



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 01:24 AM UTC

PDB ID : 2R9E / pdb_00002r9e
Title : The structure of the binary complex of citryl dehydrogenase COA and citrate synthase from the thermophilic archaeon *Thermoplasma acidophilum*
Authors : Lehmann, C.; Chen, Z.
Deposited on : 2007-09-12
Resolution : 1.95 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

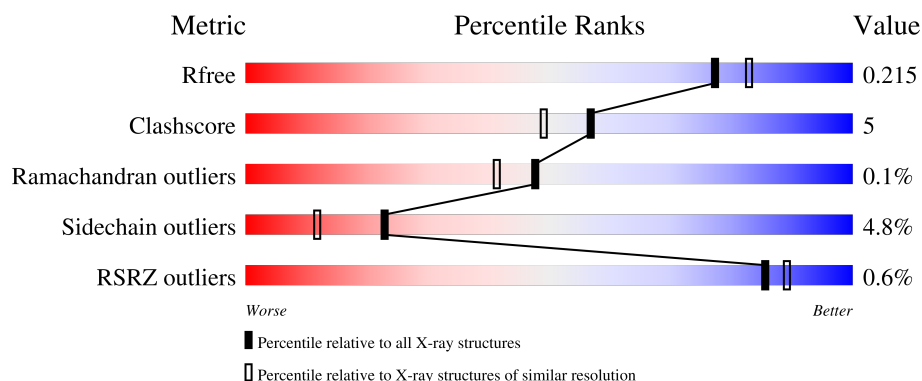
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	385	% 84% 15% ..
1	B	385	% 85% 11% ...
1	C	385	% 85% 11% ..
1	D	385	% 86% 11% ..

2 Entry composition [i](#)

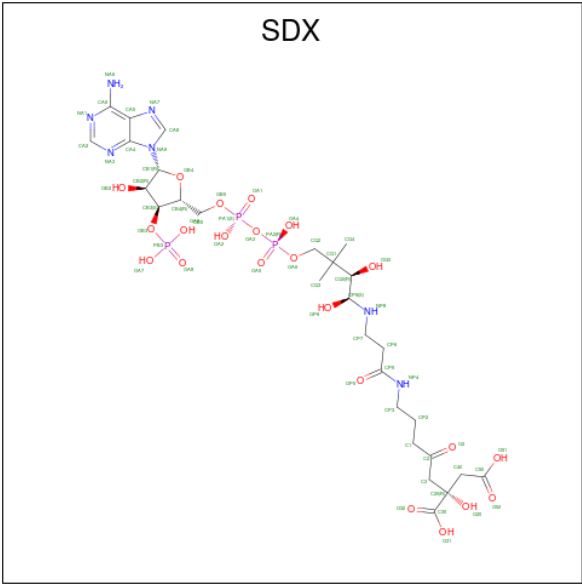
There are 3 unique types of molecules in this entry. The entry contains 13585 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	1	0
			3005	1923	508	562	12			
1	B	379	Total	C	N	O	S	0	1	0
			2989	1914	506	557	12			
1	C	379	Total	C	N	O	S	0	1	0
			2989	1914	506	557	12			
1	D	379	Total	C	N	O	S	1	1	0
			2989	1914	506	557	12			

- Molecule 2 is s-citryldethia Coenzyme A (CCD ID: SDX) (formula: C₂₈H₄₆N₇O₂₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			60	28	7	22	3		
2	B	1	Total	C	N	O	P	0	0
			60	28	7	22	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			60	28	7	22	3		
2	D	1	Total	C	N	O	P	0	0
			60	28	7	22	3		

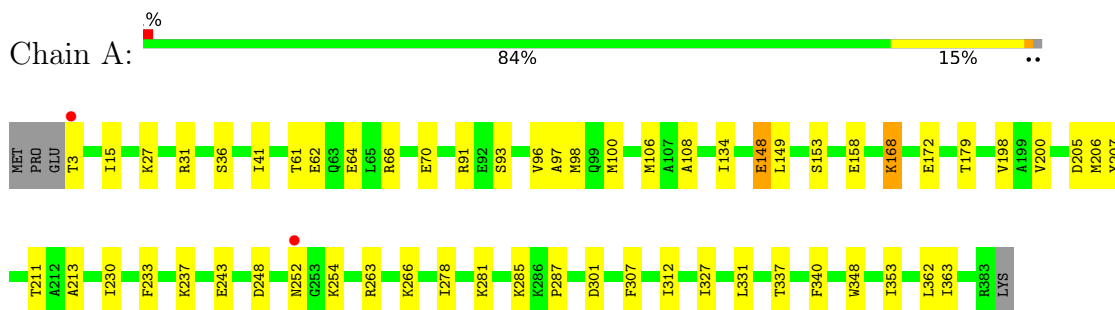
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	354	Total	O	0	0
			354	354		
3	B	335	Total	O	0	0
			335	335		
3	C	344	Total	O	0	0
			344	344		
3	D	340	Total	O	0	0
			340	340		

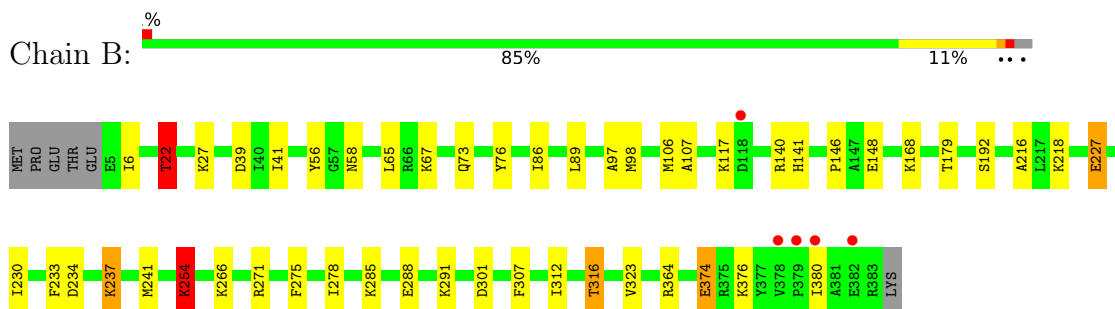
3 Residue-property plots [i](#)

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

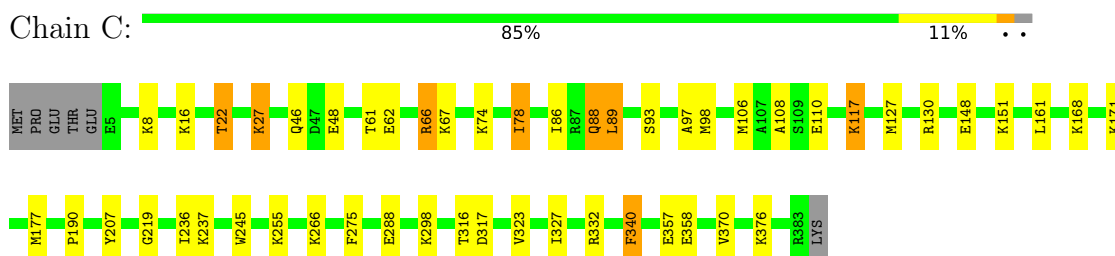
- Molecule 1: Citrate synthase



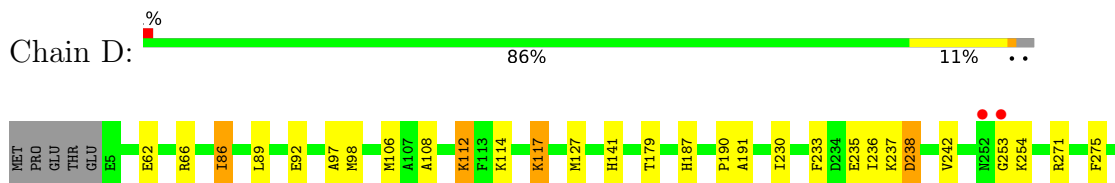
- Molecule 1: Citrate synthase



- Molecule 1: Citrate synthase



- Molecule 1: Citrate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.06Å 73.50Å 89.98Å 99.35° 98.19° 113.89°	Depositor
Resolution (Å)	33.28 – 1.95 33.28 – 1.95	Depositor EDS
% Data completeness (in resolution range)	96.8 (33.28-1.95) 96.8 (33.28-1.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.157 , 0.215 0.157 , 0.215	Depositor DCC
R_{free} test set	5292 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13585	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: SDX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	2/3072 (0.1%)	1.00	2/4153 (0.0%)
1	B	0.98	0/3056	1.03	5/4131 (0.1%)
1	C	0.94	3/3056 (0.1%)	1.01	4/4131 (0.1%)
1	D	0.96	1/3056 (0.0%)	1.01	1/4131 (0.0%)
All	All	0.97	6/12240 (0.0%)	1.01	12/16546 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	370	VAL	CA-CB	-7.57	1.44	1.54
1	C	61	THR	C-N	-6.67	1.25	1.33
1	C	62	GLU	C-N	-6.29	1.25	1.33
1	A	198	VAL	C-O	-6.02	1.17	1.24
1	A	207	TYR	C-O	-5.66	1.17	1.24
1	D	191	ALA	CA-CB	5.23	1.61	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	22	THR	CB-CA-C	-6.76	96.45	109.37
1	C	219	GLY	CA-C-N	5.92	125.54	119.56
1	C	219	GLY	C-N-CA	5.92	125.54	119.56
1	C	370	VAL	N-CA-CB	5.92	120.99	111.23
1	A	200	VAL	N-CA-CB	5.88	123.41	111.05
1	C	340	PHE	N-CA-C	-5.83	104.83	111.07
1	B	254	LYS	N-CA-C	5.56	119.36	112.47
1	B	380	ILE	N-CA-C	5.54	116.27	110.62
1	B	6	ILE	N-CA-C	5.52	116.68	108.23
1	B	316	THR	CB-CA-C	-5.50	101.32	110.68
1	A	153	SER	N-CA-C	-5.50	101.52	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	86	ILE	N-CA-C	-5.15	106.66	111.45

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	3005	0	3012	32	0
1	B	2989	0	2999	28	0
1	C	2989	0	2999	29	0
1	D	2989	0	2999	29	0
2	A	60	0	40	0	0
2	B	60	0	40	1	0
2	C	60	0	40	1	0
2	D	60	0	40	1	0
3	A	354	0	0	4	0
3	B	335	0	0	7	0
3	C	344	0	0	6	0
3	D	340	0	0	3	0
All	All	13585	0	12169	112	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 5.

All (112) 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:106:MET:CE	1:A:134:ILE:HD11	1.89	1.01
1:C:177:MET:HE2	1:C:327:ILE:HD13	1.48	0.93
1:D:86:ILE:HG23	1:D:98:MET:HE2	1.57	0.85
1:A:106:MET:HE3	1:A:134:ILE:HD11	1.59	0.84
1:D:106:MET:HE1	1:D:127:MET:SD	2.19	0.83
1:C:177:MET:CE	1:C:327:ILE:HD13	2.09	0.82
1:D:86:ILE:HG23	1:D:98:MET:CE	2.18	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ASP:O	1:B:237:LYS:HE2	1.92	0.70
1:C:66:ARG:O	1:C:66:ARG:NH2	2.23	0.70
1:C:106:MET:HE1	1:C:127:MET:SD	2.32	0.70
1:D:141:HIS:HD2	3:D:1235:HOH:O	1.75	0.68
1:D:253:GLY:O	1:D:254:LYS:HG2	1.94	0.68
1:C:177:MET:HE2	1:C:327:ILE:CD1	2.24	0.67
1:D:235:GLU:O	1:D:237:LYS:HD3	1.95	0.66
1:B:58:ASN:HB2	3:B:1078:HOH:O	1.97	0.63
1:C:8:LYS:HE3	3:C:2344:HOH:O	1.98	0.63
1:B:86:ILE:HG23	1:B:98:MET:HE2	1.82	0.62
1:A:97:ALA:HA	1:A:100:MET:HE3	1.82	0.62
1:D:271:ARG:HB2	1:D:316:THR:HG22	1.82	0.62
1:A:148:GLU:HG3	1:A:149:LEU:N	2.15	0.61
1:B:22:THR:HG21	3:B:2277:HOH:O	2.00	0.61
1:A:31:ARG:CZ	1:B:374:GLU:HG2	2.31	0.60
1:A:307:PHE:HB3	1:A:312:ILE:HB	1.85	0.59
1:A:172:GLU:OE2	1:A:285:LYS:HE3	2.02	0.58
1:D:179:THR:HG21	1:D:278:ILE:HD11	1.85	0.58
1:D:301:ASP:O	1:D:305:LYS:HG2	2.04	0.58
1:D:106:MET:CE	1:D:127:MET:SD	2.92	0.56
1:D:307:PHE:HB3	1:D:312:ILE:HB	1.88	0.55
1:B:89:LEU:O	1:B:141:HIS:HE1	1.90	0.54
1:B:86:ILE:HG23	1:B:98:MET:CE	2.37	0.54
1:C:93:SER:HB2	1:C:98:MET:HE3	1.89	0.54
1:A:106:MET:CE	1:A:134:ILE:CD1	2.77	0.54
1:B:288:GLU:H	1:B:288:GLU:CD	2.16	0.54
1:C:78:ILE:HD11	1:C:130:ARG:HB3	1.88	0.54
1:C:93:SER:HB2	1:C:98:MET:CE	2.39	0.53
1:D:114:LYS:HE2	3:D:2348:HOH:O	2.08	0.53
1:C:88:GLN:O	1:C:88:GLN:HG2	2.08	0.52
1:B:41:ILE:HD12	1:B:179:THR:HG23	1.92	0.51
1:A:106:MET:HE1	1:A:134:ILE:HD11	1.87	0.51
2:D:703:SDX:OA7	2:D:703:SDX:OB2	2.23	0.50
1:A:158:GLU:OE1	1:A:168:LYS:HE3	2.12	0.50
1:C:8:LYS:CE	3:C:2344:HOH:O	2.57	0.50
1:C:66:ARG:HG3	3:C:1838:HOH:O	2.13	0.49
1:A:206:MET:HE1	1:A:353:ILE:HD11	1.94	0.49
1:D:271:ARG:HB2	1:D:316:THR:CG2	2.42	0.48
1:C:27:LYS:HA	1:C:27:LYS:HE2	1.94	0.48
1:C:78:ILE:CD1	1:C:130:ARG:HG2	2.44	0.48
1:A:41:ILE:HG12	1:A:179:THR:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:SER:HB2	1:A:98:MET:HE3	1.95	0.47
1:D:238:ASP:HA	1:D:291:LYS:HZ2	1.80	0.47
1:B:307:PHE:HB3	1:B:312:ILE:HB	1.96	0.47
1:C:316:THR:HG23	1:C:317:ASP:OD2	2.16	0.46
1:A:15:ILE:HD11	1:A:363:ILE:HD13	1.97	0.46
1:B:266:LYS:NZ	3:B:2319:HOH:O	2.48	0.46
1:D:285:LYS:HB2	3:D:1029:HOH:O	2.15	0.46
1:D:187:HIS:O	1:D:190:PRO:HD3	2.16	0.46
1:A:179:THR:HG21	1:A:278:ILE:HD11	1.98	0.45
1:B:56:TYR:OH	3:B:1155:HOH:O	2.19	0.45
1:D:86:ILE:CG2	1:D:98:MET:HE2	2.40	0.45
1:A:61:THR:OG1	1:A:64:GLU:HG3	2.17	0.45
1:A:248:ASP:O	1:A:252:ASN:ND2	2.50	0.45
1:B:285:LYS:HA	1:B:285:LYS:HE2	1.99	0.45
1:A:205:ASP:OD1	1:B:218:LYS:HE3	2.16	0.45
1:B:67:LYS:HD3	3:B:1136:HOH:O	2.16	0.45
1:C:255:LYS:HE3	3:C:1604:HOH:O	2.17	0.45
1:D:236:ILE:HG21	1:D:242:VAL:HG22	1.99	0.45
1:B:73:GLN:HG2	1:B:76:TYR:CE1	2.52	0.45
1:B:140:ARG:HD3	1:B:146:PRO:O	2.17	0.45
3:C:1378:HOH:O	1:D:62:GLU:HG2	2.17	0.44
1:A:91:ARG:NH2	3:A:2262:HOH:O	2.31	0.44
1:B:179:THR:HG21	1:B:278:ILE:HD11	1.99	0.44
1:B:275:PHE:HD2	1:B:323:VAL:HG21	1.82	0.44
1:B:148:GLU:HG2	3:B:1776:HOH:O	2.18	0.44
1:D:112:LYS:HD2	1:D:112:LYS:HA	1.41	0.44
1:C:161:LEU:HD21	1:C:177:MET:HE3	2.00	0.44
1:A:91:ARG:HD2	3:A:2262:HOH:O	2.18	0.44
1:C:106:MET:O	1:C:110:GLU:HG2	2.18	0.44
1:C:46:GLN:HG2	1:C:48:GLU:OE1	2.17	0.43
1:A:66:ARG:O	1:A:70:GLU:HG3	2.18	0.43
1:B:89:LEU:O	1:B:141:HIS:CE1	2.71	0.43
1:D:230:ILE:HA	1:D:233:PHE:CD1	2.52	0.43
1:A:100:MET:HG2	1:A:211:THR:HG23	2.00	0.43
1:C:22:THR:HG23	1:D:369:TYR:CG	2.53	0.43
1:D:86:ILE:CG2	1:D:98:MET:CE	2.91	0.43
1:B:230:ILE:HA	1:B:233:PHE:CD2	2.54	0.43
1:C:97:ALA:CB	1:D:108:ALA:HA	2.49	0.43
1:C:117:LYS:HE2	3:C:2351:HOH:O	2.18	0.43
1:A:263:ARG:HG2	1:B:364:ARG:HB3	2.01	0.42
1:A:108:ALA:HA	1:B:97:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LEU:HD22	2:B:701:SDX:HQ4	2.01	0.42
1:D:117:LYS:O	1:D:117:LYS:HD3	2.19	0.42
1:D:89:LEU:O	1:D:141:HIS:HE1	2.03	0.42
1:A:213:ALA:HB1	1:A:348:TRP:CE2	2.55	0.42
1:A:96:VAL:HG21	1:A:337:THR:HG22	2.02	0.41
1:C:357:GLU:HG2	1:C:358:GLU:HG3	2.01	0.41
1:D:275:PHE:HD1	1:D:323:VAL:HG21	1.85	0.41
1:A:230:ILE:HA	1:A:233:PHE:CD2	2.55	0.41
1:C:86:ILE:O	1:C:89:LEU:HB2	2.20	0.41
1:C:106:MET:HE3	1:C:207:TYR:CD2	2.56	0.41
1:A:287:PRO:HG2	3:A:1553:HOH:O	2.21	0.41
1:A:340:PHE:C	1:A:340:PHE:HD2	2.29	0.41
1:B:227:GLU:HG3	3:B:1009:HOH:O	2.21	0.41
1:B:271:ARG:HB2	1:B:316:THR:HG22	2.03	0.41
1:D:373:ALA:O	1:D:375:ARG:HG3	2.21	0.41
1:B:106:MET:O	1:B:107:ALA:C	2.63	0.41
1:C:108:ALA:HA	1:D:97:ALA:CB	2.51	0.41
1:A:281:LYS:HG3	3:A:1135:HOH:O	2.21	0.40
1:C:190:PRO:HB3	2:C:702:SDX:C50	2.51	0.40
1:B:192:SER:HA	1:B:216:ALA:HB3	2.04	0.40
1:C:236:ILE:HG12	1:C:245:TRP:CG	2.57	0.40
1:C:275:PHE:HD2	1:C:323:VAL:HG21	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/385 (99%)	372 (98%)	8 (2%)	0	100	100
1	B	378/385 (98%)	369 (98%)	8 (2%)	1 (0%)	36	28
1	C	378/385 (98%)	369 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	378/385 (98%)	367 (97%)	11 (3%)	0	100	100
All	All	1514/1540 (98%)	1477 (98%)	36 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	254	LYS

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	312/315 (99%)	299 (96%)	13 (4%)	26	16
1	B	310/315 (98%)	296 (96%)	14 (4%)	24	14
1	C	310/315 (98%)	289 (93%)	21 (7%)	14	5
1	D	310/315 (98%)	299 (96%)	11 (4%)	32	22
All	All	1242/1260 (99%)	1183 (95%)	59 (5%)	23	12

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	27	LYS
1	A	36	SER
1	A	62	GLU
1	A	148	GLU
1	A	168	LYS
1	A	237	LYS
1	A	243	GLU
1	A	254	LYS
1	A	266	LYS
1	A	301	ASP
1	A	327	ILE
1	A	331	LEU

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Mol	Chain	Res	Type
1	B	22	THR
1	B	27	LYS
1	B	39	ASP
1	B	65	LEU
1	B	117	LYS
1	B	168	LYS
1	B	227	GLU
1	B	237	LYS
1	B	241	MET
1	B	254	LYS
1	B	291	LYS
1	B	301	ASP
1	B	374	GLU
1	B	376	LYS
1	C	16	LYS
1	C	22	THR
1	C	27	LYS
1	C	66	ARG
1	C	67	LYS
1	C	74	LYS
1	C	78	ILE
1	C	88	GLN
1	C	89	LEU
1	C	117	LYS
1	C	148	GLU
1	C	151	LYS
1	C	168	LYS
1	C	171	LYS
1	C	237	LYS
1	C	266	LYS
1	C	288	GLU
1	C	298	LYS
1	C	332	ARG
1	C	340	PHE
1	C	376	LYS
1	D	66	ARG
1	D	92	GLU
1	D	112	LYS
1	D	117	LYS
1	D	238	ASP
1	D	282	LEU
1	D	285	LYS

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Mol	Chain	Res	Type
1	D	310	LYS
1	D	370	VAL
1	D	376	LYS
1	D	382	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	137	ASN
1	B	73	GLN
1	B	141	HIS
1	C	137	ASN
1	D	141	HIS

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](#)

4 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	SDX	A	700	-	61,62,62	1.18	6 (9%)	82,93,93	1.91	20 (24%)
2	SDX	D	703	-	61,62,62	1.21	4 (6%)	82,93,93	1.77	17 (20%)
2	SDX	B	701	-	61,62,62	1.22	5 (8%)	82,93,93	1.54	18 (21%)
2	SDX	C	702	-	61,62,62	1.30	7 (11%)	82,93,93	1.57	15 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SDX	A	700	-	-	15/65/83/83	0/3/3/3
2	SDX	D	703	-	-	17/65/83/83	0/3/3/3
2	SDX	B	701	-	-	17/65/83/83	0/3/3/3
2	SDX	C	702	-	-	13/65/83/83	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	702	SDX	CA5-CA4	5.61	1.49	1.39
2	D	703	SDX	CA5-CA4	5.12	1.48	1.39
2	B	701	SDX	CA5-CA4	5.07	1.48	1.39
2	A	700	SDX	CA5-CA4	4.28	1.46	1.39
2	B	701	SDX	CA4-NA9	-3.11	1.31	1.37
2	A	700	SDX	CA8-NA7	2.95	1.37	1.31
2	C	702	SDX	CA5-NA7	-2.80	1.34	1.39
2	A	700	SDX	CA5-CA6	2.75	1.48	1.41
2	D	703	SDX	CA5-CA6	2.73	1.48	1.41
2	D	703	SDX	CA5-NA7	-2.71	1.34	1.39
2	C	702	SDX	CA4-NA9	-2.70	1.32	1.37
2	C	702	SDX	CA5-CA6	2.62	1.48	1.41
2	A	700	SDX	PB3-OB3	2.57	1.64	1.59
2	B	701	SDX	CA5-NA7	-2.46	1.34	1.39
2	C	702	SDX	CA8-NA7	2.44	1.36	1.31
2	A	700	SDX	C20-C30	-2.42	1.50	1.53
2	B	701	SDX	CA8-NA7	2.40	1.36	1.31
2	B	701	SDX	CA5-CA6	2.38	1.47	1.41
2	A	700	SDX	CA5-NA7	-2.31	1.34	1.39
2	D	703	SDX	PB3-OB3	2.25	1.63	1.59
2	C	702	SDX	PB3-OB3	2.13	1.63	1.59
2	C	702	SDX	CA2-NA1	2.03	1.37	1.33

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	700	SDX	CA5-CA4-NA3	-6.04	118.41	126.72
2	D	703	SDX	CA5-CA4-NA3	-5.86	118.65	126.72
2	A	700	SDX	NA3-CA4-NA9	5.28	136.15	127.17
2	A	700	SDX	NA1-CA2-NA3	-5.27	120.60	128.58
2	D	703	SDX	NA3-CA4-NA9	5.13	135.90	127.17
2	A	700	SDX	CA2-NA3-CA4	4.84	123.66	111.83
2	C	702	SDX	NA3-CA4-NA9	4.16	134.24	127.17
2	B	701	SDX	CA4-NA9-CA8	4.16	110.10	105.74
2	C	702	SDX	CA5-CA4-NA3	-4.13	121.03	126.72
2	A	700	SDX	CA4-NA9-CA8	3.98	109.92	105.74
2	C	702	SDX	CA4-NA9-CA8	3.86	109.79	105.74
2	D	703	SDX	CA4-CA5-NA7	-3.81	106.23	110.58
2	D	703	SDX	CA4-NA9-CA8	3.75	109.68	105.74
2	C	702	SDX	O31-C30-C20	3.61	120.07	113.14
2	D	703	SDX	CA2-NA3-CA4	3.61	120.64	111.83
2	B	701	SDX	NA3-CA4-NA9	3.60	133.29	127.17
2	B	701	SDX	CA5-CA4-NA3	-3.58	121.78	126.72
2	B	701	SDX	NA1-CA2-NA3	-3.54	123.23	128.58
2	D	703	SDX	CA5-NA7-CA8	3.49	108.94	103.45
2	A	700	SDX	NA9-CA8-NA7	-3.48	108.99	113.94
2	C	702	SDX	NA1-CA2-NA3	-3.19	123.75	128.58
2	A	700	SDX	OA3-PA1-OA1	3.18	120.26	110.70
2	A	700	SDX	O51-C50-C40	3.17	124.38	114.35
2	A	700	SDX	O2-C2-C3	-3.07	117.47	121.80
2	D	703	SDX	NA1-CA2-NA3	-3.05	123.97	128.58
2	A	700	SDX	CA5-NA7-CA8	3.04	108.23	103.45
2	B	701	SDX	CA2-NA1-CA6	3.03	123.72	118.73
2	C	702	SDX	O2-C2-C3	-3.02	117.54	121.80
2	A	700	SDX	CP7-CP6-CP5	-2.98	107.42	112.39
2	B	701	SDX	O52-C50-C40	-2.98	114.51	122.95
2	D	703	SDX	NA9-CA8-NA7	-2.97	109.72	113.94
2	A	700	SDX	C3-C20-C40	2.85	116.63	109.31
2	C	702	SDX	CA2-NA3-CA4	2.85	118.78	111.83
2	D	703	SDX	O51-C50-C40	2.83	123.33	114.35
2	B	701	SDX	O2-C2-C3	-2.78	117.87	121.80
2	A	700	SDX	CA4-CA5-NA7	-2.77	107.41	110.58
2	D	703	SDX	O2-C2-C3	-2.71	117.98	121.80
2	C	702	SDX	O51-C50-C40	2.71	122.92	114.35
2	C	702	SDX	OB3-PB3-OA8	-2.67	99.82	109.33
2	B	701	SDX	CA2-NA3-CA4	2.66	118.33	111.83
2	D	703	SDX	OP5-CP5-CP6	-2.58	117.35	122.02
2	C	702	SDX	CA2-NA1-CA6	2.55	122.92	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	703	SDX	O31-C30-C20	2.55	118.02	113.14
2	B	701	SDX	O51-C50-C40	2.53	122.36	114.35
2	D	703	SDX	OA3-PA1-OA1	2.51	118.25	110.70
2	A	700	SDX	OA2-PA1-OA3	-2.38	100.85	107.27
2	A	700	SDX	CA2-NA1-CA6	2.34	122.58	118.73
2	D	703	SDX	C3-C20-C30	-2.32	104.91	110.03
2	B	701	SDX	OB3-PB3-OA8	-2.30	101.15	109.33
2	B	701	SDX	NA6-CA6-NA1	2.27	123.43	118.38
2	B	701	SDX	NA9-CA8-NA7	-2.26	110.73	113.94
2	C	702	SDX	CA4-CA5-NA7	-2.23	108.03	110.58
2	A	700	SDX	O31-C30-C20	2.22	117.40	113.14
2	B	701	SDX	CP7-CP6-CP5	-2.21	108.70	112.39
2	A	700	SDX	C3-C20-C30	-2.21	105.15	110.03
2	A	700	SDX	OA7-PB3-OA9	2.20	116.07	107.80
2	B	701	SDX	CA4-CA5-NA7	-2.19	108.08	110.58
2	C	702	SDX	O52-C50-C40	-2.16	116.83	122.95
2	B	701	SDX	OA9-PB3-OA8	2.13	119.13	110.83
2	A	700	SDX	CA6-CA5-NA7	2.13	136.19	132.09
2	B	701	SDX	C20-C40-C50	2.12	119.72	113.92
2	B	701	SDX	C3-C20-C30	-2.08	105.44	110.03
2	A	700	SDX	O52-C50-C40	-2.07	117.09	122.95
2	D	703	SDX	CA6-CA5-NA7	2.06	136.06	132.09
2	C	702	SDX	NA9-CA8-NA7	-2.06	111.02	113.94
2	C	702	SDX	C3-C20-C40	2.05	114.57	109.31
2	B	701	SDX	CA4-NA9-CB1	-2.02	121.91	126.63
2	C	702	SDX	O32-C30-C20	-2.01	118.20	122.09
2	D	703	SDX	OA2-PA1-OA3	-2.01	101.84	107.27
2	D	703	SDX	PB3-OB3-CB3	-2.00	118.08	123.43

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	700	SDX	CQ2-OA6-PA2-OA5
2	B	701	SDX	CQ2-OA6-PA2-OA5
2	C	702	SDX	C40-C20-C30-O32
2	C	702	SDX	C40-C20-C30-O31
2	C	702	SDX	O20-C20-C30-O32
2	C	702	SDX	O20-C20-C30-O31
2	C	702	SDX	CQ2-OA6-PA2-OA5
2	D	703	SDX	CQ2-OA6-PA2-OA5
2	D	703	SDX	C40-C20-C3-C2

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Mol	Chain	Res	Type	Atoms
2	B	701	SDX	C40-C20-C3-C2
2	B	701	SDX	C40-C20-C30-O32
2	D	703	SDX	C30-C20-C3-C2
2	D	703	SDX	CP6-CP7-NP8-CP9
2	D	703	SDX	O20-C20-C3-C2
2	A	700	SDX	O20-C20-C30-O31
2	B	701	SDX	O20-C20-C30-O32
2	B	701	SDX	O20-C20-C30-O31
2	D	703	SDX	O20-C20-C30-O32
2	D	703	SDX	O20-C20-C30-O31
2	A	700	SDX	C40-C20-C30-O31
2	B	701	SDX	C40-C20-C30-O31
2	D	703	SDX	C40-C20-C30-O31
2	A	700	SDX	O20-C20-C3-C2
2	A	700	SDX	C40-C20-C3-C2
2	C	702	SDX	C40-C20-C3-C2
2	B	701	SDX	C30-C20-C3-C2
2	A	700	SDX	CP6-CP7-NP8-CP9
2	B	701	SDX	CP6-CP7-NP8-CP9
2	A	700	SDX	C40-C20-C30-O32
2	B	701	SDX	C3-C20-C30-O31
2	D	703	SDX	C40-C20-C30-O32
2	B	701	SDX	CQ2-OA6-PA2-OA3
2	D	703	SDX	CQ2-OA6-PA2-OA3
2	D	703	SDX	C20-C40-C50-O51
2	D	703	SDX	C20-C40-C50-O52
2	B	701	SDX	C20-C40-C50-O51
2	A	700	SDX	C30-C20-C3-C2
2	C	702	SDX	C30-C20-C3-C2
2	A	700	SDX	C3-C20-C30-O32
2	A	700	SDX	C3-C20-C30-O31
2	B	701	SDX	C3-C20-C30-O32
2	D	703	SDX	C3-C20-C30-O31
2	B	701	SDX	O20-C20-C3-C2
2	C	702	SDX	CP6-CP7-NP8-CP9
2	B	701	SDX	CB3-OB3-PB3-OA9
2	C	702	SDX	CB3-OB3-PB3-OA7
2	B	701	SDX	C20-C40-C50-O52
2	A	700	SDX	C20-C40-C50-O51
2	A	700	SDX	C20-C40-C50-O52
2	D	703	SDX	C3-C20-C30-O32
2	C	702	SDX	C20-C40-C50-O51

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Mol	Chain	Res	Type	Atoms
2	B	701	SDX	O2-C2-C3-C20
2	D	703	SDX	O2-C2-C3-C20
2	C	702	SDX	C20-C40-C50-O52
2	A	700	SDX	C1-C2-C3-C20
2	C	702	SDX	C1-C2-C3-C20
2	C	702	SDX	O20-C20-C3-C2
2	A	700	SDX	O20-C20-C30-O32
2	B	701	SDX	CB3-OB3-PB3-OA8
2	D	703	SDX	CB3-OB3-PB3-OA8
2	D	703	SDX	CB2-CB3-OB3-PB3
2	A	700	SDX	PA2-OA3-PA1-OA2

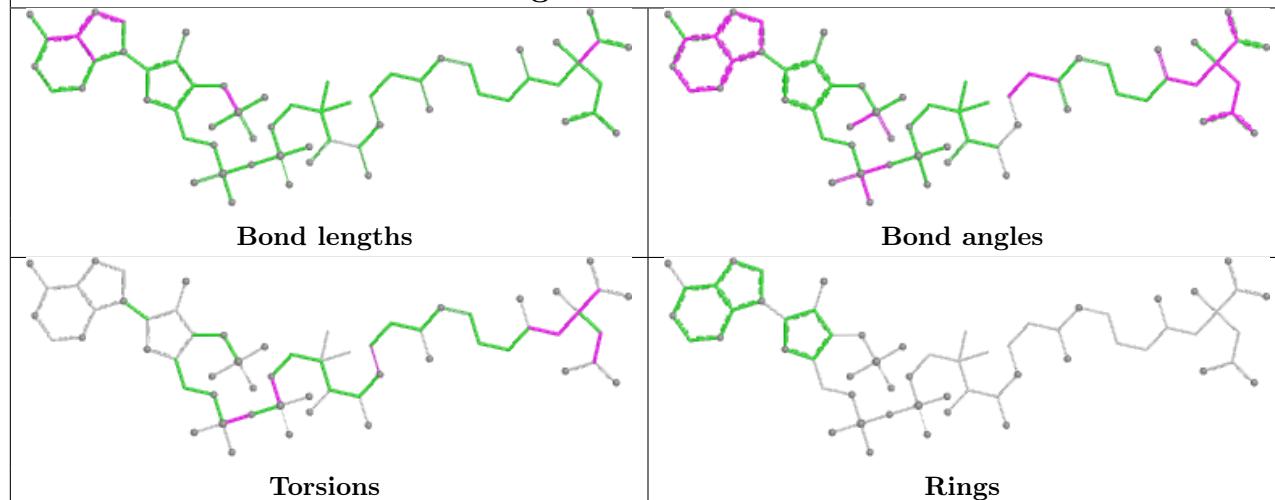
There are no ring outliers.

3 monomers are involved in 3 short contacts:

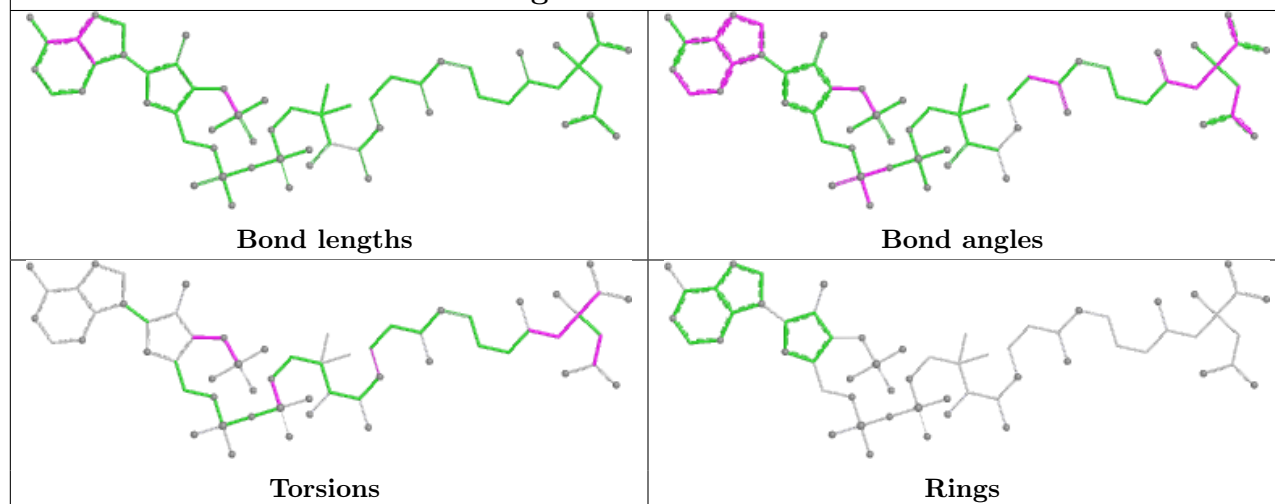
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	703	SDX	1	0
2	B	701	SDX	1	0
2	C	702	SDX	1	0

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.

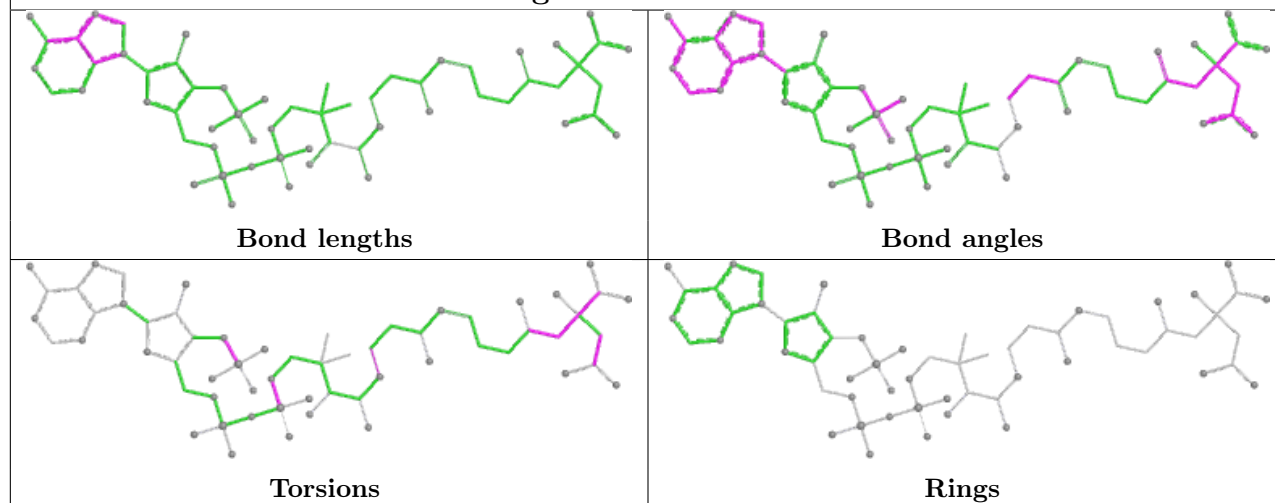
Ligand SDX A 700

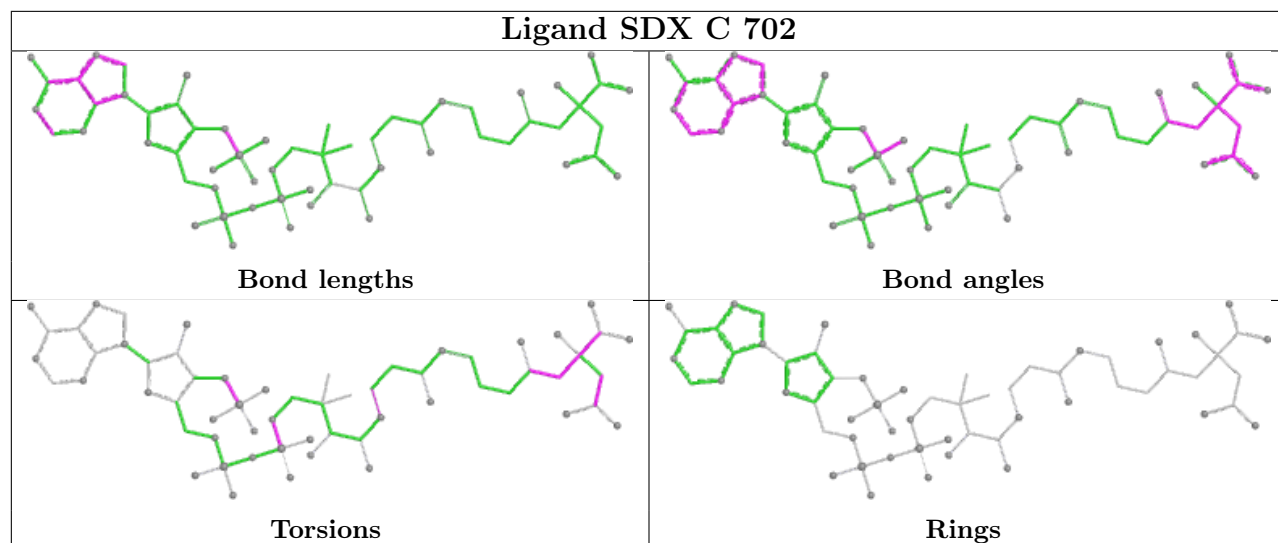


Ligand SDX D 703



Ligand SDX B 701





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	381/385 (98%)	-0.30	2 (0%) 87 90	10, 21, 34, 48	1 (0%)
1	B	379/385 (98%)	-0.25	5 (1%) 75 81	10, 21, 39, 53	1 (0%)
1	C	379/385 (98%)	-0.19	0 100 100	12, 24, 36, 45	1 (0%)
1	D	379/385 (98%)	-0.20	2 (0%) 87 90	10, 23, 41, 54	2 (0%)
All	All	1518/1540 (98%)	-0.24	9 (0%) 85 89	10, 22, 38, 54	5 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	GLU	3.1
1	D	252	ASN	3.0
1	B	380	ILE	3.0
1	A	3	THR	2.8
1	B	378	VAL	2.5
1	B	379	PRO	2.5
1	B	118	ASP	2.1
1	A	252	ASN	2.0
1	D	253	GLY	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](#)

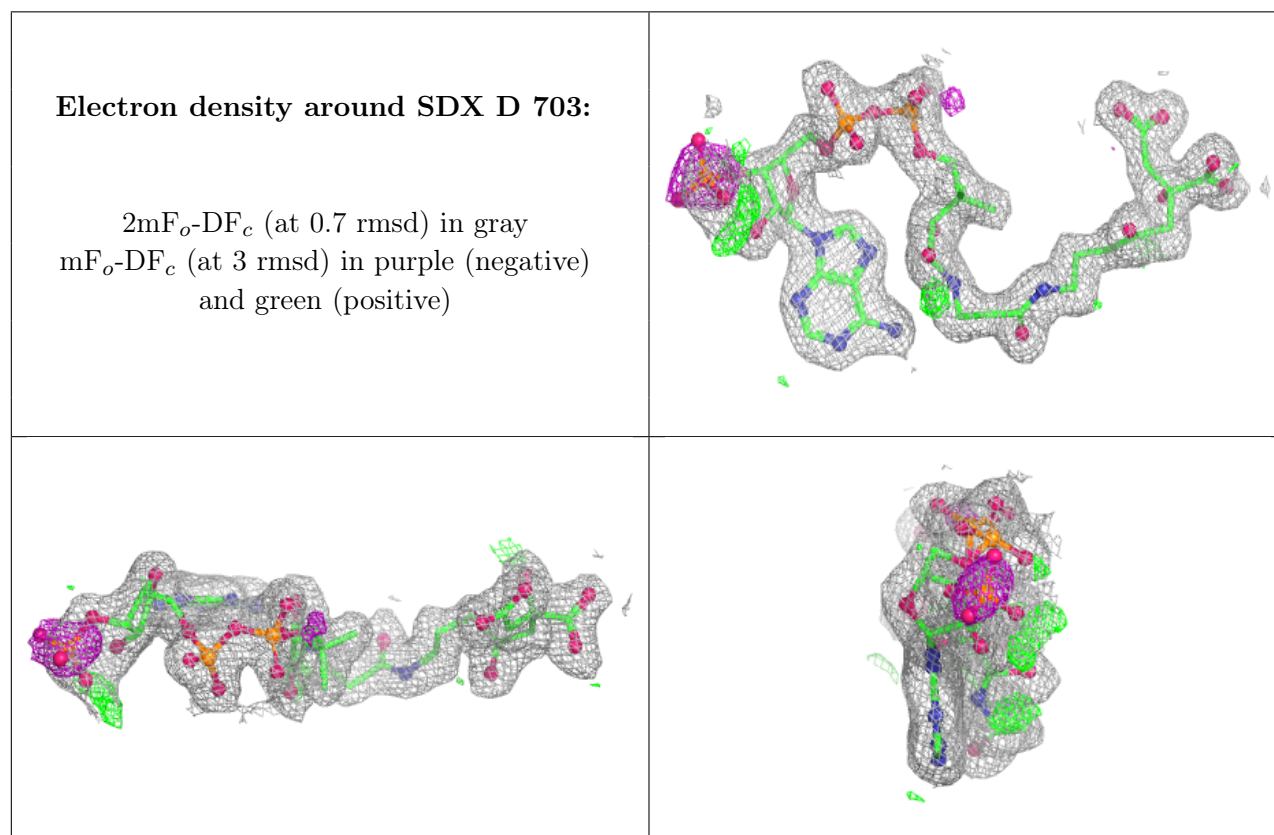
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

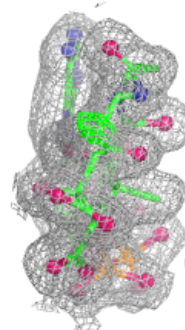
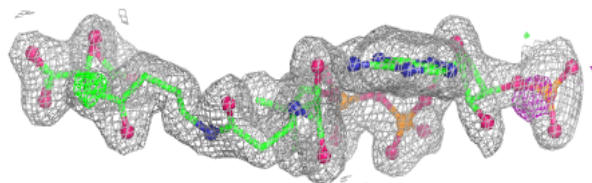
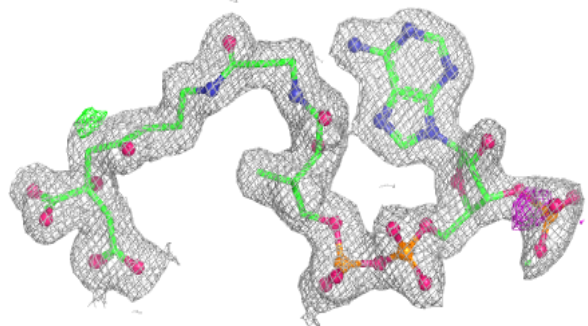
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SDX	D	703	60/60	0.95	0.07	15,23,57,59	0
2	SDX	C	702	60/60	0.96	0.06	12,21,40,43	0
2	SDX	A	700	60/60	0.97	0.06	11,20,39,42	0
2	SDX	B	701	60/60	0.97	0.05	11,18,38,41	0

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.

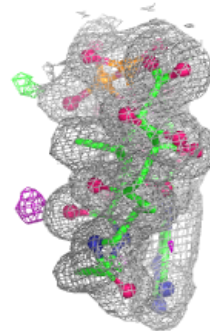
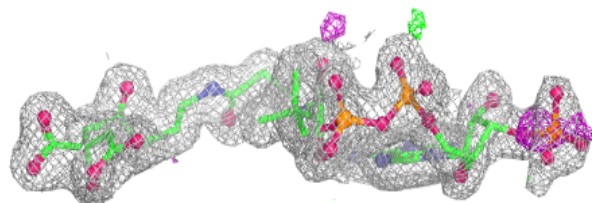
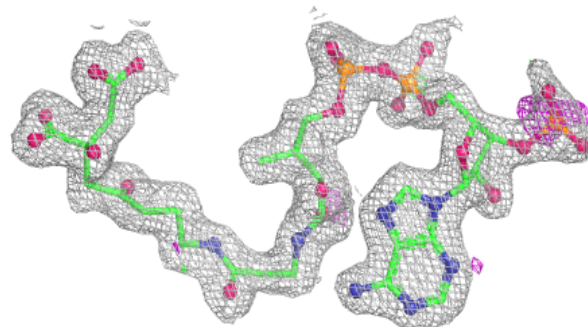


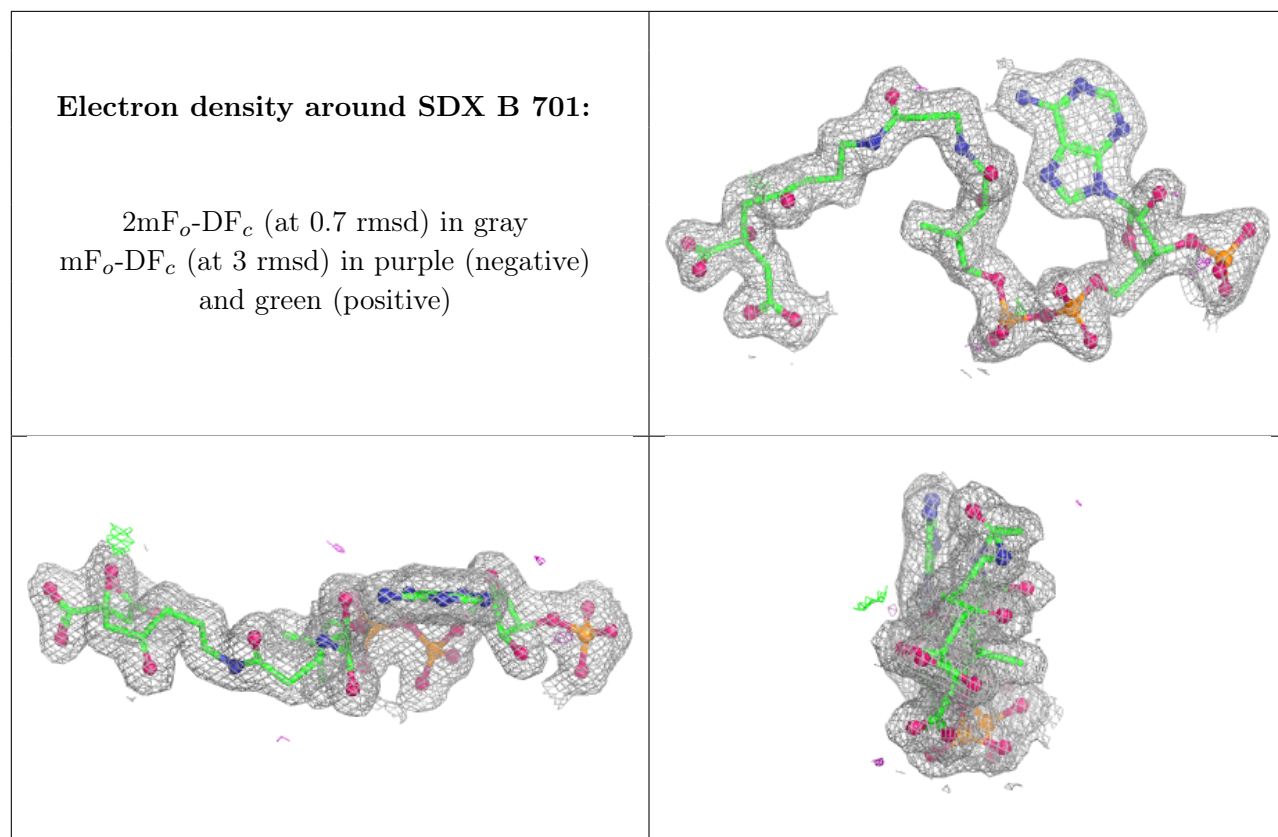
Electron density around SDX C 702:

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

**Electron density around SDX A 700:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.