



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:08 am BST

PDB ID : 1GZ6
Title : (3R)-HYDROXYACYL-COA DEHYDROGENASE FRAGMENT OF RAT
PEROXISOMAL MULTIFUNCTIONAL ENZYME TYPE 2
Authors : Haapalainen, A.M.; Hiltunen, J.K.; Glumoff, T.
Deposited on : 2002-05-16
Resolution : 2.38 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 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 : 2.11
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) : 2.11

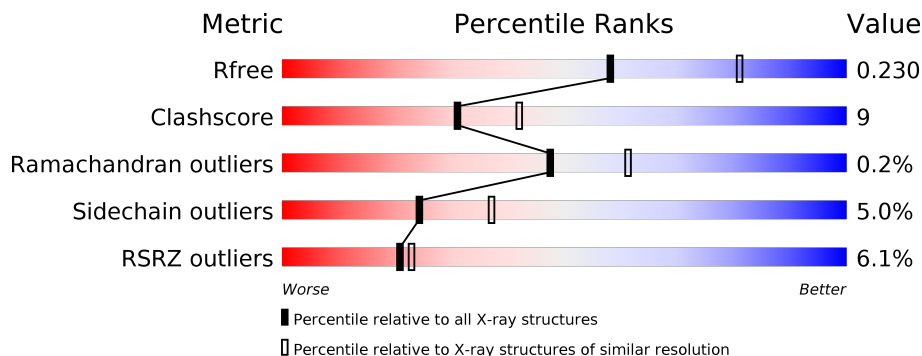
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	319	<p>4% 76% 16% • 5%</p>
1	B	319	<p>5% 72% 14% • 13%</p>
1	C	319	<p>9% 73% 16% • 10%</p>
1	D	319	<p>4% 75% 18% • 5%</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9961 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 ESTRADIOL 17 BETA-DEHYDROGENASE 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	302	Total 2302	C 1442	N 423	O 428	S 4	Se 5	54	0	1
1	B	279	Total 2135	C 1339	N 395	O 394	S 4	Se 3	47	0	1
1	C	288	Total 2204	C 1385	N 406	O 406	S 4	Se 3	59	0	1
1	D	302	Total 2302	C 1442	N 423	O 428	S 4	Se 5	43	0	1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



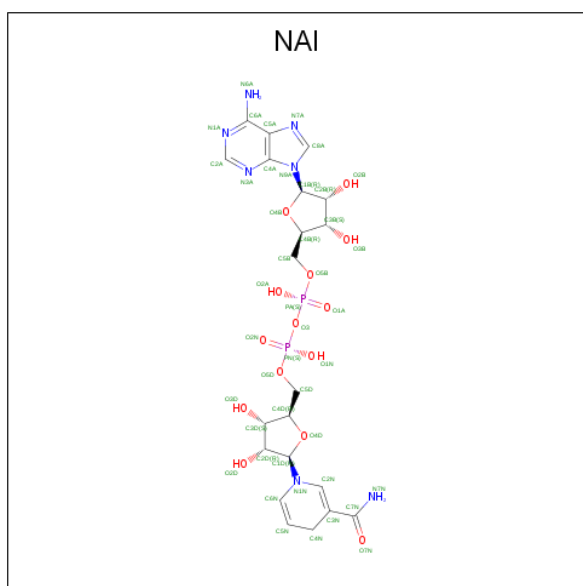
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (three-letter code: NAI) (formula: C₂₁H₂₉N₇O₁₄P₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
3	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	238	Total	O	0	0
			238	238		
4	B	176	Total	O	0	0
			176	176		

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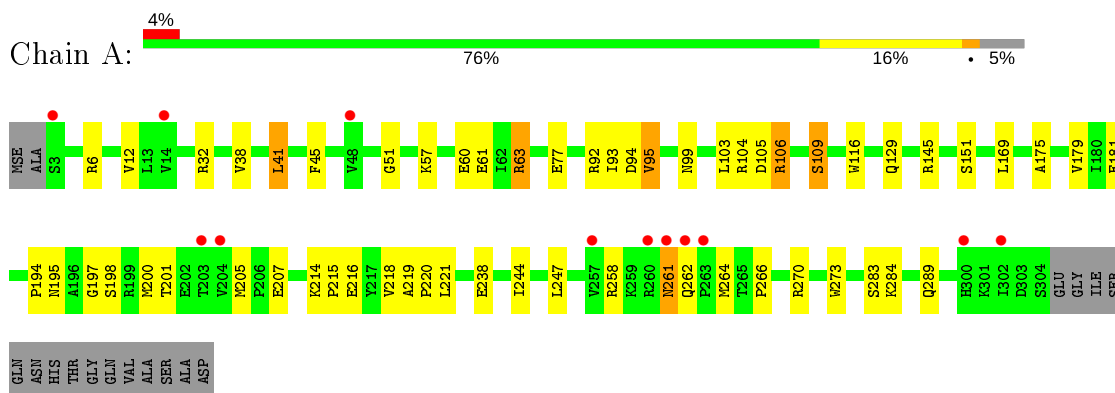
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	186	Total 186	O 186	0	0
4	D	217	Total 217	O 217	0	0

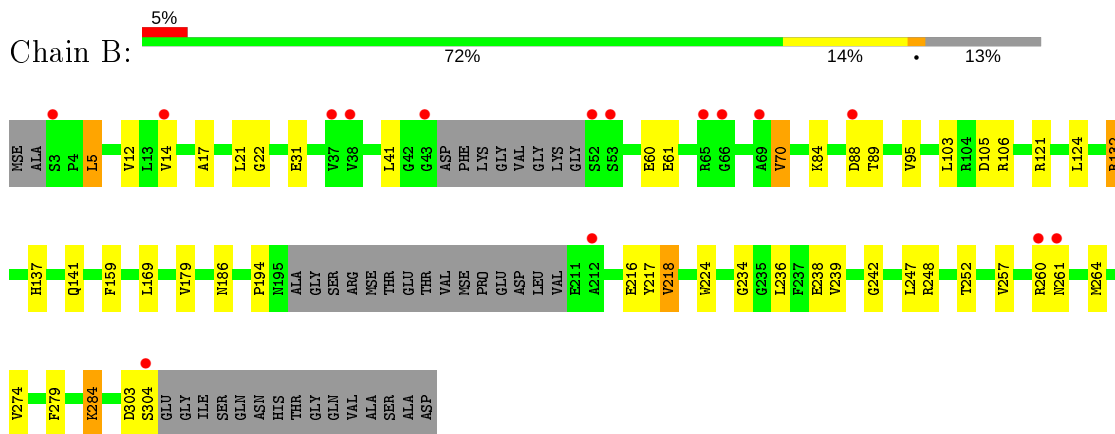
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

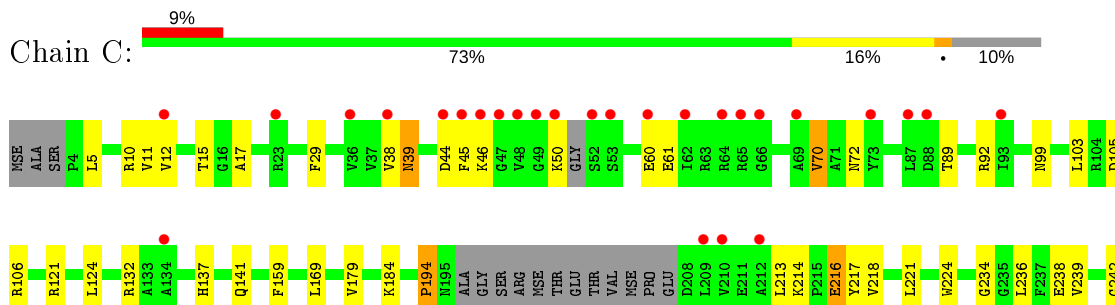
- Molecule 1: ESTRADIOL 17 BETA-DEHYDROGENASE 4

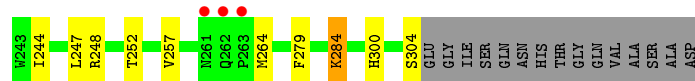


- Molecule 1: ESTRADIOL 17 BETA-DEHYDROGENASE 4

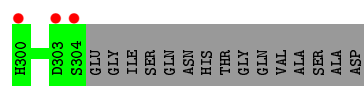
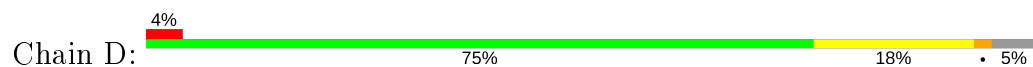


- Molecule 1: ESTRADIOL 17 BETA-DEHYDROGENASE 4





• Molecule 1: ESTRADIOL 17 BETA-DEHYDROGENASE 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.47Å 82.75Å 95.75Å 90.00° 94.20° 90.00°	Depositor
Resolution (Å)	20.00 – 2.38 19.99 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.38) 98.7 (19.99-2.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.38Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.197 , 0.236 0.192 , 0.230	Depositor DCC
R_{free} test set	2809 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtrriage
Anisotropy	0.705	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9961	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NAI, SO4

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	0/2336	0.82	7/3146 (0.2%)
1	B	0.58	2/2167 (0.1%)	0.77	5/2920 (0.2%)
1	C	0.56	2/2237 (0.1%)	0.77	5/3012 (0.2%)
1	D	0.49	0/2336	0.81	6/3146 (0.2%)
All	All	0.53	4/9076 (0.0%)	0.79	23/12224 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	VAL	CB-CG2	-11.61	1.28	1.52
1	C	70	VAL	CB-CG1	-11.52	1.28	1.52
1	B	70	VAL	CB-CG1	-11.34	1.29	1.52
1	C	70	VAL	CB-CG2	-10.88	1.30	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	ARG	NE-CZ-NH2	-11.79	114.40	120.30
1	C	70	VAL	CG1-CB-CG2	-11.14	93.08	110.90
1	A	63	ARG	NE-CZ-NH1	10.72	125.66	120.30
1	D	6	ARG	NE-CZ-NH2	-9.79	115.40	120.30
1	D	63	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	B	70	VAL	CG1-CB-CG2	-9.55	95.62	110.90
1	A	104	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	D	63	ARG	NE-CZ-NH2	9.16	124.88	120.30
1	B	121	ARG	NE-CZ-NH1	-9.04	115.78	120.30
1	D	104	ARG	NE-CZ-NH1	-8.86	115.87	120.30
1	A	104	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	A	6	ARG	NE-CZ-NH1	-8.58	116.01	120.30
1	D	6	ARG	NE-CZ-NH1	8.24	124.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	121	ARG	NE-CZ-NH2	-8.11	116.24	120.30
1	B	132	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	121	ARG	NE-CZ-NH2	8.01	124.31	120.30
1	C	132	ARG	NE-CZ-NH1	-7.90	116.35	120.30
1	D	104	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	C	121	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	C	132	ARG	NE-CZ-NH2	7.37	123.99	120.30
1	B	132	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	6	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	A	63	ARG	CD-NE-CZ	5.33	131.06	123.60

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	2302	0	2311	54	0
1	B	2135	0	2142	34	0
1	C	2204	0	2216	38	0
1	D	2302	0	2311	54	0
2	A	15	0	0	1	0
2	D	10	0	0	0	0
3	A	44	0	27	3	0
3	B	44	0	27	0	0
3	C	44	0	27	1	0
3	D	44	0	27	3	0
4	A	238	0	0	4	0
4	B	176	0	0	6	0
4	C	186	0	0	6	0
4	D	217	0	0	3	0
All	All	9961	0	9088	161	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 9.

All (161) 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:198:SER:H	1:A:201:THR:HG22	1.32	0.94
1:D:103:LEU:HG	1:D:200:MSE:HE3	1.55	0.89
1:C:242:GLY:HA2	1:D:264:MSE:CE	2.05	0.86
1:A:264:MSE:CE	1:B:242:GLY:HA2	2.05	0.86
1:A:201:THR:OG1	1:A:205:MSE:HE3	1.81	0.80
1:D:258:ARG:HB2	1:D:264:MSE:HE2	1.66	0.77
1:C:248:ARG:NH1	1:C:284:LYS:HE3	2.00	0.77
1:B:70:VAL:HG11	1:B:89:THR:HG21	1.68	0.76
1:B:248:ARG:NH1	1:B:284:LYS:HE3	2.02	0.75
1:D:198:SER:H	1:D:201:THR:HG22	1.53	0.74
1:A:258:ARG:HB2	1:A:264:MSE:HE2	1.69	0.74
1:A:264:MSE:HE1	1:B:242:GLY:HA2	1.70	0.73
1:C:242:GLY:HA2	1:D:264:MSE:HE1	1.69	0.73
1:A:238:GLU:HG3	1:A:247:LEU:HD11	1.71	0.73
1:D:12:VAL:HG13	1:D:95:VAL:HG22	1.71	0.73
1:D:238:GLU:HG3	1:D:247:LEU:HD11	1.72	0.71
1:C:70:VAL:HG11	1:C:89:THR:HG21	1.72	0.71
1:A:261:ASN:HB2	4:A:2202:HOH:O	1.89	0.71
1:D:214:LYS:HB3	1:D:216:GLU:OE2	1.91	0.70
1:A:12:VAL:HG13	1:A:95:VAL:HG22	1.72	0.70
1:A:264:MSE:HE2	1:B:242:GLY:HA2	1.74	0.70
1:A:266:PRO:HB2	1:B:5:LEU:HD23	1.75	0.69
1:D:175:ALA:O	1:D:179:VAL:HG23	1.93	0.69
1:D:201:THR:OG1	1:D:205:MSE:HE3	1.94	0.67
1:C:242:GLY:HA2	1:D:264:MSE:HE2	1.76	0.66
1:A:214:LYS:HB3	1:A:216:GLU:OE2	1.96	0.66
1:D:207:GLU:CD	1:D:207:GLU:H	1.98	0.65
1:A:92:ARG:HD3	1:A:94:ASP:OD1	1.96	0.65
1:D:198:SER:H	1:D:201:THR:CG2	2.08	0.65
1:D:92:ARG:HD3	1:D:94:ASP:OD1	1.95	0.65
1:D:215:PRO:HD2	1:D:216:GLU:OE2	1.97	0.64
1:A:215:PRO:HD2	1:A:216:GLU:OE2	1.96	0.64
1:A:258:ARG:HD3	1:A:264:MSE:HE3	1.80	0.63
1:A:214:LYS:HB3	1:A:216:GLU:HG2	1.81	0.63
1:A:258:ARG:HD3	1:A:264:MSE:CE	2.30	0.62
1:D:77:GLU:O	1:D:129:GLN:NE2	2.32	0.62
1:D:32:ARG:HG2	1:D:32:ARG:HH11	1.65	0.62
1:A:175:ALA:O	1:A:179:VAL:HG23	2.01	0.61
1:D:197:GLY:HA2	1:D:201:THR:HG21	1.81	0.61
1:A:198:SER:H	1:A:201:THR:CG2	2.10	0.61
1:D:258:ARG:HD3	1:D:264:MSE:CE	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HH11	1:A:32:ARG:HG2	1.65	0.60
1:C:304:SER:N	4:C:2180:HOH:O	2.34	0.60
1:D:93:ILE:HG23	1:D:93:ILE:O	2.02	0.59
1:D:151:SER:HB2	3:D:1305:NAI:H5N	1.86	0.58
1:B:248:ARG:HH11	1:B:284:LYS:HE3	1.69	0.58
1:D:258:ARG:HD3	1:D:264:MSE:HE3	1.85	0.58
1:A:77:GLU:O	1:A:129:GLN:NE2	2.35	0.57
1:C:45:PHE:CE1	1:C:46:LYS:HD2	2.41	0.56
1:C:248:ARG:HH11	1:C:284:LYS:HE3	1.68	0.55
1:D:198:SER:O	1:D:201:THR:HG22	2.06	0.55
1:C:300:HIS:HD2	4:C:2174:HOH:O	1.90	0.55
1:A:194:PRO:O	3:A:1306:NAI:H42N	2.07	0.55
1:B:304:SER:N	4:B:2173:HOH:O	2.40	0.54
1:B:304:SER:N	4:B:2174:HOH:O	2.40	0.54
1:A:151:SER:HB2	3:A:1306:NAI:H5N	1.88	0.54
1:A:93:ILE:HG23	1:A:93:ILE:O	2.09	0.53
1:A:197:GLY:HA2	1:A:201:THR:HG21	1.91	0.53
1:B:186:ASN:HB3	4:B:2083:HOH:O	2.07	0.53
1:C:15:THR:O	1:C:99:ASN:HB3	2.09	0.53
1:D:194:PRO:O	3:D:1305:NAI:H42N	2.08	0.53
1:A:181:GLU:HG2	1:B:159:PHE:CD2	2.43	0.53
1:A:116:TRP:HZ2	1:B:124:LEU:HG	1.74	0.52
1:D:221:LEU:HD13	1:D:244:ILE:HD13	1.92	0.52
1:C:159:PHE:CD2	1:D:181:GLU:HG2	2.44	0.52
1:D:106:ARG:HG2	1:D:106:ARG:HH11	1.75	0.51
1:A:221:LEU:HD13	1:A:244:ILE:HD13	1.92	0.51
1:C:238:GLU:HG3	1:C:247:LEU:HD11	1.93	0.50
1:C:11:VAL:CG2	1:C:92:ARG:HG3	2.41	0.50
1:A:103:LEU:HG	1:A:200:MSE:HE3	1.94	0.50
1:C:137:HIS:O	1:C:141:GLN:HG2	2.10	0.50
1:B:137:HIS:O	1:B:141:GLN:HG2	2.12	0.50
1:B:70:VAL:CG1	1:B:89:THR:HG21	2.41	0.50
1:A:106:ARG:HG2	1:A:106:ARG:HH11	1.77	0.49
1:A:109:SER:HB2	4:A:2108:HOH:O	2.12	0.49
1:C:214:LYS:HB3	1:C:216:GLU:OE2	2.12	0.49
1:C:221:LEU:HD13	1:C:244:ILE:HD13	1.94	0.49
1:B:41:LEU:HB3	4:B:2026:HOH:O	2.12	0.49
1:A:77:GLU:HA	4:A:2119:HOH:O	2.13	0.48
1:C:300:HIS:CD2	4:C:2174:HOH:O	2.65	0.48
1:C:217:TYR:CD1	1:D:264:MSE:HE3	2.48	0.48
1:C:106:ARG:HG2	1:C:106:ARG:HH11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:THR:HG22	1:B:279:PHE:HA	1.94	0.47
1:D:154:GLY:O	1:D:169:LEU:HG	2.14	0.47
1:D:95:VAL:HB	1:D:145:ARG:HB2	1.97	0.47
1:D:263:PRO:HA	4:D:2179:HOH:O	2.14	0.47
1:C:50:LYS:O	1:C:50:LYS:HG2	2.14	0.47
1:C:194:PRO:O	3:C:1304:NAI:H42N	2.14	0.47
1:D:207:GLU:N	1:D:207:GLU:CD	2.66	0.47
1:B:84:LYS:HG2	1:B:88:ASP:OD2	2.15	0.47
1:D:121:ARG:HD2	4:D:2065:HOH:O	2.13	0.47
1:B:257:VAL:CG2	1:B:264:MSE:HE3	2.45	0.47
1:D:99:ASN:HD21	3:D:1305:NAI:H51N	1.80	0.47
1:C:124:LEU:HG	1:D:116:TRP:HZ2	1.80	0.46
1:A:45:PHE:HB2	1:A:200:MSE:HG3	1.97	0.46
1:A:270:ARG:HG3	1:B:224:TRP:CH2	2.50	0.46
1:A:12:VAL:HG22	1:A:95:VAL:HG13	1.98	0.46
1:C:213:LEU:HD21	1:D:299:LEU:HD11	1.97	0.46
1:A:57:LYS:O	1:A:61:GLU:HG3	2.15	0.46
1:D:57:LYS:O	1:D:61:GLU:HG3	2.15	0.46
1:D:114:GLU:O	1:D:118:ILE:HG22	2.16	0.46
1:A:95:VAL:HB	1:A:145:ARG:HB2	1.98	0.45
1:C:11:VAL:HG21	1:C:92:ARG:HG3	1.97	0.45
1:A:38:VAL:O	1:A:38:VAL:HG22	2.16	0.45
1:D:41:LEU:O	1:D:41:LEU:HD22	2.17	0.45
1:A:41:LEU:HD22	1:A:41:LEU:O	2.17	0.45
1:C:92:ARG:NH1	4:C:2044:HOH:O	2.40	0.45
1:B:260:ARG:O	1:B:261:ASN:HB2	2.16	0.45
1:B:274:VAL:HB	4:B:2148:HOH:O	2.15	0.45
1:A:99:ASN:HD21	3:A:1306:NAI:H51N	1.82	0.45
1:B:12:VAL:HG22	1:B:95:VAL:HB	1.99	0.44
1:C:17:ALA:HB3	1:C:38:VAL:HG13	1.99	0.44
1:C:39:ASN:HB2	1:C:72:ASN:HB3	1.99	0.44
1:C:224:TRP:CH2	1:D:270:ARG:HG3	2.52	0.44
1:C:105:ASP:O	1:C:106:ARG:HG2	2.16	0.44
1:A:266:PRO:CB	1:B:5:LEU:HD23	2.44	0.44
1:B:14:VAL:HG12	1:B:17:ALA:HB2	1.99	0.44
1:D:219:ALA:HB3	1:D:220:PRO:HD3	2.00	0.44
1:D:283:SER:C	1:D:284:LYS:HD2	2.38	0.44
1:A:264:MSE:HE3	1:B:217:TYR:CD1	2.53	0.44
1:B:21:LEU:HD22	1:B:218:VAL:HG21	2.00	0.43
1:C:105:ASP:C	1:C:106:ARG:HG2	2.38	0.43
1:A:214:LYS:HG2	4:A:2164:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HG	1:A:200:MSE:CE	2.48	0.43
1:A:214:LYS:CB	1:A:216:GLU:HG2	2.48	0.43
1:B:238:GLU:HG3	1:B:247:LEU:HD11	2.00	0.43
1:B:17:ALA:HA	1:B:22:GLY:HA3	2.01	0.43
1:B:105:ASP:O	1:B:106:ARG:HG2	2.18	0.43
1:C:257:VAL:CG2	1:C:264:MSE:HE3	2.49	0.43
1:C:252:THR:HG22	1:C:279:PHE:HA	1.99	0.43
1:B:105:ASP:C	1:B:106:ARG:HG2	2.39	0.43
1:D:139:LYS:HB3	1:D:139:LYS:HE2	1.86	0.42
1:D:216:GLU:H	1:D:216:GLU:CD	2.21	0.42
1:A:283:SER:C	1:A:284:LYS:HD2	2.40	0.42
1:B:106:ARG:HG2	1:B:106:ARG:HH11	1.83	0.42
1:D:105:ASP:O	1:D:106:ARG:HD2	2.19	0.42
1:D:38:VAL:O	1:D:38:VAL:HG22	2.19	0.42
1:C:179:VAL:HG21	1:C:234:GLY:HA2	2.01	0.42
1:D:82:LEU:N	1:D:82:LEU:HD12	2.35	0.42
1:D:12:VAL:HG22	1:D:95:VAL:HG13	2.01	0.41
1:A:105:ASP:O	1:A:106:ARG:HD2	2.20	0.41
1:A:51:GLY:HA3	2:A:1305:SO4:O4	2.20	0.41
1:D:295:ILE:HD13	1:D:295:ILE:HA	1.88	0.41
1:A:219:ALA:HB3	1:A:220:PRO:HD3	2.01	0.41
1:B:132:ARG:HD3	4:B:2045:HOH:O	2.20	0.41
1:C:304:SER:N	4:C:2179:HOH:O	2.53	0.41
1:A:216:GLU:H	1:A:216:GLU:CD	2.22	0.41
1:D:205:MSE:HB3	1:D:210:VAL:HG23	2.03	0.41
1:A:273:TRP:HA	1:A:273:TRP:CE3	2.55	0.41
1:B:260:ARG:NH2	1:B:303:ASP:HA	2.36	0.41
1:A:289:GLN:O	1:D:293:GLY:HA3	2.20	0.41
1:C:213:LEU:CD2	1:D:299:LEU:HD11	2.51	0.41
1:D:60:GLU:HA	4:D:2047:HOH:O	2.21	0.41
1:A:214:LYS:HB3	1:A:216:GLU:CG	2.50	0.40
1:A:32:ARG:HG2	1:A:32:ARG:NH1	2.35	0.40
1:C:184:LYS:HB2	4:C:2097:HOH:O	2.21	0.40
1:D:262:GLN:OE1	1:D:262:GLN:HA	2.21	0.40
1:C:12:VAL:HG11	1:C:29:PHE:CD2	2.57	0.40
1:A:214:LYS:HA	1:A:215:PRO:HD3	1.85	0.40
1:B:179:VAL:HG21	1:B:234:GLY:CA	2.51	0.40
1:C:179:VAL:HG21	1:C:234:GLY:CA	2.51	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	300/319 (94%)	288 (96%)	11 (4%)	1 (0%)	41	53
1	B	273/319 (86%)	260 (95%)	13 (5%)	0	100	100
1	C	282/319 (88%)	269 (95%)	13 (5%)	0	100	100
1	D	300/319 (94%)	285 (95%)	14 (5%)	1 (0%)	41	53
All	All	1155/1276 (90%)	1102 (95%)	51 (4%)	2 (0%)	47	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	D	261	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	238/245 (97%)	227 (95%)	11 (5%)	27	40
1	B	220/245 (90%)	208 (94%)	12 (6%)	21	32
1	C	227/245 (93%)	213 (94%)	14 (6%)	18	27
1	D	238/245 (97%)	229 (96%)	9 (4%)	33	49
All	All	923/980 (94%)	877 (95%)	46 (5%)	24	37

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LEU
1	A	60	GLU
1	A	63	ARG
1	A	95	VAL
1	A	106	ARG
1	A	109	SER
1	A	169	LEU
1	A	195	ASN
1	A	207	GLU
1	A	218	VAL
1	A	262	GLN
1	B	5	LEU
1	B	31	GLU
1	B	60	GLU
1	B	61	GLU
1	B	103	LEU
1	B	169	LEU
1	B	194	PRO
1	B	216	GLU
1	B	218	VAL
1	B	236	LEU
1	B	239	VAL
1	B	284	LYS
1	C	5	LEU
1	C	10	ARG
1	C	39	ASN
1	C	44	ASP
1	C	60	GLU
1	C	61	GLU
1	C	103	LEU
1	C	169	LEU
1	C	194	PRO
1	C	216	GLU
1	C	218	VAL
1	C	236	LEU
1	C	239	VAL
1	C	284	LYS
1	D	41	LEU
1	D	60	GLU
1	D	95	VAL
1	D	106	ARG
1	D	169	LEU
1	D	195	ASN

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Mol	Chain	Res	Type
1	D	207	GLU
1	D	218	VAL
1	D	262	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	B	261	ASN
1	B	272	ASN
1	C	188	HIS
1	C	272	ASN
1	C	300	HIS
1	D	99	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 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	NAI	D	1305	-	42,48,48	1.10	3 (7%)	47,73,73	1.30	4 (8%)
2	SO4	D	1303	-	4,4,4	0.27	0	6,6,6	0.06	0
2	SO4	A	1305	-	4,4,4	0.27	0	6,6,6	0.07	0
3	NAI	C	1304	-	42,48,48	1.29	5 (11%)	47,73,73	1.30	5 (10%)
2	SO4	D	1304	-	4,4,4	0.25	0	6,6,6	0.20	0
2	SO4	A	1304	-	4,4,4	0.31	0	6,6,6	0.32	0
3	NAI	B	1304	-	42,48,48	1.20	6 (14%)	47,73,73	1.36	4 (8%)
2	SO4	A	1303	-	4,4,4	0.24	0	6,6,6	0.10	0
3	NAI	A	1306	-	42,48,48	1.18	6 (14%)	47,73,73	1.29	4 (8%)

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	NAI	D	1305	-	-	7/25/72/72	0/5/5/5
3	NAI	C	1304	-	-	6/25/72/72	0/5/5/5
3	NAI	B	1304	-	-	10/25/72/72	0/5/5/5
3	NAI	A	1306	-	-	8/25/72/72	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1306	NAI	C6N-C5N	3.06	1.38	1.33
3	C	1304	NAI	C2A-N1A	3.05	1.39	1.33
3	D	1305	NAI	C6N-C5N	3.04	1.38	1.33
3	B	1304	NAI	C7N-C3N	2.83	1.54	1.48
3	C	1304	NAI	C7N-C3N	2.82	1.54	1.48
3	C	1304	NAI	C6N-C5N	2.76	1.38	1.33
3	B	1304	NAI	C6N-C5N	2.75	1.38	1.33
3	D	1305	NAI	C6N-N1N	2.74	1.44	1.37
3	D	1305	NAI	C4N-C5N	-2.66	1.41	1.48
3	B	1304	NAI	C2A-N1A	2.62	1.38	1.33
3	C	1304	NAI	C6N-N1N	2.57	1.43	1.37
3	A	1306	NAI	C6N-N1N	2.53	1.43	1.37
3	A	1306	NAI	C2A-N1A	2.49	1.38	1.33
3	B	1304	NAI	C6N-N1N	2.36	1.43	1.37
3	A	1306	NAI	C4A-N3A	2.33	1.38	1.35
3	C	1304	NAI	C4N-C5N	-2.19	1.43	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1306	NAI	C4N-C5N	-2.13	1.43	1.48
3	B	1304	NAI	C2N-C3N	2.03	1.40	1.34
3	A	1306	NAI	PA-O2A	-2.01	1.45	1.55
3	B	1304	NAI	C4N-C5N	-2.00	1.43	1.48

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1305	NAI	C3N-C2N-N1N	-5.13	115.78	123.10
3	A	1306	NAI	C3N-C2N-N1N	-4.66	116.45	123.10
3	C	1304	NAI	C3N-C2N-N1N	-4.65	116.46	123.10
3	B	1304	NAI	C3N-C2N-N1N	-4.60	116.53	123.10
3	A	1306	NAI	C1D-N1N-C2N	-3.40	115.46	121.11
3	B	1304	NAI	O4B-C1B-C2B	-3.25	102.18	106.93
3	C	1304	NAI	C1D-N1N-C2N	-3.18	115.82	121.11
3	A	1306	NAI	O4B-C1B-C2B	-3.09	102.41	106.93
3	D	1305	NAI	C1D-N1N-C2N	-2.93	116.23	121.11
3	B	1304	NAI	C1D-N1N-C2N	-2.85	116.36	121.11
3	B	1304	NAI	C4A-C5A-N7A	2.83	112.35	109.40
3	D	1305	NAI	C4A-C5A-N7A	2.65	112.16	109.40
3	D	1305	NAI	O4B-C1B-C2B	-2.63	103.08	106.93
3	C	1304	NAI	O4B-C1B-C2B	-2.60	103.13	106.93
3	A	1306	NAI	C4A-C5A-N7A	2.54	112.05	109.40
3	C	1304	NAI	C5A-C6A-N6A	2.26	123.78	120.35
3	C	1304	NAI	C4A-C5A-N7A	2.18	111.67	109.40

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1304	NAI	O4D-C1D-N1N-C6N
3	B	1304	NAI	C5B-O5B-PA-O1A
3	B	1304	NAI	O4D-C1D-N1N-C6N
3	D	1305	NAI	O4D-C1D-N1N-C6N
3	A	1306	NAI	O4D-C1D-N1N-C6N
3	B	1304	NAI	O4D-C4D-C5D-O5D
3	B	1304	NAI	C3D-C4D-C5D-O5D
3	B	1304	NAI	PN-O3-PA-O5B
3	A	1306	NAI	PN-O3-PA-O5B
3	D	1305	NAI	C5D-O5D-PN-O3
3	B	1304	NAI	C5B-O5B-PA-O3
3	A	1306	NAI	C5D-O5D-PN-O3

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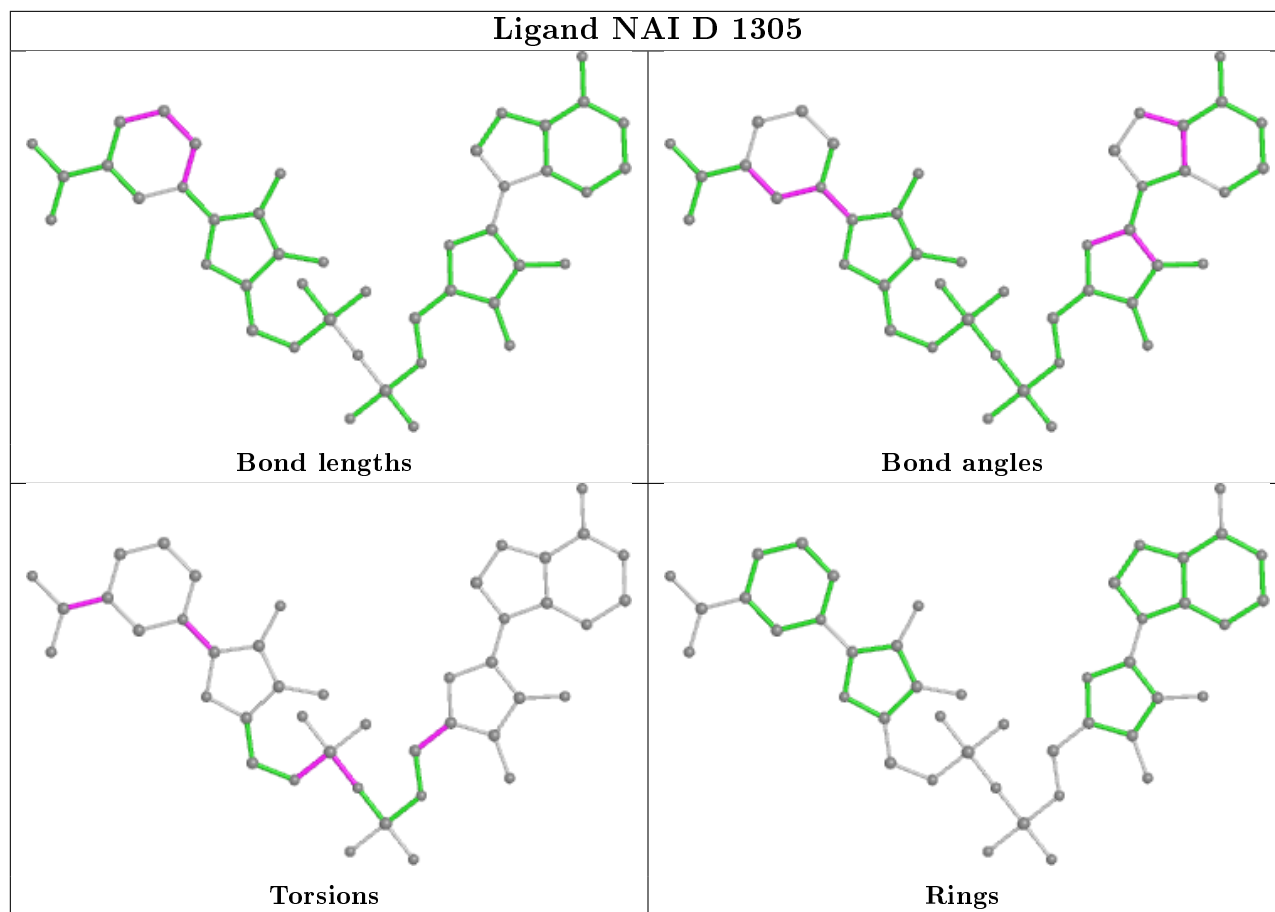
Mol	Chain	Res	Type	Atoms
3	D	1305	NAI	PA-O3-PN-O2N
3	C	1304	NAI	PA-O3-PN-O2N
3	B	1304	NAI	PA-O3-PN-O2N
3	A	1306	NAI	PA-O3-PN-O2N
3	D	1305	NAI	C5D-O5D-PN-O2N
3	C	1304	NAI	C5B-O5B-PA-O2A
3	B	1304	NAI	C5B-O5B-PA-O2A
3	A	1306	NAI	C5D-O5D-PN-O1N
3	A	1306	NAI	C5D-O5D-PN-O2N
3	D	1305	NAI	O4B-C4B-C5B-O5B
3	C	1304	NAI	O4B-C4B-C5B-O5B
3	B	1304	NAI	O4B-C4B-C5B-O5B
3	A	1306	NAI	O4B-C4B-C5B-O5B
3	C	1304	NAI	C5B-O5B-PA-O3
3	D	1305	NAI	C5D-O5D-PN-O1N
3	D	1305	NAI	C2N-C3N-C7N-N7N
3	C	1304	NAI	C2N-C3N-C7N-N7N
3	B	1304	NAI	C2N-C3N-C7N-N7N
3	A	1306	NAI	C2N-C3N-C7N-N7N

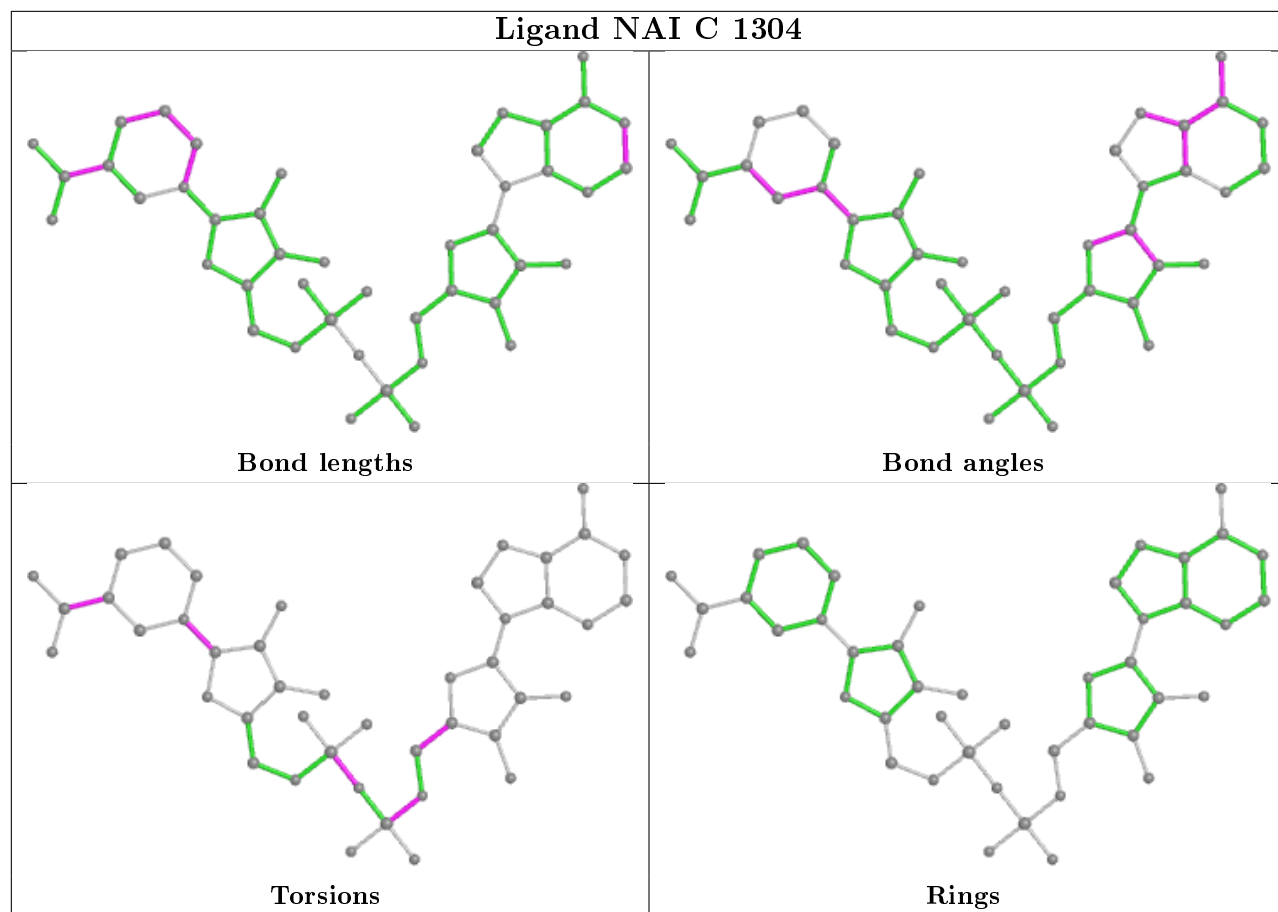
There are no ring outliers.

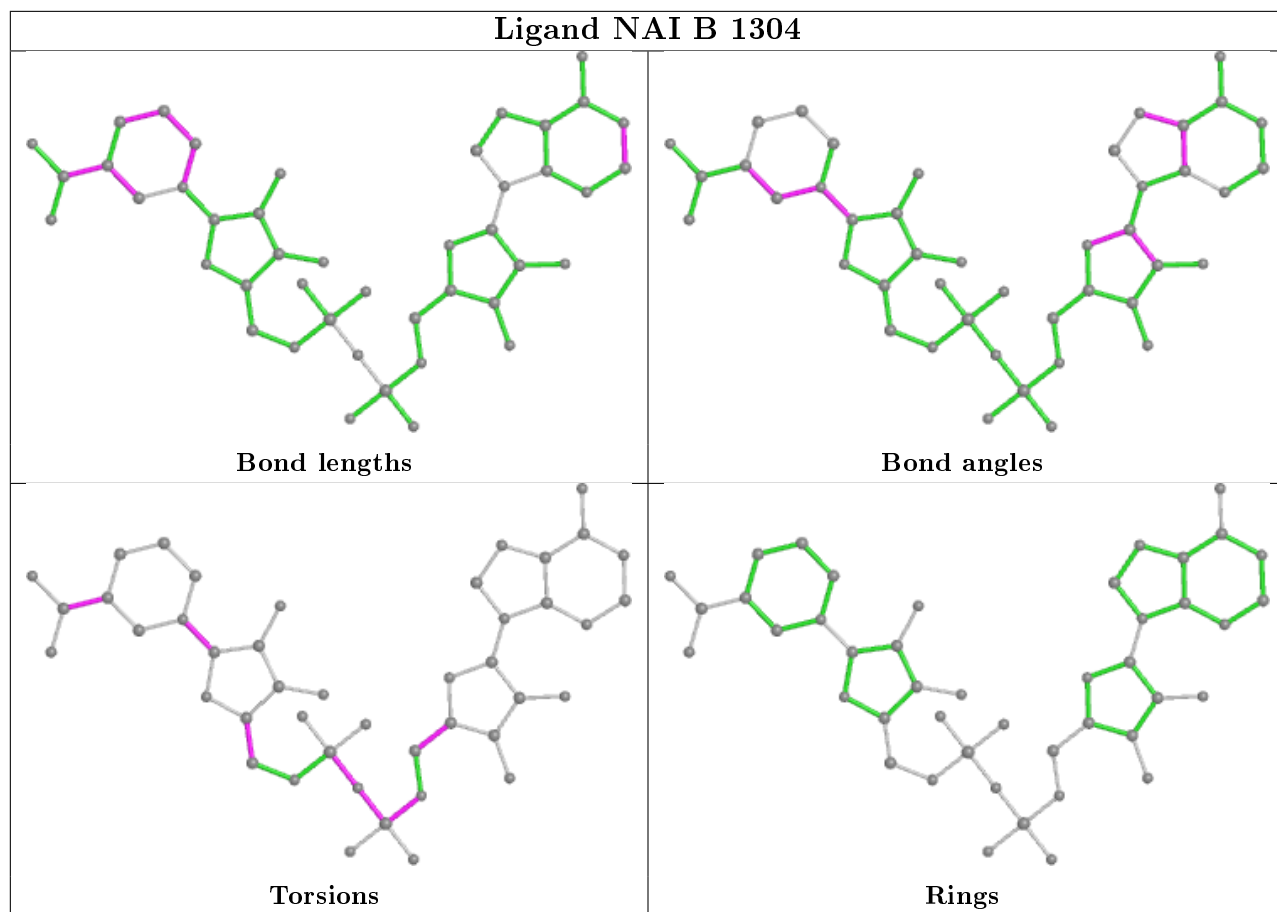
4 monomers are involved in 8 short contacts:

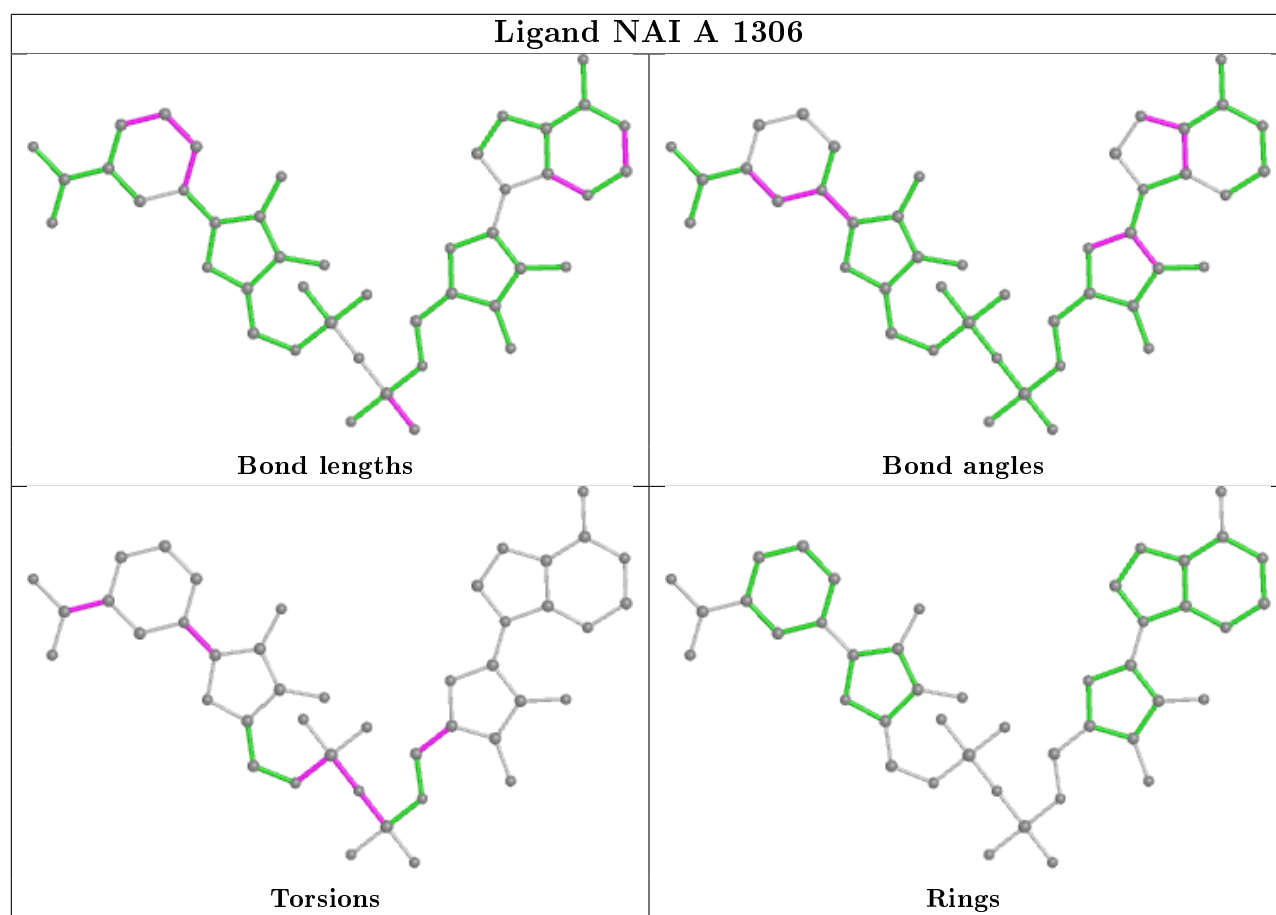
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1305	NAI	3	0
2	A	1305	SO4	1	0
3	C	1304	NAI	1	0
3	A	1306	NAI	3	0

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









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	297/319 (93%)	0.16	12 (4%) 38 41	10, 21, 40, 58	37 (12%)
1	B	276/319 (86%)	0.36	15 (5%) 25 28	9, 25, 44, 53	25 (9%)
1	C	285/319 (89%)	0.49	30 (10%) 6 7	12, 27, 50, 64	31 (10%)
1	D	297/319 (93%)	0.21	14 (4%) 31 34	10, 21, 42, 57	35 (11%)
All	All	1155/1276 (90%)	0.30	71 (6%) 21 23	9, 24, 45, 64	128 (11%)

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	261	ASN	7.7
1	C	48	VAL	6.4
1	A	204	VAL	5.4
1	D	262	GLN	5.2
1	C	45	PHE	4.9
1	D	300	HIS	4.8
1	C	52	SER	4.2
1	B	3	SER	4.2
1	B	52	SER	4.2
1	D	263	PRO	4.1
1	A	300	HIS	3.9
1	C	209	LEU	3.9
1	D	48	VAL	3.7
1	C	210	VAL	3.6
1	B	261	ASN	3.4
1	C	73	TYR	3.4
1	A	263	PRO	3.4
1	D	303	ASP	3.3
1	C	47	GLY	3.3
1	D	204	VAL	3.3
1	C	44	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	44	ASP	3.2
1	C	53	SER	3.2
1	A	3	SER	3.2
1	D	203	THR	3.1
1	B	14	VAL	3.1
1	B	43	GLY	3.1
1	C	60	GLU	3.1
1	B	212	ALA	3.1
1	C	49	GLY	3.0
1	B	69	ALA	3.0
1	A	262	GLN	2.9
1	A	260	ARG	2.9
1	D	261	ASN	2.8
1	C	87	LEU	2.7
1	A	48	VAL	2.6
1	B	260	ARG	2.5
1	C	88	ASP	2.5
1	C	69	ALA	2.4
1	C	65	ARG	2.4
1	D	304	SER	2.4
1	A	302	ILE	2.4
1	C	36	VAL	2.4
1	B	88	ASP	2.4
1	C	50	LYS	2.4
1	B	53	SER	2.4
1	B	37	VAL	2.4
1	C	261	ASN	2.3
1	B	38	VAL	2.3
1	C	64	ARG	2.3
1	C	263	PRO	2.3
1	A	14	VAL	2.3
1	C	62	ILE	2.3
1	C	66	GLY	2.2
1	C	12	VAL	2.2
1	C	134	ALA	2.2
1	D	3	SER	2.2
1	A	257	VAL	2.1
1	C	212	ALA	2.1
1	D	113	ASP	2.1
1	C	46	LYS	2.1
1	B	66	GLY	2.1
1	B	304	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	46	LYS	2.1
1	A	203	THR	2.0
1	C	93	ILE	2.0
1	C	262	GLN	2.0
1	B	65	ARG	2.0
1	C	38	VAL	2.0
1	D	42	GLY	2.0
1	C	23	ARG	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 carbohydrates in this entry.

6.4 Ligands [i](#)

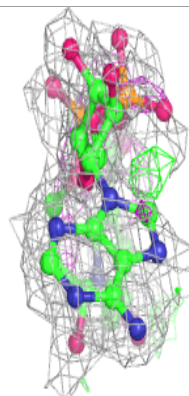
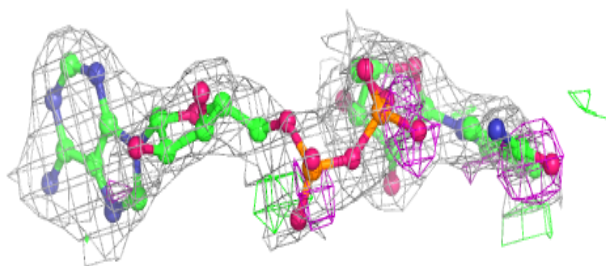
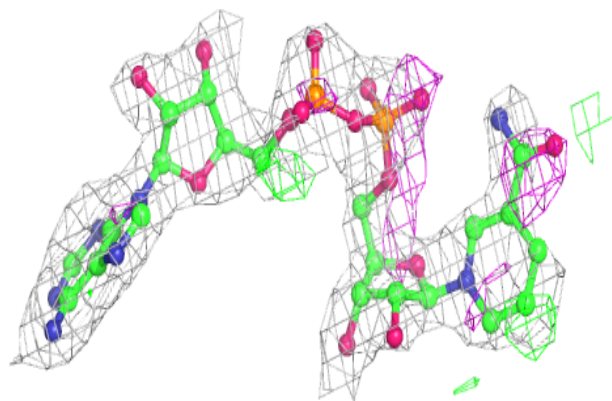
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	NAI	B	1304	44/44	0.80	0.27	28,43,56,58	0
2	SO4	A	1305	5/5	0.84	0.25	69,70,71,71	5
3	NAI	C	1304	44/44	0.87	0.24	31,41,46,49	0
2	SO4	D	1303	5/5	0.94	0.20	69,69,69,69	5
3	NAI	D	1305	44/44	0.94	0.13	18,23,28,30	0
2	SO4	A	1303	5/5	0.95	0.27	55,56,56,56	5
3	NAI	A	1306	44/44	0.95	0.12	15,21,26,33	0
2	SO4	A	1304	5/5	0.97	0.13	19,21,25,27	5
2	SO4	D	1304	5/5	0.97	0.10	24,25,26,28	5

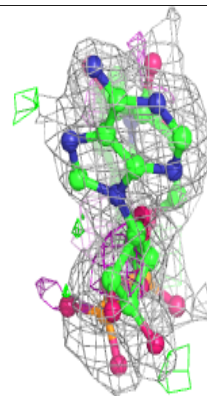
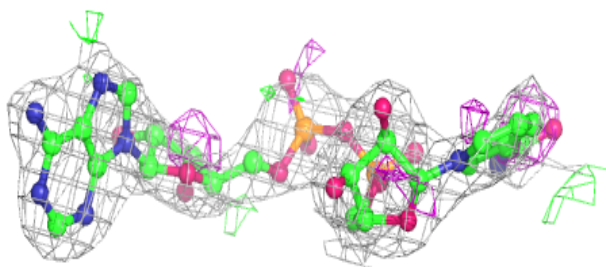
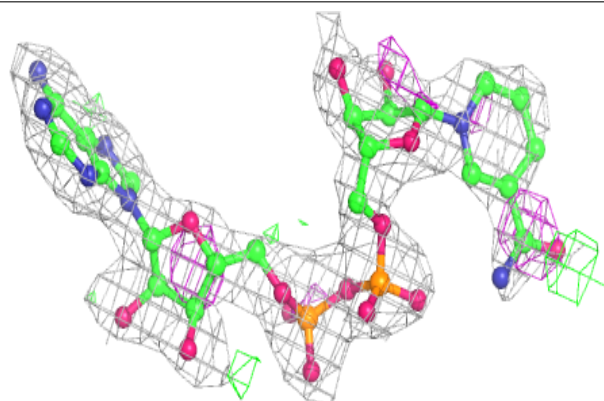
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NAI B 1304:

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

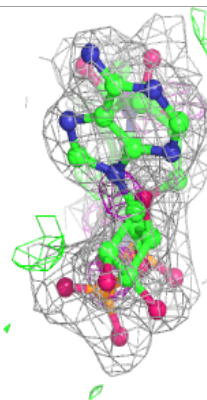
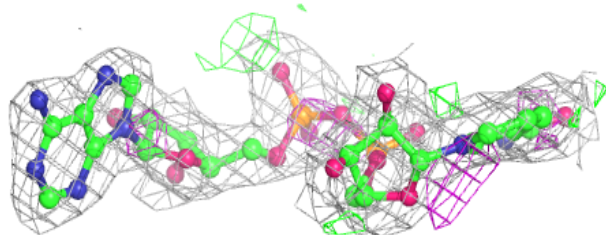
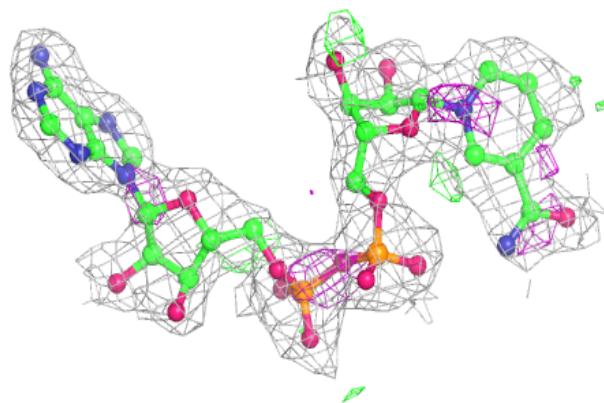
**Electron density around NAI C 1304:**

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

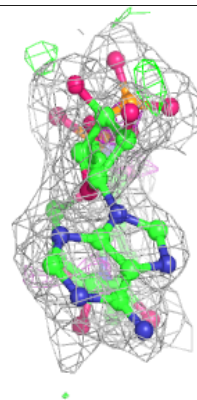
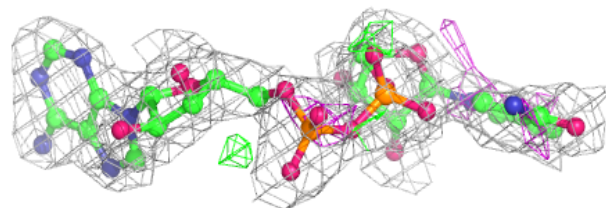
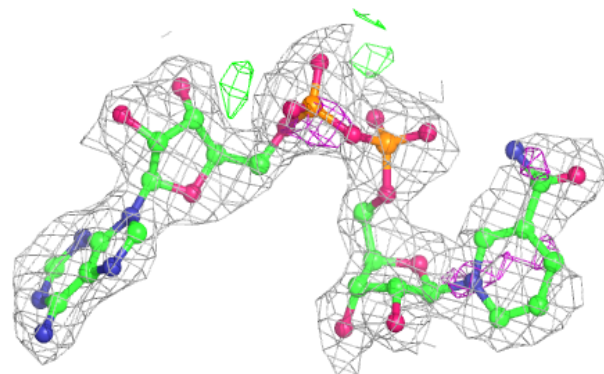


Electron density around NAI D 1305:

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

**Electron density around NAI A 1306:**

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



6.5 Other polymers

There are no such residues in this entry.