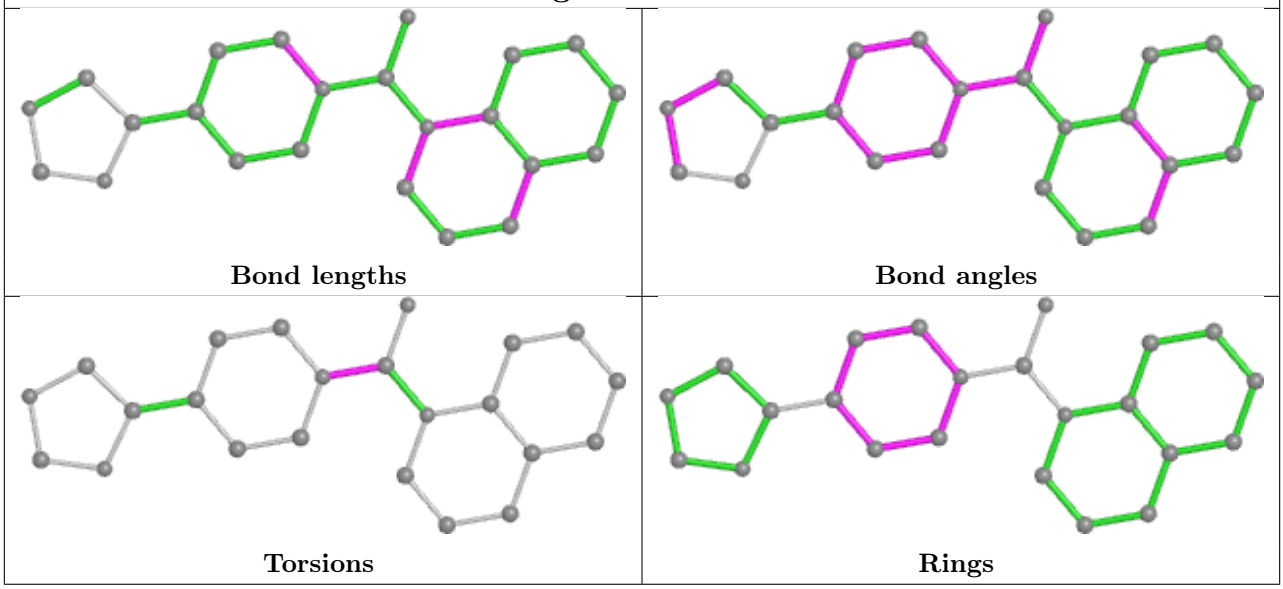


Rings

Ligand NDP C 293



Ligand S05 C 3



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, 95^{th} 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	270/286 (94%)	-0.17	13 (4%)	30	29	10, 23, 72, 100	0
1	B	266/286 (93%)	-0.17	12 (4%)	33	32	10, 25, 65, 113	0
1	C	262/286 (91%)	-0.32	5 (1%)	66	69	8, 20, 49, 62	0
1	D	258/286 (90%)	-0.10	6 (2%)	60	62	13, 29, 64, 87	0
All	All	1056/1144 (92%)	-0.19	36 (3%)	45	45	8, 24, 62, 113	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	LEU	5.9
1	A	229	GLY	5.3
1	B	280	TYR	4.9
1	A	284	TYR	4.3
1	B	263	TRP	4.2
1	D	263	TRP	4.1
1	C	263	TRP	4.1
1	B	285	ASN	3.6
1	C	279	LEU	3.6
1	D	23	LEU	3.4
1	A	263	TRP	3.4
1	B	20	GLN	3.2
1	B	284	TYR	3.2
1	B	262	LEU	3.1
1	A	233	MET	3.0
1	D	266	LEU	2.8
1	D	24	ASN	2.8
1	A	230	ILE	2.8
1	C	20	GLN	2.7
1	A	232	HIS	2.6
1	A	231	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	23	LEU	2.5
1	A	24	ASN	2.5
1	A	279	LEU	2.4
1	B	276	LEU	2.4
1	B	267	LEU	2.4
1	A	280	TYR	2.3
1	B	282	THR	2.3
1	B	261	SER	2.3
1	A	25	GLU	2.3
1	D	61	VAL	2.2
1	C	265	THR	2.1
1	B	23	LEU	2.1
1	A	234	GLN	2.1
1	D	20	GLN	2.0
1	C	280	TYR	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 monosaccharides in this entry.

6.4 Ligands (i)

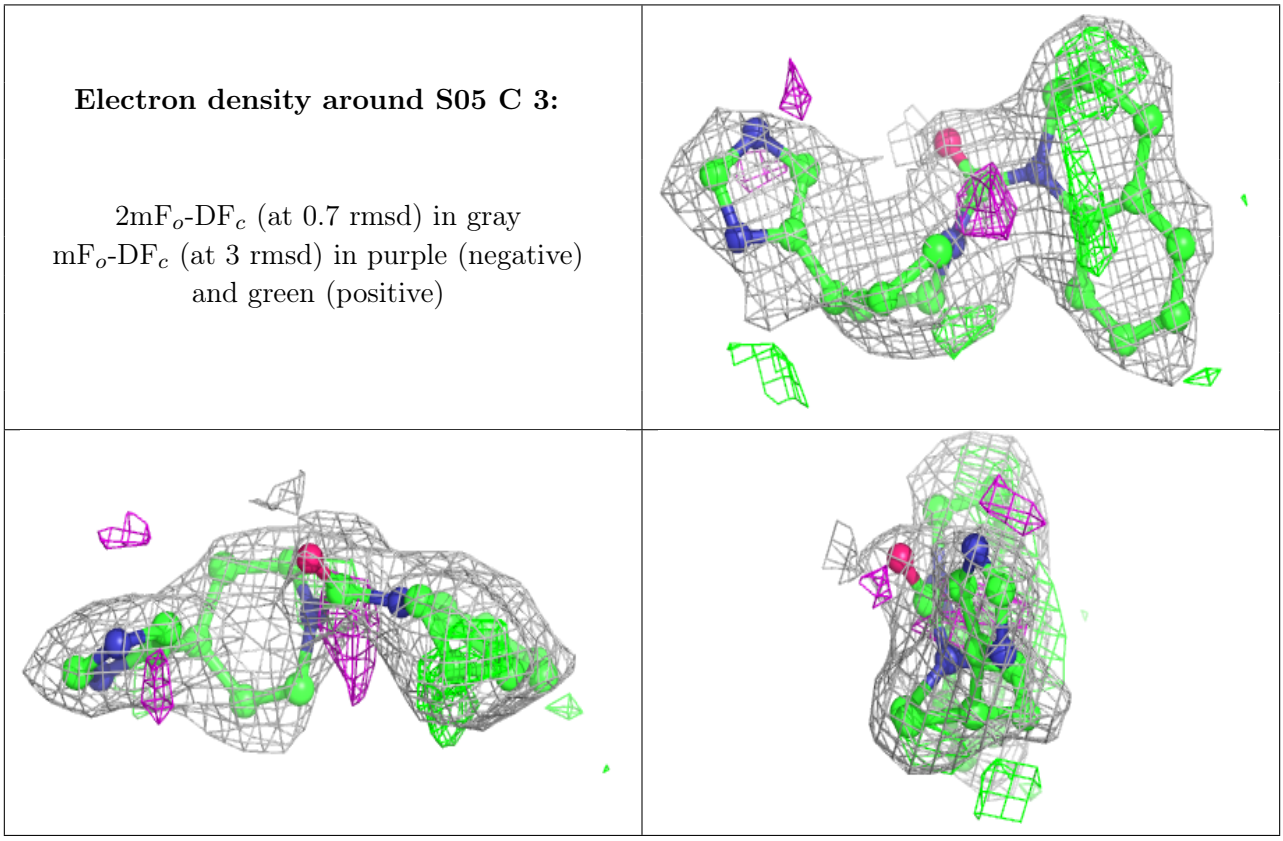
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	S05	C	3	23/23	0.81	0.25	45,50,53,53	0
2	S05	A	1	23/23	0.84	0.27	49,56,64,65	0
2	S05	B	2	23/23	0.85	0.27	55,64,67,67	0
2	S05	D	4	23/23	0.88	0.26	56,60,62,62	0
3	NDP	A	293	48/48	0.98	0.13	15,17,18,19	0
3	NDP	B	293	48/48	0.98	0.13	18,19,22,23	0
3	NDP	D	293	48/48	0.98	0.13	18,23,26,27	0
3	NDP	C	293	48/48	0.99	0.12	15,18,21,22	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.

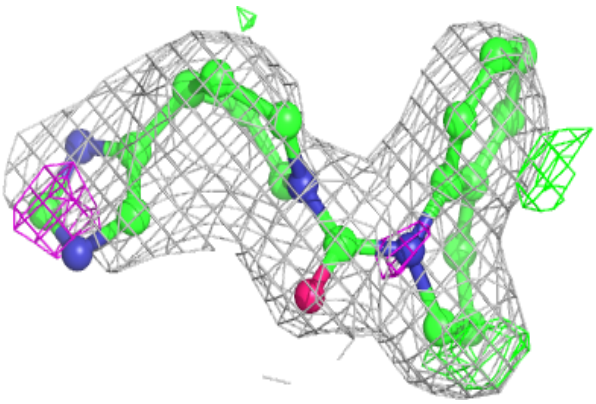
Electron density around S05 C 3:

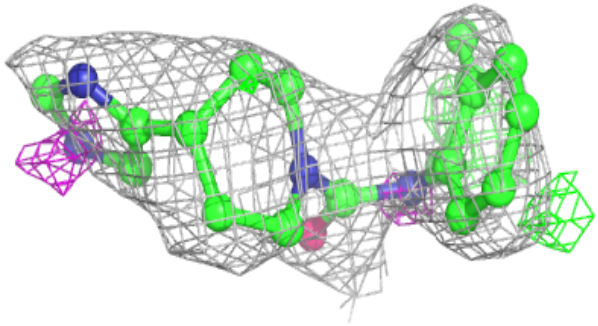
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

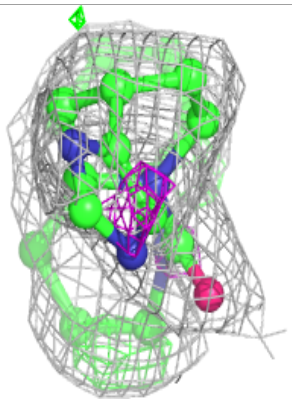


Electron density around S05 A 1:

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

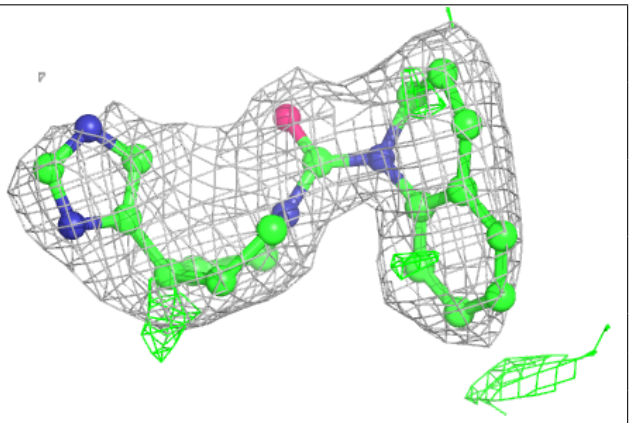


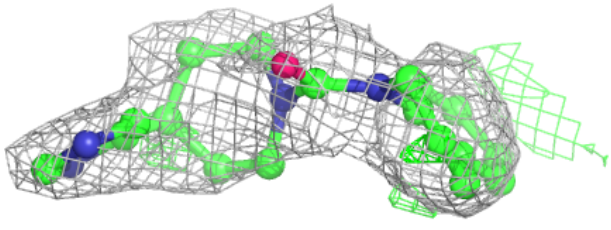


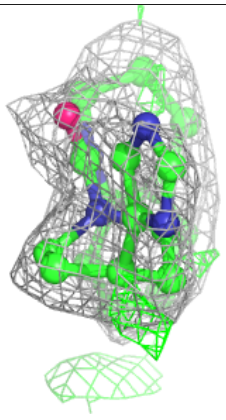


Electron density around S05 B 2:

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

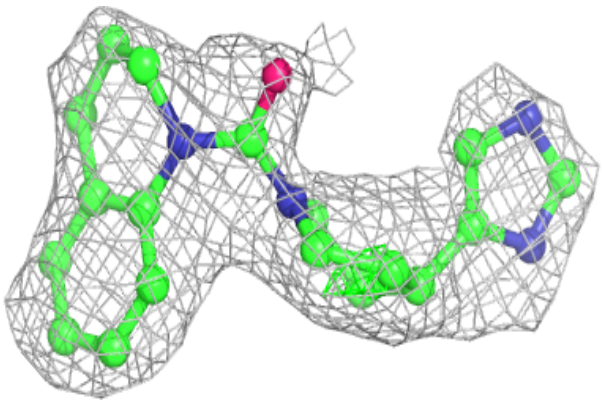


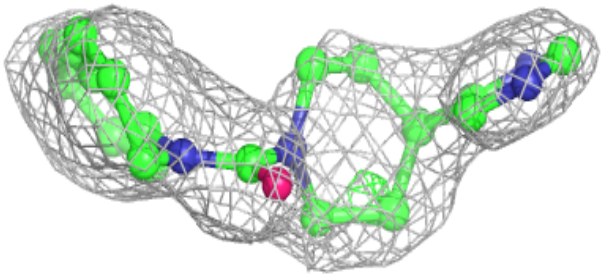


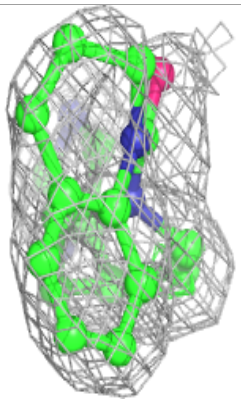


Electron density around S05 D 4:

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

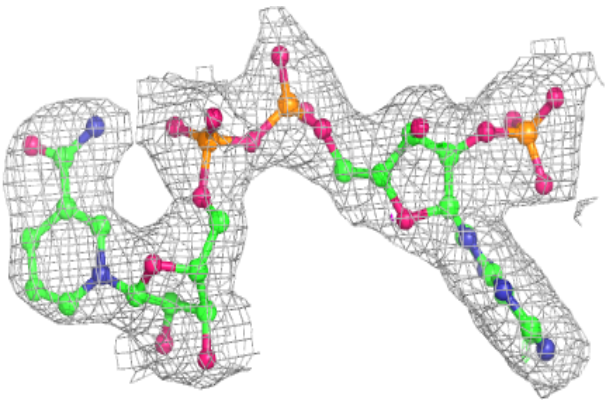


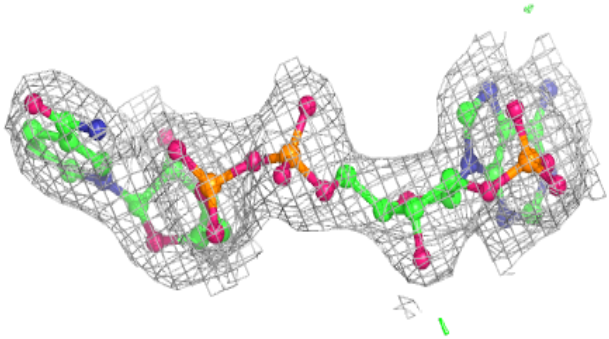


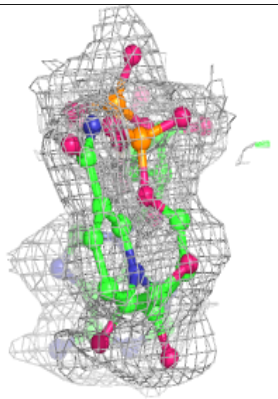


Electron density around NDP A 293:

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

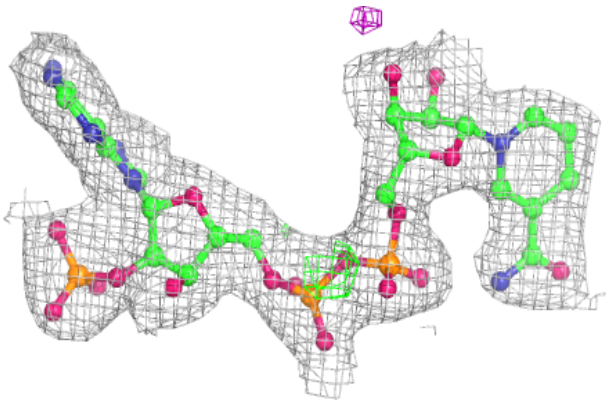


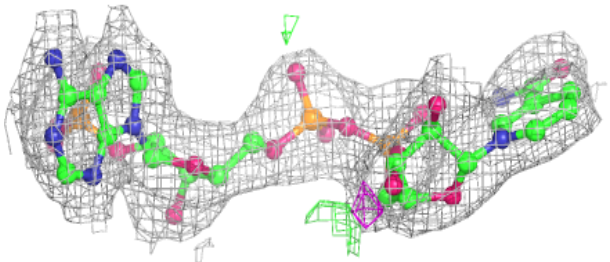


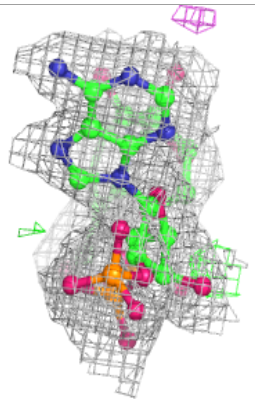


Electron density around NDP B 293:

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

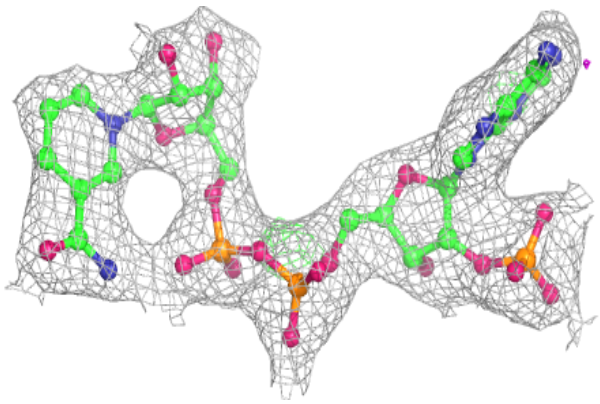


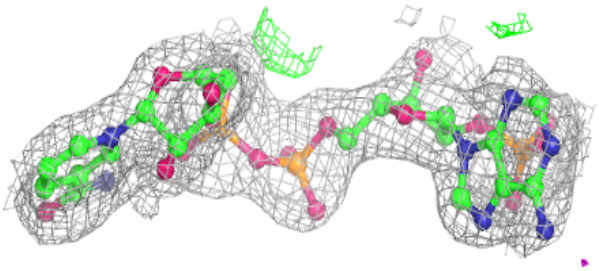


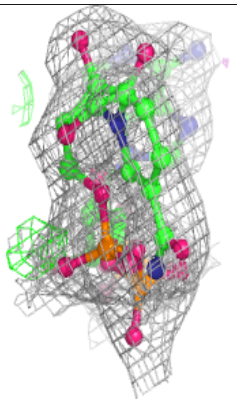


Electron density around NDP D 293:

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

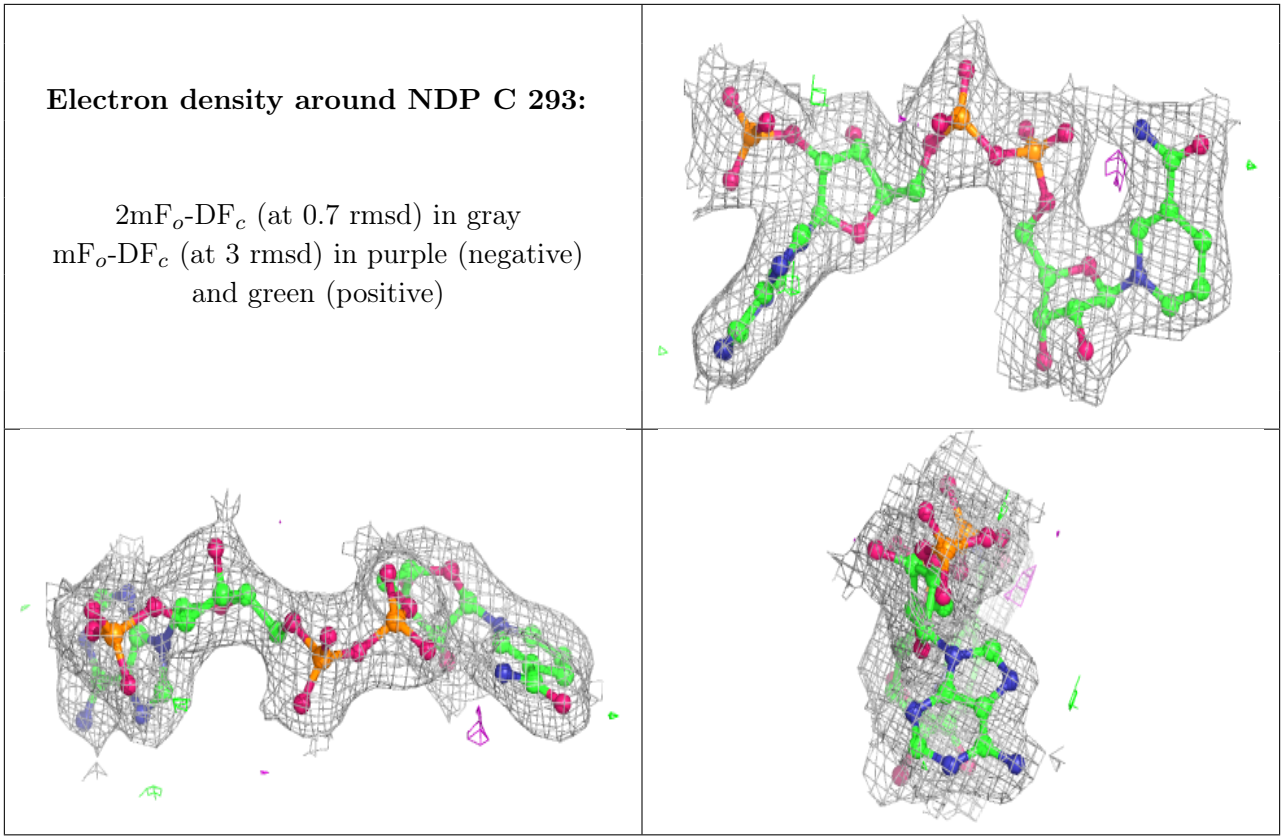






Electron density around NDP C 293:

$2mF_o$-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.