



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 30, 2025 – 05:11 pm BST

PDB ID : 8RB2 / pdb_00008rb2
Title : The crystal structure of DNA-bound human MutSbeta (MSH2_E749A/MSH3_E976A) in the canonical mismatch bound conformation with ADP bound in MSH2
Authors : Thomsen, M.; Neudegger, T.; Thieulin-Pardo, G.; Blaesse, M.; Costanzi, E.; Steinbacher, S.; Plotnikov, N.V.; Dominguez, C.; Iyer, R.R.; Wilkinson, H.A.; Monteagudo, E.; Haque, T.S.; Prasad, B.C.; Finley, M.; Boudet, J.; Vogt, T.F.; Felsenfeld, D.P.
Deposited on : 2023-12-01
Resolution : 2.53 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 Phenix2.0rc1
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11

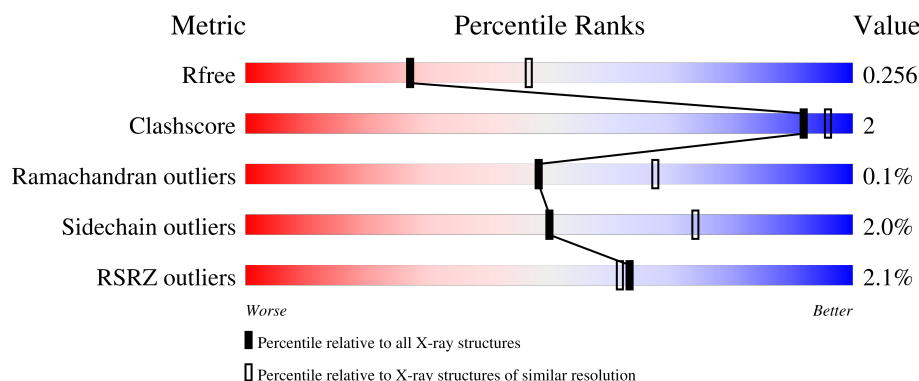
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	164625	6935 (2.54-2.50)
Clashscore	180529	7778 (2.54-2.50)
Ramachandran outliers	177936	7674 (2.54-2.50)
Sidechain outliers	177891	7676 (2.54-2.50)
RSRZ outliers	164620	6935 (2.54-2.50)

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	934	
1	E	934	
2	B	1137	

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Ideal geometry (proteins) : Engh & Huber (2001)
 Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.44

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Mol	Chain	Length	Quality of chain
2	F	1137	
3	C	24	
3	G	24	
4	D	24	
4	H	24	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29972 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 DNA mismatch repair protein Msh2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	872	Total	C	N	O	S	322	1	0
			6911	4394	1173	1308	36			
1	E	888	Total	C	N	O	S	255	6	0
			7053	4482	1195	1338	38			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	749	ALA	GLU	engineered mutation	UNP P43246
E	749	ALA	GLU	engineered mutation	UNP P43246

- Molecule 2 is a protein called DNA mismatch repair protein Msh3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	857	Total	C	N	O	S	202	3	0
			6866	4382	1172	1280	32			
2	F	844	Total	C	N	O	S	257	8	0
			6785	4333	1159	1261	32			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	79	VAL	ILE	conflict	UNP P20585
B	949	ARG	GLN	conflict	UNP P20585
B	976	ALA	GLU	engineered mutation	UNP P20585
B	1045	THR	ALA	conflict	UNP P20585
F	79	VAL	ILE	conflict	UNP P20585
F	949	ARG	GLN	conflict	UNP P20585
F	976	ALA	GLU	engineered mutation	UNP P20585
F	1045	THR	ALA	conflict	UNP P20585

- Molecule 3 is a DNA chain called DNA (5'-D(P*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP

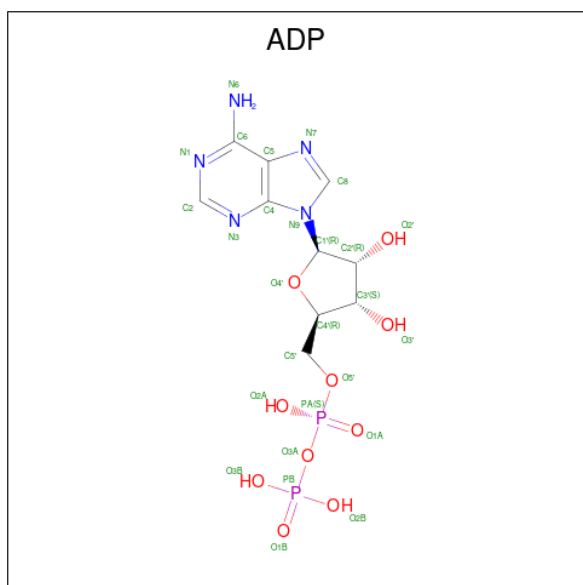
*CP*CP*GP*AP*TP*CP*GP*AP*TP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	21	Total	C	N	O	P	0	0	0
			432	205	80	126	21			
3	G	22	Total	C	N	O	P	0	0	0
			452	215	82	133	22			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP*AP*GP*AP*TP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	24	Total	C	N	O	P	1	0	0
			489	234	90	142	23			
4	H	24	Total	C	N	O	P	0	0	0
			489	234	90	142	23			

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).

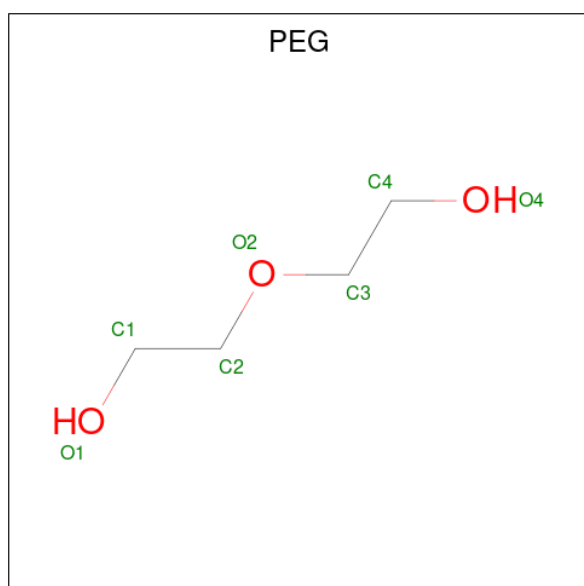


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	6	Total	Cl	0	0
			6	6		
6	B	6	Total	Cl	0	0
			6	6		
6	D	1	Total	Cl	0	0
			1	1		
6	E	3	Total	Cl	0	0
			3	3		
6	F	1	Total	Cl	0	0
			1	1		

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total	Na	0	0
			3	3		
7	E	1	Total	Na	0	0
			1	1		
7	F	1	Total	Na	0	0
			1	1		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



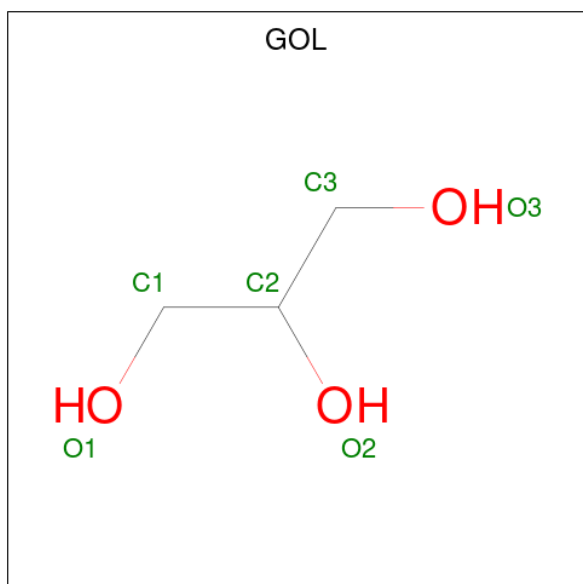
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	B	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		
9	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	E	1	Total	C	O	0	0
			4	2	2		
9	F	1	Total	C	O	0	0
			4	2	2		
9	F	1	Total	C	O	0	0
			4	2	2		
9	F	1	Total	C	O	0	0
			4	2	2		
9	G	1	Total	C	O	0	0
			4	2	2		
9	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	70	Total	O	0	0
			70	70		
11	B	98	Total	O	0	0
			98	98		

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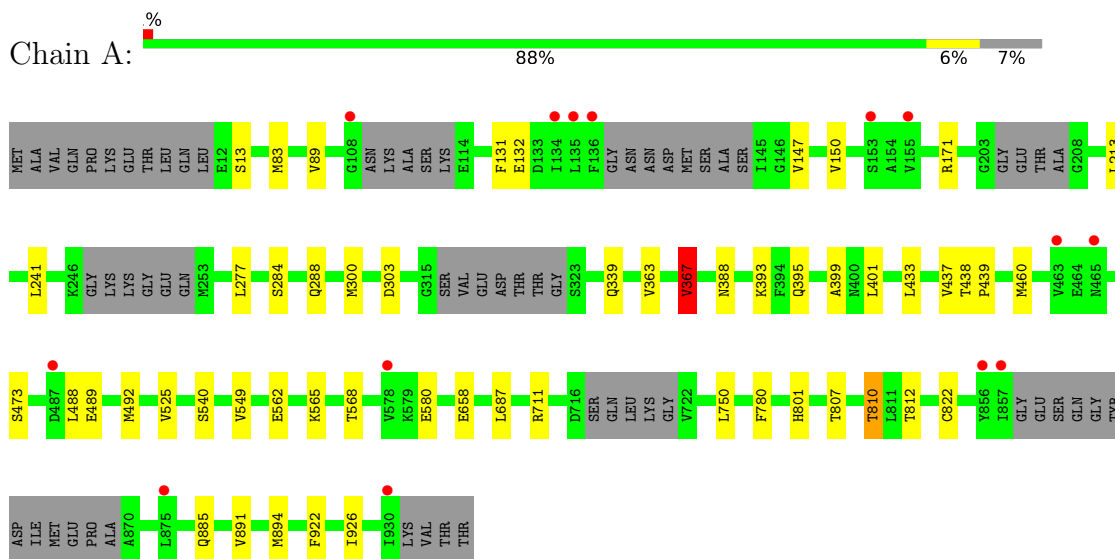
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	C	13	Total 13	O 13	0	0
11	D	17	Total 17	O 17	0	0
11	E	86	Total 86	O 86	0	0
11	F	34	Total 34	O 34	0	0
11	G	2	Total 2	O 2	0	0
11	H	10	Total 10	O 10	0	0

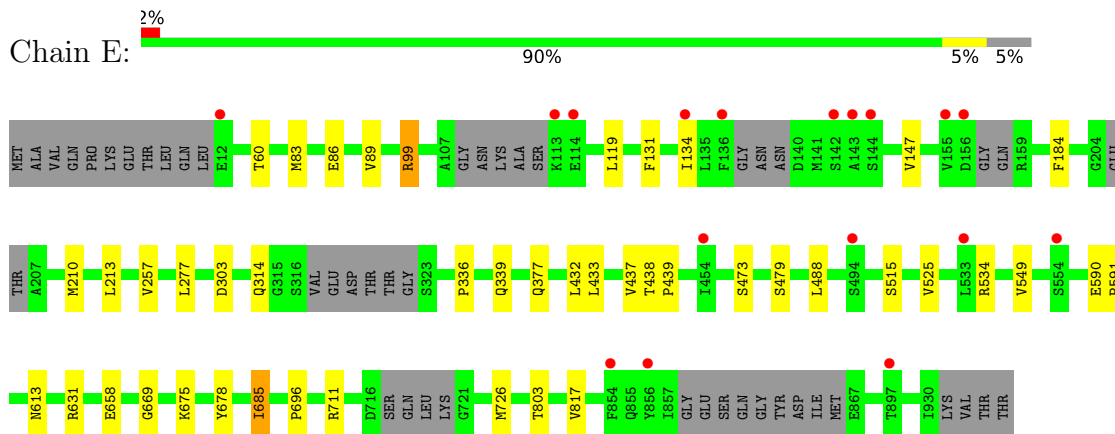
3 Residue-property plots

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.

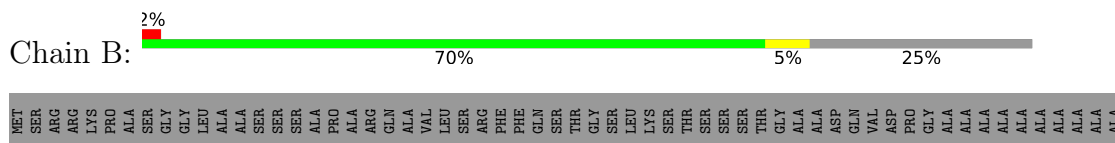
- Molecule 1: DNA mismatch repair protein Msh2



- Molecule 1: DNA mismatch repair protein Msh2



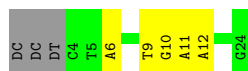
- Molecule 2: DNA mismatch repair protein Msh3





- Molecule 3: DNA (5'-D(P*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*CP*GP*AP*TP*GP*G)-3')

Chain C:  67% 21% 12%




- Molecule 3: DNA (5'-D(P*CP*TP*AP*TP*CP*TP*GP*AP*AP*GP*CP*CP*GP*AP*TP*CP*GP*AP*TP*GP*G)-3')

Chain G:  75% 17% 8%



- Molecule 4: DNA (5'-D(*TP*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP*AP*GP*AP*TP*AP*GP*G)-3')

Chain D:  88% 12%



- Molecule 4: DNA (5'-D(*TP*CP*AP*TP*CP*GP*AP*TP*CP*GP*CP*AP*GP*CP*TP*TP*CP*AP*GP*AP*TP*AP*GP*G)-3')

Chain H:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	100.61Å 104.29Å 121.07Å 110.03° 91.72° 110.21°	Depositor
Resolution (Å)	93.25 – 2.53 93.25 – 2.53	Depositor EDS
% Data completeness (in resolution range)	98.4 (93.25-2.53) 98.4 (93.25-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.211 , 0.256 0.213 , 0.256	Depositor DCC
R_{free} test set	1996 reflections (1.39%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	29972	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.78% 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: NA, PEG, CL, GOL, EDO, ADP

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	1.04	1/7021 (0.0%)	1.54	4/9458 (0.0%)
1	E	1.03	0/7180	1.53	1/9668 (0.0%)
2	B	1.03	0/6998	1.53	9/9444 (0.1%)
2	F	1.03	0/6928	1.54	9/9343 (0.1%)
3	C	0.41	0/484	0.83	0/745
3	G	0.38	0/506	0.87	0/779
4	D	0.41	0/548	0.92	1/844 (0.1%)
4	H	0.33	0/548	0.80	0/844
All	All	1.00	1/30213 (0.0%)	1.50	24/41125 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	460	MET	SD-CE	6.76	1.96	1.79

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	48	DG	C4'-C3'-O3'	6.72	120.08	110.00
2	F	517	LYS	CA-C-N	6.08	129.25	120.38
2	F	517	LYS	C-N-CA	6.08	129.25	120.38
1	A	303	ASP	CA-CB-CG	5.43	118.03	112.60
2	B	1025	VAL	CA-C-N	5.41	125.77	121.61
2	B	1025	VAL	C-N-CA	5.41	125.77	121.61
1	A	885	GLN	CA-C-N	5.39	127.81	120.54
1	A	885	GLN	C-N-CA	5.39	127.81	120.54
2	F	1025	VAL	CA-C-N	5.38	125.31	121.65
2	F	1025	VAL	C-N-CA	5.38	125.31	121.65
2	B	845	ASP	CB-CA-C	5.36	120.25	111.41
2	F	341	GLY	CA-C-N	5.34	128.82	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	341	GLY	C-N-CA	5.34	128.82	120.82
1	E	303	ASP	CA-CB-CG	5.30	117.90	112.60
2	B	1094	GLU	CA-C-N	5.26	125.94	119.99
2	B	1094	GLU	C-N-CA	5.26	125.94	119.99
1	A	367	VAL	N-CA-CB	5.23	117.27	110.57
2	F	1079	PRO	CA-C-N	5.12	125.77	120.03
2	F	1079	PRO	C-N-CA	5.12	125.77	120.03
2	B	720	GLN	CA-C-N	5.11	125.61	119.94
2	B	720	GLN	C-N-CA	5.11	125.61	119.94
2	F	1062	GLY	CA-C-O	-5.03	118.83	122.45
2	B	555	LYS	CA-C-N	5.00	127.23	120.38
2	B	555	LYS	C-N-CA	5.00	127.23	120.38

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	6911	0	6977	20	0
1	E	7053	0	7125	19	0
2	B	6866	0	6983	23	0
2	F	6785	0	6930	20	0
3	C	432	0	237	3	0
3	G	452	0	249	3	0
4	D	489	0	272	2	0
4	H	489	0	272	0	0
5	A	27	0	12	0	0
5	E	27	0	12	0	0
6	A	6	0	0	0	0
6	B	6	0	0	0	0
6	D	1	0	0	0	0
6	E	3	0	0	0	0
6	F	1	0	0	0	0
7	A	3	0	0	0	0
7	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	1	0	0	0	0
8	B	7	0	10	0	0
9	B	24	0	36	0	0
9	E	32	0	48	0	0
9	F	12	0	18	0	0
9	G	4	0	6	0	0
9	H	4	0	6	0	0
10	B	6	0	8	0	0
11	A	70	0	0	0	0
11	B	98	0	0	1	0
11	C	13	0	0	0	0
11	D	17	0	0	0	0
11	E	86	0	0	0	0
11	F	34	0	0	0	0
11	G	2	0	0	0	0
11	H	10	0	0	0	0
All	All	29972	0	29201	85	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 2.

All (85) 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)
2:B:395:PRO:HA	2:B:518:MET:HE1	1.70	0.72
1:E:89:VAL:HG11	1:E:131:PHE:CE2	2.30	0.64
1:A:89:VAL:HG11	1:A:131:PHE:CE2	2.35	0.61
2:B:906:ILE:HD11	2:B:939:MET:HE3	1.83	0.59
1:E:99[A]:ARG:HH11	1:E:99[A]:ARG:HB3	1.69	0.58
1:E:60:THR:OG1	2:F:357:ASP:OD2	2.22	0.57
2:B:563:VAL:HG21	2:B:866:VAL:HA	1.87	0.57
1:A:711:ARG:HG2	1:A:750:LEU:HD13	1.88	0.55
1:A:810:THR:HG23	1:A:812:THR:HG23	1.90	0.54
2:F:384:GLY:O	2:F:411:ARG:NH2	2.41	0.53
1:E:336:PRO:HA	1:E:339:GLN:HE21	1.73	0.52
2:B:601:LEU:HD11	2:B:841:ALA:HB1	1.91	0.52
2:F:621:ILE:HG21	2:F:645:LEU:HD21	1.91	0.52
2:B:621:ILE:HG21	2:B:645:LEU:HD21	1.92	0.51
1:A:284:SER:O	1:A:288:GLN:HG3	2.11	0.50
2:F:342:GLU:HG2	2:F:634:SER:HB3	1.93	0.50
3:G:3:DT:P	3:G:3:DT:O4'	2.70	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:285:ILE:HG21	2:F:293:HIS:CD2	2.47	0.49
2:F:952:PHE:CZ	2:F:956:LEU:HD11	2.48	0.49
2:B:889:GLU:OE2	2:B:1061:ARG:NH2	2.46	0.49
1:E:678:TYR:CD1	1:E:817:VAL:HG21	2.47	0.49
3:C:6:DA:C2	4:D:47:DA:C2	3.01	0.49
2:B:587:LEU:HD13	2:B:851:VAL:HG12	1.96	0.48
2:F:397:THR:C	2:F:626:CYS:SG	2.96	0.48
2:B:565:ASP:OD2	2:B:573:ARG:NH1	2.47	0.47
2:B:996:TYR:CE2	2:B:1001:VAL:CG2	2.98	0.47
1:A:150:VAL:HG11	1:A:213:LEU:HD21	1.97	0.47
2:F:254:TYR:O	2:F:287:THR:HG23	2.15	0.46
1:A:922:PHE:CZ	1:A:926:ILE:HD11	2.51	0.46
1:E:99[A]:ARG:HB3	1:E:99[A]:ARG:NH1	2.30	0.46
1:A:891:VAL:HA	1:A:894:MET:HE3	1.98	0.46
2:B:285:ILE:HG21	2:B:293:HIS:CD2	2.51	0.46
1:E:257:VAL:HG12	1:E:257:VAL:O	2.15	0.46
3:G:3:DT:H1'	3:G:4:DC:O4'	2.16	0.46
1:E:184:PHE:CE1	1:E:213:LEU:HD12	2.51	0.45
1:E:83:MET:HE3	2:F:271:ASN:O	2.17	0.45
2:F:397:THR:O	2:F:626:CYS:SG	2.75	0.45
1:A:363:VAL:O	1:A:367:VAL:HG13	2.17	0.45
1:A:438:THR:HB	1:A:439:PRO:HD3	1.98	0.44
2:F:889:GLU:OE2	2:F:1061:ARG:NH2	2.47	0.44
2:F:937:THR:HB	2:F:939:MET:HE3	1.99	0.44
2:B:601:LEU:HD11	2:B:841:ALA:CB	2.47	0.44
1:E:86:GLU:HG2	1:E:134:ILE:HG23	2.00	0.44
2:B:322:ARG:HD2	4:D:29:DT:OP1	2.18	0.44
2:F:866:VAL:HG12	2:F:870:LEU:HD12	2.00	0.44
1:A:147:VAL:HG21	1:A:277:LEU:HD21	2.00	0.44
2:B:231:PRO:HB2	2:B:325:LEU:HD13	1.99	0.44
2:B:235:GLN:CD	2:B:325:LEU:HD23	2.43	0.43
2:F:256:TYR:CD1	2:F:287:THR:HG22	2.53	0.43
2:F:996:TYR:CE2	2:F:1001:VAL:CG2	3.01	0.43
1:A:300:MET:HE1	1:A:687:LEU:HD12	2.01	0.43
2:B:884:LEU:HD21	2:B:892:MET:HG3	2.00	0.43
1:E:711:ARG:NE	1:E:711:ARG:HA	2.34	0.43
1:E:89:VAL:HG11	1:E:131:PHE:CD2	2.53	0.43
1:A:489:GLU:HA	1:A:492:MET:HE3	2.01	0.43
2:F:595:ASP:OD1	2:F:848:ARG:NH2	2.52	0.43
3:C:11:DA:H2''	3:C:12:DA:C8	2.54	0.43
1:E:147:VAL:HG21	1:E:277:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:564:LEU:HA	2:B:840:VAL:HG21	1.99	0.42
2:B:938:ARG:NH2	2:B:955:GLU:OE1	2.52	0.42
2:F:549:GLN:NE2	2:F:554:MET:HE3	2.34	0.42
2:F:963:ILE:HG23	2:F:996:TYR:CE2	2.54	0.42
1:A:807:THR:HB	1:A:810:THR:HB	2.01	0.42
1:E:433:LEU:HA	1:E:437:VAL:HB	2.02	0.42
2:F:548:LEU:HD21	2:F:581:THR:CG2	2.50	0.42
2:B:977:LEU:HD23	2:B:990:ALA:HA	2.01	0.42
1:E:438:THR:HB	1:E:439:PRO:HD3	2.00	0.42
1:A:488:LEU:HD11	1:A:562:GLU:HG2	2.02	0.41
2:B:1113:MET:HA	2:B:1113:MET:HE2	2.02	0.41
1:A:433:LEU:HA	1:A:437:VAL:HB	2.03	0.41
2:B:672:ILE:HA	2:B:675:ILE:HD12	2.03	0.41
1:A:565:LYS:O	1:A:568:THR:HG22	2.21	0.41
2:B:564:LEU:HD21	2:B:915:MET:HE3	2.01	0.41
1:E:669:GLY:O	1:E:675:LYS:HE3	2.20	0.41
1:E:726:MET:SD	2:F:899:MET:HE1	2.61	0.41
1:A:171:ARG:HD3	1:A:288:GLN:HB3	2.02	0.41
2:B:508:LYS:NZ	11:B:1307:HOH:O	2.54	0.41
1:A:801:HIS:CD2	1:A:822:CYS:HA	2.56	0.41
1:A:393:LYS:HB3	1:A:399:ALA:HB2	2.02	0.41
1:A:750:LEU:HB3	1:A:780:PHE:CZ	2.56	0.41
1:E:590:GLU:HB3	1:E:591:PRO:HD3	2.03	0.41
1:E:685:ILE:HD12	1:E:696:PRO:HD2	2.02	0.41
3:G:19:DC:H2"	3:G:20:DG:C8	2.56	0.41
3:C:9:DT:H2"	3:C:10:DG:N7	2.36	0.40
2:B:506:ILE:HG22	2:B:519:LEU:HD11	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	857/934 (92%)	831 (97%)	25 (3%)	1 (0%)	48	67
1	E	878/934 (94%)	856 (98%)	21 (2%)	1 (0%)	48	67
2	B	846/1137 (74%)	826 (98%)	18 (2%)	2 (0%)	44	62
2	F	834/1137 (73%)	811 (97%)	23 (3%)	0	100	100
All	All	3415/4142 (82%)	3324 (97%)	87 (2%)	4 (0%)	48	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	GLU
2	B	325	LEU
2	B	1066	ARG
1	E	534	ARG

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	759/807 (94%)	744 (98%)	15 (2%)	50	74
1	E	775/807 (96%)	757 (98%)	18 (2%)	45	70
2	B	768/998 (77%)	752 (98%)	16 (2%)	48	72
2	F	761/998 (76%)	748 (98%)	13 (2%)	56	78
All	All	3063/3610 (85%)	3001 (98%)	62 (2%)	50	74

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	SER
1	A	83	MET
1	A	241	LEU
1	A	339	GLN
1	A	367	VAL
1	A	388	ASN
1	A	395	GLN

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Mol	Chain	Res	Type
1	A	401	LEU
1	A	473	SER
1	A	525	VAL
1	A	540	SER
1	A	549	VAL
1	A	580	GLU
1	A	658	GLU
1	A	810	THR
2	B	235	GLN
2	B	344	VAL
2	B	401	VAL
2	B	404	SER
2	B	421	LEU
2	B	492	ILE
2	B	552	THR
2	B	553	ASP
2	B	557	LYS
2	B	660	ASN
2	B	731	GLN
2	B	853	GLU
2	B	894	ILE
2	B	899	MET
2	B	938	ARG
2	B	964	ARG
1	E	99[A]	ARG
1	E	99[B]	ARG
1	E	119	LEU
1	E	210	MET
1	E	314	GLN
1	E	377	GLN
1	E	432	LEU
1	E	473	SER
1	E	479	SER
1	E	488	LEU
1	E	515	SER
1	E	525	VAL
1	E	549	VAL
1	E	613	ASN
1	E	631	ARG
1	E	658	GLU
1	E	685	ILE
1	E	803	THR

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Mol	Chain	Res	Type
2	F	238	GLU
2	F	401	VAL
2	F	404	SER
2	F	540	THR
2	F	542	LEU
2	F	552	THR
2	F	605	SER
2	F	615	LEU
2	F	636	GLN
2	F	653	GLN
2	F	686	LEU
2	F	816	GLU
2	F	973	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	218	GLN
1	A	344	GLN
1	A	348	GLN
1	A	377	GLN
1	A	388	ASN
1	A	681	GLN
2	B	467	HIS
2	B	630	HIS
2	B	817	HIS
2	B	984	HIS
2	B	1027	ASN
2	B	1071	ASN
1	E	74	ASN
1	E	97	GLN
1	E	170	GLN
1	E	288	GLN
1	E	339	GLN
1	E	348	GLN
1	E	377	GLN
1	E	388	ASN
1	E	397	GLN
1	E	465	ASN
1	E	510	GLN
1	E	681	GLN

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Mol	Chain	Res	Type
2	F	549	GLN
2	F	551	GLN
2	F	566	HIS
2	F	636	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 22 are monoatomic - leaving 23 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	$\# Z > 2$
9	EDO	F	1203	-	3,3,3	0.08	0	2,2,2	0.25	0
9	EDO	E	1003	-	3,3,3	0.15	0	2,2,2	0.37	0
9	EDO	E	1008	-	3,3,3	0.09	0	2,2,2	0.26	0
9	EDO	B	1207	-	3,3,3	0.07	0	2,2,2	0.20	0
9	EDO	B	1214	-	3,3,3	0.12	0	2,2,2	0.33	0
5	ADP	A	1001	-	24,29,29	0.66	0	29,45,45	0.76	1 (3%)
9	EDO	B	1210	-	3,3,3	0.09	0	2,2,2	0.26	0
9	EDO	B	1203	-	3,3,3	0.09	0	2,2,2	0.30	0
9	EDO	B	1213	-	3,3,3	0.11	0	2,2,2	0.28	0
9	EDO	E	1011	-	3,3,3	0.15	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	F	1202	-	3,3,3	0.10	0	2,2,2	0.27	0
9	EDO	E	1013	-	3,3,3	0.12	0	2,2,2	0.29	0
10	GOL	B	1209	-	5,5,5	0.11	0	5,5,5	0.40	0
8	PEG	B	1202	-	6,6,6	0.19	0	5,5,5	0.15	0
9	EDO	B	1208	-	3,3,3	0.10	0	2,2,2	0.31	0
9	EDO	G	101	-	3,3,3	0.10	0	2,2,2	0.33	0
9	EDO	E	1010	-	3,3,3	0.11	0	2,2,2	0.45	0
9	EDO	F	1204	-	3,3,3	0.10	0	2,2,2	0.11	0
9	EDO	E	1002	-	3,3,3	0.08	0	2,2,2	0.25	0
9	EDO	E	1007	-	3,3,3	0.11	0	2,2,2	0.30	0
9	EDO	H	101	-	3,3,3	0.15	0	2,2,2	0.43	0
9	EDO	E	1009	-	3,3,3	0.06	0	2,2,2	0.12	0
5	ADP	E	1001	-	24,29,29	0.65	0	29,45,45	0.82	1 (3%)

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
9	EDO	F	1203	-	-	1/1/1/1	-
9	EDO	E	1003	-	-	1/1/1/1	-
9	EDO	E	1008	-	-	0/1/1/1	-
9	EDO	B	1207	-	-	0/1/1/1	-
9	EDO	B	1214	-	-	1/1/1/1	-
5	ADP	A	1001	-	-	2/12/32/32	0/3/3/3
9	EDO	B	1210	-	-	1/1/1/1	-
9	EDO	B	1203	-	-	0/1/1/1	-
9	EDO	B	1213	-	-	1/1/1/1	-
9	EDO	E	1011	-	-	1/1/1/1	-
9	EDO	F	1202	-	-	0/1/1/1	-
9	EDO	E	1013	-	-	1/1/1/1	-
10	GOL	B	1209	-	-	2/4/4/4	-
8	PEG	B	1202	-	-	2/4/4/4	-
9	EDO	B	1208	-	-	1/1/1/1	-
9	EDO	G	101	-	-	1/1/1/1	-
9	EDO	E	1010	-	-	1/1/1/1	-
9	EDO	F	1204	-	-	1/1/1/1	-
9	EDO	E	1002	-	-	0/1/1/1	-
9	EDO	E	1007	-	-	1/1/1/1	-
9	EDO	H	101	-	-	1/1/1/1	-
9	EDO	E	1009	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	E	1001	-	-	3/12/32/32	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1001	ADP	C5-C6-N6	2.24	123.76	120.35
5	E	1001	ADP	C5-C6-N6	2.03	123.44	120.35

There are no chirality outliers.

All (22) torsion outliers are listed below:

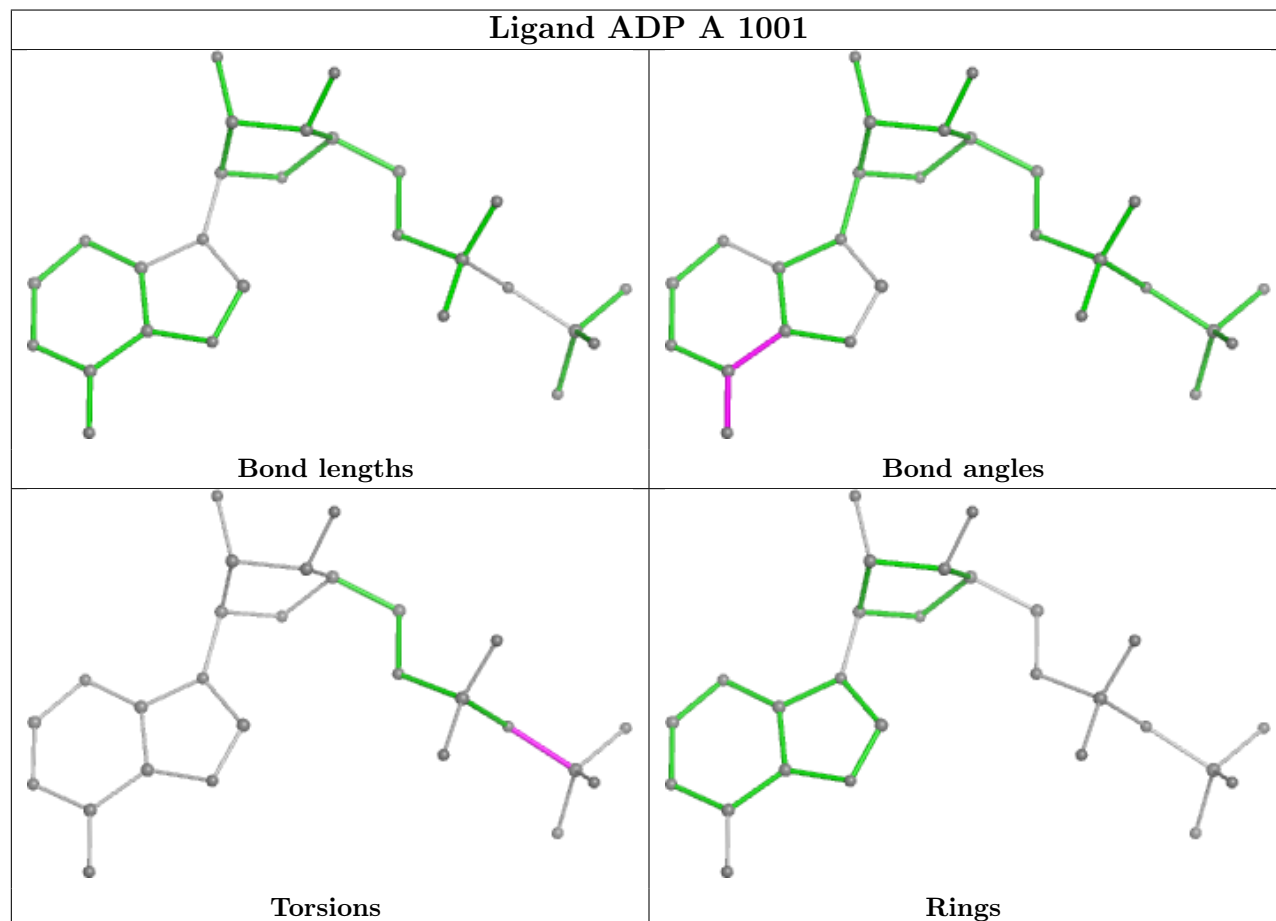
Mol	Chain	Res	Type	Atoms
5	A	1001	ADP	PA-O3A-PB-O3B
5	E	1001	ADP	PA-O3A-PB-O3B
10	B	1209	GOL	O1-C1-C2-C3
9	B	1210	EDO	O1-C1-C2-O2
10	B	1209	GOL	O1-C1-C2-O2
9	E	1003	EDO	O1-C1-C2-O2
9	E	1010	EDO	O1-C1-C2-O2
9	E	1011	EDO	O1-C1-C2-O2
8	B	1202	PEG	O2-C3-C4-O4
9	B	1213	EDO	O1-C1-C2-O2
9	B	1214	EDO	O1-C1-C2-O2
9	E	1013	EDO	O1-C1-C2-O2
9	H	101	EDO	O1-C1-C2-O2
9	E	1007	EDO	O1-C1-C2-O2
9	F	1203	EDO	O1-C1-C2-O2
9	B	1208	EDO	O1-C1-C2-O2
5	E	1001	ADP	PA-O3A-PB-O1B
8	B	1202	PEG	O1-C1-C2-O2
9	G	101	EDO	O1-C1-C2-O2
5	A	1001	ADP	PA-O3A-PB-O2B
5	E	1001	ADP	PA-O3A-PB-O2B
9	F	1204	EDO	O1-C1-C2-O2

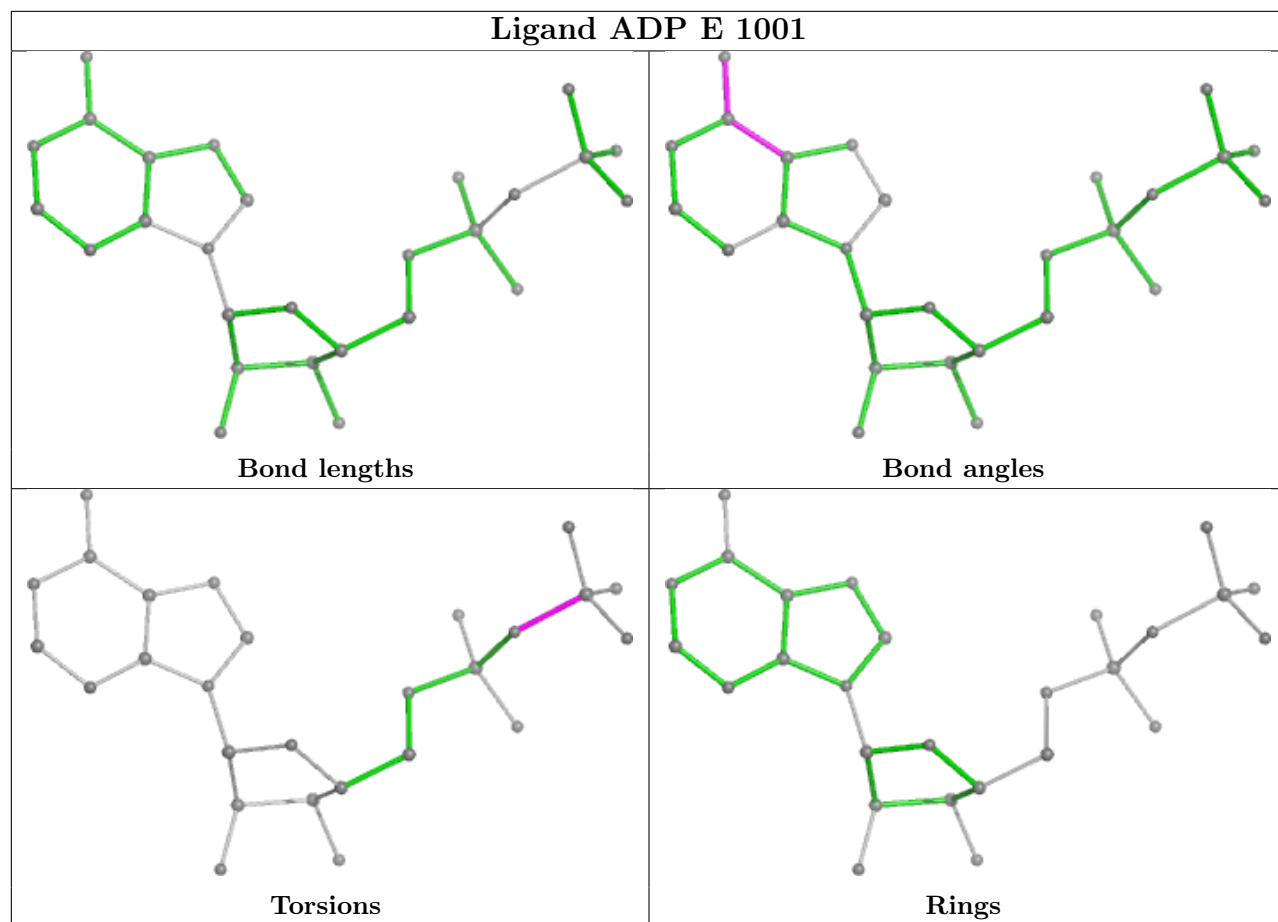
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	872/934 (93%)	0.20	14 (1%) 70 68	36, 72, 101, 131	127 (14%)
1	E	888/934 (95%)	0.16	17 (1%) 66 64	34, 70, 104, 133	110 (12%)
2	B	857/1137 (75%)	0.11	18 (2%) 63 61	37, 64, 92, 164	89 (10%)
2	F	844/1137 (74%)	0.26	24 (2%) 55 53	34, 75, 104, 141	107 (12%)
3	C	21/24 (87%)	-0.31	0 100 100	56, 76, 129, 153	0
3	G	22/24 (91%)	-0.21	0 100 100	63, 102, 151, 188	0
4	D	24/24 (100%)	-0.37	0 100 100	56, 72, 144, 165	0
4	H	24/24 (100%)	-0.14	0 100 100	67, 92, 176, 207	0
All	All	3552/4238 (83%)	0.17	73 (2%) 63 61	34, 70, 104, 207	433 (12%)

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	978	GLY	4.3
2	F	1053	VAL	3.8
2	F	489	ILE	3.7
1	E	143	ALA	3.3
2	F	710	PRO	3.3
1	A	857	ILE	3.2
1	A	135	LEU	3.2
2	F	707	SER	3.1
1	E	155	VAL	3.1
2	B	1053	VAL	3.0
2	B	360	MET	3.0
2	F	1056	LEU	2.9
2	F	360	MET	2.9
2	F	356	VAL	2.8
2	B	348	ILE	2.7
2	F	364	SER	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	448	VAL	2.7
1	A	930	ILE	2.7
2	B	488	ILE	2.7
2	B	356	VAL	2.6
2	F	677	GLU	2.6
1	E	533	LEU	2.6
2	B	407	ASP	2.6
1	A	463	VAL	2.6
2	F	492	ILE	2.5
2	F	877	TYR	2.5
1	A	108	GLY	2.4
1	A	487	ASP	2.4
1	E	854	PHE	2.4
1	E	144	SER	2.4
2	B	340	ILE	2.4
2	F	873	GLU	2.4
2	B	353	ALA	2.4
2	B	977	LEU	2.3
1	A	465	ASN	2.3
2	F	851	VAL	2.3
2	F	854	GLU	2.3
1	A	134	ILE	2.3
2	B	688	ILE	2.3
1	E	113	LYS	2.3
1	E	12	GLU	2.3
2	F	355	ASN	2.3
1	E	114	GLU	2.3
1	E	897	THR	2.2
1	A	136	PHE	2.2
2	B	354	VAL	2.2
1	E	156	ASP	2.2
2	F	361	THR	2.2
1	E	134	ILE	2.2
2	B	1034	VAL	2.2
2	F	736	ILE	2.2
1	E	856	TYR	2.2
2	F	273	TYR	2.2
1	E	136	PHE	2.2
1	A	578	VAL	2.2
1	E	142	SER	2.1
1	E	554	SER	2.1
1	E	454	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	494	SER	2.1
2	F	650	SER	2.1
2	F	578[A]	LYS	2.1
2	B	489	ILE	2.1
1	A	856	TYR	2.1
2	B	346	PRO	2.1
1	A	153	SER	2.1
1	A	155	VAL	2.1
2	F	1065	ALA	2.1
2	F	1122	TRP	2.1
2	B	479	ASP	2.1
2	B	875	ASP	2.1
2	B	486	SER	2.0
1	A	875	LEU	2.0
2	F	532	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	NA	A	1006	1/1	0.68	0.24	89,89,89,89	0
6	CL	D	101	1/1	0.71	0.13	110,110,110,110	0
9	EDO	H	101	4/4	0.72	0.14	95,98,102,104	0
9	EDO	E	1007	4/4	0.75	0.17	83,84,85,85	0
9	EDO	E	1011	4/4	0.76	0.19	95,98,99,99	0
9	EDO	E	1008	4/4	0.76	0.12	110,111,111,112	0
9	EDO	B	1213	4/4	0.77	0.15	91,92,92,92	0
10	GOL	B	1209	6/6	0.77	0.17	74,80,82,85	0

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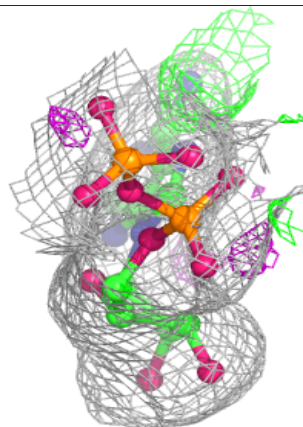
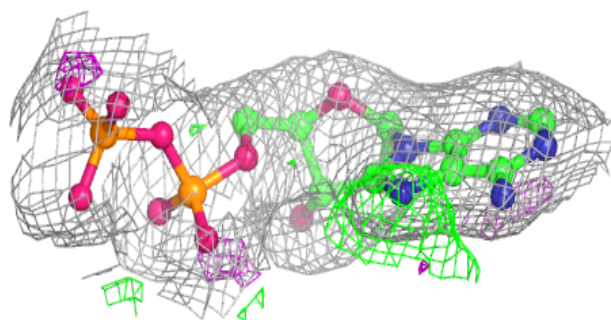
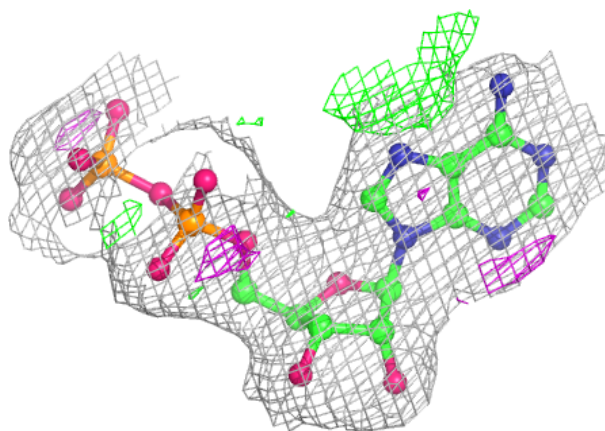
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	EDO	F	1204	4/4	0.81	0.13	70,71,71,72	0
9	EDO	E	1002	4/4	0.81	0.12	94,96,97,97	0
9	EDO	B	1208	4/4	0.81	0.15	90,90,92,93	0
9	EDO	F	1202	4/4	0.82	0.20	86,88,88,88	0
6	CL	F	1201	1/1	0.82	0.10	98,98,98,98	0
9	EDO	E	1009	4/4	0.82	0.18	93,95,96,97	0
9	EDO	B	1203	4/4	0.82	0.17	86,87,88,90	0
6	CL	A	1009	1/1	0.84	0.10	101,101,101,101	0
9	EDO	B	1214	4/4	0.85	0.18	94,96,97,98	0
9	EDO	B	1207	4/4	0.86	0.20	76,78,78,79	0
6	CL	A	1010	1/1	0.86	0.09	104,104,104,104	0
9	EDO	F	1203	4/4	0.86	0.12	79,79,80,82	0
9	EDO	G	101	4/4	0.87	0.11	114,116,116,117	0
7	NA	E	1012	1/1	0.87	0.09	65,65,65,65	0
9	EDO	B	1210	4/4	0.87	0.17	68,69,71,72	0
7	NA	F	1205	1/1	0.88	0.22	91,91,91,91	0
7	NA	A	1007	1/1	0.88	0.22	81,81,81,81	0
6	CL	B	1206	1/1	0.88	0.12	102,102,102,102	0
6	CL	B	1212	1/1	0.89	0.07	99,99,99,99	0
9	EDO	E	1013	4/4	0.89	0.15	82,86,89,91	0
8	PEG	B	1202	7/7	0.89	0.15	80,91,99,100	0
9	EDO	E	1010	4/4	0.89	0.15	91,97,98,102	0
6	CL	A	1003	1/1	0.90	0.14	105,105,105,105	0
6	CL	E	1005	1/1	0.90	0.10	86,86,86,86	0
6	CL	B	1204	1/1	0.90	0.09	91,91,91,91	0
6	CL	A	1005	1/1	0.91	0.19	91,91,91,91	0
7	NA	A	1008	1/1	0.91	0.07	55,55,55,55	0
6	CL	A	1004	1/1	0.92	0.09	99,99,99,99	0
6	CL	B	1205	1/1	0.92	0.11	107,107,107,107	0
6	CL	B	1211	1/1	0.93	0.08	106,106,106,106	0
6	CL	E	1004	1/1	0.94	0.07	96,96,96,96	0
5	ADP	E	1001	27/27	0.94	0.08	45,57,62,64	0
9	EDO	E	1003	4/4	0.94	0.11	81,83,84,85	0
5	ADP	A	1001	27/27	0.95	0.07	49,56,63,64	0
6	CL	A	1002	1/1	0.95	0.11	98,98,98,98	0
6	CL	B	1201	1/1	0.96	0.14	84,84,84,84	0
6	CL	E	1006	1/1	0.97	0.16	96,96,96,96	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.

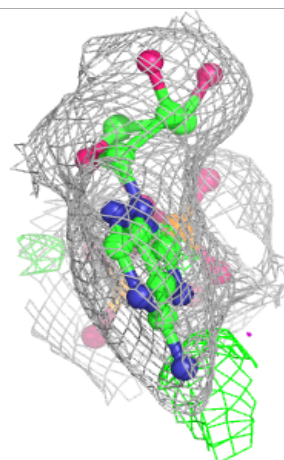
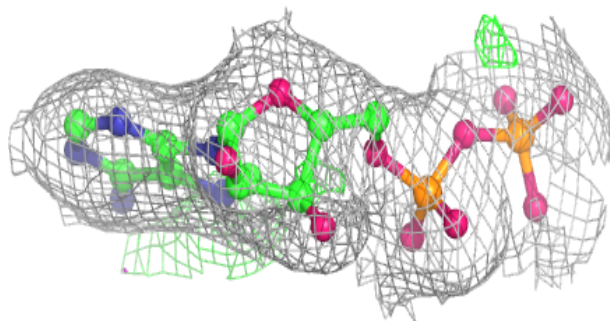
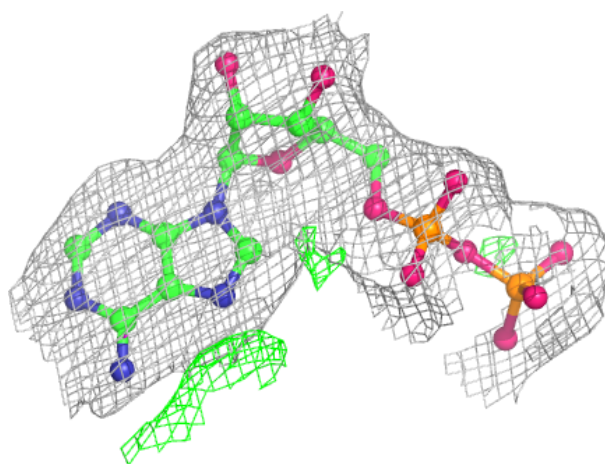
Electron density around ADP E 1001:

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



Electron density around ADP A 1001:

$2mF_o-DF_c$ (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.