



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:12 pm BST

PDB ID : 1IHX
Title : Crystal structure of two D-glyceraldehyde-3-phosphate dehydrogenase complexes: a case of asymmetry
Authors : Shen, Y.-Q.; Song, S.-Y.; Lin, Z.-J.
Deposited on : 2001-04-20
Resolution : 2.80 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

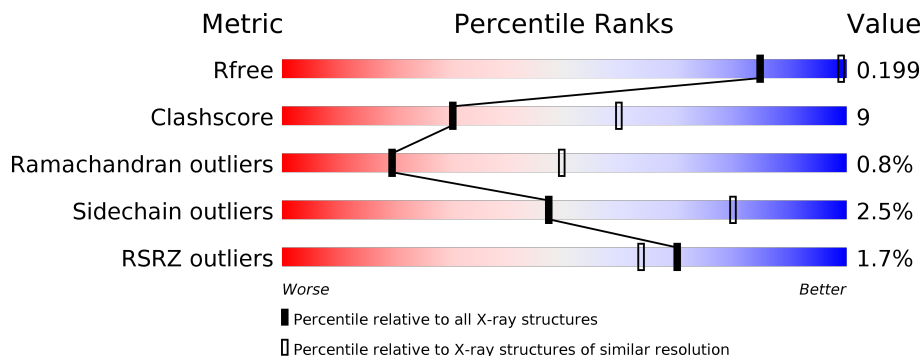
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	333	 80% 18%
1	B	333	 82% 16%
1	C	333	 78% 20%
1	D	333	 78% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10476 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 GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	333	2512	1593	421	482	16	0	0	0
1	B	333	2512	1593	421	482	16	0	0	0
1	C	333	2512	1593	421	482	16	0	0	0
1	D	333	2512	1593	421	482	16	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	THR	ALA	SEE REMARK 999	UNP P56649
A	59	VAL	ALA	SEE REMARK 999	UNP P56649
A	261	THR	ALA	SEE REMARK 999	UNP P56649
B	18	THR	ALA	SEE REMARK 999	UNP P56649
B	59	VAL	ALA	SEE REMARK 999	UNP P56649
B	261	THR	ALA	SEE REMARK 999	UNP P56649
C	18	THR	ALA	SEE REMARK 999	UNP P56649
C	59	VAL	ALA	SEE REMARK 999	UNP P56649
C	261	THR	ALA	SEE REMARK 999	UNP P56649
D	18	THR	ALA	SEE REMARK 999	UNP P56649
D	59	VAL	ALA	SEE REMARK 999	UNP P56649
D	261	THR	ALA	SEE REMARK 999	UNP P56649

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



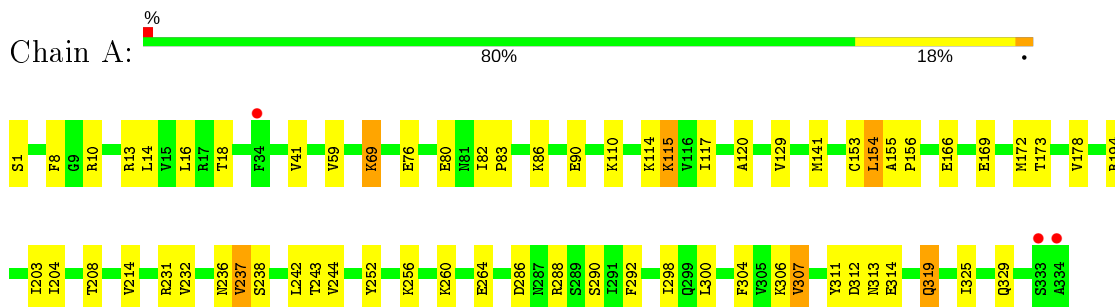
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is THIONICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: SND) (formula: C₂₁H₂₇N₇O₁₃P₂S).

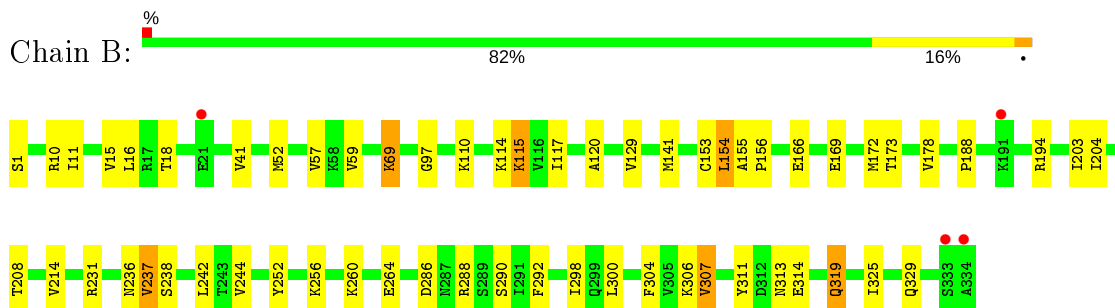
3 Residue-property plots [i](#)

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.

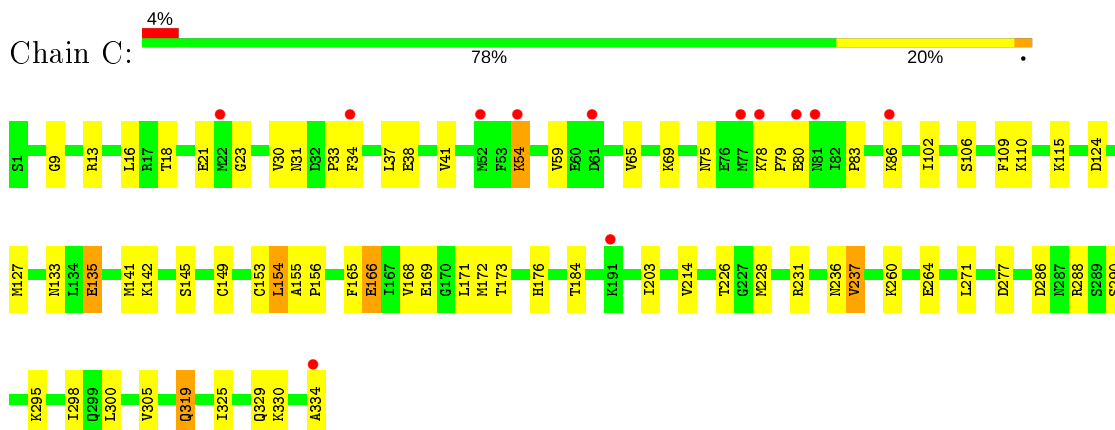
- Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE



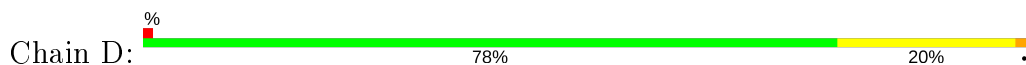
- Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE

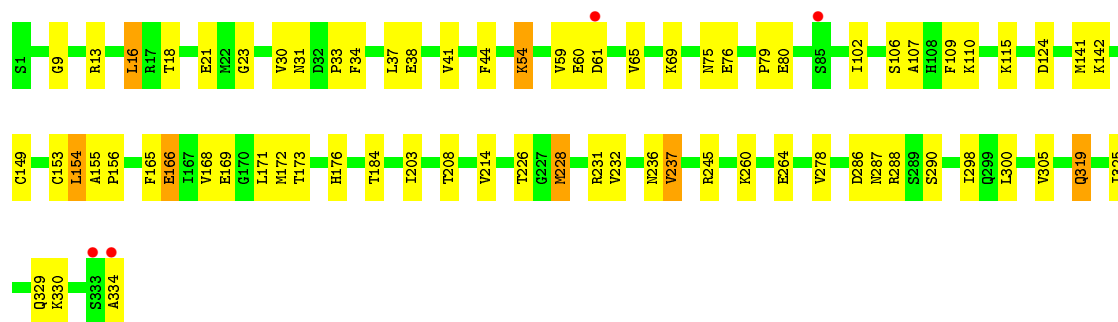


- Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE



- Molecule 1: GLYCERALDEHYDE 3-PHOSPHATE DEHYDROGENASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.41Å 100.51Å 128.44Å 90.00° 110.49° 90.00°	Depositor
Resolution (Å)	29.84 – 2.80 29.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.84-2.80) 97.9 (29.84-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.80Å)	Xtrriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.177 , 0.204 0.171 , 0.199	Depositor DCC
R_{free} test set	4424 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtrriage
Anisotropy	0.208	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 54.4	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	10476	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.19% 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: SND, 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	0.45	0/2557	0.76	4/3455 (0.1%)
1	B	0.46	0/2557	0.75	4/3455 (0.1%)
1	C	0.42	0/2557	0.63	1/3455 (0.0%)
1	D	0.43	0/2557	0.64	1/3455 (0.0%)
All	All	0.44	0/10228	0.70	10/13820 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	10	ARG	NE-CZ-NH2	-13.21	113.70	120.30
1	B	10	ARG	NE-CZ-NH1	-12.53	114.04	120.30
1	A	10	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	B	10	ARG	NE-CZ-NH2	11.79	126.19	120.30
1	B	10	ARG	CD-NE-CZ	6.69	132.97	123.60
1	D	203	ILE	N-CA-C	-6.28	94.05	111.00
1	A	10	ARG	CD-NE-CZ	6.07	132.10	123.60
1	C	203	ILE	N-CA-C	-5.99	94.83	111.00
1	A	203	ILE	N-CA-C	-5.59	95.92	111.00
1	B	203	ILE	N-CA-C	-5.54	96.03	111.00

There are no chirality outliers.

There are no planarity outliers.

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	2512	0	2537	48	0
1	B	2512	0	2537	45	0
1	C	2512	0	2537	56	0
1	D	2512	0	2537	54	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
3	A	36	0	20	1	0
3	B	36	0	20	2	0
3	C	44	0	26	3	0
3	D	44	0	26	2	0
4	A	61	0	0	3	0
4	B	68	0	0	2	0
4	C	50	0	0	1	0
4	D	49	0	0	3	0
All	All	10476	0	10240	191	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 (191) 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:80:GLU:HB2	1:A:110:LYS:HD3	1.32	1.05
1:B:120:ALA:HB2	3:B:336:SND:O3D	1.79	0.83
1:D:168:VAL:HG12	1:D:169:GLU:HG2	1.59	0.83
1:D:154:LEU:HD13	1:D:214:VAL:HG21	1.62	0.82
1:C:154:LEU:HD13	1:C:214:VAL:HG21	1.61	0.82
1:A:80:GLU:CB	1:A:110:LYS:HD3	2.12	0.80
1:B:154:LEU:HD13	1:B:214:VAL:HG21	1.64	0.80
1:A:154:LEU:HD13	1:A:214:VAL:HG21	1.67	0.76
1:C:168:VAL:HG12	1:C:169:GLU:HG2	1.67	0.75
1:C:80:GLU:HB2	1:C:110:LYS:HD3	1.68	0.74
1:C:149:CYS:HB3	3:C:337:SND:H4N	1.69	0.73
1:C:33:PRO:HG2	1:C:34:PHE:CD1	2.25	0.72
1:D:286:ASP:OD2	1:D:288:ARG:HD3	1.89	0.71
1:C:286:ASP:OD2	1:C:288:ARG:HD3	1.90	0.71
1:D:33:PRO:HG2	1:D:34:PHE:CD1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:VAL:HG21	1:C:59:VAL:HG23	1.72	0.69
1:D:41:VAL:HG21	1:D:59:VAL:HG23	1.74	0.69
1:A:69:LYS:HB2	1:A:69:LYS:NZ	2.07	0.68
1:A:153:CYS:HA	1:A:290:SER:HB2	1.76	0.68
1:C:33:PRO:HG2	1:C:34:PHE:HD1	1.58	0.67
1:D:33:PRO:HG2	1:D:34:PHE:HD1	1.60	0.67
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.78	0.65
1:B:153:CYS:HA	1:B:290:SER:HB2	1.78	0.64
1:B:69:LYS:HB2	1:B:69:LYS:NZ	2.13	0.63
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.82	0.62
1:C:115:LYS:HE2	1:C:141:MET:O	2.00	0.62
1:D:171:LEU:HD23	1:D:226:THR:HG23	1.82	0.61
1:C:171:LEU:HD23	1:C:226:THR:HG23	1.83	0.61
1:A:286:ASP:OD2	1:A:288:ARG:HD3	2.00	0.61
1:A:114:LYS:O	1:A:115:LYS:HD2	2.00	0.60
1:D:115:LYS:HE2	1:D:141:MET:O	2.01	0.60
1:B:114:LYS:O	1:B:115:LYS:HD2	2.01	0.59
1:A:172:MET:HG2	1:A:173:THR:N	2.16	0.58
1:D:149:CYS:HB3	3:D:338:SND:H4N	1.86	0.58
1:B:286:ASP:OD2	1:B:288:ARG:HD3	2.03	0.58
1:C:83:PRO:CB	1:C:86:LYS:HG3	2.33	0.58
1:A:292:PHE:CE1	1:A:307:VAL:HG22	2.39	0.57
1:D:155:ALA:HB3	1:D:156:PRO:HD3	1.86	0.57
1:C:153:CYS:HA	1:C:290:SER:HB2	1.87	0.57
1:B:292:PHE:CE1	1:B:307:VAL:HG22	2.40	0.57
1:A:312:ASP:O	4:A:563:HOH:O	2.17	0.56
1:A:231:ARG:NH2	4:A:551:HOH:O	2.37	0.56
1:B:172:MET:HG2	1:B:173:THR:N	2.20	0.56
1:D:287:ASN:HB2	4:D:535:HOH:O	2.06	0.56
1:A:83:PRO:O	1:A:86:LYS:HB2	2.06	0.55
1:B:252:TYR:CE2	1:B:256:LYS:HD2	2.42	0.55
1:C:102:ILE:HG13	1:C:124:ASP:OD2	2.07	0.55
1:B:169:GLU:HB2	1:C:300:LEU:CD2	2.36	0.55
1:C:38:GLU:OE2	1:C:38:GLU:N	2.39	0.54
1:D:208:THR:HA	2:D:504:SO4:O2	2.08	0.54
1:D:330:LYS:O	1:D:334:ALA:HB2	2.08	0.53
1:C:83:PRO:HB3	1:C:86:LYS:HG3	1.89	0.53
1:A:286:ASP:OD1	1:A:288:ARG:NH1	2.41	0.53
1:B:286:ASP:OD1	1:B:288:ARG:NH1	2.42	0.53
1:D:153:CYS:HA	1:D:290:SER:HB2	1.91	0.53
1:A:252:TYR:CE2	1:A:256:LYS:HD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ARG:HD3	1:D:278:VAL:O	2.08	0.52
1:C:54:LYS:H	1:C:54:LYS:HD2	1.75	0.52
1:D:165:PHE:O	1:D:166:GLU:HB3	2.09	0.52
1:A:292:PHE:HE1	1:A:307:VAL:HG22	1.75	0.52
1:D:109:PHE:CZ	1:D:142:LYS:HB3	2.44	0.52
1:D:171:LEU:CD2	1:D:226:THR:HG23	2.40	0.52
1:B:231:ARG:NH2	4:B:573:HOH:O	2.42	0.52
1:C:165:PHE:O	1:C:166:GLU:HB3	2.10	0.52
1:A:236:ASN:O	1:A:237:VAL:HB	2.10	0.52
1:D:54:LYS:H	1:D:54:LYS:HD2	1.74	0.52
1:D:102:ILE:HG13	1:D:124:ASP:OD2	2.09	0.51
1:C:109:PHE:CZ	1:C:142:LYS:HB3	2.44	0.51
1:C:33:PRO:HB3	1:C:75:ASN:O	2.11	0.51
1:B:178:VAL:HG11	1:D:184:THR:HB	1.91	0.51
1:D:102:ILE:HD11	1:D:124:ASP:O	2.10	0.51
1:C:330:LYS:O	1:C:334:ALA:HB2	2.10	0.51
1:A:115:LYS:HE2	1:A:141:MET:O	2.11	0.51
1:B:188:PRO:HD3	4:D:538:HOH:O	2.09	0.51
1:D:172:MET:HG2	1:D:173:THR:N	2.24	0.51
1:B:194:ARG:NH2	1:C:295:LYS:HB2	2.25	0.51
1:A:41:VAL:HG21	1:A:59:VAL:HG23	1.93	0.51
1:C:155:ALA:HB3	1:C:156:PRO:HD3	1.92	0.50
1:A:243:THR:HG23	1:D:171:LEU:HD12	1.92	0.50
1:B:18:THR:HG21	1:B:319:GLN:HA	1.93	0.50
1:A:18:THR:HG21	1:A:319:GLN:HA	1.92	0.50
1:D:9:GLY:HA3	3:D:338:SND:O5B	2.11	0.50
1:A:178:VAL:HG11	1:C:184:THR:HB	1.94	0.50
1:D:38:GLU:N	1:D:38:GLU:OE2	2.42	0.50
1:A:69:LYS:HZ3	1:A:69:LYS:HB2	1.77	0.50
1:B:231:ARG:HH21	1:B:231:ARG:HG3	1.76	0.50
1:A:232:VAL:HG11	1:D:232:VAL:HG11	1.92	0.49
1:B:97:GLY:HA3	3:B:336:SND:H2D	1.93	0.49
1:B:41:VAL:HG21	1:B:59:VAL:HG23	1.94	0.49
1:D:236:ASN:O	1:D:237:VAL:HB	2.13	0.49
1:C:176:HIS:HB3	1:C:231:ARG:HD3	1.95	0.49
1:B:115:LYS:HE2	1:B:141:MET:O	2.13	0.49
1:C:171:LEU:CD2	1:C:226:THR:HG23	2.42	0.49
1:B:292:PHE:HE1	1:B:307:VAL:HG22	1.77	0.49
1:C:109:PHE:HZ	1:C:142:LYS:HB3	1.77	0.48
1:C:41:VAL:CG2	1:C:59:VAL:HG23	2.42	0.48
1:A:69:LYS:HZ2	1:A:69:LYS:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ASN:O	1:B:237:VAL:HB	2.13	0.48
1:C:133:ASN:HA	1:C:135:GLU:OE1	2.14	0.48
1:C:83:PRO:HB2	1:C:86:LYS:HG3	1.94	0.48
1:B:69:LYS:HZ3	1:B:69:LYS:HB2	1.79	0.48
1:C:18:THR:HG21	1:C:319:GLN:HA	1.94	0.48
1:A:300:LEU:HD23	1:A:304:PHE:HD2	1.79	0.48
1:C:37:LEU:HD21	1:C:59:VAL:HG13	1.94	0.48
1:D:41:VAL:CG2	1:D:59:VAL:HG23	2.42	0.48
1:C:172:MET:HG2	1:C:173:THR:N	2.28	0.47
1:B:172:MET:CE	1:B:208:THR:HG21	2.45	0.47
1:D:109:PHE:HZ	1:D:142:LYS:HB3	1.78	0.47
1:B:52:MET:HE2	1:B:52:MET:HB3	1.69	0.47
1:C:102:ILE:HD11	1:C:124:ASP:O	2.14	0.47
1:B:298:ILE:HG13	1:B:306:LYS:HB3	1.96	0.47
1:D:176:HIS:HB3	1:D:231:ARG:HD3	1.97	0.47
1:C:31:ASN:ND2	3:C:337:SND:H2A	2.30	0.47
1:C:260:LYS:O	1:C:264:GLU:HG3	2.14	0.47
1:C:31:ASN:HD22	3:C:337:SND:H2A	1.80	0.47
1:D:18:THR:HG21	1:D:319:GLN:HA	1.96	0.46
1:A:298:ILE:HG13	1:A:306:LYS:HB3	1.97	0.46
1:B:69:LYS:HG2	4:B:548:HOH:O	2.16	0.46
1:B:194:ARG:HG2	1:C:277:ASP:HB3	1.97	0.46
1:A:325:ILE:O	1:A:329:GLN:HG3	2.15	0.46
1:B:300:LEU:HD23	1:B:304:PHE:HD2	1.81	0.46
1:D:106:SER:HA	1:D:109:PHE:CD2	2.50	0.46
1:D:33:PRO:HB3	1:D:75:ASN:O	2.16	0.46
1:A:231:ARG:HH21	1:A:231:ARG:HG3	1.79	0.46
1:A:242:LEU:HG	1:A:244:VAL:HG13	1.98	0.45
1:B:325:ILE:O	1:B:329:GLN:HG3	2.17	0.45
1:D:37:LEU:HD21	1:D:59:VAL:HG13	1.97	0.45
1:A:238:SER:HB2	1:A:311:TYR:CZ	2.51	0.45
1:A:204:ILE:HB	1:A:231:ARG:HB2	1.98	0.45
1:B:252:TYR:CD2	1:B:256:LYS:HD2	2.51	0.45
1:C:106:SER:HA	1:C:109:PHE:CD2	2.52	0.45
1:B:238:SER:HB2	1:B:311:TYR:CZ	2.52	0.45
1:C:271:LEU:HD12	1:C:290:SER:O	2.16	0.45
1:A:120:ALA:HB2	3:A:335:SND:O3D	2.17	0.45
4:A:550:HOH:O	1:D:245:ARG:HG3	2.16	0.44
1:D:80:GLU:HB2	1:D:110:LYS:HG3	1.98	0.44
1:A:172:MET:CE	1:A:208:THR:HG21	2.47	0.44
1:A:169:GLU:HB2	1:D:300:LEU:CD2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:ARG:HH21	1:C:295:LYS:HB2	1.83	0.44
1:C:21:GLU:C	1:C:23:GLY:H	2.21	0.44
1:C:236:ASN:O	1:C:237:VAL:HB	2.17	0.44
1:B:129:VAL:HG11	1:B:155:ALA:HB3	2.00	0.44
1:A:80:GLU:HB2	1:A:110:LYS:CD	2.24	0.44
1:B:169:GLU:HB2	1:C:300:LEU:HD21	1.98	0.44
1:A:252:TYR:CD2	1:A:256:LYS:HD2	2.53	0.44
1:D:9:GLY:O	1:D:13:ARG:HB2	2.17	0.44
1:A:117:ILE:N	1:A:117:ILE:HD12	2.33	0.43
1:B:11:ILE:O	1:B:15:VAL:HG23	2.19	0.43
1:D:30:VAL:HG12	1:D:31:ASN:N	2.34	0.43
1:B:204:ILE:HB	1:B:231:ARG:HB2	1.99	0.43
1:D:13:ARG:NH1	4:D:538:HOH:O	2.51	0.43
1:C:34:PHE:N	1:C:34:PHE:CD1	2.86	0.43
1:A:83:PRO:HB3	1:A:86:LYS:HG3	2.00	0.43
1:C:286:ASP:OD1	1:C:288:ARG:NH1	2.51	0.43
1:C:65:VAL:HA	1:C:69:LYS:O	2.19	0.43
1:D:65:VAL:HA	1:D:69:LYS:O	2.19	0.43
1:D:228:MET:HB2	1:D:228:MET:HE3	1.94	0.42
1:B:231:ARG:HG3	1:B:231:ARG:NH2	2.33	0.42
1:B:242:LEU:HG	1:B:244:VAL:HG13	2.01	0.42
1:D:21:GLU:C	1:D:23:GLY:H	2.22	0.42
1:B:41:VAL:HG13	1:B:57:VAL:HG12	2.00	0.42
1:D:260:LYS:O	1:D:264:GLU:HG3	2.19	0.42
1:A:8:PHE:CE2	1:A:13:ARG:HG2	2.55	0.42
1:A:129:VAL:HG11	1:A:155:ALA:HB3	2.01	0.42
1:D:34:PHE:N	1:D:34:PHE:CD1	2.87	0.42
1:A:8:PHE:CZ	1:A:13:ARG:HG2	2.55	0.42
1:C:298:ILE:O	1:C:305:VAL:HG23	2.20	0.42
1:C:78:LYS:HA	1:C:79:PRO:HD3	1.91	0.42
1:A:76:GLU:HB2	1:A:82:ILE:HG12	2.01	0.42
1:B:260:LYS:O	1:B:264:GLU:HG3	2.19	0.42
1:B:300:LEU:HD13	1:C:226:THR:HG22	2.02	0.42
1:C:30:VAL:HG12	1:C:31:ASN:N	2.35	0.42
1:C:325:ILE:O	1:C:329:GLN:HG3	2.20	0.42
1:D:286:ASP:OD1	1:D:288:ARG:NH1	2.53	0.42
1:D:60:GLU:O	1:D:61:ASP:HB2	2.20	0.42
1:A:231:ARG:HG3	1:A:231:ARG:NH2	2.36	0.41
1:A:260:LYS:O	1:A:264:GLU:HG3	2.21	0.41
1:B:110:LYS:HB3	1:B:110:LYS:HE3	1.87	0.41
1:C:13:ARG:HD2	4:C:525:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ILE:O	1:D:305:VAL:HG23	2.21	0.41
1:D:325:ILE:O	1:D:329:GLN:HG3	2.21	0.41
1:D:76:GLU:OE2	1:D:76:GLU:HA	2.21	0.41
1:D:171:LEU:HD23	1:D:226:THR:CG2	2.49	0.41
1:A:14:LEU:HA	1:A:14:LEU:HD23	1.87	0.41
1:D:16:LEU:HD13	1:D:44:PHE:CE1	2.56	0.41
1:C:9:GLY:O	1:C:13:ARG:HB2	2.21	0.41
1:C:83:PRO:HB3	1:C:86:LYS:CG	2.51	0.40
1:D:79:PRO:HB2	1:D:107:ALA:CB	2.51	0.40
1:B:117:ILE:HD12	1:B:117:ILE:N	2.35	0.40
1:A:90:GLU:OE2	1:A:114:LYS:HE2	2.22	0.40
1:C:127:MET:HG2	1:C:145:SER:HB3	2.03	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	331/333 (99%)	313 (95%)	15 (4%)	3 (1%)	17	46
1	B	331/333 (99%)	313 (95%)	15 (4%)	3 (1%)	17	46
1	C	331/333 (99%)	304 (92%)	25 (8%)	2 (1%)	25	56
1	D	331/333 (99%)	305 (92%)	24 (7%)	2 (1%)	25	56
All	All	1324/1332 (99%)	1235 (93%)	79 (6%)	10 (1%)	19	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	ASN
1	B	313	ASN
1	A	237	VAL

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Mol	Chain	Res	Type
1	B	237	VAL
1	C	237	VAL
1	D	237	VAL
1	A	166	GLU
1	B	166	GLU
1	C	166	GLU
1	D	166	GLU

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	272/272 (100%)	264 (97%)	8 (3%)	42	76
1	B	272/272 (100%)	264 (97%)	8 (3%)	42	76
1	C	272/272 (100%)	266 (98%)	6 (2%)	52	83
1	D	272/272 (100%)	267 (98%)	5 (2%)	59	86
All	All	1088/1088 (100%)	1061 (98%)	27 (2%)	47	80

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	16	LEU
1	A	69	LYS
1	A	115	LYS
1	A	154	LEU
1	A	307	VAL
1	A	314	GLU
1	A	319	GLN
1	B	1	SER
1	B	16	LEU
1	B	69	LYS
1	B	115	LYS
1	B	154	LEU
1	B	307	VAL

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Mol	Chain	Res	Type
1	B	314	GLU
1	B	319	GLN
1	C	16	LEU
1	C	54	LYS
1	C	135	GLU
1	C	154	LEU
1	C	228	MET
1	C	319	GLN
1	D	16	LEU
1	D	54	LYS
1	D	154	LEU
1	D	228	MET
1	D	319	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	81	ASN
1	A	146	ASN
1	A	268	GLN
1	A	313	ASN
1	B	50	HIS
1	B	146	ASN
1	B	201	GLN
1	B	268	GLN
1	C	146	ASN
1	C	268	GLN
1	D	146	ASN
1	D	268	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 carbohydrates in this entry.

5.6 Ligand geometry i

12 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	SND	B	336	-	33,39,48	1.05	2 (6%)	38,60,73	1.13	4 (10%)
2	SO4	C	503	-	4,4,4	1.79	1 (25%)	6,6,6	0.66	0
3	SND	C	337	-	42,48,48	4.47	9 (21%)	49,73,73	1.27	4 (8%)
2	SO4	D	504	-	4,4,4	1.82	1 (25%)	6,6,6	0.39	0
2	SO4	A	505	-	4,4,4	1.94	1 (25%)	6,6,6	0.45	0
3	SND	D	338	-	42,48,48	4.54	9 (21%)	49,73,73	1.22	2 (4%)
2	SO4	A	501	-	4,4,4	1.66	1 (25%)	6,6,6	0.68	0
2	SO4	D	508	-	4,4,4	2.01	2 (50%)	6,6,6	0.59	0
2	SO4	B	506	-	4,4,4	2.09	2 (50%)	6,6,6	0.39	0
3	SND	A	335	-	33,39,48	1.03	3 (9%)	38,60,73	1.04	3 (7%)
2	SO4	B	502	-	4,4,4	1.71	1 (25%)	6,6,6	0.62	0
2	SO4	C	507	-	4,4,4	2.00	1 (25%)	6,6,6	0.59	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	SND	B	336	-	-	5/18/54/62	0/4/4/5
3	SND	C	337	-	-	12/26/62/62	0/5/5/5
3	SND	D	338	-	-	8/26/62/62	0/5/5/5
3	SND	A	335	-	-	6/18/54/62	0/4/4/5

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	338	SND	C7N-S7N	-26.98	1.23	1.67
3	C	337	SND	C7N-S7N	-26.62	1.24	1.67
3	D	338	SND	C2N-N1N	7.07	1.43	1.35
3	C	337	SND	C2N-N1N	7.00	1.43	1.35
3	D	338	SND	O4D-C1D	4.12	1.46	1.41
3	C	337	SND	O4D-C1D	3.59	1.46	1.41
3	D	338	SND	C3N-C7N	3.21	1.56	1.49
3	C	337	SND	C2A-N3A	2.90	1.36	1.32
3	B	336	SND	C2A-N1A	2.89	1.39	1.33
3	D	338	SND	C6N-N1N	2.86	1.42	1.35
3	C	337	SND	O4B-C1B	2.86	1.45	1.41
3	A	335	SND	C2A-N1A	2.76	1.39	1.33
3	C	337	SND	C6N-N1N	2.67	1.41	1.35
2	C	507	SO4	O2-S	2.65	1.60	1.46
3	D	338	SND	C7N-N7N	2.64	1.35	1.32
2	A	505	SO4	O2-S	2.62	1.60	1.46
3	C	337	SND	C3N-C7N	2.62	1.55	1.49
2	D	508	SO4	O2-S	2.57	1.59	1.46
2	B	506	SO4	O2-S	2.56	1.59	1.46
2	D	504	SO4	O2-S	2.47	1.59	1.46
3	D	338	SND	C2A-N3A	2.39	1.35	1.32
3	D	338	SND	O4B-C1B	2.38	1.44	1.41
3	C	337	SND	C5A-N7A	-2.32	1.31	1.39
2	B	502	SO4	O2-S	2.29	1.58	1.46
3	B	336	SND	C4A-N3A	2.29	1.38	1.35
2	C	503	SO4	O2-S	2.28	1.58	1.46
2	A	501	SO4	O2-S	2.26	1.58	1.46
3	C	337	SND	C7N-N7N	2.18	1.34	1.32
3	A	335	SND	PN-O2N	-2.09	1.45	1.55
2	D	508	SO4	O4-S	2.08	1.65	1.47
3	D	338	SND	C5A-N7A	-2.08	1.32	1.39
3	A	335	SND	C2B-C1B	-2.05	1.50	1.53
2	B	506	SO4	O4-S	2.03	1.64	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	338	SND	N3A-C2A-N1A	-4.62	121.46	128.68
3	C	337	SND	N3A-C2A-N1A	-4.44	121.74	128.68
3	C	337	SND	C4A-C5A-N7A	3.87	113.44	109.40
3	D	338	SND	C4A-C5A-N7A	3.74	113.30	109.40
3	A	335	SND	C1B-N9A-C4A	-3.00	121.37	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	336	SND	C1B-N9A-C4A	-2.97	121.43	126.64
3	B	336	SND	O4D-C4D-C3D	2.58	110.22	105.11
3	B	336	SND	C3D-C2D-C1D	2.38	105.94	101.42
3	A	335	SND	O4D-C4D-C3D	2.34	109.75	105.11
3	A	335	SND	C5A-C6A-N6A	2.16	123.64	120.35
3	B	336	SND	C5A-C6A-N6A	2.16	123.64	120.35
3	C	337	SND	C4N-C3N-C7N	-2.09	118.40	121.06
3	C	337	SND	N6A-C6A-N1A	2.04	122.80	118.57

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	336	SND	C5B-O5B-PA-O1A
3	C	337	SND	O4D-C1D-N1N-C2N
3	C	337	SND	O4D-C1D-N1N-C6N
3	C	337	SND	C2D-C1D-N1N-C2N
3	C	337	SND	C2D-C1D-N1N-C6N
3	C	337	SND	C2N-C3N-C7N-N7N
3	D	338	SND	O4D-C1D-N1N-C2N
3	D	338	SND	O4D-C1D-N1N-C6N
3	A	335	SND	C5B-O5B-PA-O1A
3	A	335	SND	C5B-O5B-PA-O2A
3	A	335	SND	PN-O3-PA-O5B
3	B	336	SND	O4B-C4B-C5B-O5B
3	A	335	SND	O4B-C4B-C5B-O5B
3	A	335	SND	C3B-C4B-C5B-O5B
3	C	337	SND	C2N-C3N-C7N-S7N
3	C	337	SND	C4N-C3N-C7N-S7N
3	C	337	SND	C4N-C3N-C7N-N7N
3	B	336	SND	C3B-C4B-C5B-O5B
3	D	338	SND	PN-O3-PA-O1A
3	B	336	SND	C5B-O5B-PA-O3
3	C	337	SND	C5D-O5D-PN-O3
3	A	335	SND	C5B-O5B-PA-O3
3	B	336	SND	C5B-O5B-PA-O2A
3	C	337	SND	PN-O3-PA-O2A
3	D	338	SND	PN-O3-PA-O2A
3	D	338	SND	O4B-C4B-C5B-O5B
3	C	337	SND	O4B-C4B-C5B-O5B
3	D	338	SND	C2D-C1D-N1N-C2N
3	D	338	SND	C2D-C1D-N1N-C6N

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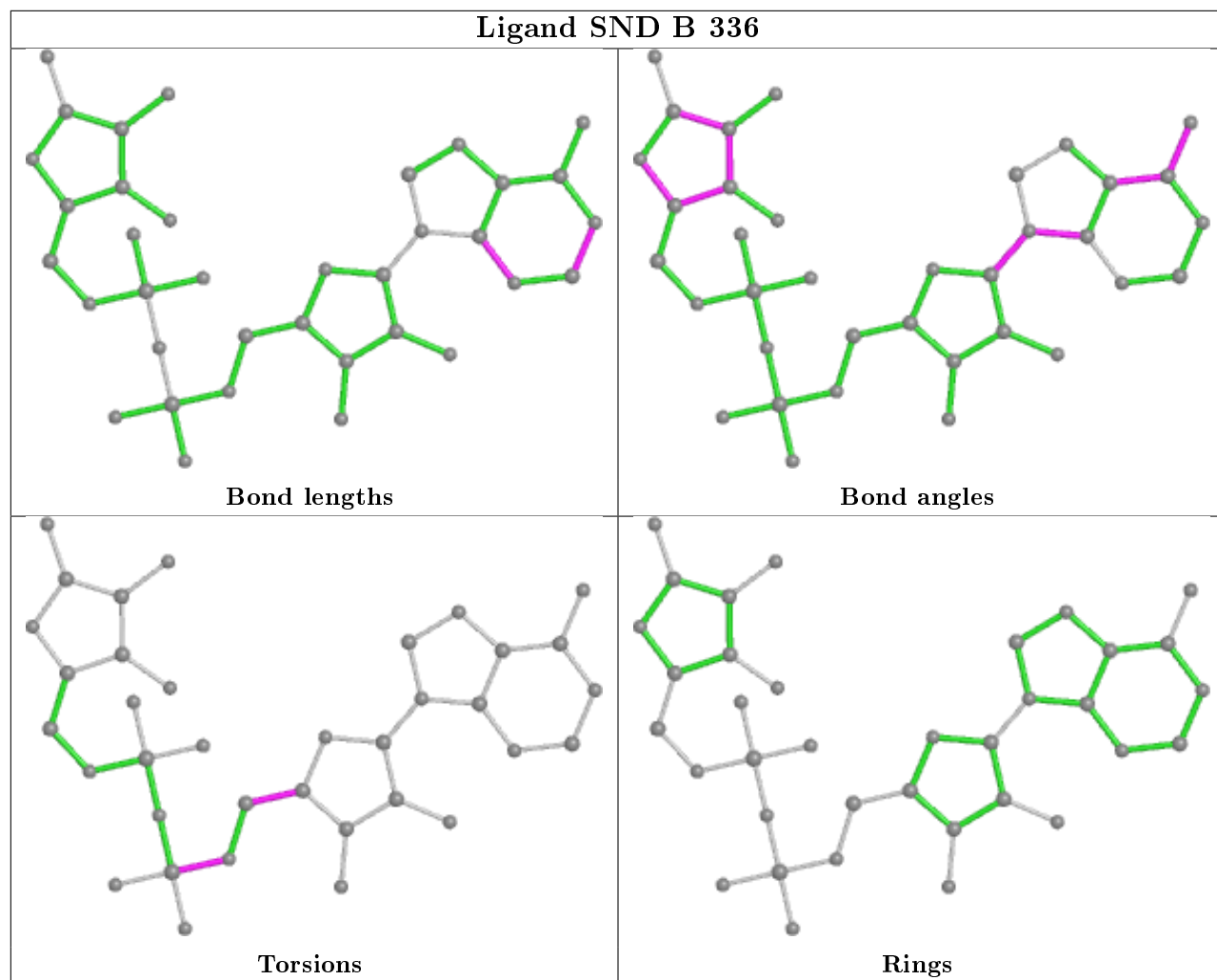
Mol	Chain	Res	Type	Atoms
3	C	337	SND	C5D-O5D-PN-O1N
3	D	338	SND	C5D-O5D-PN-O1N

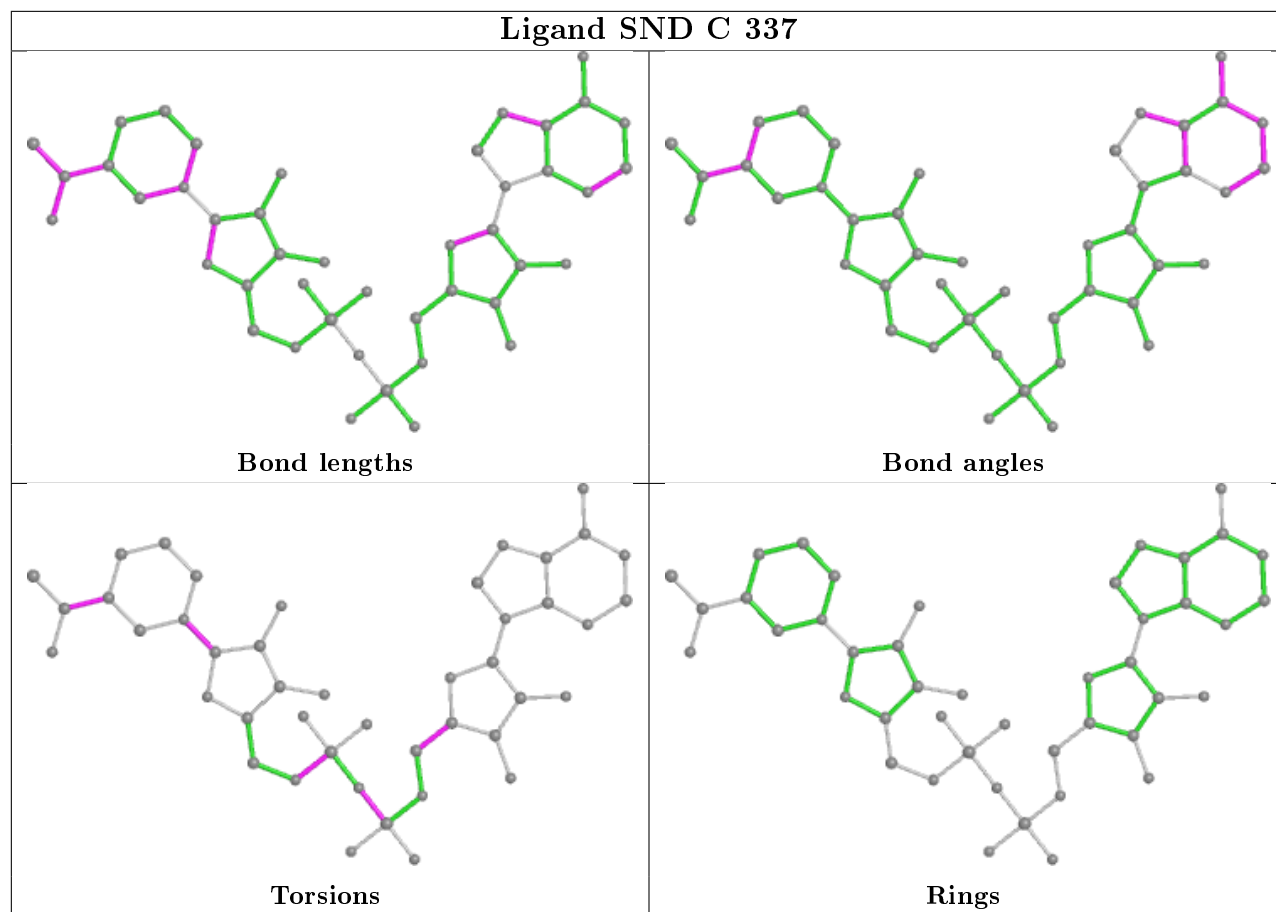
There are no ring outliers.

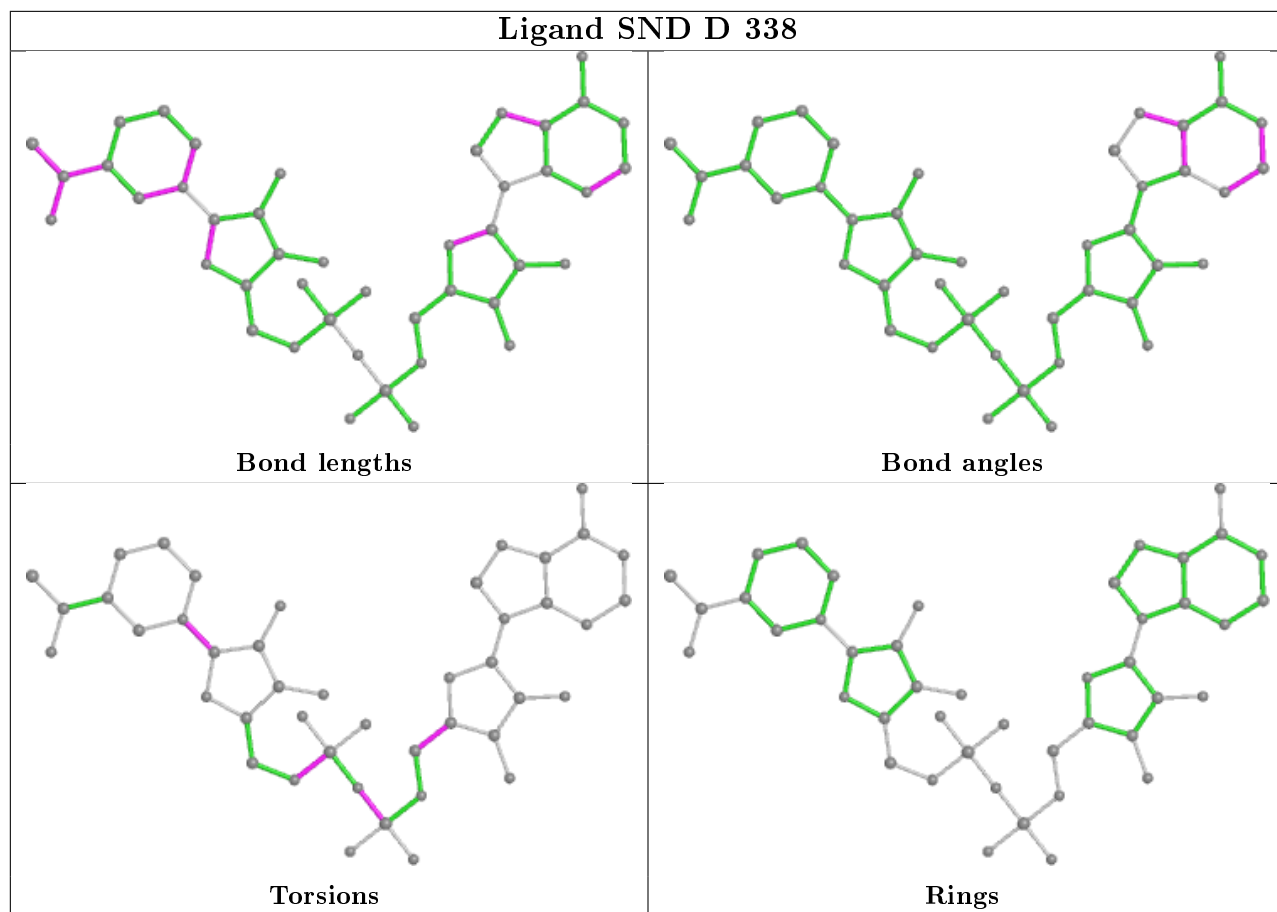
5 monomers are involved in 9 short contacts:

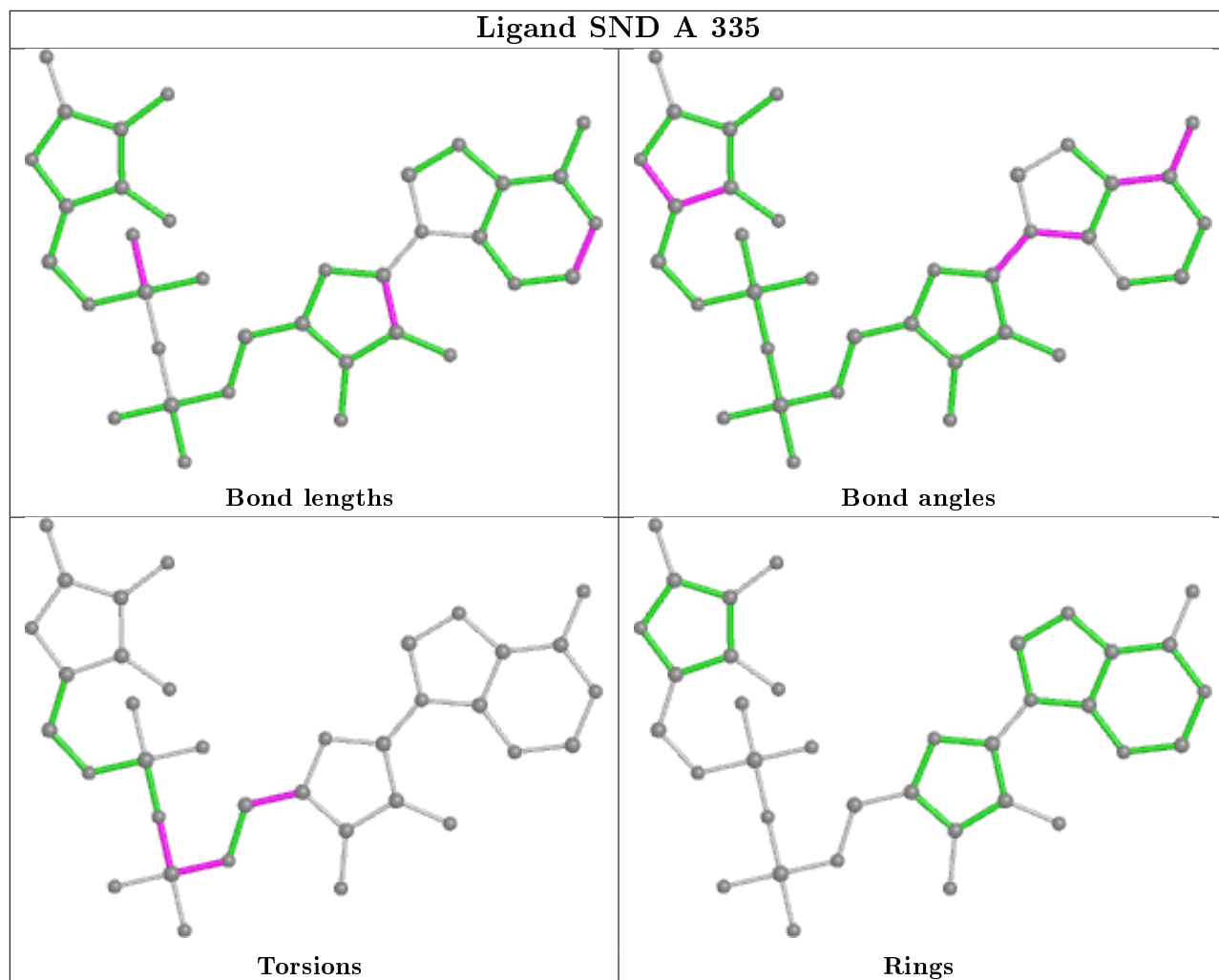
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	336	SND	2	0
3	C	337	SND	3	0
2	D	504	SO4	1	0
3	D	338	SND	2	0
3	A	335	SND	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	333/333 (100%)	-0.56	3 (0%) 84 80	12, 26, 45, 69	0
1	B	333/333 (100%)	-0.61	4 (1%) 79 73	13, 24, 42, 67	0
1	C	333/333 (100%)	-0.28	12 (3%) 42 32	16, 31, 67, 84	0
1	D	333/333 (100%)	-0.28	4 (1%) 79 73	13, 31, 64, 82	0
All	All	1332/1332 (100%)	-0.43	23 (1%) 70 63	12, 27, 60, 84	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	334	ALA	10.4
1	C	334	ALA	6.9
1	A	334	ALA	6.2
1	B	334	ALA	6.0
1	C	81	ASN	4.3
1	D	333	SER	3.8
1	C	77	MET	3.4
1	C	61	ASP	3.0
1	C	78	LYS	3.0
1	C	80	GLU	2.9
1	A	333	SER	2.8
1	D	61	ASP	2.6
1	B	333	SER	2.5
1	B	191	LYS	2.5
1	C	52	MET	2.5
1	C	191	LYS	2.5
1	A	34	PHE	2.5
1	C	86	LYS	2.5
1	C	34	PHE	2.3
1	D	85	SER	2.2
1	B	21	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	54	LYS	2.0
1	C	22	MET	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](#)

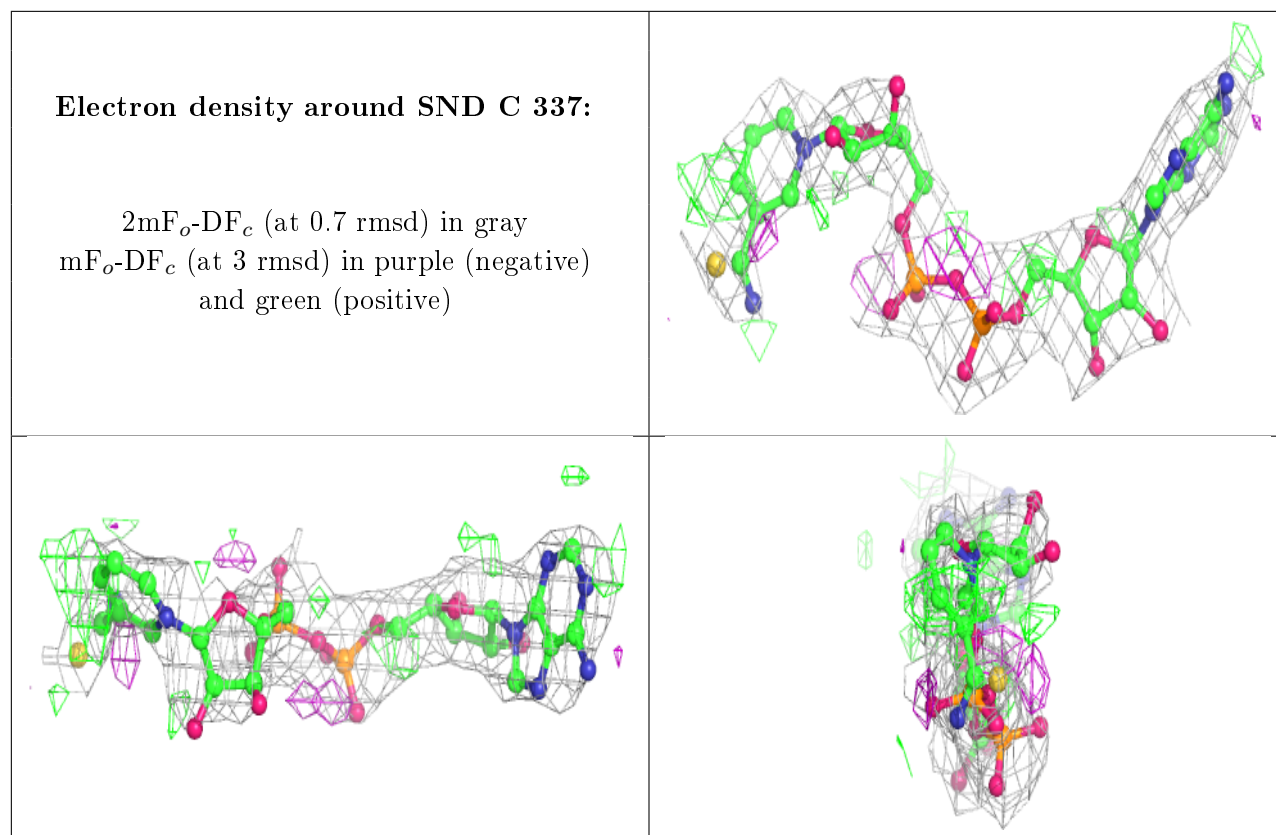
There are no carbohydrates in this entry.

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.

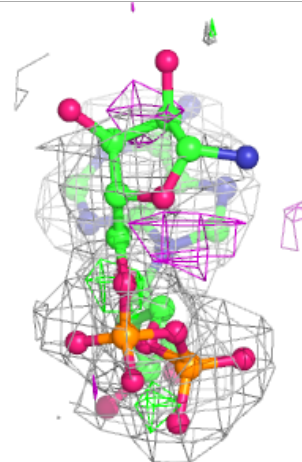
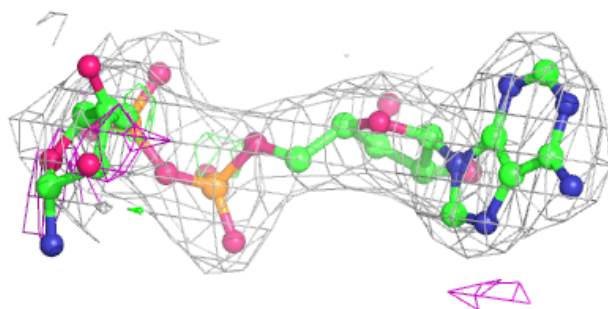
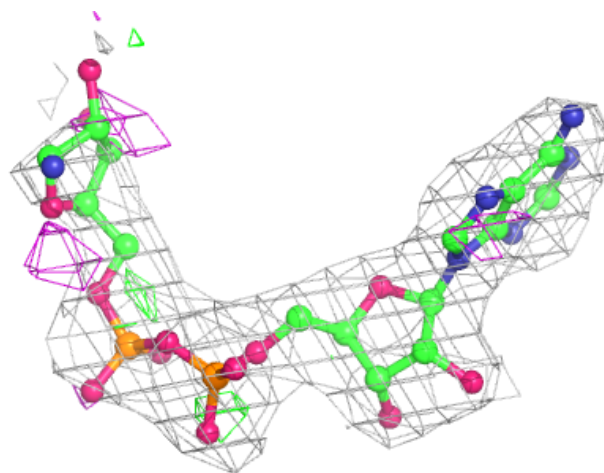
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SND	C	337	44/44	0.89	0.23	54,63,87,92	0
2	SO4	B	506	5/5	0.91	0.54	22,23,25,47	0
2	SO4	C	507	5/5	0.91	0.52	24,24,26,46	0
2	SO4	D	508	5/5	0.92	0.42	23,23,24,44	0
2	SO4	A	505	5/5	0.93	0.47	23,23,25,44	0
3	SND	B	336	36/44	0.94	0.18	29,37,79,80	0
3	SND	A	335	36/44	0.94	0.18	36,41,90,91	0
2	SO4	D	504	5/5	0.94	0.33	22,22,24,39	0
2	SO4	C	503	5/5	0.95	0.27	22,22,24,40	0
3	SND	D	338	44/44	0.95	0.17	44,51,69,76	0
2	SO4	B	502	5/5	0.96	0.20	21,21,23,37	0
2	SO4	A	501	5/5	0.96	0.23	22,22,23,38	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.



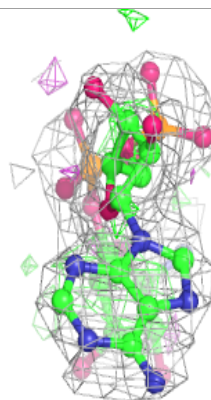
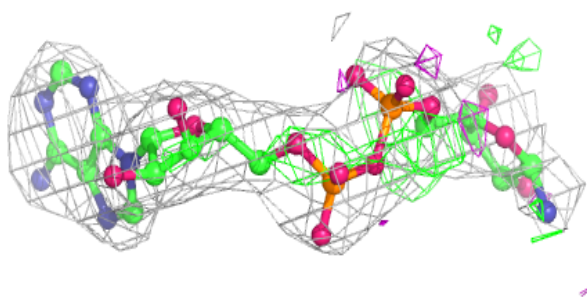
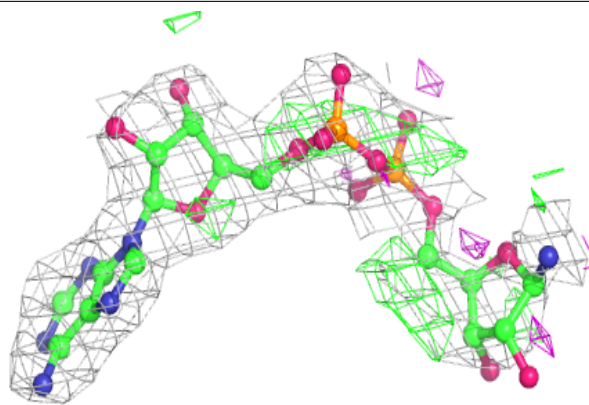
Electron density around SND B 336:

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

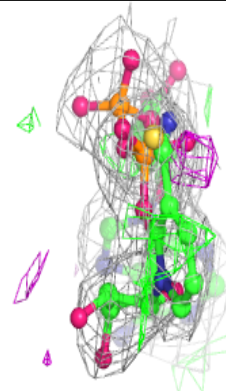
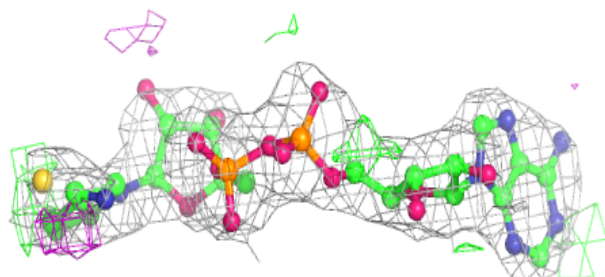
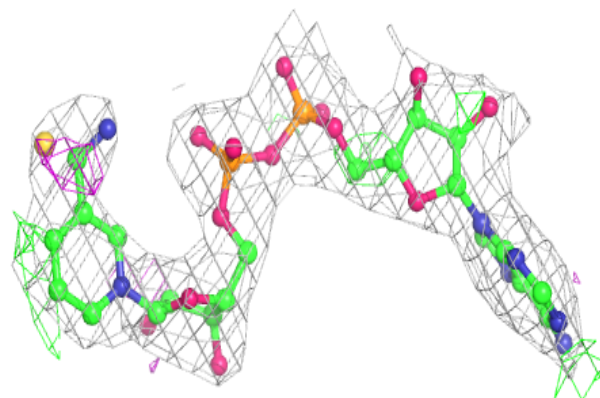


Electron density around SND A 335:

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

**Electron density around SND D 338:**

$2mF_o-DF_c$ (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.