Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 10:51 PM EDT

PDB ID	:	3G49
Title	:	N-(Pyridin-2-yl) Arylsulfonamide Inhibitors of 11b-Hydroxysteroid Dehydrogenase Type 1: Discovery of PF-915275
Authors	:	Pauly, T.A.
Deposited on	:	2009-02-03
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

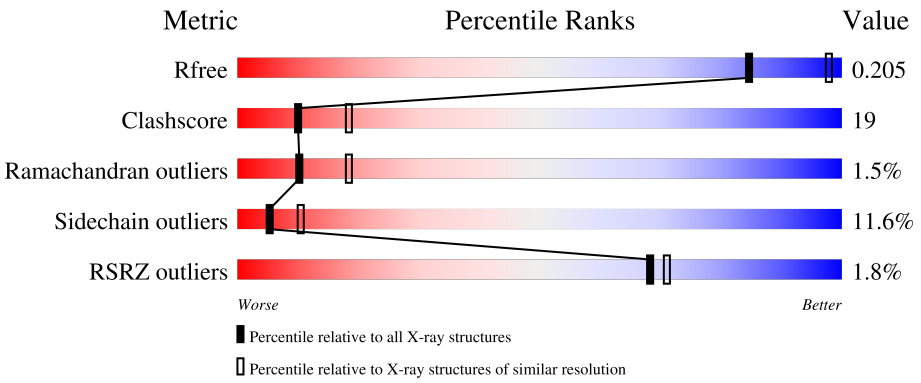
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	277	60% 25% 10% 5%
1	B	277	3% 56% 34% 5% 5%
1	C	277	2% 56% 30% 6% • 5%
1	D	277	2% 55% 31% 9% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	3G4	A	2004	-	-	X	-
3	3G4	D	2007	-	-	X	-

2 Entry composition (i)

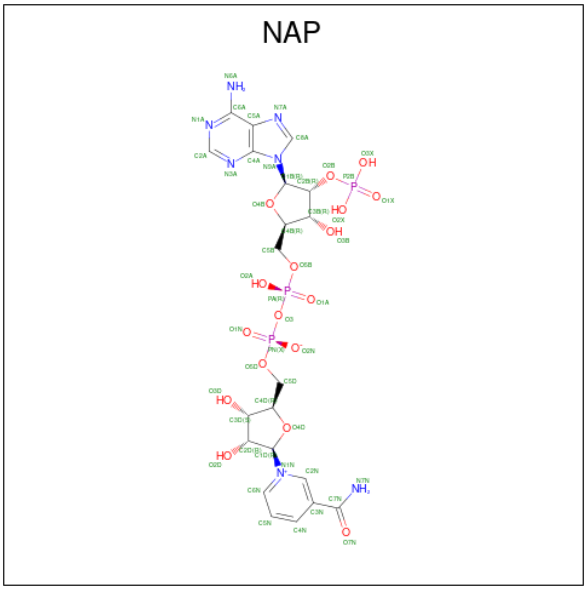
There are 4 unique types of molecules in this entry. The entry contains 8480 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 11-beta-hydroxysteroid dehydrogenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	263	2017	1296	337	369	15	0	0	0
1	B	263	2017	1296	337	369	15	0	0	0
1	C	263	2017	1296	337	369	15	0	0	0
1	D	263	2017	1296	337	369	15	0	0	0

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



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

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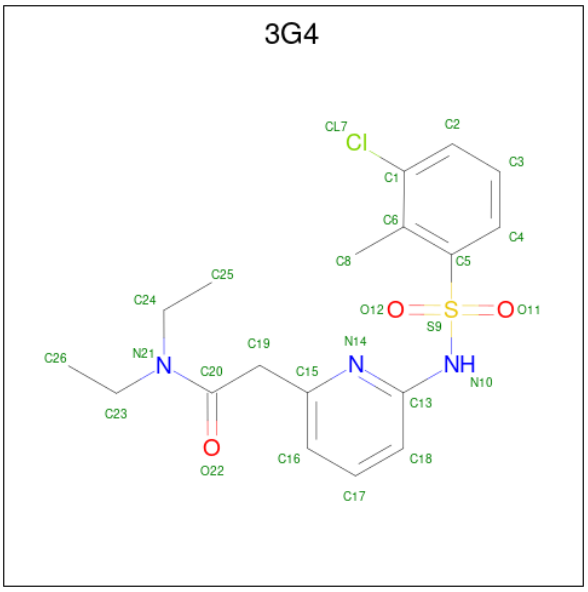
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	48	21	7	17	3	0	0
2	D	1	48	21	7	17	3	0	0

- Molecule 3 is 2-(6-{[(3-chloro-2-methylphenyl)sulfonyl]amino}pyridin-2-yl)-N,N-diethylacetamide (three-letter code: 3G4) (formula: $C_{18}H_{22}ClN_3O_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Cl	N	O	S		
3	A	1	26	18	1	3	3	1	0	0
3	D	1	26	18	1	3	3	1	0	0

- Molecule 4 is water.

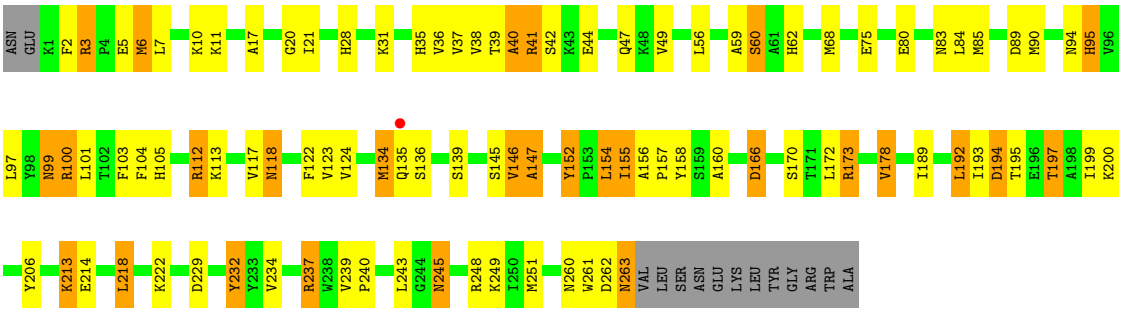
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	46	46	46	0	0
4	B	28	28	28	0	0
4	C	48	48	48	0	0
4	D	46	46	46	0	0

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.

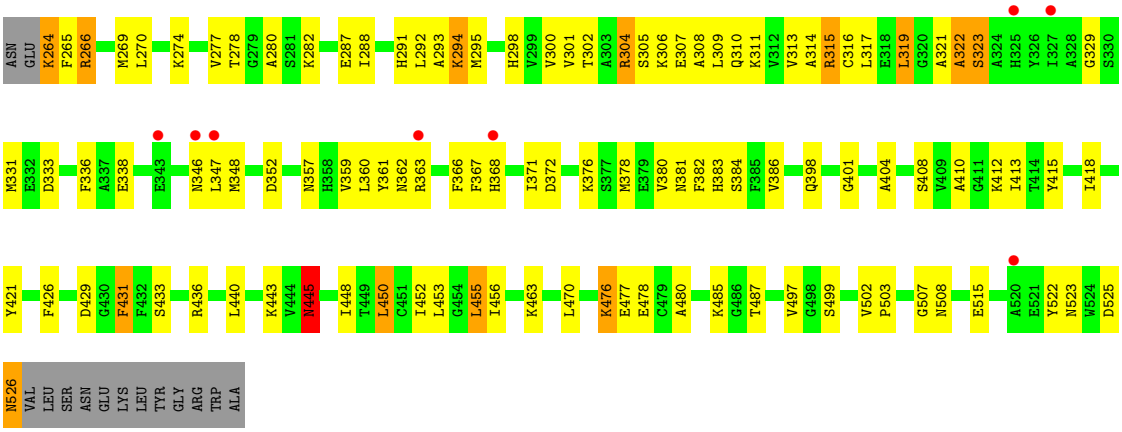
• Molecule 1: 11-beta-hydroxysteroid dehydrogenase 1

Chain A:



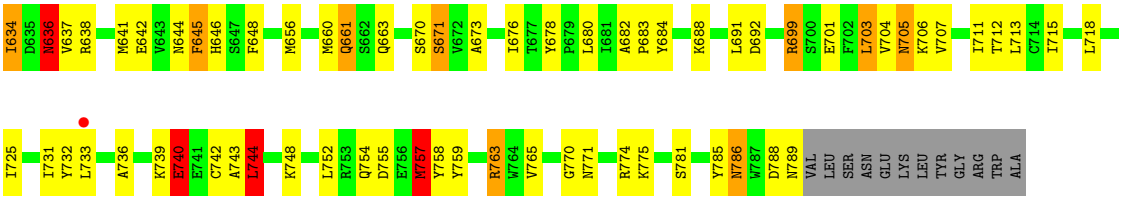
• Molecule 1: 11-beta-hydroxysteroid dehydrogenase 1

Chain B:



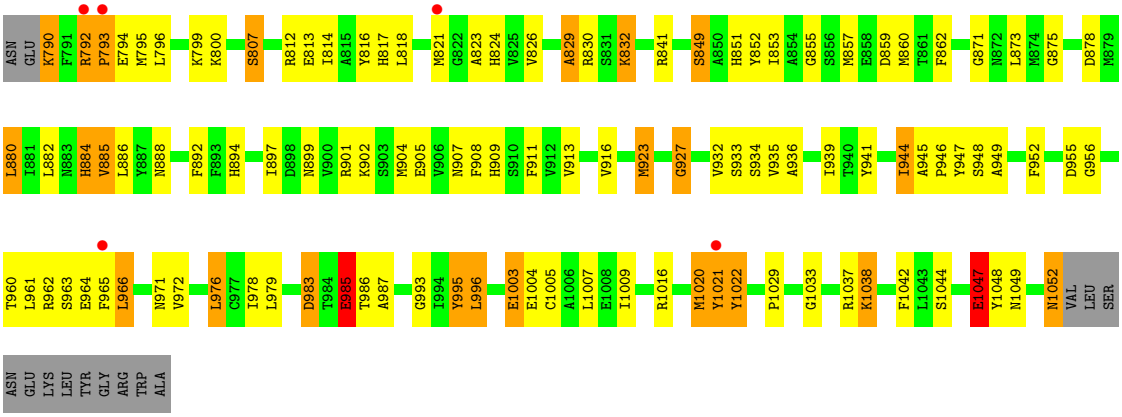
• Molecule 1: 11-beta-hydroxysteroid dehydrogenase 1

Chain C:



- Molecule 1: 11-beta-hydroxysteroid dehydrogenase 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.21Å 83.60Å 179.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.27 – 2.50 41.28 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.8 (41.27-2.50) 91.8 (41.28-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.1.24, CNS	Depositor
R, R_{free}	0.189 , 0.225 0.212 , 0.205	Depositor DCC
R_{free} test set	1935 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.408	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 50.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8480	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3G4, NAP

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	1.58	12/2056 (0.6%)	1.46	20/2777 (0.7%)
1	B	1.55	12/2056 (0.6%)	1.38	13/2777 (0.5%)
1	C	1.57	17/2056 (0.8%)	1.41	18/2777 (0.6%)
1	D	1.58	11/2056 (0.5%)	1.45	25/2777 (0.9%)
All	All	1.57	52/8224 (0.6%)	1.43	76/11108 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	733	LEU	C-O	8.51	1.39	1.23
1	A	158	TYR	CB-CG	-6.82	1.41	1.51
1	A	173	ARG	CD-NE	6.08	1.56	1.46
1	C	701	GLU	CD-OE2	5.96	1.32	1.25
1	D	885	VAL	CB-CG1	5.92	1.65	1.52
1	C	684	TYR	CD2-CE2	-5.91	1.30	1.39
1	B	421	TYR	CD1-CE1	5.87	1.48	1.39
1	B	294	LYS	CB-CG	5.85	1.68	1.52
1	C	624	TYR	CD2-CE2	5.85	1.48	1.39
1	A	232	TYR	CD1-CE1	5.83	1.48	1.39
1	A	117	VAL	CA-CB	5.81	1.67	1.54
1	B	463	LYS	CE-NZ	-5.81	1.34	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	152	TYR	CE2-CZ	5.75	1.46	1.38
1	A	178	VAL	CB-CG2	5.72	1.64	1.52
1	B	421	TYR	CD2-CE2	5.69	1.47	1.39
1	C	781	SER	CB-OG	5.68	1.49	1.42
1	C	763	ARG	NE-CZ	5.67	1.40	1.33
1	C	789	ASN	CB-CG	5.67	1.64	1.51
1	B	346	ASN	C-O	5.65	1.34	1.23
1	A	104	PHE	C-O	5.63	1.34	1.23
1	A	123	VAL	CB-CG1	-5.61	1.41	1.52
1	D	841	ARG	NE-CZ	5.59	1.40	1.33
1	A	42	SER	CA-CB	5.53	1.61	1.52
1	B	445	ASN	CB-CG	5.51	1.63	1.51
1	C	757	MET	SD-CE	-5.49	1.47	1.77
1	D	987	ALA	CA-CB	-5.43	1.41	1.52
1	B	366	PHE	C-O	5.42	1.33	1.23
1	D	816	TYR	CD1-CE1	-5.38	1.31	1.39
1	D	902	LYS	C-O	-5.38	1.13	1.23
1	D	964	GLU	CD-OE1	5.37	1.31	1.25
1	C	624	TYR	CB-CG	5.32	1.59	1.51
1	A	36	VAL	CB-CG1	5.30	1.64	1.52
1	B	367	PHE	CB-CG	-5.27	1.42	1.51
1	C	754	GLN	CD-OE1	5.27	1.35	1.24
1	B	264	LYS	CD-CE	5.25	1.64	1.51
1	B	368	HIS	CB-CG	5.25	1.59	1.50
1	D	993	GLY	C-O	5.24	1.32	1.23
1	A	134	MET	SD-CE	5.22	2.07	1.77
1	B	295	MET	CG-SD	5.22	1.94	1.81
1	D	813	GLU	CD-OE1	5.15	1.31	1.25
1	C	661	GLN	CD-NE2	5.15	1.45	1.32
1	C	765	VAL	CB-CG2	5.13	1.63	1.52
1	C	625	ASN	C-N	5.13	1.45	1.34
1	B	264	LYS	CE-NZ	5.12	1.61	1.49
1	D	830	ARG	CZ-NH2	-5.12	1.26	1.33
1	C	684	TYR	CG-CD1	-5.10	1.32	1.39
1	A	49	VAL	CB-CG2	5.08	1.63	1.52
1	C	736	ALA	CA-CB	-5.08	1.41	1.52
1	D	1021	TYR	C-N	-5.03	1.22	1.34
1	D	1042	PHE	CE1-CZ	5.02	1.46	1.37
1	C	663	GLN	CG-CD	-5.01	1.39	1.51
1	C	758	TYR	CE2-CZ	5.00	1.45	1.38

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	ARG	NE-CZ-NH2	16.72	128.66	120.30
1	D	962	ARG	NE-CZ-NH2	-12.70	113.95	120.30
1	A	173	ARG	NE-CZ-NH1	-12.68	113.96	120.30
1	D	962	ARG	NE-CZ-NH1	12.10	126.35	120.30
1	C	699	ARG	NE-CZ-NH2	9.37	124.99	120.30
1	A	166	ASP	CB-CG-OD2	8.99	126.39	118.30
1	C	703	LEU	CB-CG-CD2	8.91	126.14	111.00
1	A	248	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	B	525	ASP	CB-CG-OD2	8.36	125.82	118.30
1	B	450	LEU	CB-CG-CD2	8.18	124.91	111.00
1	C	692	ASP	CB-CG-OD1	7.71	125.24	118.30
1	A	112	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	C	733	LEU	O-C-N	-7.30	110.79	123.20
1	C	763	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	C	529	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	D	841	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	625	ASN	N-CA-CB	-6.82	98.33	110.60
1	D	955	ASP	CB-CG-OD1	6.54	124.19	118.30
1	D	1021	TYR	CB-CA-C	-6.47	97.45	110.40
1	D	995	TYR	CB-CA-C	-6.47	97.46	110.40
1	A	229	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	455	LEU	CB-CG-CD2	-6.16	100.53	111.00
1	C	615	ASP	CB-CG-OD2	6.16	123.84	118.30
1	C	636	ASN	CB-CA-C	6.14	122.69	110.40
1	D	1021	TYR	CA-C-O	-6.12	107.24	120.10
1	D	1016	ARG	NE-CZ-NH2	6.12	123.36	120.30
1	D	859	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	100	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	B	372	ASP	CB-CG-OD2	5.97	123.68	118.30
1	D	966	LEU	CB-CG-CD1	-5.93	100.92	111.00
1	A	192	LEU	CB-CA-C	-5.88	99.03	110.20
1	D	793	PRO	N-CD-CG	-5.87	94.40	103.20
1	A	263	ASN	CA-C-O	5.83	132.34	120.10
1	D	1016	ARG	CG-CD-NE	5.83	124.04	111.80
1	A	194	ASP	CB-CG-OD2	5.80	123.52	118.30
1	D	904	MET	CG-SD-CE	5.79	109.47	100.20
1	D	812	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	C	601	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	D	878	ASP	CB-CG-OD2	5.71	123.44	118.30
1	C	744	LEU	CA-CB-CG	5.62	128.22	115.30
1	D	830	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	248	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	31	LYS	N-CA-CB	5.52	120.53	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	956	GLY	N-CA-C	-5.50	99.35	113.10
1	A	192	LEU	CA-CB-CG	5.48	127.91	115.30
1	B	515	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	D	1016	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	A	41	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	245	ASN	CB-CA-C	5.34	121.09	110.40
1	B	361	TYR	N-CA-CB	5.33	120.20	110.60
1	D	821	MET	CB-CA-C	5.32	121.05	110.40
1	D	965	PHE	CB-CA-C	5.32	121.03	110.40
1	A	89	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	549	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	431	PHE	CB-CA-C	5.30	121.01	110.40
1	C	645	PHE	CB-CA-C	5.30	121.00	110.40
1	D	985	GLU	CB-CA-C	5.30	120.99	110.40
1	A	135	GLN	CB-CA-C	5.29	120.98	110.40
1	C	527	LYS	CB-CA-C	5.29	120.98	110.40
1	B	378	MET	CG-SD-CE	5.26	108.61	100.20
1	A	56	LEU	N-CA-C	5.23	125.13	111.00
1	B	347	LEU	CB-CG-CD1	5.23	119.89	111.00
1	C	755	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	515	GLU	CG-CD-OE2	5.18	128.66	118.30
1	B	440	LEU	CA-CB-CG	-5.16	103.43	115.30
1	C	740	GLU	N-CA-CB	5.16	119.88	110.60
1	D	923	MET	CG-SD-CE	5.10	108.36	100.20
1	D	1022	TYR	N-CA-C	-5.10	97.24	111.00
1	D	880	LEU	CA-CB-CG	5.08	126.97	115.30
1	C	703	LEU	CB-CG-CD1	-5.07	102.37	111.00
1	D	905	GLU	CB-CA-C	-5.07	100.26	110.40
1	A	218	LEU	CB-CG-CD2	5.07	119.61	111.00
1	B	331	MET	CG-SD-CE	-5.06	92.11	100.20
1	C	625	ASN	CA-C-N	5.05	128.30	117.20
1	A	262	ASP	CB-CA-C	-5.00	100.40	110.40
1	B	362	ASN	CB-CA-C	-5.00	100.40	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	507	GLY	Peptide
1	D	927	GLY	Peptide

5.2 Too-close contacts (i)

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	2017	0	2053	78	0
1	B	2017	0	2050	64	0
1	C	2017	0	2050	84	0
1	D	2017	0	2050	93	0
2	A	48	0	25	5	0
2	B	48	0	25	2	0
2	C	48	0	25	2	0
2	D	48	0	25	2	0
3	A	26	0	22	15	0
3	D	26	0	22	14	0
4	A	46	0	0	2	0
4	B	28	0	0	2	0
4	C	48	0	0	2	0
4	D	46	0	0	5	0
All	All	8480	0	8347	316	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 (316) 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:A:134:MET:SD	1:A:134:MET:CE	2.07	1.41
1:D:985:GLU:HB3	4:D:2239:HOH:O	1.11	1.23
1:B:526:ASN:N	1:B:526:ASN:HD22	1.60	1.00
1:C:527:LYS:C	1:C:527:LYS:HD3	1.83	0.98
1:D:892:PHE:HB2	1:D:894:HIS:HE1	1.28	0.98
1:B:360:LEU:H	1:B:381:ASN:HD21	1.13	0.96
1:D:857:MET:HG3	1:D:884:HIS:CD2	2.02	0.94
1:D:888:ASN:HD21	1:D:899:ASN:HD21	0.96	0.94
1:C:631:HIS:CE1	1:C:633:GLU:OE2	2.22	0.93
1:B:363:ARG:NH1	4:B:2283:HOH:O	2.05	0.90
1:D:888:ASN:ND2	1:D:899:ASN:HD21	1.68	0.90
3:A:2004:3G4:O11	3:A:2004:3G4:H8	1.72	0.88
1:C:594:MET:HG3	1:C:621:HIS:CD2	2.11	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:561:HIS:CE1	1:C:585:ALA:HB1	2.09	0.86
1:D:792:ARG:O	1:D:795:MET:HG3	1.75	0.85
1:A:3:ARG:O	1:A:6:MET:HG3	1.77	0.84
1:B:526:ASN:HD22	1:B:526:ASN:H	1.21	0.84
3:D:2007:3G4:H8	3:D:2007:3G4:O11	1.77	0.84
1:C:594:MET:HG3	1:C:621:HIS:HD2	1.43	0.83
1:C:774:ARG:HG3	1:D:939:ILE:HG22	1.62	0.80
1:C:561:HIS:ND1	1:C:585:ALA:HB3	1.97	0.79
1:D:888:ASN:HD21	1:D:899:ASN:ND2	1.78	0.79
1:A:206:TYR:CD1	3:A:2004:3G4:CL7	2.73	0.78
1:C:631:HIS:HE1	1:C:633:GLU:OE2	1.66	0.78
1:A:95:HIS:ND1	1:A:122:PHE:HE1	1.81	0.78
1:A:206:TYR:CE1	3:A:2004:3G4:CL7	2.74	0.78
1:A:124:VAL:HG22	1:B:371:ILE:HD13	1.66	0.75
1:A:95:HIS:CE1	1:A:122:PHE:CE1	2.74	0.75
1:A:68:MET:HG3	1:A:95:HIS:CD2	2.22	0.75
1:C:561:HIS:ND1	1:C:585:ALA:CB	2.50	0.75
1:A:95:HIS:CE1	1:A:122:PHE:HE1	2.05	0.74
1:B:526:ASN:N	1:B:526:ASN:ND2	2.33	0.74
1:D:892:PHE:HB2	1:D:894:HIS:CE1	2.20	0.74
1:A:95:HIS:HD1	1:A:122:PHE:HE1	1.36	0.73
1:A:11:LYS:HE3	1:A:85:MET:O	1.89	0.72
1:D:995:TYR:CD2	3:D:2007:3G4:CL7	2.79	0.72
1:A:28:HIS:HE1	1:A:214:GLU:O	1.74	0.71
1:D:824:HIS:ND1	1:D:849:SER:HB2	2.05	0.71
1:C:570:GLU:H	1:C:570:GLU:CD	1.94	0.71
1:A:146:VAL:HG11	1:A:152:TYR:OH	1.90	0.70
1:A:160:ALA:HB2	1:B:431:PHE:HB2	1.72	0.70
1:C:786:ASN:C	1:C:786:ASN:HD22	1.94	0.70
1:D:947:TYR:CZ	3:D:2007:3G4:H19	2.25	0.70
1:B:304:ARG:HB2	2:B:2003:NAP:O1X	1.91	0.70
1:C:527:LYS:C	1:C:527:LYS:CD	2.57	0.70
1:C:623:LEU:H	1:C:644:ASN:HD21	1.40	0.70
1:B:523:ASN:OD1	1:B:526:ASN:ND2	2.25	0.69
1:C:638:ARG:HA	1:D:909:HIS:HE1	1.56	0.69
1:A:197:THR:HG21	2:A:2002:NAP:O1A	1.94	0.68
1:D:860:MET:SD	1:D:913:VAL:HG21	2.34	0.68
1:B:526:ASN:H	1:B:526:ASN:ND2	1.89	0.68
1:C:554:HIS:CE1	1:C:744:LEU:HB2	2.29	0.68
1:C:646:HIS:HE1	1:D:901:ARG:HA	1.59	0.68
1:D:1049:ASN:ND2	1:D:1052:ASN:OD1	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1044:SER:HA	1:D:1047:GLU:HG2	1.77	0.67
1:D:817:HIS:CE1	1:D:1007:LEU:HB2	2.30	0.67
1:C:671:SER:HB2	1:C:673:ALA:H	1.59	0.67
1:B:412:LYS:HG2	1:B:452:ILE:HD12	1.78	0.66
1:A:35:HIS:CD2	1:A:59:ALA:HB3	2.31	0.66
1:D:857:MET:HG3	1:D:884:HIS:NE2	2.12	0.65
1:B:410:ALA:HB2	1:B:415:TYR:CD1	2.32	0.65
1:C:732:TYR:CE2	1:D:1047:GLU:HB3	2.31	0.65
1:A:206:TYR:CG	3:A:2004:3G4:CL7	2.87	0.65
1:D:944:ILE:HD13	3:D:2007:3G4:H3	1.78	0.64
1:C:561:HIS:CE1	1:C:585:ALA:CB	2.79	0.64
1:C:561:HIS:HE1	1:C:585:ALA:HB1	1.62	0.64
1:A:239:VAL:N	1:A:240:PRO:CD	2.61	0.64
1:B:300:VAL:HG23	1:B:348:MET:SD	2.37	0.64
1:A:194:ASP:HA	1:A:199:ILE:HD11	1.78	0.63
1:C:625:ASN:HD21	1:C:636:ASN:ND2	1.96	0.63
1:D:886:LEU:H	1:D:907:ASN:HD21	1.47	0.62
1:D:947:TYR:CE2	3:D:2007:3G4:H19	2.35	0.62
1:A:206:TYR:CZ	3:A:2004:3G4:CL7	2.90	0.62
1:B:313:VAL:O	1:B:314:ALA:C	2.38	0.62
1:D:1005:CYS:O	1:D:1009:ILE:HG13	2.00	0.61
1:D:851:HIS:CD2	1:D:873:LEU:HD22	2.35	0.61
1:D:857:MET:HG3	1:D:884:HIS:HD2	1.62	0.61
1:D:884:HIS:CE1	1:D:911:PHE:CE1	2.88	0.61
1:C:625:ASN:HD21	1:C:636:ASN:HD21	1.49	0.61
1:D:1044:SER:HA	1:D:1047:GLU:CG	2.31	0.61
1:C:562:VAL:O	1:C:562:VAL:HG23	2.01	0.60
1:C:570:GLU:N	1:C:570:GLU:OE1	2.35	0.60
1:A:103:PHE:HB2	1:A:105:HIS:HE1	1.67	0.60
3:A:2004:3G4:H26B	3:A:2004:3G4:C15	2.31	0.60
1:B:278:THR:O	1:B:357:ASN:HB3	2.02	0.60
1:C:699:ARG:O	1:C:703:LEU:HG	2.02	0.59
1:D:1020:MET:HE1	1:D:1022:TYR:HB2	1.83	0.59
3:D:2007:3G4:H19	3:D:2007:3G4:H26A	1.84	0.59
1:A:146:VAL:HG12	1:A:152:TYR:HE1	1.67	0.59
3:A:2004:3G4:H18	3:A:2004:3G4:C5	2.33	0.59
1:D:1021:TYR:CG	1:D:1029:PRO:HB3	2.37	0.59
1:C:699:ARG:NH2	4:C:2393:HOH:O	2.36	0.58
1:B:270:LEU:HD23	1:B:292:LEU:HD22	1.86	0.58
1:B:497:VAL:HG21	1:B:502:VAL:HG12	1.86	0.58
1:D:884:HIS:ND1	1:D:911:PHE:HE1	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TYR:HB3	1:B:522:TYR:OH	2.02	0.58
1:B:360:LEU:N	1:B:381:ASN:HD21	1.95	0.57
3:D:2007:3G4:H23A	3:D:2007:3G4:C15	2.33	0.57
1:C:636:ASN:C	1:C:636:ASN:HD22	2.07	0.57
1:D:884:HIS:HD1	1:D:911:PHE:HE1	1.52	0.57
1:D:935:VAL:HG23	1:D:979:LEU:O	2.03	0.57
1:B:293:ALA:HB2	1:B:316:CYS:HB3	1.85	0.57
1:B:523:ASN:CG	1:B:526:ASN:HD21	2.08	0.57
1:B:380:VAL:O	1:B:384:SER:OG	2.23	0.57
1:B:412:LYS:NZ	1:B:429:ASP:OD2	2.33	0.57
1:B:265:PHE:CD1	1:B:269:MET:CE	2.88	0.57
1:A:156:ALA:HB3	1:A:157:PRO:HD3	1.86	0.56
1:C:627:LEU:N	1:C:627:LEU:HD23	2.18	0.56
1:D:884:HIS:CE1	1:D:911:PHE:HE1	2.23	0.56
1:B:523:ASN:CG	1:B:526:ASN:ND2	2.60	0.56
1:C:774:ARG:HG3	1:D:939:ILE:CG2	2.32	0.56
1:C:616:MET:SD	1:C:618:ILE:HD11	2.46	0.56
1:D:945:ALA:N	1:D:946:PRO:CD	2.68	0.55
1:A:118:ASN:N	1:A:118:ASN:ND2	2.54	0.55
1:D:995:TYR:C	1:D:996:LEU:HD23	2.26	0.55
1:D:960:THR:O	1:D:961:LEU:C	2.43	0.55
1:D:892:PHE:CB	1:D:894:HIS:HE1	2.12	0.55
1:D:936:ALA:HA	1:D:939:ILE:O	2.07	0.55
1:A:195:THR:HA	1:A:213:LYS:HE2	1.88	0.55
1:A:206:TYR:CD2	3:A:2004:3G4:CL7	2.97	0.55
1:A:118:ASN:N	1:A:118:ASN:HD22	2.05	0.54
1:C:551:ILE:HG13	1:C:743:ALA:HB1	1.87	0.54
1:D:1005:CYS:HB2	1:D:1022:TYR:CE2	2.42	0.54
3:D:2007:3G4:H23A	3:D:2007:3G4:C16	2.37	0.54
1:A:166:ASP:O	1:A:170:SER:HB2	2.07	0.54
1:C:532:MET:O	1:C:536:LYS:HE3	2.07	0.54
1:D:947:TYR:CZ	3:D:2007:3G4:C19	2.90	0.54
1:B:436:ARG:NH1	1:B:448:ILE:O	2.41	0.54
1:B:329:GLY:HA3	1:B:336:PHE:CZ	2.42	0.54
1:A:95:HIS:ND1	1:A:122:PHE:CE1	2.68	0.54
1:C:625:ASN:O	1:C:626:ARG:C	2.46	0.54
1:A:39:THR:O	1:A:40:ALA:HB2	2.09	0.53
1:B:429:ASP:O	1:B:433:SER:HB2	2.07	0.53
1:A:62:HIS:ND1	1:A:84:LEU:HD22	2.24	0.53
1:D:1021:TYR:CD1	1:D:1029:PRO:HB3	2.44	0.53
1:D:855:GLY:HA3	1:D:862:PHE:CE1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:MET:HA	1:A:139:SER:O	2.08	0.52
1:C:554:HIS:HE1	1:C:740:GLU:O	1.92	0.52
1:D:995:TYR:CG	3:D:2007:3G4:CL7	2.99	0.52
1:A:260:ASN:HB2	1:B:470:LEU:HD11	1.92	0.52
1:D:852:TYR:CD1	1:D:852:TYR:C	2.81	0.52
1:A:35:HIS:CD2	1:A:59:ALA:CB	2.93	0.52
1:D:944:ILE:HG13	1:D:944:ILE:O	2.09	0.52
1:A:2:PHE:CD2	1:A:222:LYS:HE2	2.45	0.52
1:C:527:LYS:HD3	1:C:528:PHE:N	2.23	0.52
4:C:2072:HOH:O	1:D:897:ILE:HD11	2.10	0.51
1:B:359:VAL:CG1	2:B:2003:NAP:H3D	2.41	0.51
1:C:594:MET:CG	1:C:621:HIS:CD2	2.90	0.51
1:A:206:TYR:CE2	3:A:2004:3G4:CL7	3.01	0.51
1:D:985:GLU:CB	4:D:2239:HOH:O	1.98	0.51
1:B:502:VAL:N	1:B:503:PRO:HD2	2.26	0.51
1:D:985:GLU:HA	4:D:2239:HOH:O	2.10	0.51
1:A:146:VAL:HG12	1:A:147:ALA:N	2.24	0.51
1:C:634:ILE:HD12	1:D:916:VAL:HG21	1.93	0.51
1:D:880:LEU:HD11	1:D:882:LEU:HD21	1.92	0.51
1:D:985:GLU:CA	4:D:2239:HOH:O	2.49	0.51
1:A:44:GLU:CD	1:A:44:GLU:H	2.15	0.50
1:C:634:ILE:CD1	1:D:916:VAL:HG21	2.42	0.50
3:A:2004:3G4:C5	3:A:2004:3G4:C18	2.89	0.50
1:B:291:HIS:HE1	1:B:477:GLU:O	1.94	0.50
1:D:888:ASN:ND2	1:D:899:ASN:ND2	2.49	0.50
1:C:786:ASN:HD21	1:C:788:ASP:HB2	1.76	0.50
1:B:485:LYS:HD2	4:B:2278:HOH:O	2.12	0.50
1:A:68:MET:HG3	1:A:95:HIS:NE2	2.27	0.49
1:B:308:ALA:HA	1:B:311:LYS:HE2	1.94	0.49
1:C:621:HIS:HD1	1:C:648:PHE:HE1	1.58	0.49
1:C:671:SER:HB2	1:C:673:ALA:N	2.27	0.49
1:A:100:ARG:HD3	4:A:2308:HOH:O	2.11	0.49
1:A:263:ASN:ND2	4:A:2235:HOH:O	2.42	0.49
1:B:386:VAL:HG13	1:B:431:PHE:CZ	2.47	0.49
1:A:11:LYS:HD3	1:A:85:MET:O	2.13	0.49
1:A:35:HIS:ND1	1:A:60:SER:OG	2.46	0.49
1:C:543:ALA:HB3	1:C:564:VAL:HB	1.94	0.49
1:C:676:ILE:HG22	1:D:1037:ARG:HG3	1.94	0.49
1:A:166:ASP:O	1:A:170:SER:CB	2.60	0.49
1:B:502:VAL:N	1:B:503:PRO:CD	2.76	0.49
1:C:617:LEU:HD21	1:C:619:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:786:ASN:HB2	1:D:996:LEU:HD11	1.94	0.48
1:A:194:ASP:OD1	1:A:213:LYS:HG2	2.14	0.48
1:B:380:VAL:HG12	1:B:381:ASN:HD22	1.77	0.48
1:A:44:GLU:HA	1:A:47:GLN:NE2	2.29	0.48
1:C:621:HIS:CE1	1:C:648:PHE:CE1	3.02	0.48
1:A:7:LEU:HD11	1:A:90:MET:CE	2.44	0.48
1:B:360:LEU:H	1:B:381:ASN:ND2	1.96	0.48
1:C:682:ALA:N	1:C:683:PRO:HD2	2.28	0.48
1:B:277:VAL:HG12	1:B:280:ALA:HB2	1.96	0.48
1:A:21:ILE:HD11	1:A:193:ILE:HG21	1.95	0.48
1:A:97:LEU:H	1:A:118:ASN:ND2	2.11	0.48
1:D:1052:ASN:N	1:D:1052:ASN:ND2	2.61	0.48
1:B:410:ALA:HB2	1:B:415:TYR:HD1	1.76	0.47
1:B:301:VAL:HG23	1:B:309:LEU:HD22	1.96	0.47
1:D:948:SER:O	1:D:949:ALA:C	2.49	0.47
1:B:265:PHE:CD1	1:B:269:MET:HE1	2.49	0.47
1:B:280:ALA:HB3	1:B:301:VAL:HB	1.96	0.47
1:D:996:LEU:HD23	1:D:996:LEU:N	2.30	0.47
1:C:757:MET:HE1	1:C:759:TYR:HB2	1.96	0.47
1:A:146:VAL:HG22	1:A:243:LEU:HD11	1.97	0.47
1:C:713:LEU:HD13	1:C:715:ILE:HD11	1.97	0.47
1:D:829:ALA:O	1:D:855:GLY:N	2.44	0.47
1:D:886:LEU:N	1:D:907:ASN:HD21	2.09	0.47
1:A:7:LEU:HD11	1:A:90:MET:HE3	1.97	0.47
1:B:266:ARG:O	1:B:269:MET:HE2	2.15	0.47
1:B:270:LEU:HD23	1:B:292:LEU:CD2	2.45	0.46
1:C:527:LYS:HD3	1:C:527:LYS:O	2.12	0.46
1:C:627:LEU:N	1:C:627:LEU:CD2	2.78	0.46
1:D:976:LEU:HD13	1:D:978:ILE:HD11	1.97	0.46
1:A:6:MET:O	1:A:7:LEU:HD22	2.15	0.46
1:C:621:HIS:ND1	1:C:648:PHE:HE1	2.13	0.46
1:D:1021:TYR:OH	1:D:1033:GLY:CA	2.63	0.46
1:B:333:ASP:OD1	1:B:333:ASP:C	2.52	0.46
1:C:527:LYS:CD	1:C:527:LYS:O	2.64	0.46
1:C:682:ALA:N	1:C:683:PRO:CD	2.79	0.46
1:A:37:VAL:HG23	1:A:85:MET:SD	2.56	0.46
1:B:382:PHE:O	1:B:383:HIS:C	2.54	0.46
1:C:538:VAL:HG22	1:C:616:MET:HB3	1.96	0.46
1:A:97:LEU:H	1:A:118:ASN:HD21	1.63	0.46
1:B:321:ALA:C	1:B:323:SER:N	2.69	0.46
1:C:699:ARG:NH1	1:C:711:ILE:HG22	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:731:ILE:N	1:C:731:ILE:HD12	2.31	0.46
1:D:792:ARG:HD2	1:D:793:PRO:HD2	1.97	0.46
1:B:497:VAL:HG23	1:B:497:VAL:O	2.15	0.45
1:C:636:ASN:ND2	1:C:636:ASN:C	2.70	0.45
2:A:2002:NAP:H2D	3:A:2004:3G4:H19A	1.97	0.45
1:B:315:ARG:O	1:B:319:LEU:HG	2.16	0.45
1:D:908:PHE:O	1:D:911:PHE:HB2	2.15	0.45
1:A:17:ALA:HB3	1:A:38:VAL:HB	1.97	0.45
1:B:455:LEU:O	1:B:456:ILE:HD13	2.15	0.45
1:A:7:LEU:HA	1:A:10:LYS:HG3	1.97	0.45
1:B:497:VAL:HG21	1:B:502:VAL:CG1	2.46	0.45
1:A:197:THR:CG2	2:A:2002:NAP:O1A	2.63	0.45
1:A:199:ILE:O	1:A:200:LYS:C	2.55	0.45
1:A:239:VAL:N	1:A:240:PRO:HD2	2.32	0.45
1:D:944:ILE:CD1	3:D:2007:3G4:H3	2.44	0.45
1:A:41:ARG:HB2	2:A:2002:NAP:O1X	2.17	0.45
1:C:568:SER:HB2	1:C:571:ALA:HB3	2.00	0.45
1:C:732:TYR:CE2	1:D:1047:GLU:CB	2.99	0.44
1:D:884:HIS:HE1	1:D:911:PHE:CD1	2.35	0.44
1:C:562:VAL:O	1:C:562:VAL:CG2	2.64	0.44
1:C:705:ASN:HB3	1:C:707:VAL:HG23	1.98	0.44
1:B:404:ALA:HB2	1:B:487:THR:HG21	1.98	0.44
1:B:410:ALA:HA	1:B:413:ILE:O	2.17	0.44
1:D:790:LYS:HE3	1:D:792:ARG:HH22	1.82	0.44
1:B:352:ASP:O	1:B:401:GLY:HA3	2.18	0.44
1:C:688:LYS:O	1:C:691:LEU:HB2	2.18	0.44
1:C:678:TYR:HB3	1:D:1048:TYR:OH	2.18	0.44
1:C:528:PHE:HB2	1:C:752:LEU:HD11	2.00	0.44
1:D:927:GLY:O	1:D:972:VAL:HA	2.18	0.43
1:D:933:SER:OG	1:D:934:SER:N	2.51	0.43
1:D:892:PHE:CB	1:D:894:HIS:CE1	2.96	0.43
1:C:786:ASN:C	1:C:786:ASN:ND2	2.66	0.43
1:D:935:VAL:HB	3:D:2007:3G4:O12	2.18	0.43
1:A:145:SER:HB3	3:A:2004:3G4:HN10	1.84	0.43
1:C:631:HIS:ND1	1:C:633:GLU:OE2	2.49	0.43
1:C:637:VAL:HA	1:C:683:PRO:HB3	2.00	0.43
1:D:799:LYS:O	1:D:823:ALA:HB1	2.19	0.43
1:D:851:HIS:HD2	1:D:873:LEU:HD22	1.81	0.43
1:A:11:LYS:CE	1:A:85:MET:O	2.63	0.43
1:A:251:MET:HB3	1:B:413:ILE:HD13	1.99	0.43
1:D:853:ILE:HD13	1:D:853:ILE:HG21	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:832:LYS:H	1:D:832:LYS:CD	2.32	0.43
1:A:5:GLU:CD	1:A:5:GLU:H	2.21	0.43
1:A:172:LEU:O	1:A:173:ARG:C	2.53	0.43
1:A:189:ILE:HB	1:A:232:TYR:CD1	2.54	0.43
3:A:2004:3G4:H25A	3:A:2004:3G4:H26A	2.00	0.43
2:D:2001:NAP:H2A	4:D:2017:HOH:O	2.19	0.43
1:D:947:TYR:OH	3:D:2007:3G4:N14	2.45	0.43
1:B:321:ALA:C	1:B:323:SER:H	2.22	0.42
1:D:1038:LYS:HB3	1:D:1038:LYS:HE2	1.86	0.42
1:C:563:VAL:HG11	1:C:607:ALA:HB2	2.01	0.42
1:A:62:HIS:N	1:A:62:HIS:CD2	2.87	0.42
1:C:671:SER:HB3	2:C:2000:NAP:H5N	2.00	0.42
1:C:770:GLY:O	1:C:771:ASN:C	2.57	0.42
1:D:817:HIS:NE2	1:D:1003:GLU:HG2	2.34	0.42
3:D:2007:3G4:H25A	3:D:2007:3G4:H23	1.76	0.42
1:A:237:ARG:O	1:A:237:ARG:HG3	2.19	0.42
1:D:832:LYS:HB2	1:D:832:LYS:HE2	1.94	0.42
1:A:154:LEU:C	1:A:155:ILE:HG23	2.40	0.42
1:C:670:SER:O	2:C:2000:NAP:H6N	2.20	0.42
1:B:445:ASN:H	1:B:445:ASN:HD22	1.67	0.42
1:C:550:GLU:HG3	1:C:739:LYS:HG3	2.01	0.42
1:C:571:ALA:O	1:C:575:VAL:HG23	2.19	0.42
1:D:790:LYS:CE	1:D:792:ARG:HH22	2.33	0.42
1:B:298:HIS:CE1	1:B:322:ALA:HB1	2.55	0.41
1:D:814:ILE:O	1:D:818:LEU:HG	2.20	0.41
1:A:3:ARG:O	1:A:6:MET:CG	2.60	0.41
1:A:173:ARG:HH11	1:A:173:ARG:HD3	1.50	0.41
3:A:2004:3G4:O11	3:A:2004:3G4:C8	2.56	0.41
1:C:528:PHE:CD1	1:C:748:LYS:HE2	2.55	0.41
1:D:826:VAL:HA	1:D:851:HIS:O	2.20	0.41
1:B:288:ILE:HG13	1:B:480:ALA:HB1	2.02	0.41
1:B:415:TYR:HB2	1:B:418:ILE:HD11	2.03	0.41
1:D:807:SER:OG	2:D:2001:NAP:O3B	2.29	0.41
1:D:871:GLY:O	1:D:875:GLY:N	2.53	0.41
1:B:287:GLU:HG3	1:B:476:LYS:HB2	2.03	0.41
1:C:638:ARG:O	1:C:642:GLU:HG2	2.21	0.41
1:A:44:GLU:HA	1:A:47:GLN:HE21	1.85	0.41
3:A:2004:3G4:H23	3:A:2004:3G4:H19	1.91	0.41
1:C:529:ARG:HH11	1:C:529:ARG:HG3	1.86	0.41
1:C:625:ASN:ND2	1:C:636:ASN:ND2	2.64	0.41
1:C:641:MET:SD	1:C:645:PHE:CD1	3.14	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:885:VAL:HG21	1:D:947:TYR:HE2	1.86	0.41
1:D:944:ILE:O	1:D:944:ILE:CG1	2.66	0.41
1:A:94:ASN:O	2:A:2002:NAP:H4D	2.21	0.40
1:A:154:LEU:O	1:A:155:ILE:HG23	2.21	0.40
1:A:178:VAL:HG11	1:A:261:TRP:CZ3	2.56	0.40
1:C:670:SER:HB3	1:C:715:ILE:HD13	2.03	0.40
1:C:785:TYR:OH	1:D:941:TYR:HB3	2.21	0.40
1:D:882:LEU:O	1:D:932:VAL:HG23	2.21	0.40
1:A:99:ASN:HD22	1:A:99:ASN:HA	1.66	0.40
1:A:234:VAL:HG21	1:A:239:VAL:HG12	2.03	0.40
1:B:293:ALA:O	1:B:294:LYS:C	2.59	0.40
1:B:317:LEU:HA	1:B:317:LEU:HD23	1.81	0.40
1:C:623:LEU:H	1:C:644:ASN:ND2	2.12	0.40
1:D:1004:GLU:HB3	1:D:1022:TYR:OH	2.21	0.40
1:C:533:LEU:O	1:C:536:LYS:HB2	2.21	0.40
1:C:565:THR:O	1:C:566:ALA:HB2	2.21	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	261/277 (94%)	233 (89%)	23 (9%)	5 (2%)	8 13
1	B	261/277 (94%)	228 (87%)	29 (11%)	4 (2%)	10 18
1	C	261/277 (94%)	238 (91%)	20 (8%)	3 (1%)	14 26
1	D	261/277 (94%)	244 (94%)	13 (5%)	4 (2%)	10 18
All	All	1044/1108 (94%)	943 (90%)	85 (8%)	16 (2%)	10 18

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	LEU
1	B	322	ALA
1	A	20	GLY
1	C	742	CYS
1	B	319	LEU
1	C	680	LEU
1	B	323	SER
1	D	983	ASP
1	D	985	GLU
1	A	147	ALA
1	C	633	GLU
1	A	40	ALA
1	D	829	ALA
1	D	1047	GLU
1	A	155	ILE
1	B	508	ASN

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	214/226 (95%)	193 (90%)	21 (10%)	8 15
1	B	214/226 (95%)	190 (89%)	24 (11%)	6 11
1	C	214/226 (95%)	185 (86%)	29 (14%)	3 7
1	D	214/226 (95%)	189 (88%)	25 (12%)	5 10
All	All	856/904 (95%)	757 (88%)	99 (12%)	5 10

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	6	MET
1	A	60	SER
1	A	75	GLU
1	A	80	GLU
1	A	83	ASN

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Mol	Chain	Res	Type
1	A	95	HIS
1	A	99	ASN
1	A	101	LEU
1	A	112	ARG
1	A	113	LYS
1	A	118	ASN
1	A	136	SER
1	A	146	VAL
1	A	192	LEU
1	A	197	THR
1	A	213	LYS
1	A	218	LEU
1	A	237	ARG
1	A	245	ASN
1	A	249	LYS
1	B	264	LYS
1	B	266	ARG
1	B	274	LYS
1	B	282	LYS
1	B	302	THR
1	B	304	ARG
1	B	305	SER
1	B	306	LYS
1	B	307	GLU
1	B	310	GLN
1	B	315	ARG
1	B	338	GLU
1	B	376	LYS
1	B	398	GLN
1	B	408	SER
1	B	426	PHE
1	B	443	LYS
1	B	445	ASN
1	B	450	LEU
1	B	453	LEU
1	B	476	LYS
1	B	478	GLU
1	B	499	SER
1	B	526	ASN
1	C	527	LYS
1	C	529	ARG
1	C	568	SER

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Mol	Chain	Res	Type
1	C	569	LYS
1	C	570	GLU
1	C	621	HIS
1	C	622	VAL
1	C	623	LEU
1	C	626	ARG
1	C	627	LEU
1	C	631	HIS
1	C	634	ILE
1	C	636	ASN
1	C	656	MET
1	C	660	MET
1	C	661	GLN
1	C	671	SER
1	C	704	VAL
1	C	705	ASN
1	C	706	LYS
1	C	712	THR
1	C	718	LEU
1	C	725	ILE
1	C	740	GLU
1	C	744	LEU
1	C	757	MET
1	C	763	ARG
1	C	775	LYS
1	C	786	ASN
1	D	790	LYS
1	D	792	ARG
1	D	794	GLU
1	D	796	LEU
1	D	800	LYS
1	D	807	SER
1	D	832	LYS
1	D	849	SER
1	D	884	HIS
1	D	923	MET
1	D	944	ILE
1	D	952	PHE
1	D	963	SER
1	D	966	LEU
1	D	971	ASN
1	D	976	LEU

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Mol	Chain	Res	Type
1	D	983	ASP
1	D	985	GLU
1	D	986	THR
1	D	996	LEU
1	D	1003	GLU
1	D	1020	MET
1	D	1038	LYS
1	D	1047	GLU
1	D	1052	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	HIS
1	A	47	GLN
1	A	62	HIS
1	A	83	ASN
1	A	99	ASN
1	A	118	ASN
1	A	182	ASN
1	A	245	ASN
1	A	260	ASN
1	B	291	HIS
1	B	373	ASN
1	B	381	ASN
1	B	445	ASN
1	B	526	ASN
1	C	554	HIS
1	C	588	HIS
1	C	609	ASN
1	C	631	HIS
1	C	636	ASN
1	C	644	ASN
1	C	646	HIS
1	C	786	ASN
1	D	883	ASN
1	D	888	ASN
1	D	894	HIS
1	D	907	ASN
1	D	909	HIS
1	D	1049	ASN
1	D	1052	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)

6 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	3G4	A	2004	-	27,27,27	2.94	6 (22%)	36,38,38	2.25	7 (19%)
2	NAP	C	2000	-	46,52,52	1.80	7 (15%)	61,80,80	2.02	16 (26%)
2	NAP	B	2003	-	46,52,52	2.07	10 (21%)	61,80,80	2.42	17 (27%)
2	NAP	A	2002	-	46,52,52	1.84	11 (23%)	61,80,80	2.89	16 (26%)
2	NAP	D	2001	-	46,52,52	1.51	7 (15%)	61,80,80	1.90	16 (26%)
3	3G4	D	2007	-	27,27,27	3.45	8 (29%)	36,38,38	2.06	7 (19%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3G4	A	2004	-	-	6/23/23/23	0/2/2/2
2	NAP	C	2000	-	-	7/31/67/67	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAP	B	2003	-	-	4/31/67/67	0/5/5/5
2	NAP	A	2002	-	-	4/31/67/67	0/5/5/5
2	NAP	D	2001	-	-	5/31/67/67	0/5/5/5
3	3G4	D	2007	-	-	10/23/23/23	0/2/2/2

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2007	3G4	C19-C20	-10.41	1.40	1.52
3	A	2004	3G4	C19-C20	-9.10	1.42	1.52
3	D	2007	3G4	C5-S9	-8.99	1.65	1.77
2	C	2000	NAP	C4A-N3A	8.74	1.47	1.35
3	D	2007	3G4	S9-N10	-8.43	1.50	1.63
3	A	2004	3G4	C5-S9	-8.33	1.66	1.77
2	B	2003	NAP	C4A-N3A	7.72	1.46	1.35
2	B	2003	NAP	PA-O3	7.37	1.67	1.59
3	A	2004	3G4	S9-N10	-6.68	1.53	1.63
2	A	2002	NAP	C4A-N3A	5.77	1.43	1.35
2	A	2002	NAP	PA-O3	5.16	1.65	1.59
2	D	2001	NAP	C4A-N3A	4.77	1.42	1.35
3	D	2007	3G4	C6-C5	-4.15	1.37	1.41
2	A	2002	NAP	PN-O3	3.76	1.63	1.59
2	D	2001	NAP	O4D-C4D	-3.54	1.37	1.45
2	D	2001	NAP	C2A-N3A	3.03	1.36	1.32
2	A	2002	NAP	C1B-N9A	-2.92	1.42	1.49
3	D	2007	3G4	C13-N14	-2.88	1.28	1.34
2	D	2001	NAP	PA-O3	2.80	1.62	1.59
3	A	2004	3G4	O12-S9	2.80	1.46	1.43
2	B	2003	NAP	C2A-N1A	2.74	1.38	1.33
2	B	2003	NAP	C7N-N7N	2.73	1.38	1.33
2	C	2000	NAP	C2A-N3A	2.64	1.36	1.32
3	A	2004	3G4	C1-C6	-2.57	1.35	1.39
2	C	2000	NAP	C7N-N7N	2.57	1.37	1.33
2	B	2003	NAP	C2A-N3A	2.53	1.36	1.32
2	C	2000	NAP	P2B-O2B	2.50	1.63	1.59
3	D	2007	3G4	C4-C5	2.47	1.42	1.39
2	D	2001	NAP	C2D-C3D	-2.42	1.46	1.53
2	A	2002	NAP	PN-O1N	2.37	1.59	1.50
2	A	2002	NAP	C3D-C4D	-2.35	1.47	1.53
2	D	2001	NAP	O4B-C4B	-2.35	1.39	1.45
2	C	2000	NAP	C3B-C2B	-2.34	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2002	NAP	O5B-C5B	-2.33	1.35	1.44
2	A	2002	NAP	C3B-C2B	-2.32	1.47	1.53
3	D	2007	3G4	C1-C6	2.30	1.43	1.39
2	D	2001	NAP	O4B-C1B	-2.26	1.37	1.40
3	D	2007	3G4	O22-C20	-2.22	1.18	1.23
2	B	2003	NAP	O4D-C4D	-2.17	1.40	1.45
2	A	2002	NAP	C5A-N7A	-2.17	1.32	1.39
2	B	2003	NAP	C8A-N7A	2.17	1.38	1.34
2	B	2003	NAP	C6N-N1N	-2.15	1.30	1.35
2	B	2003	NAP	PN-O3	-2.13	1.57	1.59
3	A	2004	3G4	C3-C4	2.10	1.42	1.38
2	B	2003	NAP	O3D-C3D	2.10	1.48	1.43
2	C	2000	NAP	C1B-N9A	-2.09	1.44	1.49
2	A	2002	NAP	P2B-O2B	2.08	1.63	1.59
2	C	2000	NAP	O5B-C5B	-2.02	1.36	1.44
2	A	2002	NAP	C2N-N1N	-2.00	1.32	1.35

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2002	NAP	O4B-C1B-N9A	15.02	128.66	108.75
3	A	2004	3G4	O12-S9-O11	-8.41	109.31	119.52
2	A	2002	NAP	N3A-C2A-N1A	-8.04	117.76	128.67
2	B	2003	NAP	N3A-C2A-N1A	-7.67	118.26	128.67
3	D	2007	3G4	O12-S9-O11	-7.42	110.51	119.52
3	D	2007	3G4	C13-N14-C15	6.68	122.80	118.16
2	B	2003	NAP	O2N-PN-O3	-6.03	90.97	107.27
2	B	2003	NAP	C4D-O4D-C1D	5.98	115.40	109.92
2	D	2001	NAP	O4B-C1B-N9A	5.92	116.59	108.75
2	B	2003	NAP	O3-PA-O1A	-5.53	94.07	110.70
3	A	2004	3G4	C13-N14-C15	5.44	121.94	118.16
2	C	2000	NAP	N3A-C2A-N1A	-5.38	121.37	128.67
3	A	2004	3G4	O22-C20-N21	-5.07	113.09	122.12
2	A	2002	NAP	C4D-O4D-C1D	4.83	114.35	109.92
2	A	2002	NAP	O3B-C3B-C2B	-4.70	98.03	111.19
2	A	2002	NAP	O3B-C3B-C4B	-4.65	97.73	111.08
2	C	2000	NAP	O3B-C3B-C2B	-4.63	98.24	111.19
2	C	2000	NAP	O4B-C1B-N9A	4.56	114.80	108.75
2	D	2001	NAP	O2N-PN-O1N	4.36	132.73	112.44
2	B	2003	NAP	O4B-C1B-N9A	4.18	114.29	108.75
2	A	2002	NAP	O3D-C3D-C4D	-4.18	99.07	111.08
2	D	2001	NAP	C4A-C5A-N7A	-4.17	104.93	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2003	NAP	C3N-C7N-N7N	4.12	122.81	117.74
2	D	2001	NAP	N3A-C2A-N1A	-4.07	123.15	128.67
2	A	2002	NAP	C2B-C3B-C4B	3.95	110.48	101.99
2	B	2003	NAP	O2A-PA-O3	3.94	117.92	107.27
2	B	2003	NAP	C4A-C5A-N7A	-3.90	105.21	109.34
2	C	2000	NAP	O2X-P2B-O2B	3.87	120.91	105.85
2	B	2003	NAP	O7N-C7N-C3N	-3.61	115.18	119.60
2	B	2003	NAP	O3B-C3B-C4B	-3.61	100.72	111.08
2	C	2000	NAP	O3X-P2B-O2B	-3.60	91.83	105.85
2	A	2002	NAP	O2B-C2B-C1B	3.57	122.61	110.05
2	D	2001	NAP	O2B-C2B-C1B	3.54	122.49	110.05
2	C	2000	NAP	O4B-C1B-C2B	3.43	112.46	106.61
2	A	2002	NAP	O7N-C7N-N7N	3.41	127.54	122.62
2	D	2001	NAP	O3X-P2B-O2B	-3.37	92.71	105.85
2	D	2001	NAP	O3B-C3B-C4B	-3.34	101.50	111.08
3	A	2004	3G4	C8-C6-C1	-3.24	117.96	121.86
2	C	2000	NAP	O2D-C2D-C3D	3.23	122.17	111.82
2	C	2000	NAP	O7N-C7N-C3N	-3.15	115.74	119.60
2	A	2002	NAP	C4A-C5A-N7A	-3.15	106.01	109.34
2	B	2003	NAP	O2A-PA-O1A	3.11	126.89	112.44
2	D	2001	NAP	O3X-P2B-O1X	3.03	122.63	110.83
2	C	2000	NAP	O5B-PA-O1A	-3.01	97.00	108.94
2	C	2000	NAP	C2B-C3B-C4B	2.98	108.40	101.99
2	B	2003	NAP	O3-PN-O1N	2.95	119.59	110.70
2	C	2000	NAP	C4B-O4B-C1B	-2.95	107.22	109.92
2	A	2002	NAP	O7N-C7N-C3N	-2.90	116.06	119.60
3	D	2007	3G4	C4-C5-C6	-2.87	118.51	121.19
2	A	2002	NAP	C2D-C3D-C4D	2.85	108.11	102.61
2	B	2003	NAP	O2B-C2B-C1B	2.79	119.84	110.05
2	D	2001	NAP	O3-PN-O1N	-2.78	102.34	110.70
2	C	2000	NAP	C4A-C5A-N7A	-2.75	106.43	109.34
3	A	2004	3G4	O22-C20-C19	2.72	125.94	121.61
3	D	2007	3G4	O22-C20-C19	2.71	125.92	121.61
2	B	2003	NAP	C5N-C4N-C3N	-2.64	117.77	120.36
2	D	2001	NAP	C1B-N9A-C4A	-2.63	122.01	126.64
2	A	2002	NAP	O2A-PA-O1A	2.63	124.67	112.44
2	C	2000	NAP	O2A-PA-O1A	2.62	124.62	112.44
2	B	2003	NAP	C2D-C3D-C4D	2.48	107.39	102.61
2	D	2001	NAP	C2D-C3D-C4D	2.45	107.35	102.61
2	B	2003	NAP	O4B-C1B-C2B	2.39	110.68	106.61
2	D	2001	NAP	O5D-PN-O1N	-2.35	99.63	108.94
2	A	2002	NAP	O2A-PA-O5B	-2.31	97.11	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2001	NAP	O4B-C4B-C3B	2.31	109.73	105.15
3	D	2007	3G4	O22-C20-N21	-2.28	118.07	122.12
2	C	2000	NAP	C1B-N9A-C4A	-2.25	122.69	126.64
2	D	2001	NAP	C2B-C1B-N9A	2.24	117.52	112.56
2	C	2000	NAP	O3X-P2B-O2X	2.20	116.06	107.80
2	B	2003	NAP	O2X-P2B-O1X	2.20	119.40	110.83
2	D	2001	NAP	C5B-C4B-C3B	-2.18	107.36	115.21
2	C	2000	NAP	O2B-P2B-O1X	-2.18	101.58	109.33
2	A	2002	NAP	C2B-C1B-N9A	-2.17	107.73	112.56
2	A	2002	NAP	C6N-N1N-C1D	-2.07	115.67	119.73
3	D	2007	3G4	C8-C6-C1	-2.07	119.36	121.86
3	D	2007	3G4	C6-C5-S9	2.04	123.83	122.02
3	A	2004	3G4	C4-C5-C6	-2.04	119.29	121.19
2	D	2001	NAP	O3-PA-O1A	-2.02	104.62	110.70
3	A	2004	3G4	C5-S9-N10	2.00	109.66	107.30

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2003	NAP	C5B-O5B-PA-O1A
2	C	2000	NAP	C5B-O5B-PA-O1A
2	C	2000	NAP	C5B-O5B-PA-O3
2	C	2000	NAP	C5D-O5D-PN-O2N
2	D	2001	NAP	C5D-O5D-PN-O2N
3	A	2004	3G4	C6-C5-S9-O12
3	A	2004	3G4	C6-C5-S9-N10
3	D	2007	3G4	C6-C5-S9-O12
3	D	2007	3G4	C6-C5-S9-N10
3	A	2004	3G4	C25-C24-N21-C20
3	A	2004	3G4	C4-C5-S9-O12
3	D	2007	3G4	C4-C5-S9-O12
3	D	2007	3G4	C6-C5-S9-O11
3	A	2004	3G4	C25-C24-N21-C23
3	D	2007	3G4	C25-C24-N21-C20
3	A	2004	3G4	C4-C5-S9-N10
3	D	2007	3G4	C4-C5-S9-N10
3	D	2007	3G4	C25-C24-N21-C23
2	C	2000	NAP	O4B-C4B-C5B-O5B
2	D	2001	NAP	C1B-C2B-O2B-P2B
2	A	2002	NAP	PN-O3-PA-O2A
2	A	2002	NAP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	D	2001	NAP	C5D-O5D-PN-O3
2	D	2001	NAP	PN-O3-PA-O1A
2	A	2002	NAP	O4D-C1D-N1N-C2N
2	C	2000	NAP	O4D-C1D-N1N-C6N
3	D	2007	3G4	C13-N10-S9-O11
2	B	2003	NAP	O4B-C4B-C5B-O5B
2	A	2002	NAP	O4D-C4D-C5D-O5D
3	D	2007	3G4	C4-C5-S9-O11
2	B	2003	NAP	PN-O3-PA-O1A
2	C	2000	NAP	PN-O3-PA-O1A
2	C	2000	NAP	PN-O3-PA-O2A
2	D	2001	NAP	PN-O3-PA-O2A
2	B	2003	NAP	C1B-C2B-O2B-P2B
3	D	2007	3G4	C15-C19-C20-N21

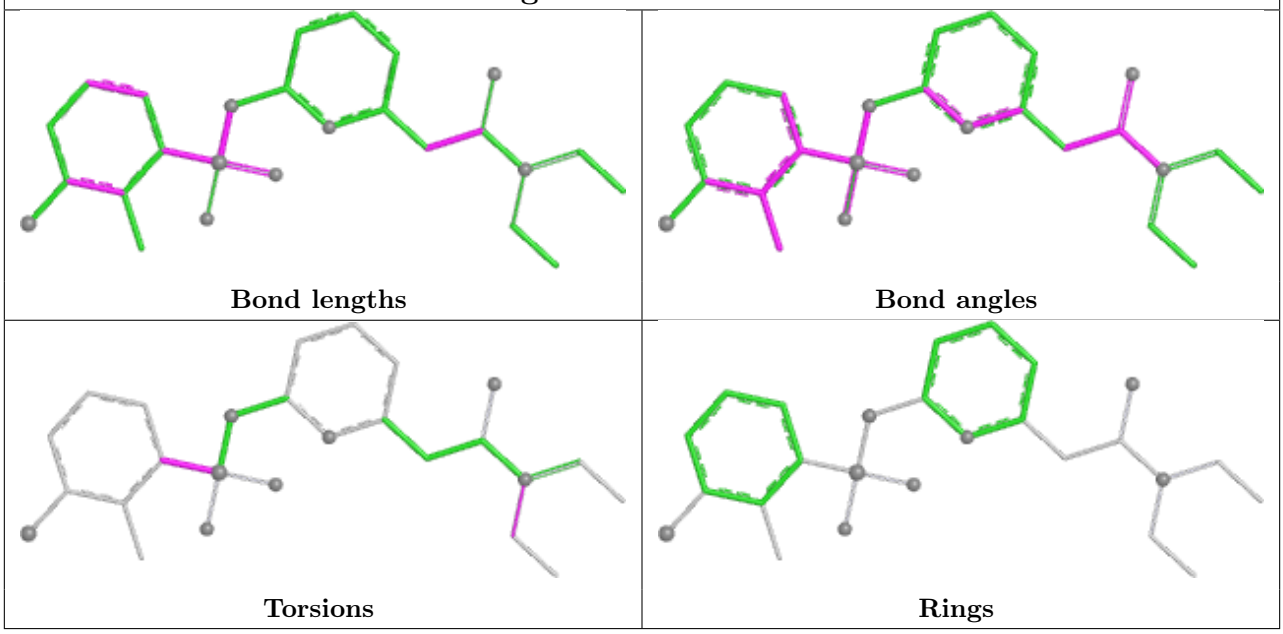
There are no ring outliers.

6 monomers are involved in 39 short contacts:

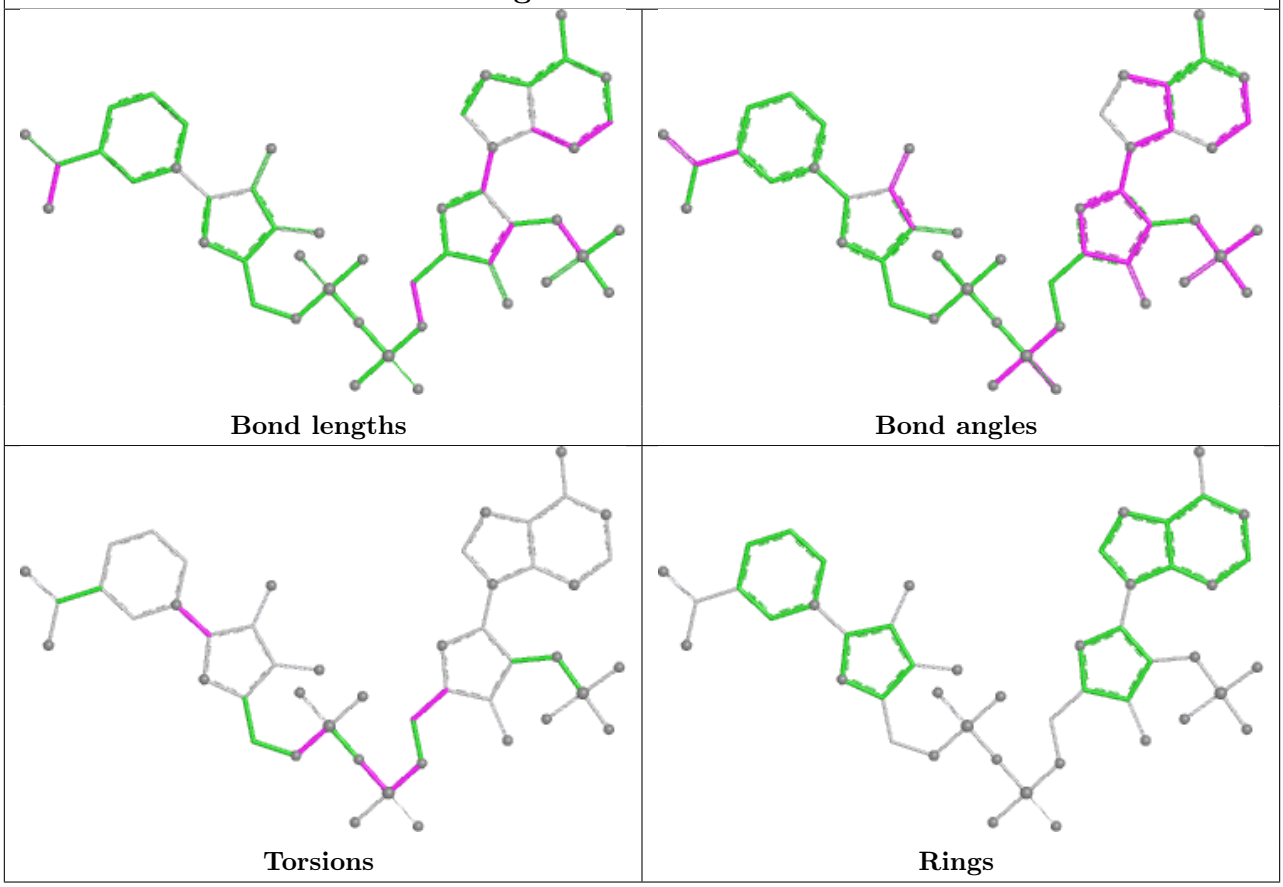
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2004	3G4	15	0
2	C	2000	NAP	2	0
2	B	2003	NAP	2	0
2	A	2002	NAP	5	0
2	D	2001	NAP	2	0
3	D	2007	3G4	14	0

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.

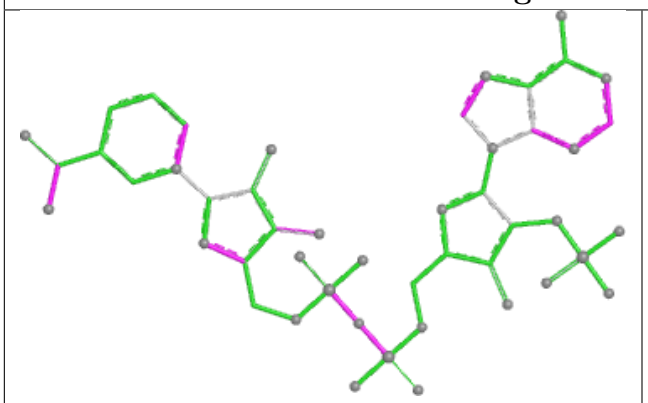
Ligand 3G4 A 2004



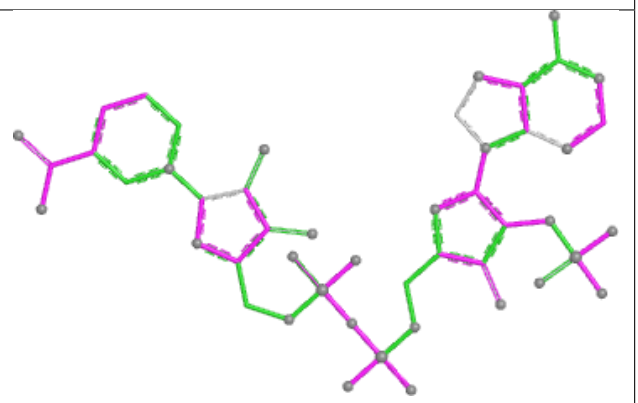
Ligand NAP C 2000



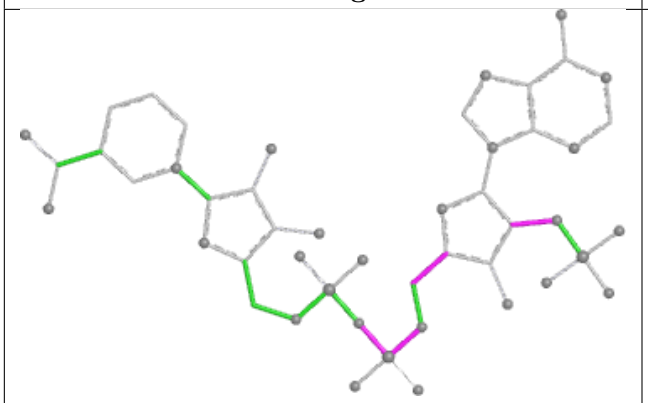
Ligand NAP B 2003



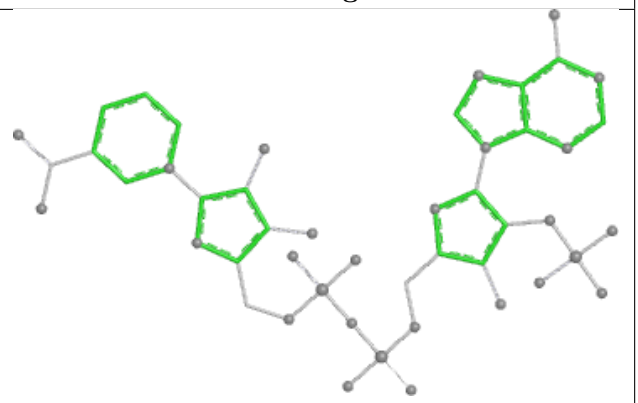
Bond lengths



Bond angles

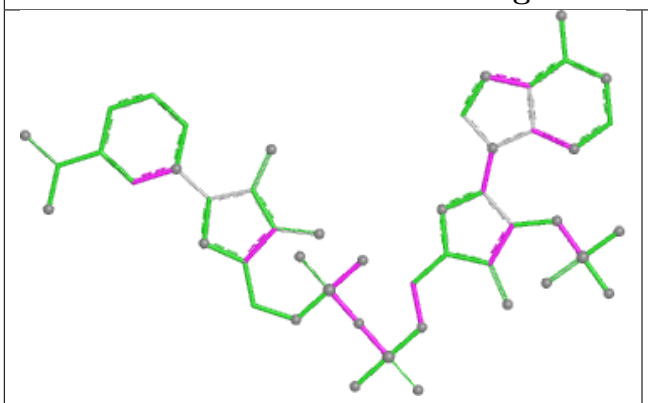


Torsions

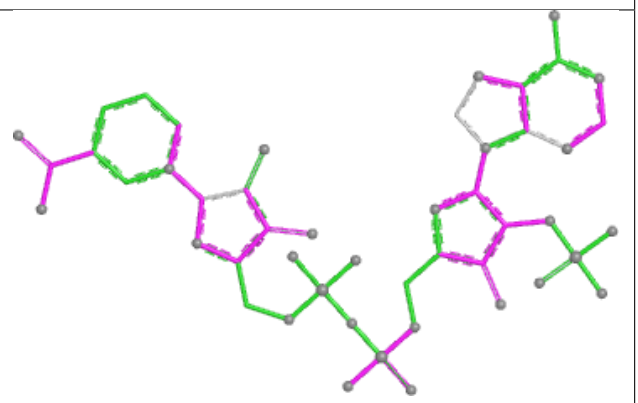


Rings

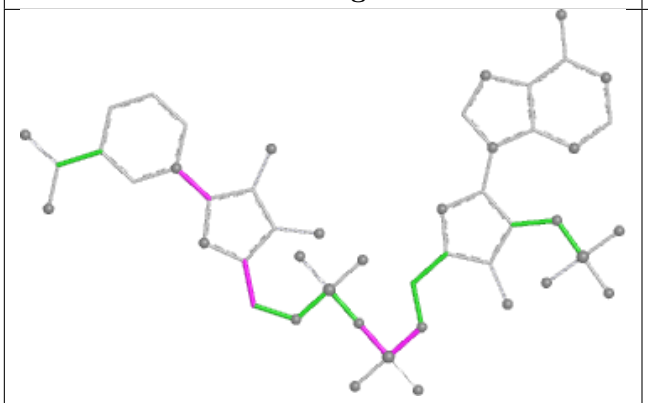
Ligand NAP A 2002



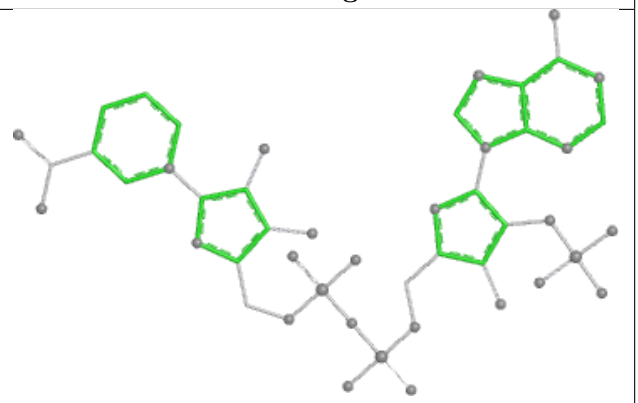
Bond lengths



Bond angles

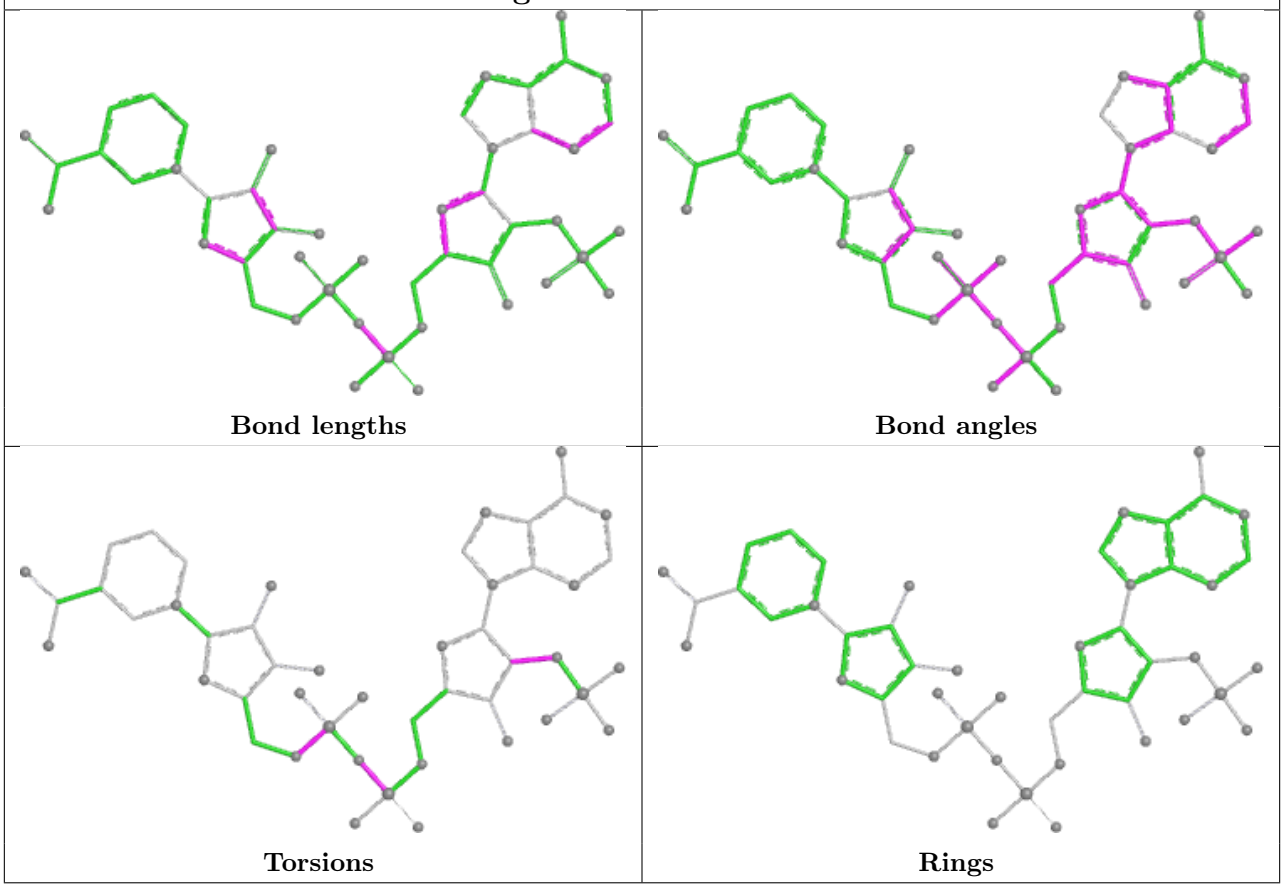


Torsions

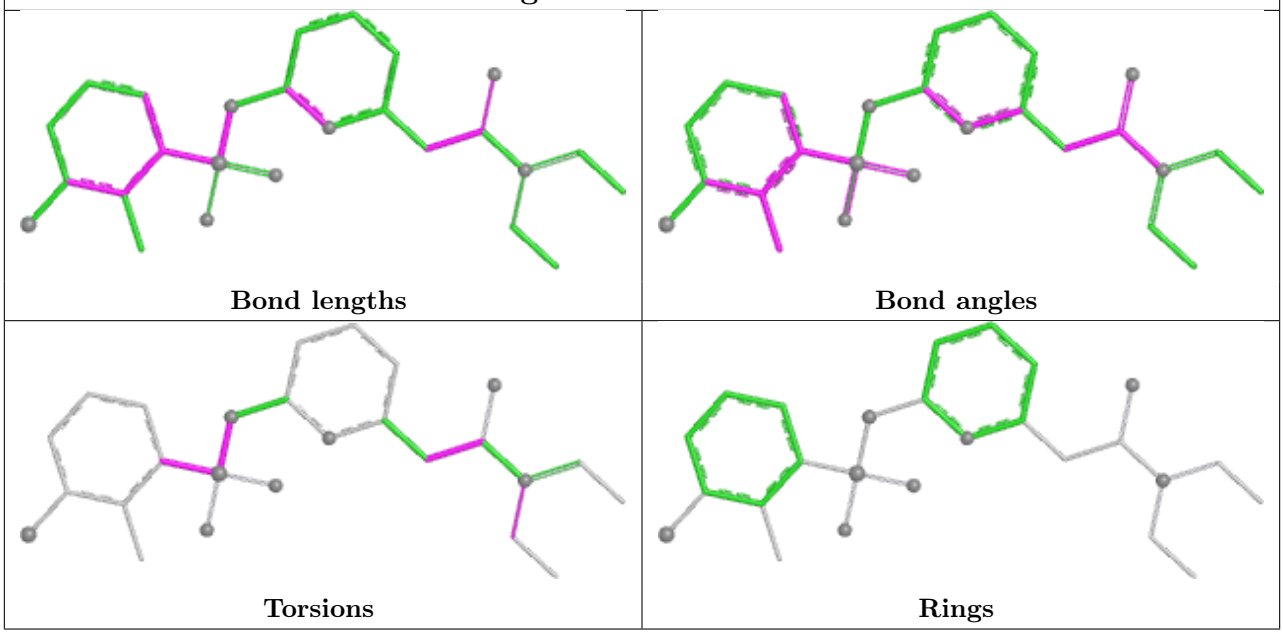


Rings

Ligand NAP D 2001



Ligand 3G4 D 2007



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	263/277 (94%)	-0.13	1 (0%)	92	93	17, 29, 41, 56	0
1	B	263/277 (94%)	0.10	8 (3%)	50	53	16, 32, 45, 51	0
1	C	263/277 (94%)	0.08	5 (1%)	66	69	16, 31, 45, 60	0
1	D	263/277 (94%)	-0.02	5 (1%)	66	69	16, 28, 41, 56	0
All	All	1052/1108 (94%)	0.01	19 (1%)	68	71	16, 30, 44, 60	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	733	LEU	5.5
1	B	363	ARG	3.9
1	D	1021	TYR	3.7
1	D	792	ARG	3.0
1	B	325	HIS	2.8
1	B	520	ALA	2.6
1	C	626	ARG	2.5
1	D	821	MET	2.5
1	B	347	LEU	2.4
1	C	624	TYR	2.2
1	C	529	ARG	2.2
1	B	346	ASN	2.2
1	D	793	PRO	2.2
1	C	527	LYS	2.1
1	D	965	PHE	2.1
1	B	368	HIS	2.1
1	A	135	GLN	2.1
1	B	327	ILE	2.1
1	B	343	GLU	2.1

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)

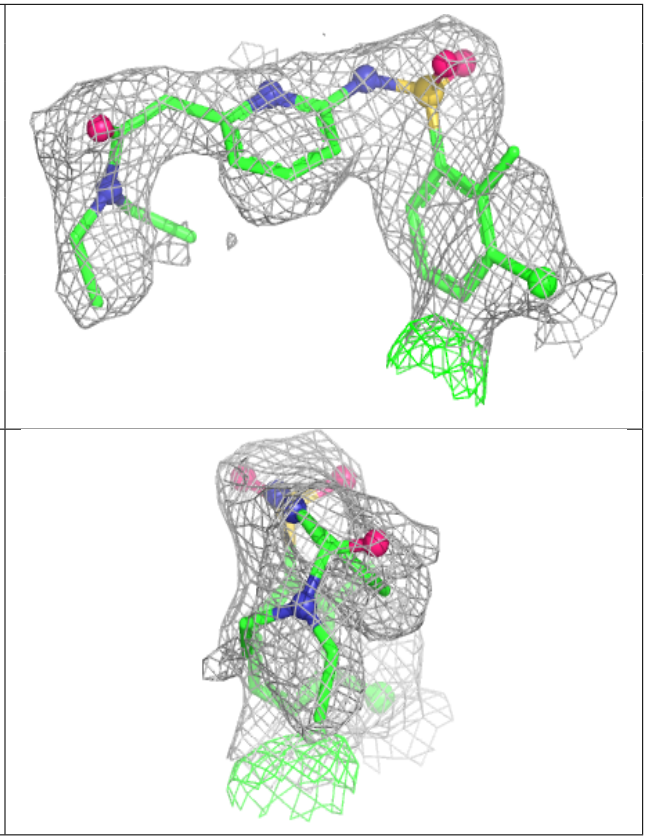
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	3G4	A	2004	26/26	0.88	0.20	41,48,60,67	0
3	3G4	D	2007	26/26	0.91	0.20	29,38,60,68	0
2	NAP	C	2000	48/48	0.97	0.12	18,26,36,39	0
2	NAP	D	2001	48/48	0.97	0.13	11,22,28,30	0
2	NAP	A	2002	48/48	0.97	0.12	15,25,29,32	0
2	NAP	B	2003	48/48	0.97	0.13	15,27,33,42	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.

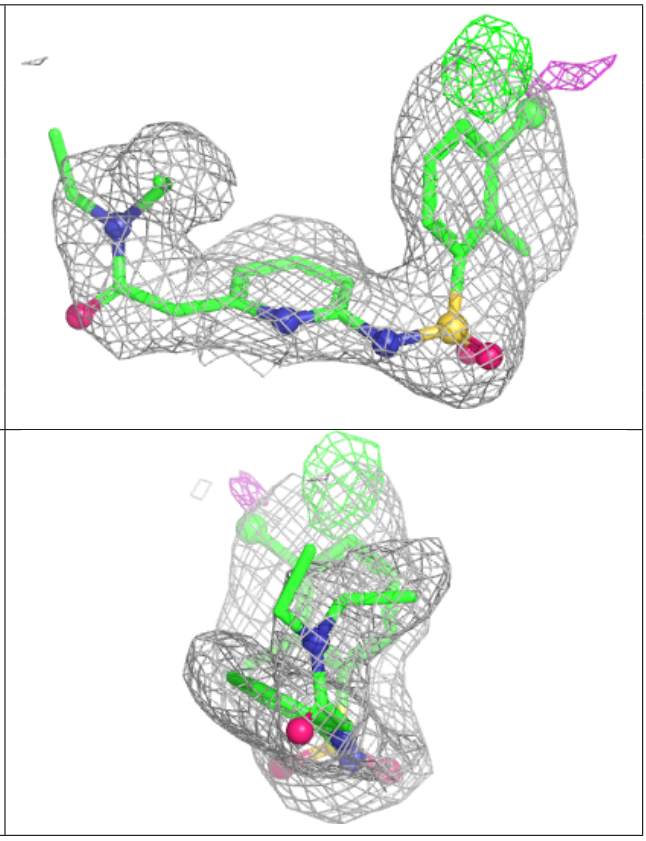
Electron density around 3G4 A 2004:

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



Electron density around 3G4 D 2007:

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



Electron density around NAP C 2000:

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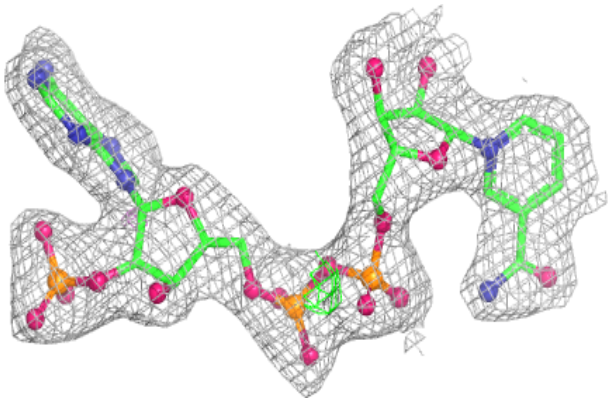
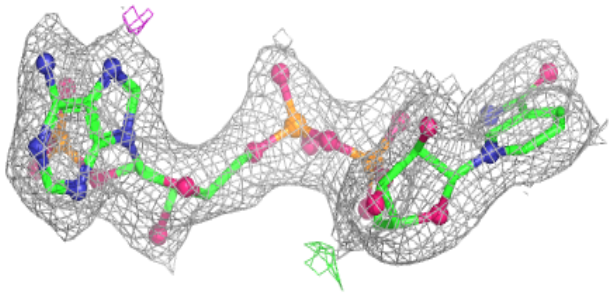
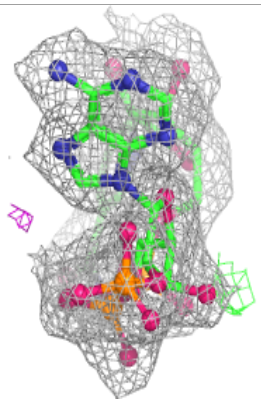
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

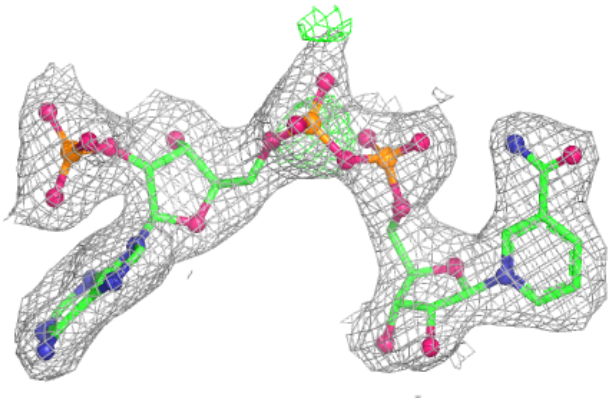


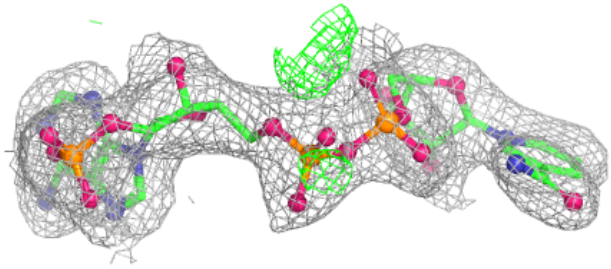


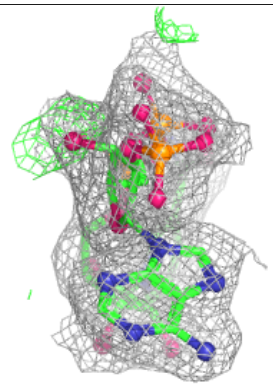


Electron density around NAP D 2001:

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







Electron density around NAP A 2002:

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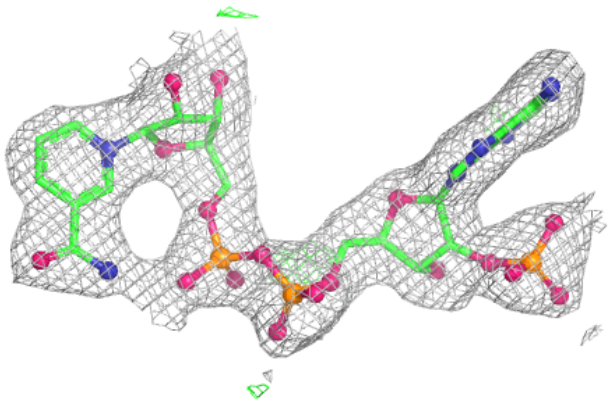
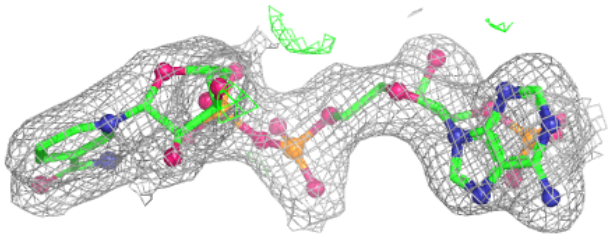
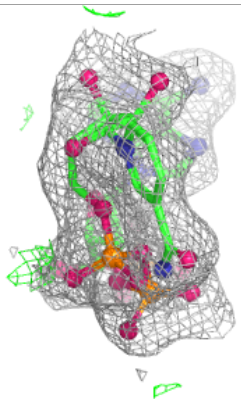
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NAP B 2003:

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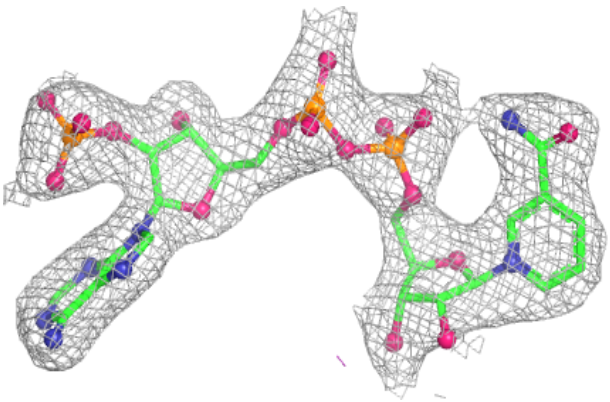
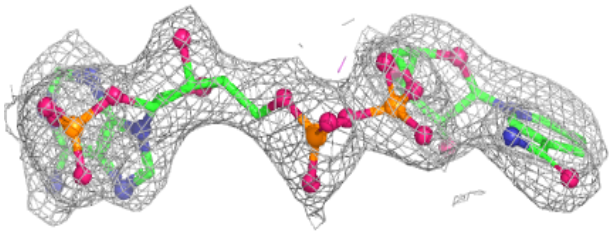
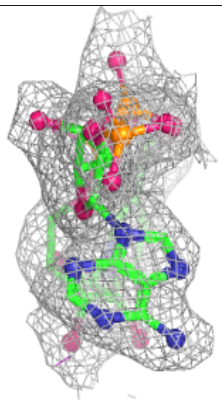
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.