



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:13 PM UTC

PDB ID : 1GZ6 / pdb_00001gz6
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

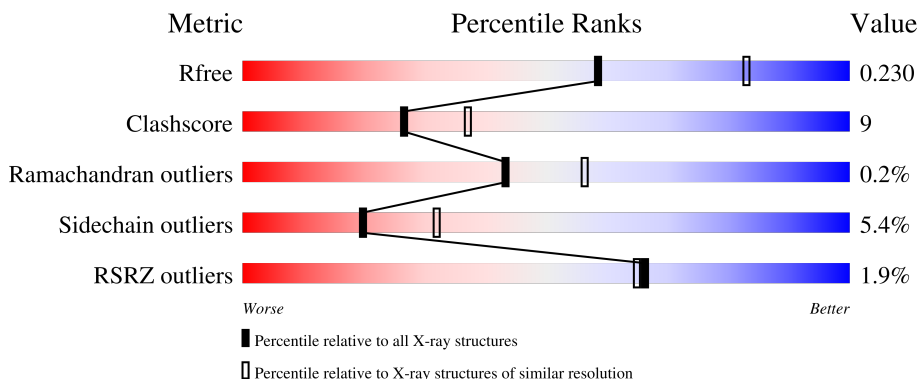
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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}	180053	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	319	
1	B	319	
1	C	319	
1	D	319	

2 Entry composition [i](#)

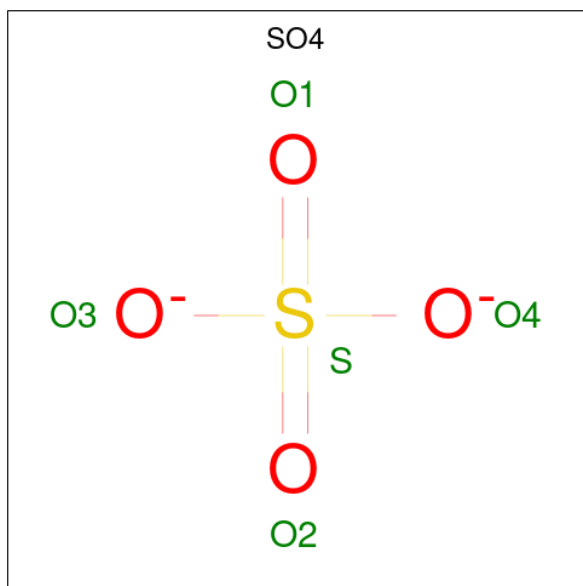
There are 4 unique types of molecules in this entry. The entry contains 9961 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



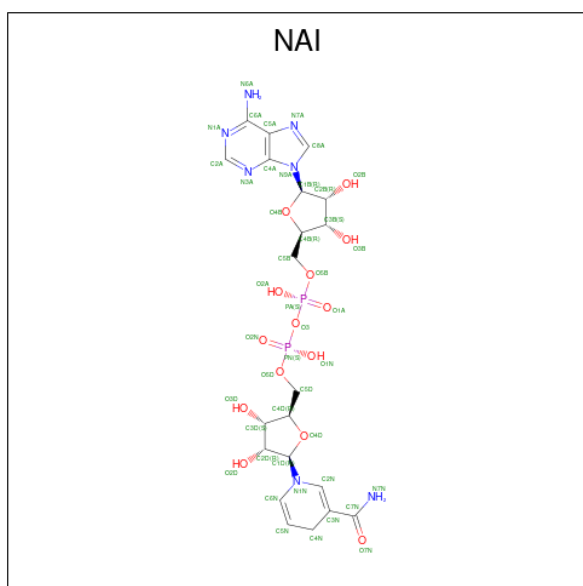
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

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 (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



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

- 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		

Continued on next page...

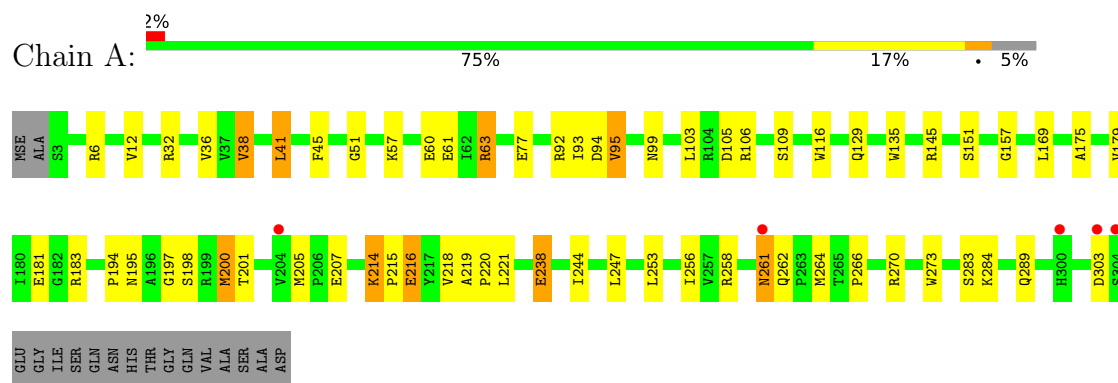
Continued from previous page...

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

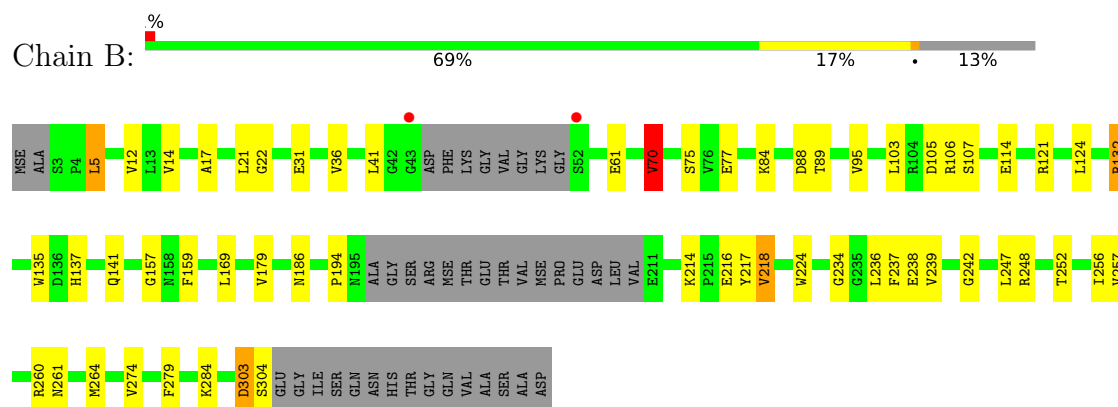
3 Residue-property plots

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.

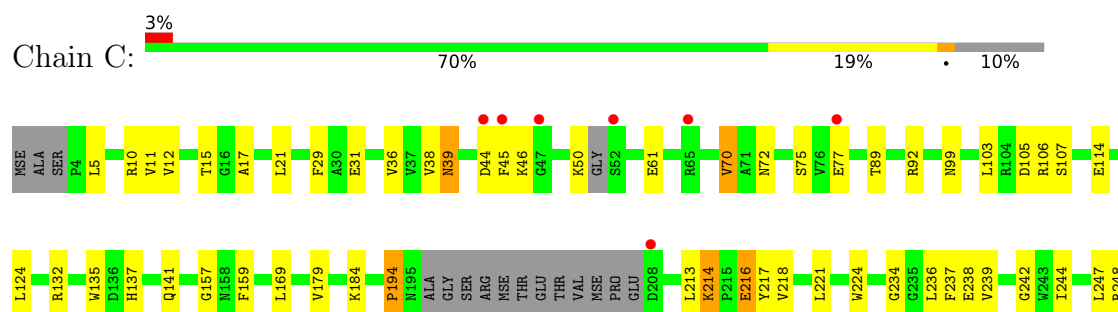
• Molecule 1: ESTRADIOL 17 BETA-DEHYDROGENASE 4

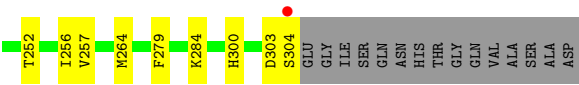


• Molecule 1: ESTRADIOL 17 BETA-DEHYDROGENASE 4

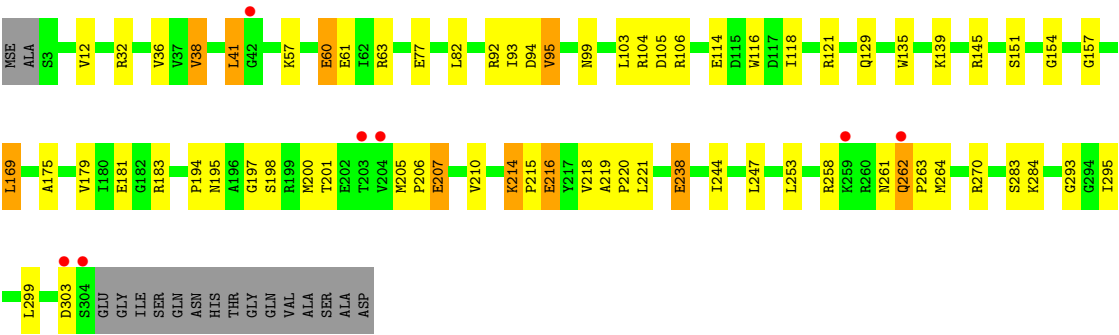


• Molecule 1: ESTRADIOL 17 BETA-DEHYDROGENASE 4





● 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 20.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.6 (20.00-2.38) 98.9 (20.00-2.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.54 (at 2.38Å)	Xtriage
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	Xtriage
Anisotropy	0.705	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9961	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage'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	0.64	1/2336 (0.0%)	1.06	11/3146 (0.3%)
1	B	0.60	3/2167 (0.1%)	1.00	10/2920 (0.3%)
1	C	0.60	3/2237 (0.1%)	1.02	10/3012 (0.3%)
1	D	0.60	1/2336 (0.0%)	1.06	11/3146 (0.3%)
All	All	0.61	8/9076 (0.1%)	1.03	42/12224 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	VAL	CB-CG2	-7.29	1.28	1.52
1	C	70	VAL	CB-CG1	-7.24	1.28	1.52
1	B	70	VAL	CB-CG1	-7.13	1.29	1.52
1	C	70	VAL	CB-CG2	-6.83	1.30	1.52
1	B	303	ASP	C-N	-5.91	1.25	1.33
1	C	303	ASP	C-N	-5.70	1.25	1.33
1	A	303	ASP	C-N	-5.26	1.25	1.33
1	D	303	ASP	C-N	-5.16	1.26	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	36	VAL	N-CA-C	8.51	120.84	108.58
1	A	214	LYS	N-CA-C	8.15	119.99	109.64
1	C	70	VAL	CG1-CB-CG2	-8.05	93.08	110.80
1	D	36	VAL	N-CA-C	7.86	119.17	108.17
1	C	36	VAL	N-CA-C	7.78	119.49	108.36
1	A	36	VAL	N-CA-C	7.52	118.70	108.17
1	B	135	TRP	N-CA-C	7.20	119.80	111.02
1	C	135	TRP	N-CA-C	7.13	119.72	111.02
1	B	70	VAL	CG1-CB-CG2	-6.90	95.62	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	ILE	N-CA-C	-6.57	98.18	108.23
1	D	63	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	C	256	ILE	N-CA-C	-6.20	98.74	108.23
1	B	107	SER	N-CA-C	-6.13	101.20	110.28
1	D	214	LYS	N-CA-C	6.13	117.62	109.83
1	D	63	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	B	237	PHE	N-CA-C	5.96	118.84	108.76
1	A	253	LEU	N-CA-C	-5.96	104.85	111.71
1	D	135	TRP	N-CA-C	5.94	118.27	111.02
1	B	214	LYS	N-CA-C	5.94	116.88	109.57
1	C	107	SER	N-CA-C	-5.91	101.53	110.28
1	D	238	GLU	N-CA-C	-5.88	100.12	109.76
1	C	214	LYS	N-CA-C	5.84	117.89	109.48
1	C	237	PHE	N-CA-C	5.83	118.61	108.76
1	B	121	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	B	157	GLY	N-CA-C	-5.71	105.48	112.68
1	A	135	TRP	N-CA-C	5.70	117.98	111.02
1	B	121	ARG	NE-CZ-NH2	5.67	124.31	119.20
1	D	104	ARG	NE-CZ-NH1	-5.63	115.87	121.50
1	D	253	LEU	N-CA-C	-5.62	105.24	111.71
1	A	238	GLU	N-CA-C	-5.61	100.56	109.76
1	C	157	GLY	N-CA-C	-5.55	105.69	112.68
1	A	6	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	D	104	ARG	NE-CZ-NH2	5.44	124.10	119.20
1	A	183	ARG	N-CA-C	5.43	117.65	111.02
1	D	183	ARG	N-CA-C	5.38	117.56	111.11
1	A	63	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	C	132	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	A	157	GLY	N-CA-C	-5.24	106.08	112.68
1	A	6	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	C	132	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	A	256	ILE	N-CA-C	-5.12	99.74	107.73
1	D	157	GLY	N-CA-C	-5.08	106.28	112.68

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	53	0
1	B	2135	0	2142	35	0
1	C	2204	0	2216	40	0
1	D	2302	0	2311	55	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	164	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 (164) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:207:GLU:H	1:D:207:GLU:CD	1.98	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:A:92:ARG:HD3	1:A:94:ASP:OD1	1.96	0.65
1:D:92:ARG:HD3	1:D:94:ASP:OD1	1.95	0.65
1:D:198:SER:H	1:D:201:THR:CG2	2.08	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
1:A:32:ARG:HG2	1:A:32:ARG:HH11	1.65	0.60
1:C:304:SER:N	4:C:2180:HOH:O	2.34	0.60
1:D:93:ILE:O	1:D:93:ILE:HG23	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:93:ILE:HG23	1:A:93:ILE:O	2.09	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:11:VAL:CG2	1:C:92:ARG:HG3	2.41	0.50
1:C:238:GLU:HG3	1:C:247:LEU:HD11	1.93	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:109:SER:HB2	4:A:2108:HOH:O	2.12	0.49
1:D:207:GLU:CD	1:D:207:GLU:N	2.66	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:D:283:SER:C	1:D:284:LYS:HD2	2.38	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:105:ASP:C	1:C:106:ARG:HG2	2.38	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
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:B:105:ASP:C	1:B:106:ARG:HG2	2.39	0.47
1:D:216:GLU:CD	1:D:216:GLU:H	2.21	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:A:283:SER:C	1:A:284:LYS:HD2	2.40	0.47
1:C:194:PRO:O	3:C:1304:NAI:H42N	2.14	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:A:216:GLU:H	1:A:216:GLU:CD	2.22	0.47
1:C:124:LEU:HG	1:D:116:TRP:HZ2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PHE:HB2	1:A:200:MSE:HG3	1.97	0.46
1:A:12:VAL:HG22	1:A:95:VAL:HG13	1.98	0.46
1:A:270:ARG:HG3	1:B:224:TRP:CH2	2.50	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:HG22	1:A:38:VAL:O	2.16	0.45
1:D:41:LEU:HD22	1:D:41:LEU:O	2.17	0.45
1:A:41:LEU:O	1:A:41:LEU:HD22	2.17	0.45
1:C:92:ARG:NH1	4:C:2044:HOH:O	2.40	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:75:SER:C	1:C:77:GLU:N	2.75	0.44
1:C:224:TRP:CH2	1:D:270:ARG:HG3	2.52	0.44
1:B:260:ARG:O	1:B:261:ASN:HB2	2.16	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: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:A:214:LYS:HG2	4:A:2164:HOH:O	2.18	0.43
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:252:THR:HG22	1:C:279:PHE:HA	1.99	0.43
1:C:257:VAL:CG2	1:C:264:MSE:HE3	2.49	0.43
1:D:139:LYS:HE2	1:D:139:LYS:HB3	1.86	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:B:75:SER:C	1:B:77:GLU:N	2.77	0.42
1:C:179:VAL:HG21	1:C:234:GLY:HA2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LEU:HD12	1:D:82:LEU:N	2.35	0.42
1:D:12:VAL:HG22	1:D:95:VAL:HG13	2.01	0.41
1:A:51:GLY:HA3	2:A:1305:SO4:O4	2.20	0.41
1:A:105:ASP:O	1:A:106:ARG:HD2	2.20	0.41
1:C:216:GLU:H	1:C:216:GLU:CD	2.27	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:D:205:MSE:HB3	1:D:210:VAL:HG23	2.03	0.41
1:A:273:TRP:CE3	1:A:273:TRP:HA	2.55	0.41
1:A:289:GLN:O	1:D:293:GLY:HA3	2.20	0.41
1:B:260:ARG:NH2	1:B:303:ASP:HA	2.36	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:D:205:MSE:O	1:D:206:PRO:C	2.64	0.41
1:A:32:ARG:HG2	1:A:32:ARG:NH1	2.35	0.40
1:A:214:LYS:HB3	1:A:216:GLU:CG	2.50	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%)	36 48

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	36	48
All	All	1155/1276 (90%)	1102 (95%)	51 (4%)	2 (0%)	43	56

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	ASN
1	D	261	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	238/245 (97%)	226 (95%)	12 (5%)	22	35
1	B	220/245 (90%)	207 (94%)	13 (6%)	18	28
1	C	227/245 (93%)	212 (93%)	15 (7%)	15	24
1	D	238/245 (97%)	228 (96%)	10 (4%)	26	42
All	All	923/980 (94%)	873 (95%)	50 (5%)	20	32

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	VAL
1	A	41	LEU
1	A	60	GLU
1	A	63	ARG
1	A	95	VAL
1	A	169	LEU
1	A	195	ASN
1	A	200	MSE
1	A	207	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	216	GLU
1	A	218	VAL
1	A	262	GLN
1	B	5	LEU
1	B	31	GLU
1	B	61	GLU
1	B	70	VAL
1	B	103	LEU
1	B	114	GLU
1	B	132	ARG
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	C	5	LEU
1	C	10	ARG
1	C	21	LEU
1	C	31	GLU
1	C	39	ASN
1	C	44	ASP
1	C	61	GLU
1	C	103	LEU
1	C	114	GLU
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	D	38	VAL
1	D	41	LEU
1	D	60	GLU
1	D	95	VAL
1	D	169	LEU
1	D	195	ASN
1	D	207	GLU
1	D	216	GLU
1	D	218	VAL
1	D	262	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	158	ASN
1	A	161	GLN
1	B	158	ASN
1	B	188	HIS
1	B	261	ASN
1	B	281	ASN
1	C	158	ASN
1	C	188	HIS
1	C	272	ASN
1	C	300	HIS
1	D	99	ASN
1	D	158	ASN
1	D	161	GLN

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 oligosaccharides 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
2	SO4	A	1305	-	4,4,4	0.38	0	6,6,6	0.11	0
2	SO4	D	1303	-	4,4,4	0.38	0	6,6,6	0.10	0
3	NAI	B	1304	-	47,48,48	1.34	7 (14%)	64,73,73	1.39	4 (6%)
3	NAI	D	1305	-	47,48,48	1.13	3 (6%)	64,73,73	1.36	4 (6%)
3	NAI	C	1304	-	47,48,48	1.39	7 (14%)	64,73,73	1.35	4 (6%)
2	SO4	A	1303	-	4,4,4	0.35	0	6,6,6	0.13	0
3	NAI	A	1306	-	47,48,48	1.25	7 (14%)	64,73,73	1.38	4 (6%)
2	SO4	A	1304	-	4,4,4	0.41	0	6,6,6	0.31	0
2	SO4	D	1304	-	4,4,4	0.36	0	6,6,6	0.23	0

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	A	1306	-	-	9/29/72/72	0/5/5/5
3	NAI	D	1305	-	-	7/29/72/72	0/5/5/5
3	NAI	C	1304	-	-	6/29/72/72	0/5/5/5
3	NAI	B	1304	-	-	11/29/72/72	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1304	NAI	PA-O3	-3.28	1.56	1.59
3	C	1304	NAI	C2A-N1A	3.17	1.39	1.33
3	C	1304	NAI	C8A-N7A	3.00	1.37	1.31
3	B	1304	NAI	C8A-N7A	2.92	1.37	1.31
3	B	1304	NAI	C7N-C3N	2.83	1.54	1.48
3	D	1305	NAI	C6N-N1N	2.83	1.44	1.37
3	C	1304	NAI	C7N-C3N	2.82	1.54	1.48
3	C	1304	NAI	PA-O3	-2.73	1.56	1.59
3	B	1304	NAI	C2A-N1A	2.73	1.38	1.33
3	D	1305	NAI	C4N-C5N	-2.73	1.41	1.49
3	C	1304	NAI	C6N-N1N	2.66	1.43	1.37
3	A	1306	NAI	C6N-N1N	2.62	1.43	1.37
3	A	1306	NAI	C2A-N1A	2.60	1.38	1.33
3	B	1304	NAI	C6N-N1N	2.44	1.43	1.37
3	A	1306	NAI	C4A-N3A	2.38	1.38	1.34
3	C	1304	NAI	C5A-C4A	2.33	1.43	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1306	NAI	C8A-N7A	2.32	1.36	1.31
3	C	1304	NAI	C4N-C5N	-2.25	1.43	1.49
3	D	1305	NAI	C8A-N7A	2.24	1.36	1.31
3	A	1306	NAI	C4N-C5N	-2.19	1.43	1.49
3	A	1306	NAI	PA-O3	-2.18	1.57	1.59
3	B	1304	NAI	C4N-C5N	-2.06	1.43	1.49
3	B	1304	NAI	C5A-C4A	2.05	1.42	1.39
3	A	1306	NAI	PA-O2A	-2.04	1.45	1.55

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1306	NAI	C6N-N1N-C2N	6.97	126.78	119.32
3	B	1304	NAI	C6N-N1N-C2N	6.91	126.71	119.32
3	C	1304	NAI	C6N-N1N-C2N	6.90	126.70	119.32
3	D	1305	NAI	C6N-N1N-C2N	6.77	126.56	119.32
3	D	1305	NAI	C3N-C2N-N1N	-5.06	115.78	123.20
3	A	1306	NAI	C3N-C2N-N1N	-4.60	116.45	123.20
3	C	1304	NAI	C3N-C2N-N1N	-4.60	116.46	123.20
3	B	1304	NAI	C3N-C2N-N1N	-4.55	116.53	123.20
3	A	1306	NAI	C1D-N1N-C2N	-3.45	115.46	121.14
3	C	1304	NAI	C1D-N1N-C2N	-3.23	115.82	121.14
3	D	1305	NAI	C1D-N1N-C2N	-2.98	116.23	121.14
3	B	1304	NAI	C1D-N1N-C2N	-2.90	116.36	121.14
3	C	1304	NAI	O2A-PA-O3	2.13	113.03	107.27
3	A	1306	NAI	O2A-PA-O3	2.12	112.99	107.27
3	B	1304	NAI	O4B-C1B-C2B	-2.07	102.18	106.62
3	D	1305	NAI	O2A-PA-O3	2.03	112.77	107.27

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1306	NAI	C5D-O5D-PN-O2N
3	B	1304	NAI	C5B-O5B-PA-O1A
3	B	1304	NAI	C5B-O5B-PA-O3
3	B	1304	NAI	O4D-C1D-N1N-C6N
3	C	1304	NAI	O4D-C1D-N1N-C6N
3	D	1305	NAI	C5D-O5D-PN-O2N
3	A	1306	NAI	O4D-C1D-N1N-C6N
3	D	1305	NAI	O4D-C1D-N1N-C6N
3	B	1304	NAI	O4D-C4D-C5D-O5D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	1304	NAI	C3D-C4D-C5D-O5D
3	A	1306	NAI	PN-O3-PA-O5B
3	B	1304	NAI	PN-O3-PA-O5B
3	A	1306	NAI	PA-O3-PN-O2N
3	B	1304	NAI	PA-O3-PN-O2N
3	C	1304	NAI	PA-O3-PN-O2N
3	D	1305	NAI	PA-O3-PN-O2N
3	A	1306	NAI	C5D-O5D-PN-O3
3	A	1306	NAI	C5D-O5D-PN-O1N
3	B	1304	NAI	C5B-O5B-PA-O2A
3	C	1304	NAI	C5B-O5B-PA-O2A
3	D	1305	NAI	C5D-O5D-PN-O3
3	A	1306	NAI	C2N-C3N-C7N-N7N
3	B	1304	NAI	C2N-C3N-C7N-N7N
3	C	1304	NAI	C2N-C3N-C7N-N7N
3	D	1305	NAI	C2N-C3N-C7N-N7N
3	B	1304	NAI	O4B-C4B-C5B-O5B
3	C	1304	NAI	O4B-C4B-C5B-O5B
3	D	1305	NAI	O4B-C4B-C5B-O5B
3	A	1306	NAI	O4B-C4B-C5B-O5B
3	A	1306	NAI	PA-O3-PN-O1N
3	B	1304	NAI	PA-O3-PN-O1N
3	C	1304	NAI	PA-O3-PN-O1N
3	D	1305	NAI	PA-O3-PN-O1N

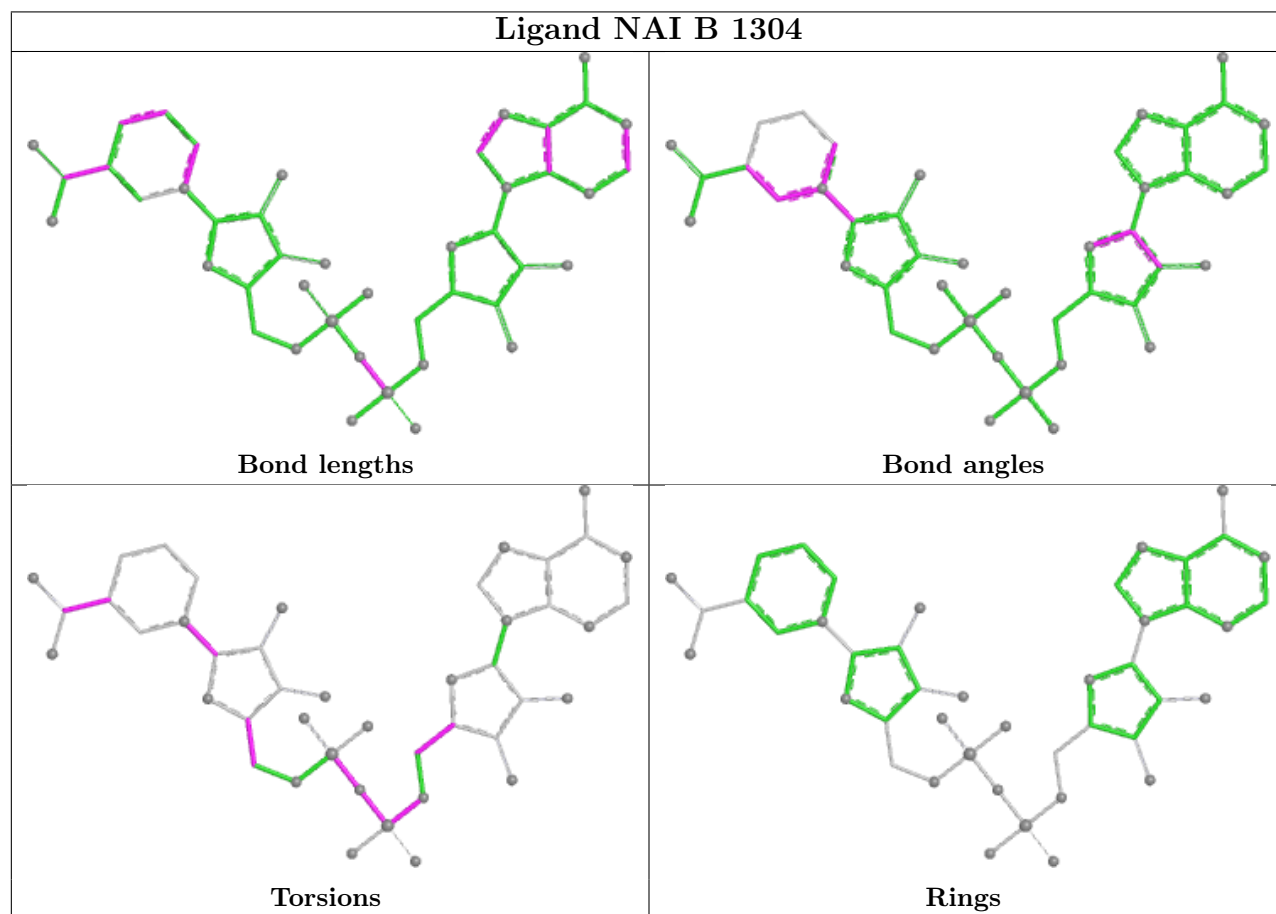
There are no ring outliers.

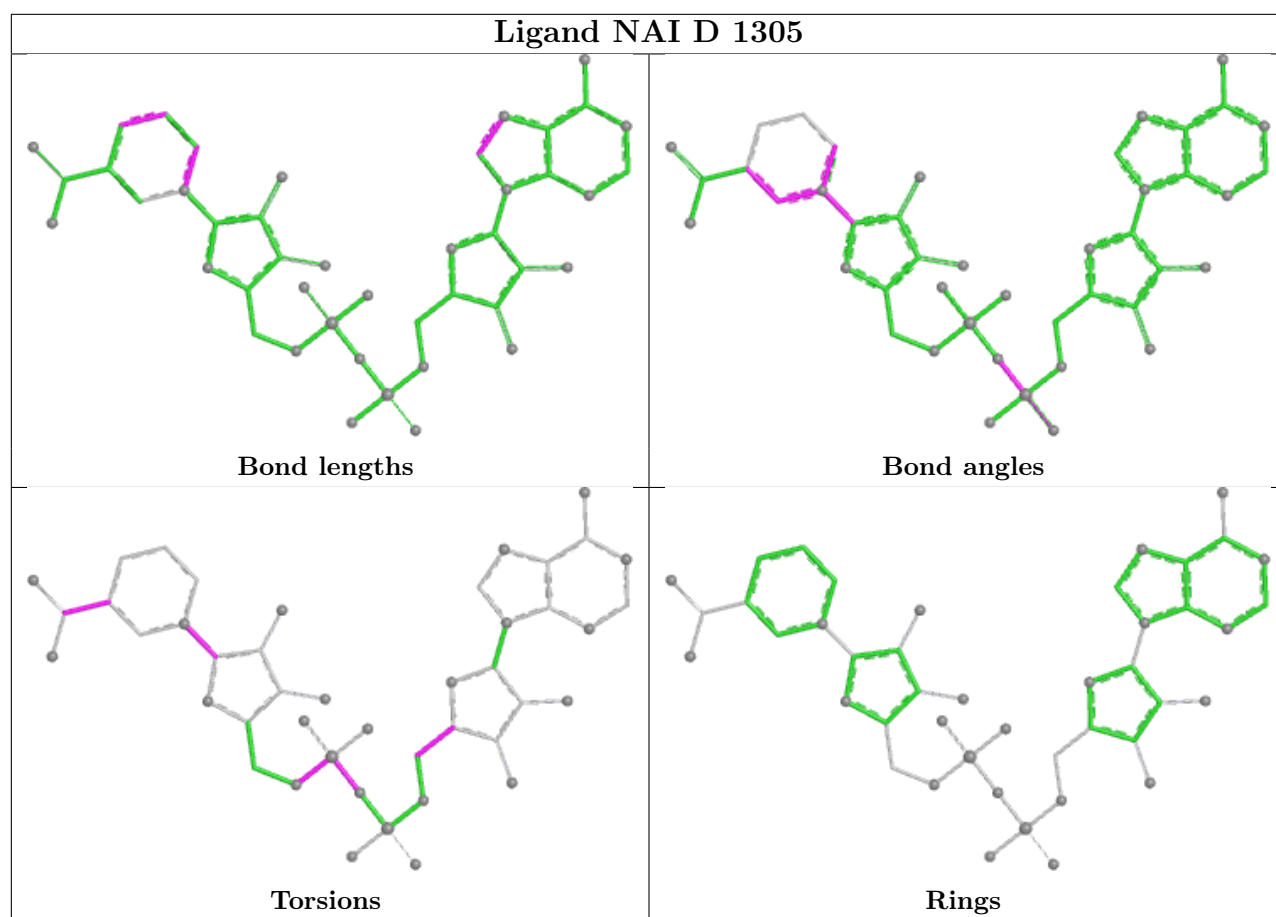
4 monomers are involved in 8 short contacts:

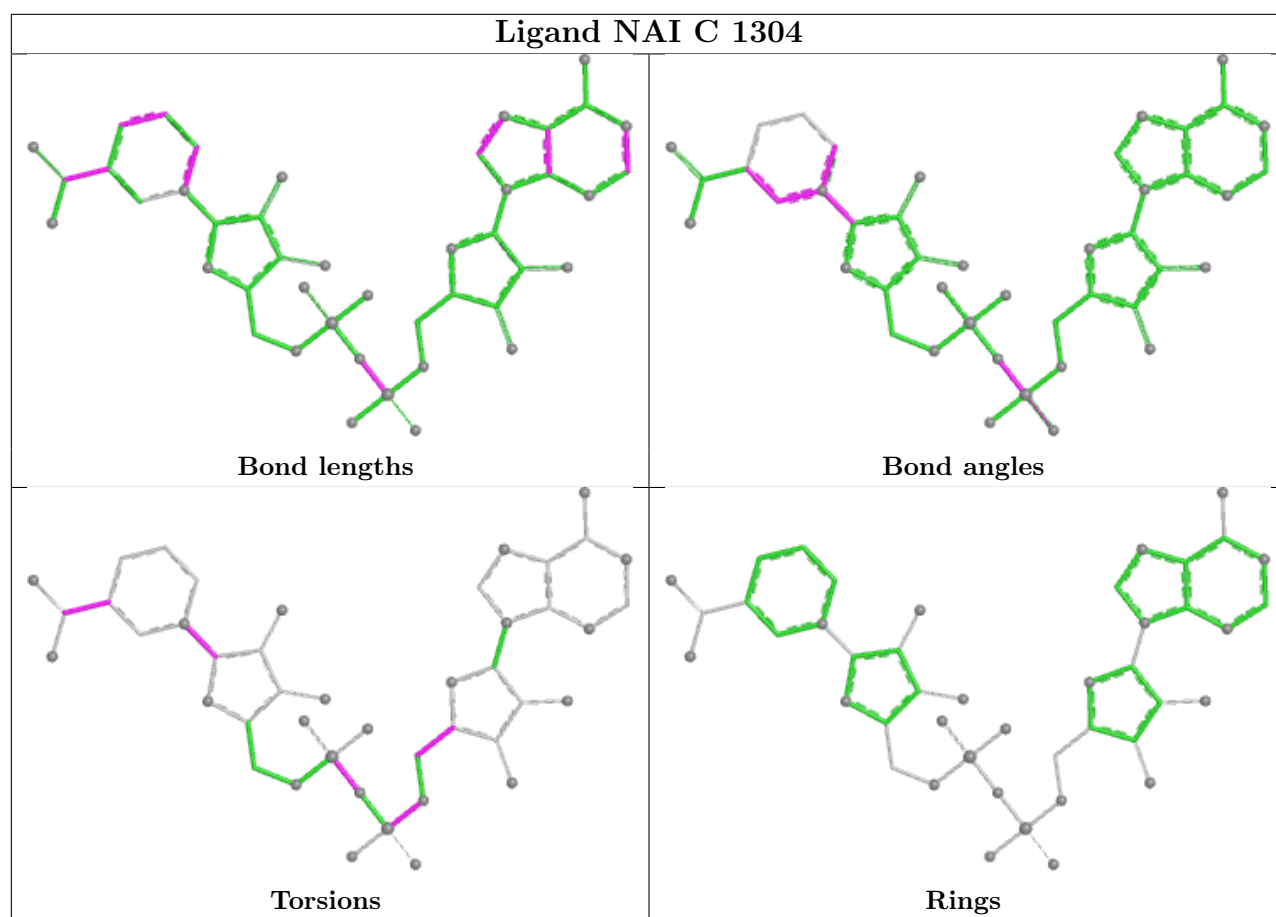
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1305	SO4	1	0
3	D	1305	NAI	3	0
3	C	1304	NAI	1	0
3	A	1306	NAI	3	0

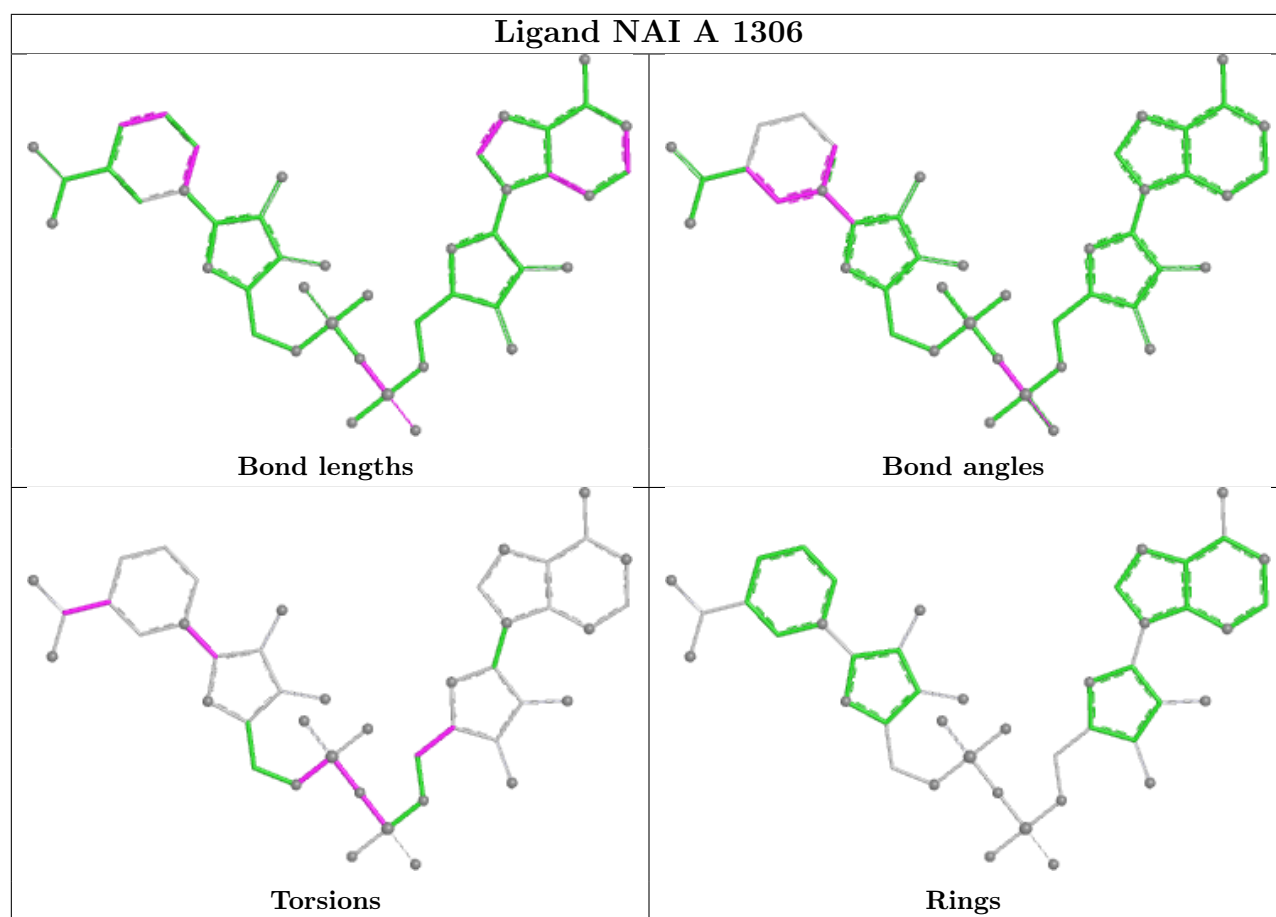
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	297/319 (93%)	-0.17	5 (1%) 69 68	10, 20, 37, 54	37 (12%)
1	B	276/319 (86%)	-0.02	2 (0%) 84 83	9, 24, 42, 53	25 (9%)
1	C	285/319 (89%)	0.08	8 (2%) 55 54	12, 25, 45, 64	31 (10%)
1	D	297/319 (93%)	-0.12	7 (2%) 59 59	10, 20, 38, 53	35 (11%)
All	All	1155/1276 (90%)	-0.06	22 (1%) 66 65	9, 23, 42, 64	128 (11%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	45	PHE	6.6
1	D	262	GLN	4.9
1	A	204	VAL	3.9
1	D	203	THR	3.6
1	A	261	ASN	3.3
1	A	304	SER	3.2
1	C	77	GLU	3.1
1	C	52	SER	3.1
1	C	304	SER	2.9
1	D	304	SER	2.8
1	B	43	GLY	2.6
1	D	204	VAL	2.6
1	D	42	GLY	2.4
1	D	303	ASP	2.3
1	D	259	LYS	2.3
1	C	47	GLY	2.2
1	C	44	ASP	2.2
1	A	303	ASP	2.1
1	C	65	ARG	2.1
1	C	208	ASP	2.1
1	B	52	SER	2.0
1	A	300	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

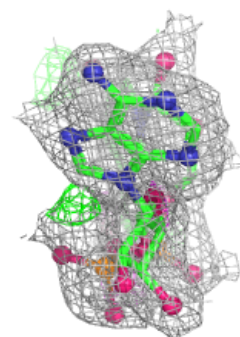
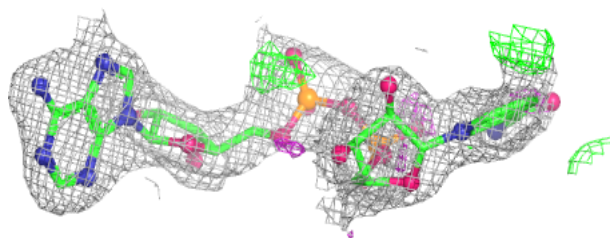
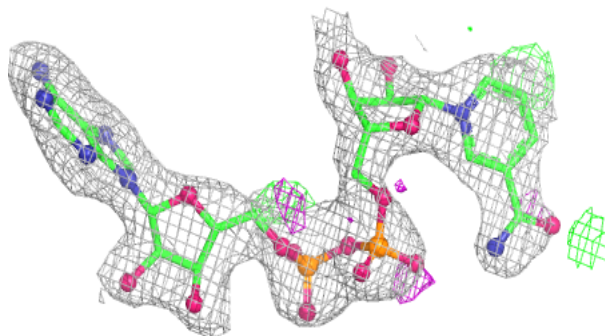
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1305	5/5	0.80	0.19	69,70,71,71	5
2	SO4	D	1303	5/5	0.84	0.13	69,69,69,69	5
3	NAI	B	1304	44/44	0.85	0.12	28,43,56,58	0
2	SO4	A	1303	5/5	0.88	0.12	55,56,56,56	5
3	NAI	C	1304	44/44	0.92	0.09	31,41,46,49	0
3	NAI	D	1305	44/44	0.95	0.07	18,23,28,30	0
3	NAI	A	1306	44/44	0.96	0.07	15,21,26,33	0
2	SO4	A	1304	5/5	0.96	0.09	19,21,25,27	5
2	SO4	D	1304	5/5	0.97	0.07	24,25,26,28	5

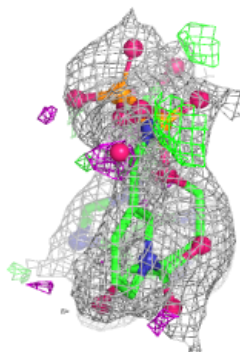
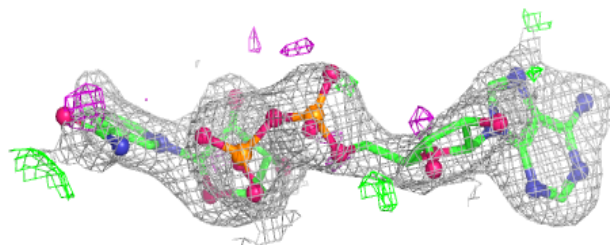
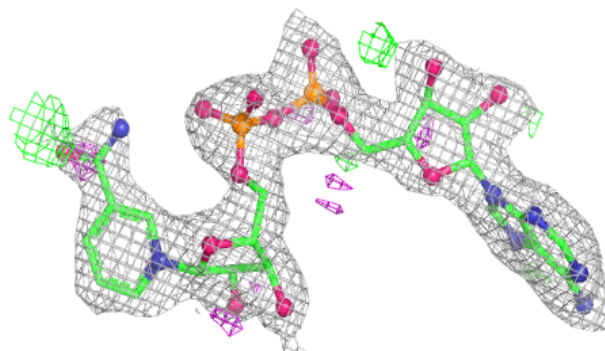
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

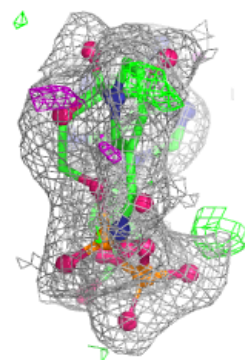
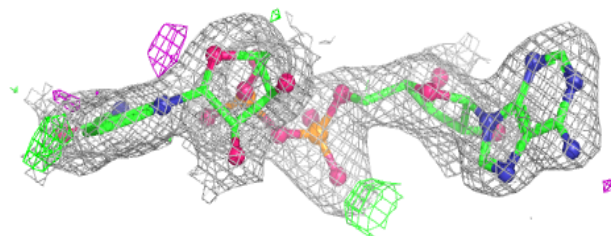
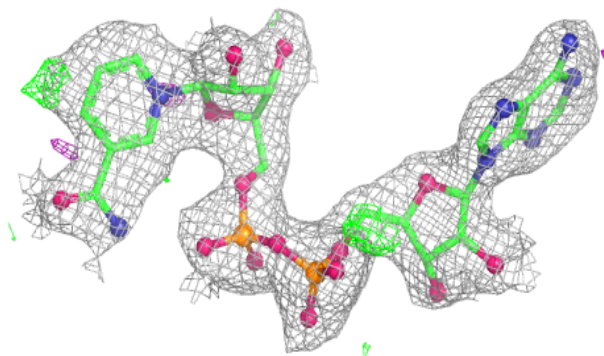
**Electron density around NAI C 1304:**

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

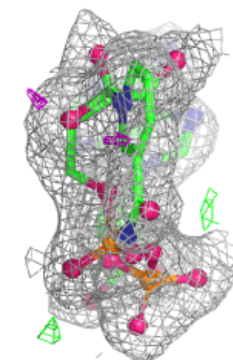
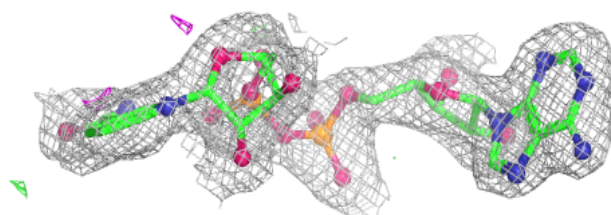
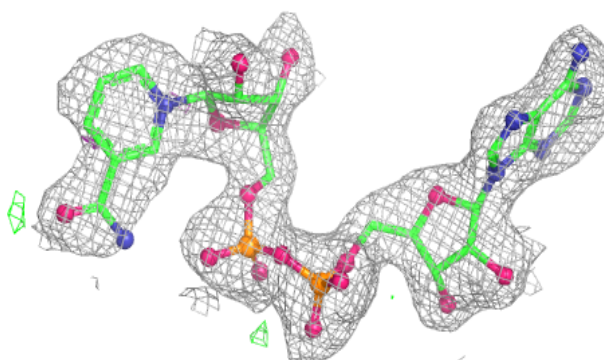


Electron density around NAI D 1305:

$2mF_o-DF_c$ (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.