



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:38 PM EDT

PDB ID : 4KTV / pdb_00004ktv
Title : Structural insights of MAT enzymes: MATa2b complexed with adenosine and pyrophosphate
Authors : Murray, B.; Antonyuk, S.V.; Marina, A.; Lu, S.C.; Mato, J.M.; Hasnain, S.S.; Rojas, A.L.
Deposited on : 2013-05-21
Resolution : 3.30 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:

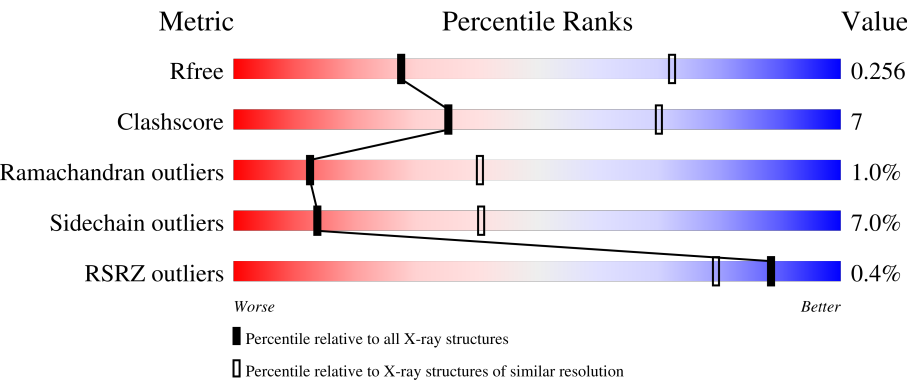
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	396	72%18%9%
1	B	396	74%20%9%
1	C	396	74%15%9%
1	D	396	78%17%9%

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Mol	Chain	Length	Quality of chain
2	E	327	72%20%6%
2	F	327	% 61%24%5%10%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16508 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 S-adenosylmethionine synthase isoform type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2822	1790	492	529	11			
1	B	381	Total	C	N	O	S	0	0	0
			2963	1872	518	562	11			
1	C	361	Total	C	N	O	S	0	0	0
			2815	1785	491	528	11			
1	D	381	Total	C	N	O	S	0	0	0
			2963	1872	518	562	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP P31153
B	0	SER	-	expression tag	UNP P31153
C	0	SER	-	expression tag	UNP P31153
D	0	SER	-	expression tag	UNP P31153

- Molecule 2 is a protein called Methionine adenosyltransferase 2 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	309	Total	C	N	O	S	0	0	0
			2448	1546	446	446	10			
2	F	295	Total	C	N	O	S	0	1	0
			2359	1493	431	425	10			

There are 8 discrepancies between the modelled and reference sequences:

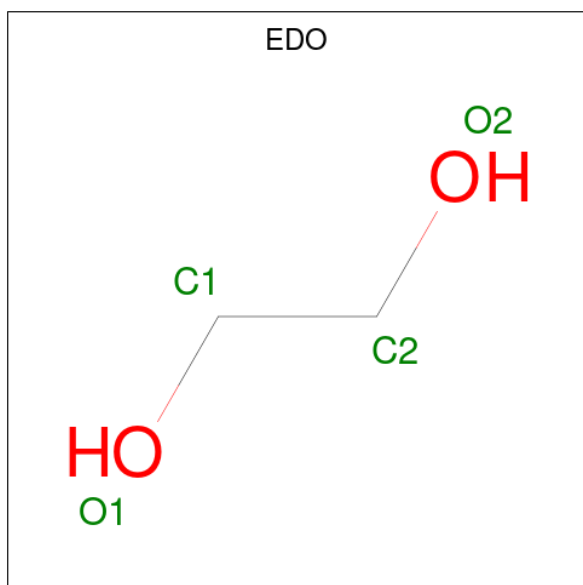
Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	GLY	-	expression tag	UNP Q9NZL9
E	-2	SER	-	expression tag	UNP Q9NZL9
E	-1	HIS	-	expression tag	UNP Q9NZL9
E	0	MET	-	expression tag	UNP Q9NZL9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	GLY	-	expression tag	UNP Q9NZL9
F	-2	SER	-	expression tag	UNP Q9NZL9
F	-1	HIS	-	expression tag	UNP Q9NZL9
F	0	MET	-	expression tag	UNP Q9NZL9

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



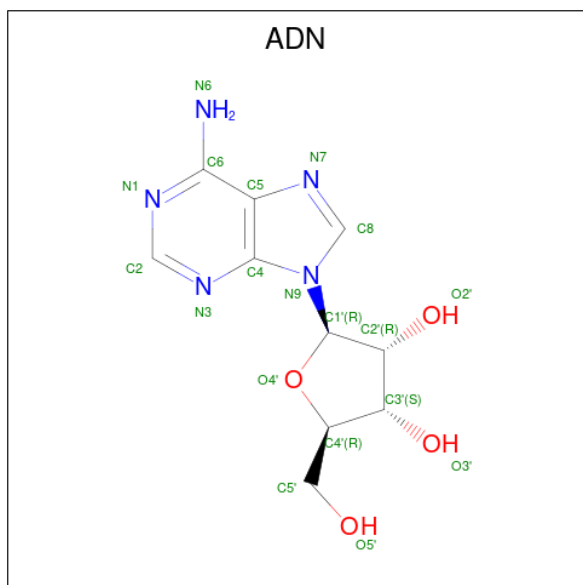
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0

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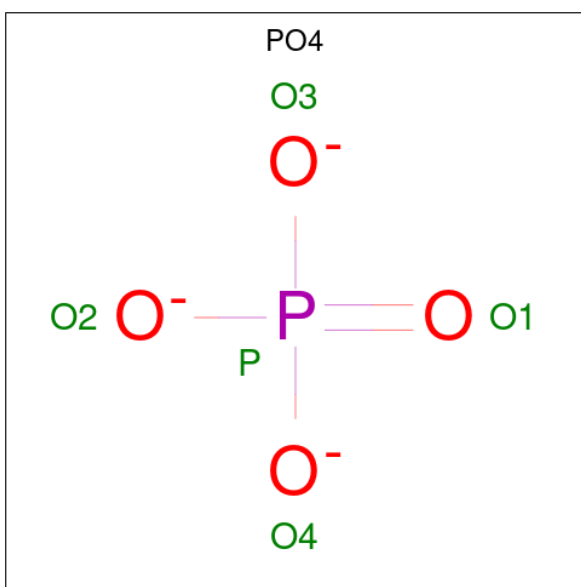
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ADENOSINE (CCD ID: ADN) (formula: $C_{10}H_{13}N_5O_4$).



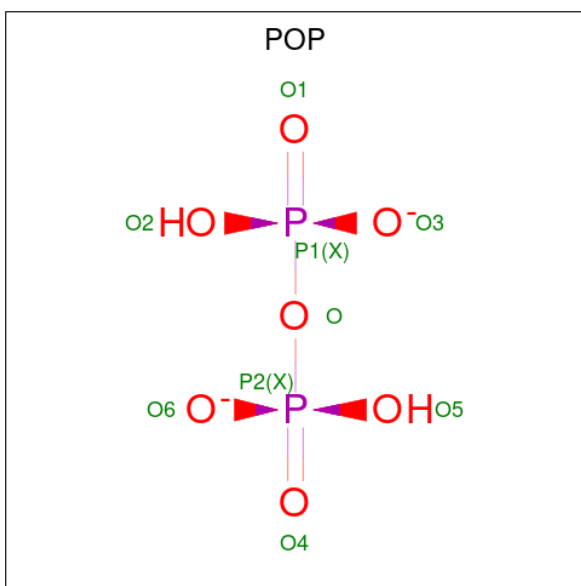
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			19	10	5	4		
4	C	1	Total	C	N	O	0	0
			19	10	5	4		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 6 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	O	P	0	0
			9	7	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total Mg 1 1	0	0

- Molecule 8 is water.

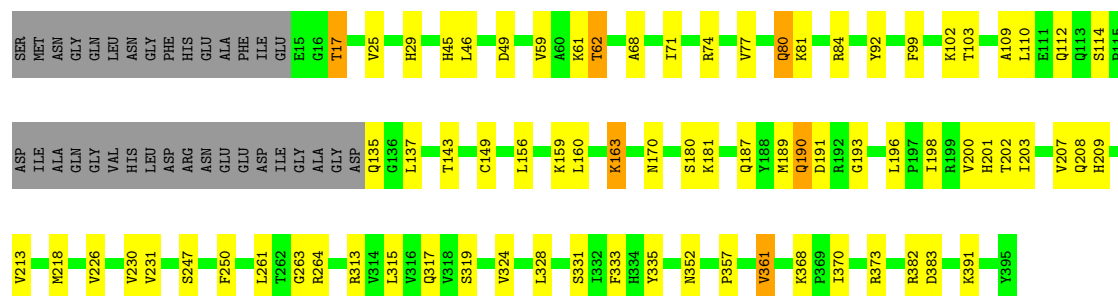
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	7	Total O 7 7	0	0
8	B	8	Total O 8 8	0	0
8	C	4	Total O 4 4	0	0
8	D	13	Total O 13 13	0	0
8	E	3	Total O 3 3	0	0
8	F	2	Total O 2 2	0	0

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.

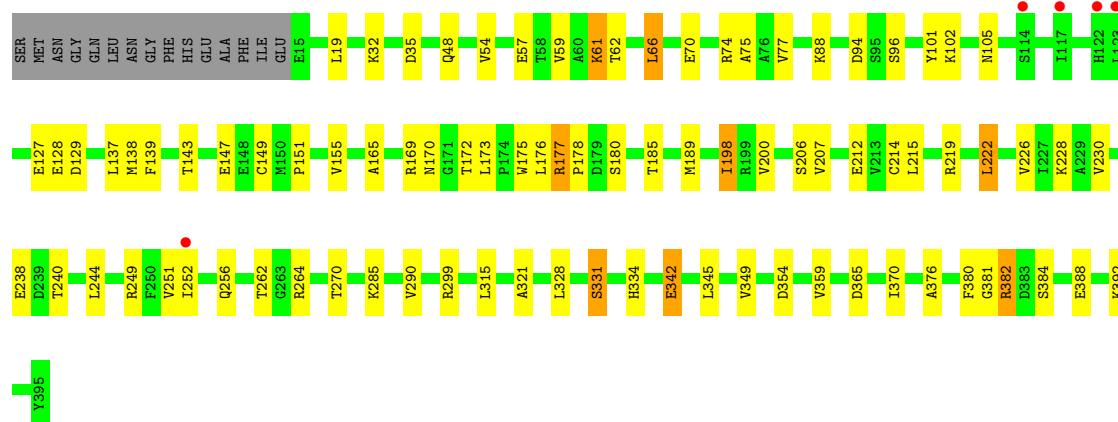
• Molecule 1: S-adenosylmethionine synthase isoform type-2

Chain A: 



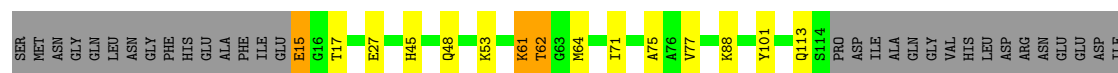
• Molecule 1: S-adenosylmethionine synthase isoform type-2

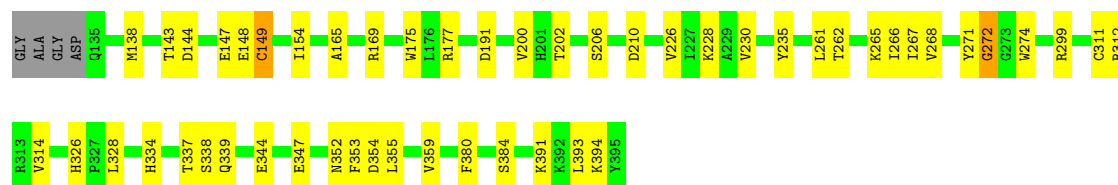
Chain B: 



• Molecule 1: S-adenosylmethionine synthase isoform type-2

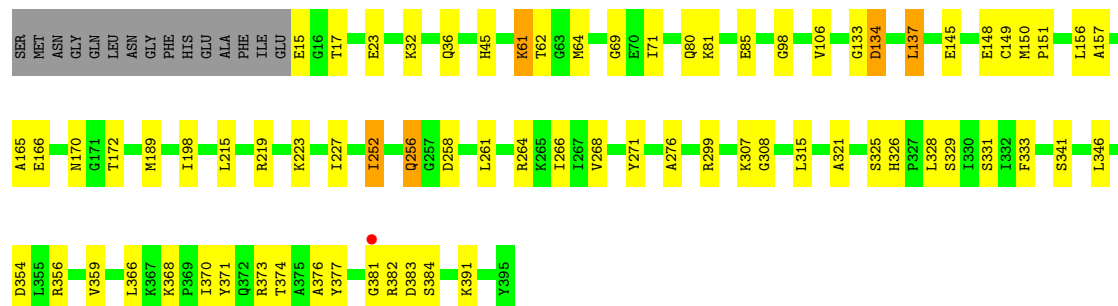
Chain C: 





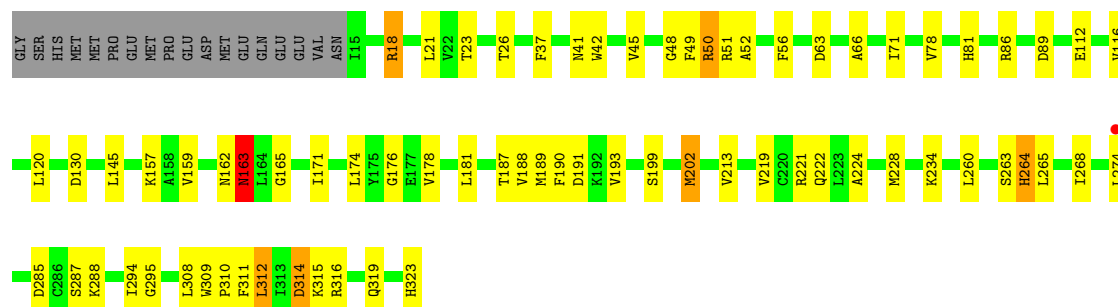
- Molecule 1: S-adenosylmethionine synthase isoform type-2

Chain D: 78% 17% . .



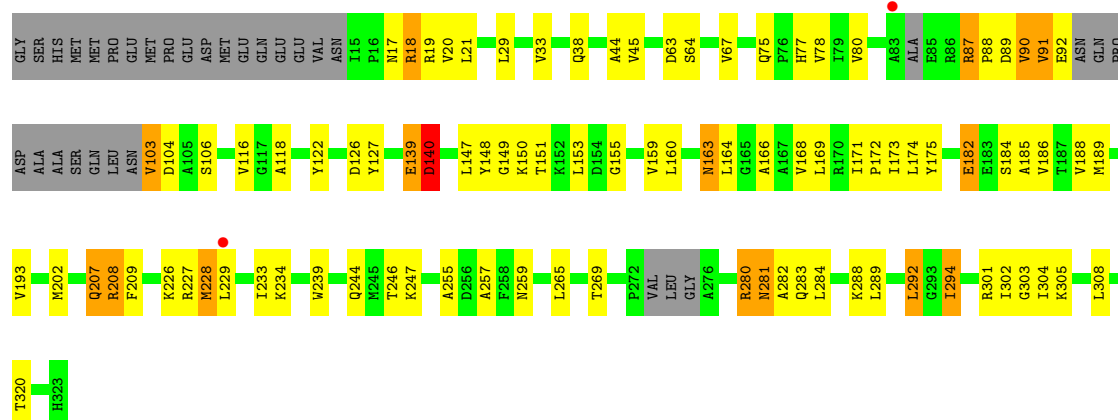
- Molecule 2: Methionine adenosyltransferase 2 subunit beta

Chain E: 72% 20% . 6%



- Molecule 2: Methionine adenosyltransferase 2 subunit beta

Chain F: 61% 24% 5% 10%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.09Å 116.57Å 299.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	108.87 – 3.30 108.87 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (108.87-3.30) 99.8 (108.87-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0029, PHENIX	Depositor
R, R_{free}	0.176 , 0.260 0.177 , 0.256	Depositor DCC
R_{free} test set	1949 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.3	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 74.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16508	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, MG, POP, ADN, PO4

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	0.58	0/2879	0.87	2/3893 (0.1%)
1	B	0.60	1/3022 (0.0%)	0.88	2/4088 (0.0%)
1	C	0.58	0/2871	0.85	1/3881 (0.0%)
1	D	0.60	0/3022	0.86	1/4088 (0.0%)
2	E	0.56	0/2507	0.83	0/3401
2	F	0.58	0/2417	0.87	1/3271 (0.0%)
All	All	0.59	1/16718 (0.0%)	0.86	7/22622 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	THR	CA-C	7.27	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	GLY	N-CA-C	6.29	118.63	110.45
1	C	314	VAL	N-CA-C	6.23	116.04	108.06
1	A	213	VAL	N-CA-C	6.06	117.24	109.30
1	A	170	ASN	CB-CA-C	-5.81	100.98	110.85
1	B	178	PRO	N-CA-C	5.48	120.96	113.84
2	F	209	PHE	N-CA-C	5.22	116.28	108.76
1	B	198	ILE	CB-CA-C	-5.06	107.41	111.71

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	2822	0	2832	43	0
1	B	2963	0	2956	40	0
1	C	2815	0	2825	30	0
1	D	2963	0	2956	42	0
2	E	2448	0	2418	38	0
2	F	2359	0	2335	61	0
3	A	8	0	12	0	0
3	B	16	0	24	1	0
3	C	8	0	12	0	0
3	D	12	0	18	2	0
3	E	4	0	6	0	0
4	A	19	0	13	2	0
4	C	19	0	13	0	0
5	A	5	0	0	0	0
6	C	9	0	0	0	0
7	D	1	0	0	0	0
8	A	7	0	0	0	0
8	B	8	0	0	0	0
8	C	4	0	0	0	0
8	D	13	0	0	0	0
8	E	3	0	0	0	0
8	F	2	0	0	0	0
All	All	16508	0	16420	242	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 7.

All (242) 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:189:MET:HB2	1:A:198:ILE:HD11	1.66	0.77
1:D:189:MET:HB2	1:D:198:ILE:HD11	1.67	0.77
1:A:25:VAL:HG12	1:A:181:LYS:HG2	1.64	0.77
1:C:200:VAL:HG23	1:C:235:TYR:HB3	1.72	0.72
1:D:150:MET:HA	1:D:150:MET:HE2	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:GLN:HB2	1:C:75:ALA:HB2	1.72	0.71
2:F:168:VAL:HG12	2:F:168:VAL:O	1.92	0.70
2:F:88:PRO:HA	2:F:89:ASP:C	2.19	0.68
1:A:156:LEU:HD22	1:A:231:VAL:HG22	1.77	0.65
1:D:150:MET:HE3	1:D:299:ARG:CZ	2.25	0.65
1:A:45:HIS:CD2	1:A:77:VAL:HG21	2.32	0.65
2:F:126:ASP:HB3	2:F:284:LEU:HD21	1.79	0.65
1:D:321:ALA:HB2	1:D:328:LEU:HD11	1.78	0.64
2:E:78:VAL:HG21	2:E:224:ALA:HB1	1.79	0.64
1:C:45:HIS:CD2	1:C:77:VAL:HG21	2.32	0.64
2:E:174:LEU:HD13	2:E:213:VAL:HG12	1.79	0.63
2:F:103:VAL:N	2:F:104:ASP:HA	2.14	0.63
2:F:227:ARG:O	2:F:228:MET:HE3	1.98	0.62
2:F:226:LYS:O	2:F:226:LYS:HD3	1.99	0.62
1:A:59:VAL:HG21	1:B:59:VAL:HG21	1.83	0.61
1:A:373:ARG:O	1:A:382:ARG:NH2	2.34	0.60
1:A:109:ALA:HB1	1:B:61:LYS:HE2	1.83	0.59
2:E:228:MET:HE2	2:E:228:MET:HA	1.84	0.59
2:F:19:ARG:NH1	2:F:75:GLN:O	2.35	0.59
1:D:189:MET:HE2	1:D:198:ILE:HD11	1.85	0.58
1:B:200:VAL:O	1:B:240:THR:HG23	2.04	0.57
2:F:184:SER:O	2:F:188:VAL:HG13	2.03	0.57
1:A:370:ILE:HB	1:A:373:ARG:HE	1.69	0.57
1:B:376:ALA:O	1:B:382:ARG:NH2	2.37	0.57
1:A:261:LEU:HD11	1:B:57:GLU:HB3	1.87	0.57
1:C:261:LEU:HB3	1:D:261:LEU:HD13	1.87	0.57
1:B:334:HIS:CD2	1:B:342:GLU:HG3	2.39	0.57
1:C:267:ILE:HG22	1:C:272:GLY:HA2	1.87	0.57
1:A:352:ASN:O	1:A:391:LYS:HE3	2.05	0.56
1:A:137:LEU:HD11	1:A:317:GLN:CG	2.36	0.56
2:E:116:VAL:HG12	2:E:116:VAL:O	2.06	0.56
2:E:176:GLY:O	2:E:178:VAL:HG13	2.06	0.55
1:D:61:LYS:HG2	1:D:64:MET:HE2	1.88	0.55
2:E:219:VAL:HG22	2:E:295:GLY:HA2	1.88	0.55
1:D:252:ILE:HG23	1:D:252:ILE:O	2.07	0.55
2:E:18:ARG:NH1	2:E:41:ASN:O	2.40	0.55
2:F:173:ILE:HD11	2:F:185:ALA:HB3	1.89	0.55
2:F:207:GLN:HA	2:F:246:THR:HG22	1.87	0.55
1:B:189:MET:HB2	1:B:198:ILE:HD11	1.88	0.54
2:F:63:ASP:O	2:F:67:VAL:HG23	2.07	0.54
1:A:137:LEU:HD11	1:A:317:GLN:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:GLY:O	1:D:256:GLN:HG2	2.07	0.54
1:B:48:GLN:HB2	1:B:75:ALA:HB2	1.88	0.54
1:A:59:VAL:HG22	1:A:261:LEU:HD22	1.89	0.54
1:B:345:LEU:O	1:B:349:VAL:HG23	2.08	0.54
2:F:257:ALA:HB1	2:F:305:LYS:HD2	1.90	0.53
1:D:346:LEU:HD22	3:D:403:EDO:H12	1.89	0.53
2:F:20:VAL:HA	2:F:78:VAL:O	2.08	0.53
2:F:116:VAL:HG12	2:F:116:VAL:O	2.09	0.53
1:D:307:LYS:O	1:D:308:GLY:C	2.51	0.53
1:D:150:MET:HE1	1:D:271:TYR:CD1	2.43	0.52
2:F:87:ARG:O	2:F:89:ASP:HB3	2.09	0.52
2:F:292:LEU:N	2:F:292:LEU:HD22	2.24	0.52
2:E:23:THR:OG1	2:E:81:HIS:HA	2.10	0.52
2:E:37:PHE:CZ	2:E:221:ARG:HA	2.44	0.52
1:B:94:ASP:OD2	1:B:96:SER:HB2	2.10	0.52
2:F:182:GLU:HA	2:F:188:VAL:HG12	1.91	0.52
1:C:45:HIS:CE1	1:C:71:ILE:HG21	2.45	0.51
1:B:74:ARG:HB2	1:B:74:ARG:CZ	2.40	0.51
1:C:143:THR:O	1:C:149:CYS:HA	2.11	0.51
2:F:155:GLY:O	2:F:159:VAL:HG23	2.09	0.51
1:A:59:VAL:HG22	1:A:261:LEU:CD2	2.41	0.51
1:C:262:THR:O	1:D:264:ARG:NH1	2.44	0.51
1:D:150:MET:HE3	1:D:299:ARG:NH1	2.25	0.51
1:B:151:PRO:O	1:B:155:VAL:HG23	2.11	0.51
1:D:170:ASN:OD1	1:D:170:ASN:C	2.54	0.51
1:D:346:LEU:HD22	3:D:403:EDO:C1	2.41	0.51
1:B:88:LYS:HG3	1:B:101:TYR:CE1	2.45	0.51
2:E:49:PHE:O	2:E:50:ARG:C	2.54	0.50
2:F:226:LYS:O	2:F:226:LYS:CD	2.60	0.50
1:A:200:VAL:HG11	1:A:203:ILE:HD11	1.93	0.50
1:C:311:CYS:HB3	1:C:338:SER:HB2	1.93	0.50
1:A:143:THR:O	1:A:149:CYS:HA	2.12	0.50
2:F:122:TYR:CD1	2:F:159:VAL:HG21	2.46	0.50
1:B:381:GLY:H	1:B:388:GLU:CD	2.19	0.50
1:C:226:VAL:O	1:C:230:VAL:HG23	2.11	0.50
1:D:45:HIS:CE1	1:D:71:ILE:HG21	2.46	0.50
2:E:71:ILE:HG22	2:E:116:VAL:HG21	1.94	0.50
1:A:160:LEU:HD23	1:A:230:VAL:HG21	1.94	0.50
2:F:163:ASN:ND2	2:F:166:ALA:HB2	2.27	0.50
2:E:202:MET:HE3	2:E:202:MET:HA	1.94	0.49
1:B:331:SER:HA	3:B:401:EDO:C2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:21:LEU:HD12	2:F:45:VAL:O	2.12	0.49
1:C:144:ASP:OD2	1:C:312:ARG:HB3	2.12	0.49
2:E:52:ALA:HB1	2:E:56:PHE:HB2	1.93	0.49
2:E:120:LEU:HD23	2:E:159:VAL:HG13	1.94	0.49
2:F:103:VAL:N	2:F:104:ASP:CA	2.75	0.49
2:F:160:LEU:HD11	2:F:168:VAL:HG21	1.95	0.49
2:E:188:VAL:C	2:E:190:PHE:H	2.20	0.49
1:D:165:ALA:O	1:D:166:GLU:C	2.56	0.49
2:E:315:LYS:O	2:E:319:GLN:HG3	2.11	0.49
2:F:168:VAL:O	2:F:168:VAL:CG1	2.60	0.49
1:B:176:LEU:C	1:B:177:ARG:HG2	2.38	0.49
1:A:209:HIS:CD2	1:A:218:MET:HE1	2.48	0.48
2:F:169:LEU:HD11	2:F:239:TRP:HB3	1.95	0.48
2:F:281:ASN:OD1	2:F:282:ALA:N	2.46	0.48
1:B:226:VAL:O	1:B:230:VAL:HG23	2.12	0.48
2:F:288:LYS:O	2:F:292:LEU:HD21	2.13	0.48
1:D:23:GLU:O	1:D:268:VAL:HG22	2.13	0.48
1:A:61:LYS:O	1:A:62:THR:C	2.56	0.48
2:E:309:TRP:HA	2:E:312:LEU:HD22	1.94	0.48
1:C:202:THR:HG21	1:D:328:LEU:HD13	1.94	0.48
1:C:334:HIS:O	1:C:337:THR:OG1	2.29	0.48
2:F:292:LEU:HD22	2:F:292:LEU:H	1.77	0.48
1:C:265:LYS:HB3	1:C:268:VAL:HB	1.95	0.48
2:E:287:SER:O	2:E:288:LYS:C	2.57	0.48
1:B:165:ALA:HB1	1:B:169:ARG:HH21	1.79	0.48
1:D:80:GLN:HE22	1:D:106:VAL:HB	1.78	0.47
2:F:173:ILE:HD12	2:F:208:ARG:NH1	2.29	0.47
1:C:354:ASP:HB3	1:C:359:VAL:HG11	1.95	0.47
1:A:109:ALA:HB1	1:B:61:LYS:CE	2.45	0.47
1:D:354:ASP:HB3	1:D:359:VAL:HG11	1.97	0.47
1:D:366:LEU:O	1:D:371:TYR:OH	2.28	0.47
2:F:104:ASP:OD2	2:F:104:ASP:C	2.57	0.47
1:A:193:GLY:O	1:A:313:ARG:NH1	2.48	0.47
1:A:370:ILE:HB	1:A:373:ARG:NE	2.28	0.47
1:C:15:GLU:N	1:C:15:GLU:CD	2.72	0.47
1:D:156:LEU:O	1:D:157:ALA:C	2.58	0.47
1:B:48:GLN:HB2	1:B:75:ALA:CB	2.45	0.46
1:D:326:HIS:CD2	1:D:356:ARG:HD3	2.50	0.46
1:C:353:PHE:HB3	1:C:355:LEU:HD21	1.96	0.46
2:F:227:ARG:HD3	2:F:233:ILE:HB	1.95	0.46
1:B:66:LEU:C	1:B:66:LEU:HD23	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:SER:HB3	1:A:207:VAL:HG23	1.98	0.46
2:E:130:ASP:HB2	2:E:145:LEU:HD21	1.98	0.46
2:F:33:VAL:HG11	2:F:80:VAL:HG11	1.97	0.46
2:E:18:ARG:HB2	2:E:42:TRP:CE3	2.51	0.46
2:F:139:GLU:O	2:F:140:ASP:O	2.33	0.46
2:E:163:ASN:C	2:E:163:ASN:HD22	2.23	0.46
2:F:89:ASP:O	2:F:91:VAL:HG23	2.16	0.46
1:B:54:VAL:O	1:B:285:LYS:HA	2.16	0.46
1:B:299:ARG:HG2	1:B:380:PHE:CD1	2.51	0.46
1:D:215:LEU:HD23	1:D:219:ARG:NH2	2.31	0.46
1:B:180:SER:HB3	1:B:207:VAL:HG23	1.98	0.46
1:B:321:ALA:HB2	1:B:328:LEU:HD21	1.98	0.45
1:D:137:LEU:N	1:D:137:LEU:HD23	2.30	0.45
2:F:280:ARG:O	2:F:281:ASN:CB	2.64	0.45
2:E:21:LEU:HD12	2:E:45:VAL:O	2.16	0.45
2:F:18:ARG:CZ	2:F:18:ARG:HB2	2.46	0.45
2:F:89:ASP:O	2:F:90:VAL:C	2.59	0.45
1:B:215:LEU:HG	1:B:219:ARG:HE	1.81	0.45
1:D:370:ILE:HB	1:D:373:ARG:HD2	1.98	0.45
1:B:165:ALA:HB1	1:B:169:ARG:NH2	2.31	0.45
1:A:247:SER:CB	4:A:403:ADN:N1	2.80	0.45
1:A:74:ARG:CZ	1:A:74:ARG:HB2	2.47	0.45
2:F:88:PRO:HA	2:F:90:VAL:N	2.32	0.45
2:F:202:MET:CE	2:F:265:LEU:HD22	2.47	0.45
2:F:226:LYS:HE2	2:F:292:LEU:HG	1.98	0.45
1:C:48:GLN:HB2	1:C:75:ALA:CB	2.44	0.45
1:C:175:TRP:HB2	1:C:210:ASP:OD1	2.17	0.45
2:E:181:LEU:HD21	2:E:311:PHE:CG	2.52	0.44
1:A:163:LYS:HG2	1:A:226:VAL:HG13	1.99	0.44
1:B:143:THR:O	1:B:149:CYS:HA	2.17	0.44
1:C:271:TYR:O	1:C:274:TRP:N	2.48	0.44
2:E:48:GLY:O	2:E:52:ALA:HB2	2.17	0.44
2:F:189:MET:O	2:F:193:VAL:HG23	2.18	0.44
2:F:246:THR:O	2:F:247:LYS:C	2.60	0.44
1:D:133:GLY:O	1:D:134:ASP:HB2	2.17	0.44
1:D:223:LYS:HA	1:D:227:ILE:HD12	1.99	0.44
2:E:188:VAL:O	2:E:190:PHE:N	2.51	0.44
1:B:35:ASP:HA	1:B:262:THR:HG23	1.98	0.44
1:C:299:ARG:HG2	1:C:380:PHE:CD1	2.53	0.44
2:E:285:ASP:C	2:E:285:ASP:OD1	2.61	0.44
1:A:71:ILE:O	1:A:112:GLN:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:165:ALA:HB1	1:C:169:ARG:NH2	2.33	0.44
2:E:222:GLN:HB3	2:E:294:ILE:HG23	2.00	0.44
2:F:294:ILE:O	2:F:294:ILE:HG22	2.18	0.44
1:B:138:MET:SD	1:B:138:MET:N	2.91	0.44
1:D:150:MET:HG3	1:D:381:GLY:HA3	2.00	0.44
2:F:92:GLU:HB3	2:F:147:LEU:HD12	2.00	0.44
1:B:354:ASP:CG	1:B:359:VAL:HG21	2.44	0.43
2:E:199:SER:HA	2:E:264:HIS:HB2	2.00	0.43
1:C:61:LYS:O	1:C:62:THR:C	2.61	0.43
1:A:201:HIS:ND1	1:A:202:THR:OG1	2.44	0.43
2:E:263:SER:C	2:E:265:LEU:N	2.75	0.43
2:F:38:GLN:HB2	2:F:44:ALA:HB3	2.01	0.43
1:D:145:GLU:CD	1:D:151:PRO:HA	2.42	0.43
2:E:314:ASP:OD2	2:E:314:ASP:N	2.46	0.43
2:F:302:ILE:O	2:F:303:GLY:C	2.62	0.43
2:F:304:ILE:HG13	2:F:308:LEU:HD12	1.99	0.43
2:F:175:TYR:HB3	2:F:186:VAL:HG21	2.00	0.43
1:A:190:GLN:HE21	1:A:191:ASP:N	2.17	0.43
1:C:391:LYS:O	1:C:393:LEU:HD22	2.18	0.43
1:D:376:ALA:O	1:D:377:TYR:HB2	2.18	0.43
1:A:46:LEU:HA	1:A:49:ASP:O	2.18	0.43
1:C:165:ALA:HB1	1:C:169:ARG:HH21	1.84	0.43
1:C:352:ASN:HD21	1:C:394:LYS:H	1.66	0.43
1:D:81:LYS:O	1:D:85:GLU:HG2	2.18	0.43
1:D:150:MET:HE1	1:D:271:TYR:CE1	2.53	0.43
1:A:208:GLN:HA	1:A:250:PHE:O	2.19	0.42
2:F:87:ARG:HD3	2:F:184:SER:HA	2.00	0.42
1:D:383:ASP:O	1:D:384:SER:HB2	2.19	0.42
2:F:148:TYR:O	2:F:149:GLY:C	2.61	0.42
2:E:165:GLY:HA2	2:E:234:LYS:HB2	2.00	0.42
2:E:309:TRP:N	2:E:310:PRO:CD	2.82	0.42
1:A:25:VAL:HG12	1:A:181:LYS:CG	2.43	0.42
1:B:222:LEU:O	1:B:226:VAL:HB	2.20	0.42
1:B:66:LEU:HD23	1:B:66:LEU:O	2.19	0.42
1:B:170:ASN:OD1	1:B:172:THR:HG22	2.19	0.42
1:D:276:ALA:HB2	2:E:323:HIS:CE1	2.54	0.42
1:A:357:PRO:O	1:A:361:VAL:HG13	2.20	0.42
1:A:261:LEU:HD12	1:A:264:ARG:HH11	1.85	0.42
2:F:29:LEU:O	2:F:33:VAL:HG23	2.20	0.42
1:A:92:TYR:HB3	1:A:99:PHE:HB3	2.03	0.41
1:B:105:ASN:CG	1:C:64:MET:HB2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:GLU:OE2	1:C:169:ARG:NH2	2.44	0.41
2:F:104:ASP:C	2:F:106:SER:N	2.78	0.41
2:F:289:LEU:HD11	2:F:294:ILE:HG21	2.03	0.41
2:E:130:ASP:CB	2:E:145:LEU:HD21	2.50	0.41
2:E:191:ASP:OD1	2:E:316:ARG:NH2	2.41	0.41
2:F:126:ASP:CB	2:F:284:LEU:HD21	2.49	0.41
1:A:80:GLN:HG3	1:A:84:ARG:HE	1.85	0.41
1:B:19:LEU:HD22	1:B:185:THR:HG22	2.02	0.41
1:C:88:LYS:HG3	1:C:101:TYR:CE1	2.55	0.41
2:E:162:ASN:O	2:E:163:ASN:HB2	2.20	0.41
1:A:17:THR:HG21	1:A:187:GLN:HE21	1.86	0.41
1:A:29:HIS:CD2	4:A:403:ADN:O2'	2.73	0.41
1:A:103:THR:O	1:D:62:THR:HG22	2.21	0.41
1:B:94:ASP:OD2	1:B:96:SER:CB	2.69	0.41
2:F:171:ILE:CD1	2:F:174:LEU:HD11	2.50	0.41
2:E:63:ASP:OD2	2:E:66:ALA:HB2	2.21	0.41
1:A:263:GLY:O	1:B:264:ARG:HD3	2.20	0.41
1:B:173:LEU:HD22	1:B:175:TRP:CZ2	2.56	0.41
2:F:207:GLN:HG2	2:F:244:GLN:HE21	1.86	0.41
2:F:227:ARG:C	2:F:228:MET:HE3	2.46	0.41
1:B:139:PHE:CD1	1:B:315:LEU:HD11	2.56	0.41
1:C:266:ILE:HD11	1:D:266:ILE:HD11	2.03	0.41
1:D:36:GLN:HE21	1:D:36:GLN:HB2	1.71	0.41
1:D:315:LEU:HB3	1:D:333:PHE:HB2	2.02	0.41
2:F:77:HIS:O	2:F:118:ALA:HA	2.21	0.40
1:D:374:THR:C	1:D:376:ALA:H	2.29	0.40
2:F:288:LYS:O	2:F:292:LEU:CD2	2.68	0.40
1:A:71:ILE:HD12	1:A:110:LEU:HD13	2.03	0.40
1:A:315:LEU:HD23	1:A:333:PHE:HD2	1.86	0.40
2:F:255:ALA:O	2:F:259:ASN:N	2.55	0.40
1:A:68:ALA:C	1:A:110:LEU:HD23	2.47	0.40
2:E:187:THR:HG22	2:E:308:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	358/396 (90%)	330 (92%)	26 (7%)	2 (1%)	21	52
1	B	379/396 (96%)	349 (92%)	29 (8%)	1 (0%)	36	65
1	C	357/396 (90%)	322 (90%)	33 (9%)	2 (1%)	21	52
1	D	379/396 (96%)	343 (90%)	33 (9%)	3 (1%)	16	45
2	E	307/327 (94%)	281 (92%)	22 (7%)	4 (1%)	9	35
2	F	288/327 (88%)	238 (83%)	42 (15%)	8 (3%)	4	21
All	All	2068/2238 (92%)	1863 (90%)	185 (9%)	20 (1%)	12	40

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	272	GLY
2	E	50	ARG
2	E	163	ASN
2	F	140	ASP
1	A	335	TYR
1	C	62	THR
1	D	134	ASP
2	F	281	ASN
1	A	62	THR
1	D	172	THR
2	E	189	MET
2	F	234	LYS
2	F	283	GLN
2	F	127	TYR
1	D	252	ILE
2	E	264	HIS
2	F	90	VAL
2	F	172	PRO
1	B	252	ILE
2	F	91	VAL

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	302/328 (92%)	285 (94%)	17 (6%)	19	47
1	B	316/328 (96%)	285 (90%)	31 (10%)	7	28
1	C	301/328 (92%)	281 (93%)	20 (7%)	15	43
1	D	316/328 (96%)	300 (95%)	16 (5%)	21	50
2	E	262/279 (94%)	246 (94%)	16 (6%)	17	45
2	F	253/279 (91%)	230 (91%)	23 (9%)	9	31
All	All	1750/1870 (94%)	1627 (93%)	123 (7%)	14	41

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	80	GLN
1	A	81	LYS
1	A	102	LYS
1	A	114	SER
1	A	135	GLN
1	A	159	LYS
1	A	163	LYS
1	A	190	GLN
1	A	196	LEU
1	A	319	SER
1	A	324	VAL
1	A	328	LEU
1	A	331	SER
1	A	361	VAL
1	A	368	LYS
1	A	383	ASP
1	B	32	LYS
1	B	61	LYS
1	B	62	THR
1	B	66	LEU
1	B	70	GLU
1	B	77	VAL
1	B	102	LYS
1	B	127	GLU
1	B	128	GLU

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Mol	Chain	Res	Type
1	B	129	ASP
1	B	137	LEU
1	B	147	GLU
1	B	177	ARG
1	B	206	SER
1	B	212	GLU
1	B	214	CYS
1	B	222	LEU
1	B	228	LYS
1	B	238	GLU
1	B	244	LEU
1	B	249	ARG
1	B	251	VAL
1	B	256	GLN
1	B	290	VAL
1	B	331	SER
1	B	342	GLU
1	B	365	ASP
1	B	370	ILE
1	B	382	ARG
1	B	384	SER
1	B	392	LYS
1	C	15	GLU
1	C	17	THR
1	C	53	LYS
1	C	61	LYS
1	C	113	GLN
1	C	138	MET
1	C	147	GLU
1	C	148	GLU
1	C	149	CYS
1	C	154	ILE
1	C	177	ARG
1	C	191	ASP
1	C	206	SER
1	C	228	LYS
1	C	326	HIS
1	C	328	LEU
1	C	339	GLN
1	C	344	GLU
1	C	347	GLU
1	C	384	SER

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Mol	Chain	Res	Type
1	D	15	GLU
1	D	17	THR
1	D	32	LYS
1	D	61	LYS
1	D	137	LEU
1	D	148	GLU
1	D	149	CYS
1	D	256	GLN
1	D	258	ASP
1	D	325	SER
1	D	329	SER
1	D	331	SER
1	D	341	SER
1	D	368	LYS
1	D	382	ARG
1	D	391	LYS
2	E	18	ARG
2	E	26	THR
2	E	51	ARG
2	E	86	ARG
2	E	89	ASP
2	E	112	GLU
2	E	157	LYS
2	E	163	ASN
2	E	171	ILE
2	E	193	VAL
2	E	202	MET
2	E	260	LEU
2	E	268	ILE
2	E	274	LEU
2	E	312	LEU
2	E	314	ASP
2	F	17	ASN
2	F	18	ARG
2	F	64	SER
2	F	87	ARG
2	F	103	VAL
2	F	139	GLU
2	F	140	ASP
2	F	150	LYS
2	F	151	THR
2	F	153	LEU

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Mol	Chain	Res	Type
2	F	163	ASN
2	F	164	LEU
2	F	182	GLU
2	F	207	GLN
2	F	208	ARG
2	F	228	MET
2	F	229	LEU
2	F	269	THR
2	F	280	ARG
2	F	292	LEU
2	F	294	ILE
2	F	301	ARG
2	F	320	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	161	ASN
1	A	187	GLN
1	A	190	GLN
1	A	243	HIS
1	B	29	HIS
1	B	113	GLN
1	B	190	GLN
1	C	45	HIS
1	C	89	HIS
1	C	113	GLN
1	C	339	GLN
1	C	352	ASN
1	D	36	GLN
1	D	112	GLN
1	D	113	GLN
1	D	135	GLN
1	D	208	GLN
1	D	256	GLN
2	E	41	ASN
2	E	65	ASN
2	E	77	HIS
2	E	100	GLN
2	E	163	ASN
2	F	40	ASN

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Mol	Chain	Res	Type
2	F	43	HIS
2	F	108	ASN
2	F	163	ASN
2	F	244	GLN
2	F	264	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](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 for Mogul analysis.

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	EDO	C	402	-	3,3,3	0.53	0	2,2,2	0.26	0
3	EDO	B	403	-	3,3,3	0.37	0	2,2,2	0.44	0
3	EDO	B	404	-	3,3,3	0.46	0	2,2,2	0.28	0
3	EDO	D	403	-	3,3,3	0.38	0	2,2,2	0.54	0
3	EDO	B	402	-	3,3,3	0.41	0	2,2,2	0.35	0
3	EDO	D	402	-	3,3,3	0.56	0	2,2,2	0.21	0
3	EDO	A	401	-	3,3,3	0.46	0	2,2,2	0.26	0
5	PO4	A	404	-	4,4,4	0.83	0	6,6,6	0.62	0
3	EDO	A	402	-	3,3,3	0.52	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	D	401	-	3,3,3	0.46	0	2,2,2	0.39	0
3	EDO	E	401	-	3,3,3	0.41	0	2,2,2	0.39	0
4	ADN	A	403	-	21,21,21	1.58	5 (23%)	31,31,31	1.99	10 (32%)
3	EDO	B	401	-	3,3,3	0.44	0	2,2,2	0.54	0
6	POP	C	404	7	6,8,8	0.72	0	12,13,13	1.05	0
3	EDO	C	401	-	3,3,3	0.35	0	2,2,2	0.41	0
4	ADN	C	403	-	21,21,21	1.58	5 (23%)	31,31,31	1.98	7 (22%)

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	EDO	C	402	-	-	1/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-
3	EDO	B	404	-	-	0/1/1/1	-
3	EDO	D	403	-	-	1/1/1/1	-
3	EDO	B	402	-	-	1/1/1/1	-
3	EDO	D	402	-	-	0/1/1/1	-
3	EDO	A	401	-	-	1/1/1/1	-
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	D	401	-	-	1/1/1/1	-
3	EDO	E	401	-	-	0/1/1/1	-
4	ADN	A	403	-	-	4/6/22/22	0/3/3/3
3	EDO	B	401	-	-	0/1/1/1	-
6	POP	C	404	7	-	0/6/6/6	-
3	EDO	C	401	-	-	1/1/1/1	-
4	ADN	C	403	-	-	5/6/22/22	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	ADN	C5-C4	4.98	1.48	1.39
4	C	403	ADN	C5-C4	4.83	1.47	1.39
4	C	403	ADN	C5-N7	-2.63	1.34	1.39
4	A	403	ADN	C5-C6	2.61	1.48	1.41
4	A	403	ADN	C8-N7	2.49	1.36	1.31
4	C	403	ADN	C8-N7	2.47	1.36	1.31
4	C	403	ADN	C5-C6	2.24	1.47	1.41
4	A	403	ADN	C5-N7	-2.13	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	ADN	C4-N9	-2.11	1.33	1.37
4	C	403	ADN	C4-N9	-2.03	1.33	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	403	ADN	C5-C4-N3	-5.60	119.01	126.72
4	A	403	ADN	C5-C4-N3	-4.58	120.41	126.72
4	C	403	ADN	N3-C4-N9	4.49	134.81	127.17
4	A	403	ADN	N3-C2-N1	-4.14	122.31	128.58
4	A	403	ADN	N3-C4-N9	3.87	133.74	127.17
4	C	403	ADN	C2-N3-C4	3.51	120.40	111.83
4	A	403	ADN	C2-N3-C4	3.44	120.23	111.83
4	C	403	ADN	N3-C2-N1	-3.40	123.44	128.58
4	A	403	ADN	C2-N1-C6	3.05	123.74	118.73
4	A	403	ADN	C4-N9-C8	2.88	108.76	105.74
4	A	403	ADN	C4-C5-N7	-2.66	107.54	110.58
4	C	403	ADN	C4-C5-N7	-2.40	107.84	110.58
4	A	403	ADN	C6-C5-N7	2.14	136.21	132.09
4	A	403	ADN	C5-N7-C8	2.11	106.77	103.45
4	C	403	ADN	N6-C6-N1	2.11	123.07	118.38
4	A	403	ADN	N9-C8-N7	-2.01	111.08	113.94
4	C	403	ADN	C4-N9-C8	2.00	107.84	105.74

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403	ADN	C3'-C4'-C5'-O5'
4	A	403	ADN	O4'-C4'-C5'-O5'
4	C	403	ADN	O4'-C4'-C5'-O5'
4	C	403	ADN	C3'-C4'-C5'-O5'
3	B	403	EDO	O1-C1-C2-O2
3	A	402	EDO	O1-C1-C2-O2
4	A	403	ADN	C2'-C1'-N9-C8
4	C	403	ADN	C2'-C1'-N9-C8
3	C	402	EDO	O1-C1-C2-O2
3	D	401	EDO	O1-C1-C2-O2
3	B	402	EDO	O1-C1-C2-O2
3	D	403	EDO	O1-C1-C2-O2
4	A	403	ADN	O4'-C1'-N9-C8
4	C	403	ADN	O4'-C1'-N9-C8

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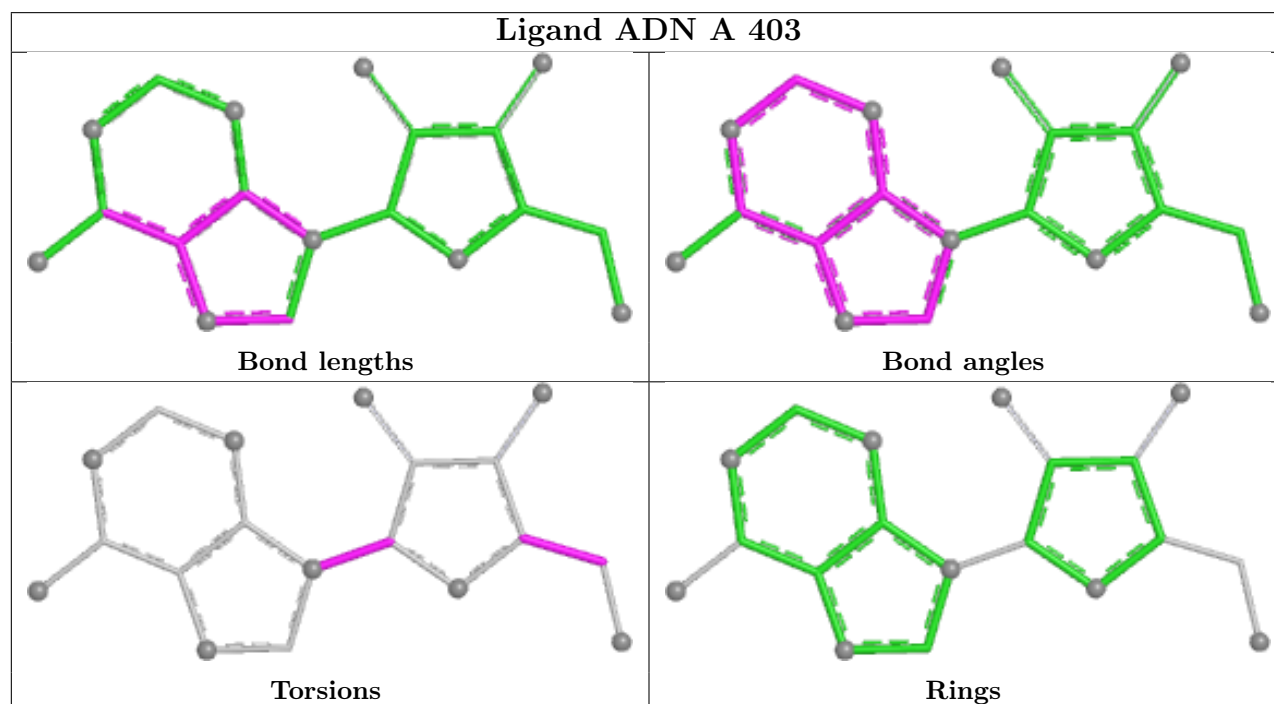
Mol	Chain	Res	Type	Atoms
4	C	403	ADN	C2'-C1'-N9-C4
3	A	401	EDO	O1-C1-C2-O2
3	C	401	EDO	O1-C1-C2-O2

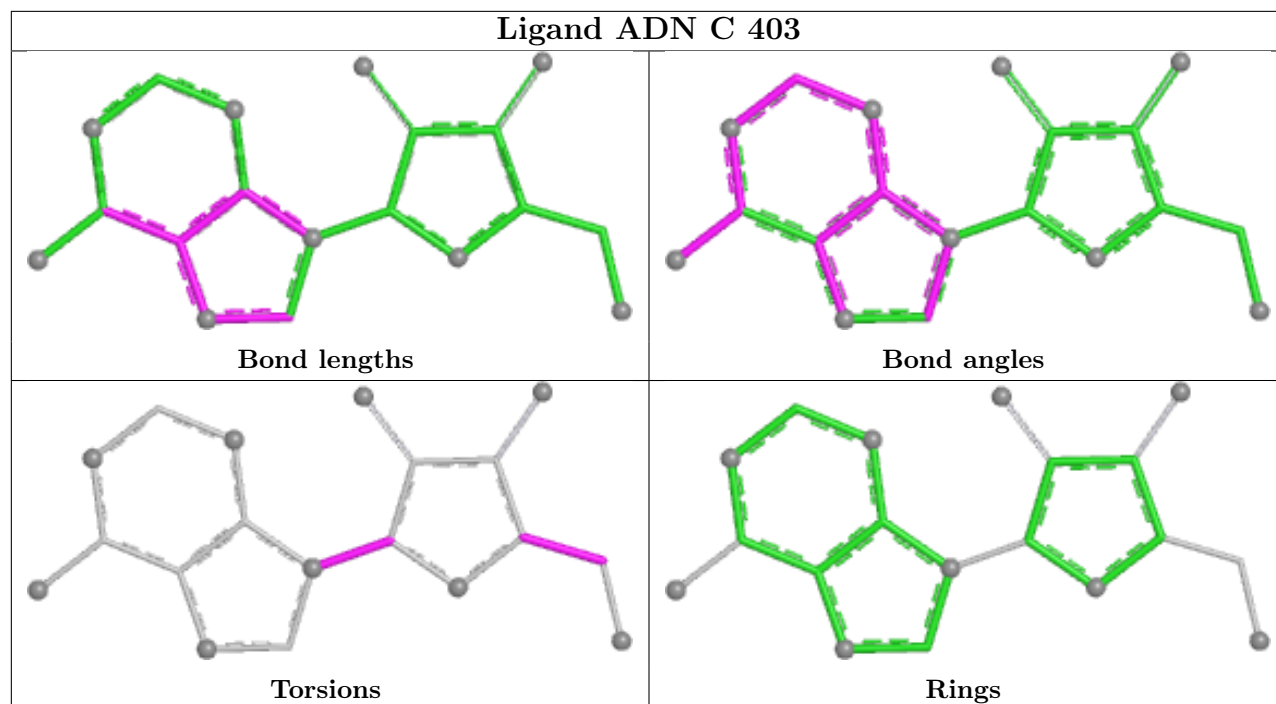
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	EDO	2	0
4	A	403	ADN	2	0
3	B	401	EDO	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	362/396 (91%)	-0.56	0 100 100	41, 59, 85, 110	0
1	B	381/396 (96%)	-0.49	5 (1%) 75 56	45, 61, 103, 159	0
1	C	361/396 (91%)	-0.39	0 100 100	42, 67, 96, 133	0
1	D	381/396 (96%)	-0.61	1 (0%) 90 82	41, 55, 83, 116	0
2	E	309/327 (94%)	-0.48	1 (0%) 90 82	45, 67, 93, 118	0
2	F	295/327 (90%)	0.02	2 (0%) 84 70	38, 100, 132, 150	1 (0%)
All	All	2089/2238 (93%)	-0.44	9 (0%) 88 79	38, 64, 111, 159	1 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	HIS	2.5
1	B	117	ILE	2.5
2	F	83	ALA	2.5
1	B	114	SER	2.4
1	B	123	LEU	2.4
1	D	381	GLY	2.4
1	B	252	ILE	2.2
2	F	229	LEU	2.2
2	E	274	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

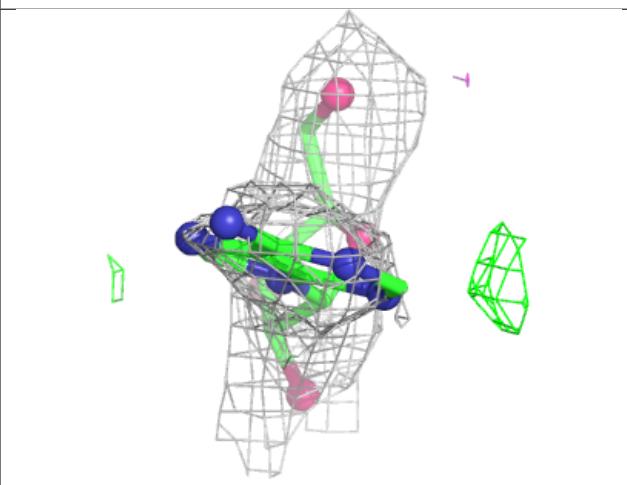
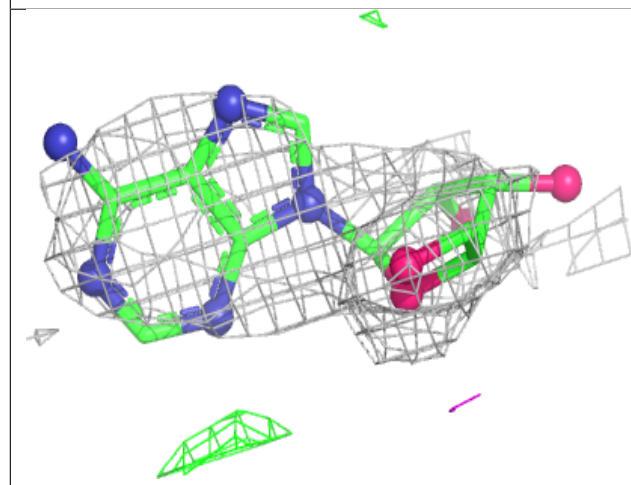
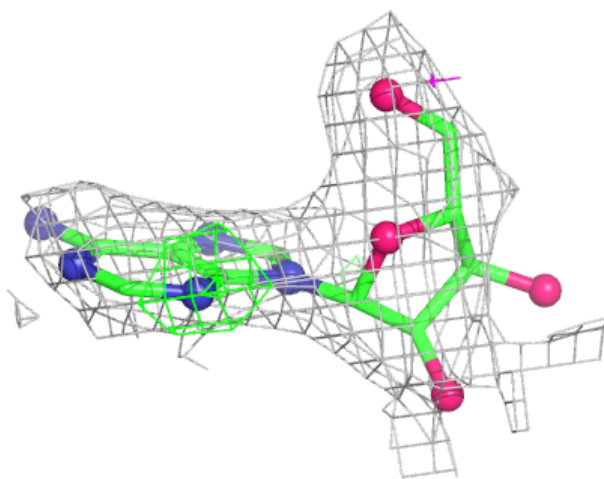
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	EDO	C	402	4/4	0.59	0.17	90,98,98,99	0
5	PO4	A	404	5/5	0.76	0.10	119,125,132,133	0
6	POP	C	404	9/9	0.84	0.11	111,113,140,146	0
7	MG	D	404	1/1	0.84	0.09	49,49,49,49	0
3	EDO	A	402	4/4	0.88	0.14	71,74,75,76	0
4	ADN	A	403	19/19	0.89	0.16	97,127,138,138	0
3	EDO	B	401	4/4	0.89	0.12	54,57,60,64	0
3	EDO	B	404	4/4	0.90	0.17	85,87,90,93	0
3	EDO	D	402	4/4	0.90	0.22	67,68,68,71	0
3	EDO	D	403	4/4	0.91	0.13	62,64,64,64	0
3	EDO	E	401	4/4	0.91	0.14	43,47,49,53	0
3	EDO	A	401	4/4	0.91	0.15	69,69,71,71	0
4	ADN	C	403	19/19	0.93	0.10	51,67,71,71	0
3	EDO	B	403	4/4	0.93	0.22	81,81,82,85	0
3	EDO	D	401	4/4	0.95	0.10	68,68,68,68	0
3	EDO	B	402	4/4	0.96	0.14	58,58,58,59	0
3	EDO	C	401	4/4	0.96	0.10	65,67,68,74	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.

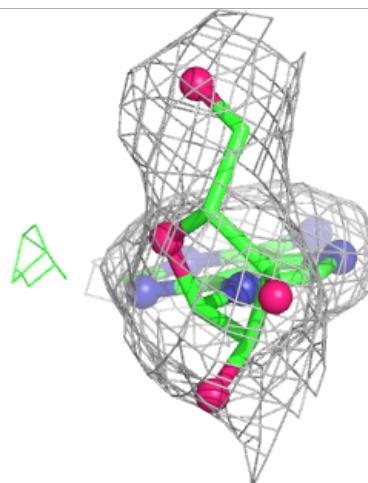
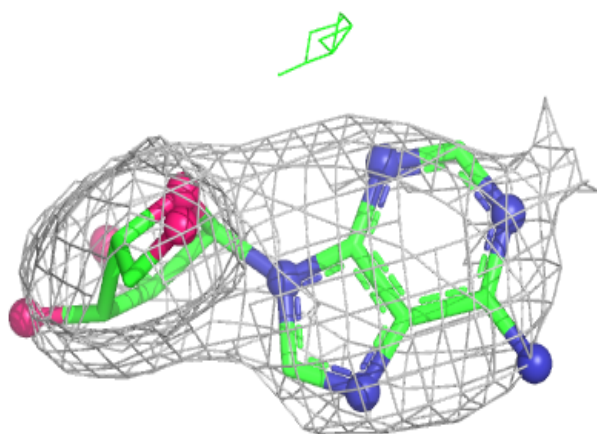
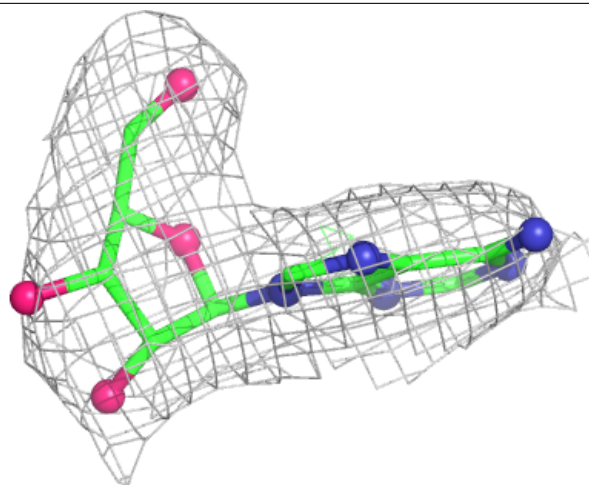
Electron density around ADN A 403:

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



Electron density around ADN C 403:

$2mF_o-DF_c$ (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.