



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 11, 2024 – 01:59 PM EST

PDB ID : 3CMT
Title : Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors : Chen, Z.; Yang, H.; Pavletich, N.P.
Deposited on : 2008-03-24
Resolution : 3.15 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

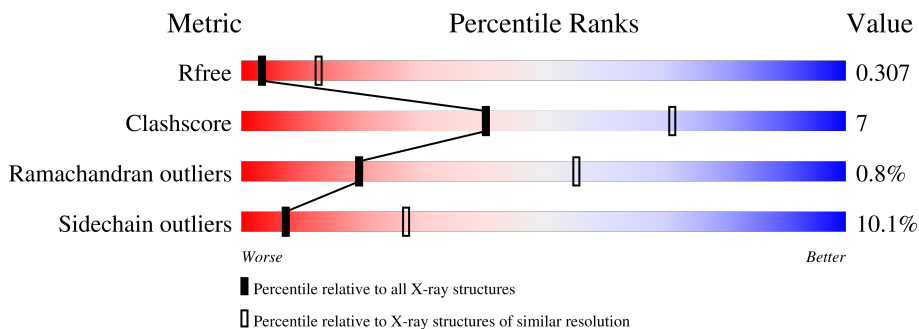
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)

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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	15	13% (green), 47% (yellow), 20% (orange), 20% (grey)
1	E	15	13% (green), 40% (yellow), 27% (orange), 20% (grey)
2	C	6	67% (green), 33% (yellow)
2	F	6	50% (green), 50% (yellow)
3	A	1706	78% (green), 13% (yellow), 6% (orange), 3% (grey)
3	D	1706	78% (green), 13% (yellow), 6% (orange), 3% (grey)

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 25312 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 DNA chain called DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	12	Total 236	C 115	N 32	O 77	P 12	0	0	0
1	E	12	Total 236	C 115	N 32	O 77	P 12	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	6	Total 130	C 60	N 27	O 37	P 6	3	0	0
2	F	6	Total 130	C 60	N 27	O 37	P 6	3	0	0

- Molecule 3 is a protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	1609	Total 12125	C 7622	N 2100	O 2347	S 56	0	0	0
3	D	1609	Total 12125	C 7622	N 2101	O 2345	S 57	0	0	0

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	linker	UNP P0A7G6
A	27	ALA	-	linker	UNP P0A7G6
A	28	MET	-	linker	UNP P0A7G6
A	29	HIS	-	linker	UNP P0A7G6
A	986	THR	-	linker	UNP P0A7G6
A	987	GLY	-	linker	UNP P0A7G6
A	988	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	989	THR	-	linker	UNP P0A7G6
A	990	GLY	-	linker	UNP P0A7G6
A	991	SER	-	linker	UNP P0A7G6
A	992	GLY	-	linker	UNP P0A7G6
A	993	THR	-	linker	UNP P0A7G6
A	994	THR	-	linker	UNP P0A7G6
A	995	GLY	-	linker	UNP P0A7G6
A	996	SER	-	linker	UNP P0A7G6
A	997	THR	-	linker	UNP P0A7G6
A	998	GLY	-	linker	UNP P0A7G6
A	999	SER	-	linker	UNP P0A7G6
A	1000	MET	-	linker	UNP P0A7G6
A	1986	THR	-	linker	UNP P0A7G6
A	1987	GLY	-	linker	UNP P0A7G6
A	1988	SER	-	linker	UNP P0A7G6
A	1989	THR	-	linker	UNP P0A7G6
A	1990	GLY	-	linker	UNP P0A7G6
A	1991	SER	-	linker	UNP P0A7G6
A	1992	MET	-	linker	UNP P0A7G6
A	1993	GLY	-	linker	UNP P0A7G6
A	1994	HIS	-	linker	UNP P0A7G6
A	1995	THR	-	linker	UNP P0A7G6
A	1996	THR	-	linker	UNP P0A7G6
A	1997	GLY	-	linker	UNP P0A7G6
A	1998	SER	-	linker	UNP P0A7G6
A	1999	MET	-	linker	UNP P0A7G6
A	2000	SER	-	linker	UNP P0A7G6
A	2985	THR	-	linker	UNP P0A7G6
A	2986	GLY	-	linker	UNP P0A7G6
A	2987	SER	-	linker	UNP P0A7G6
A	2988	THR	-	linker	UNP P0A7G6
A	2989	GLY	-	linker	UNP P0A7G6
A	2990	SER	-	linker	UNP P0A7G6
A	2991	ALA	-	linker	UNP P0A7G6
A	2992	SER	-	linker	UNP P0A7G6
A	2993	GLY	-	linker	UNP P0A7G6
A	2994	SER	-	linker	UNP P0A7G6
A	2995	SER	-	linker	UNP P0A7G6
A	2996	THR	-	linker	UNP P0A7G6
A	2997	GLY	-	linker	UNP P0A7G6
A	2998	SER	-	linker	UNP P0A7G6
A	2999	MET	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	3000	SER	-	linker	UNP P0A7G6
A	3986	THR	-	linker	UNP P0A7G6
A	3987	GLY	-	linker	UNP P0A7G6
A	3988	SER	-	linker	UNP P0A7G6
A	3989	THR	-	linker	UNP P0A7G6
A	3990	GLY	-	linker	UNP P0A7G6
A	3991	SER	-	linker	UNP P0A7G6
A	3992	MET	-	linker	UNP P0A7G6
A	3993	SER	-	linker	UNP P0A7G6
A	3994	GLY	-	linker	UNP P0A7G6
A	3995	ARG	-	linker	UNP P0A7G6
A	3996	THR	-	linker	UNP P0A7G6
A	3997	GLY	-	linker	UNP P0A7G6
A	3998	SER	-	linker	UNP P0A7G6
A	3999	MET	-	linker	UNP P0A7G6
A	4000	SER	-	linker	UNP P0A7G6
D	26	GLY	-	linker	UNP P0A7G6
D	27	ALA	-	linker	UNP P0A7G6
D	28	MET	-	linker	UNP P0A7G6
D	29	HIS	-	linker	UNP P0A7G6
D	986	THR	-	linker	UNP P0A7G6
D	987	GLY	-	linker	UNP P0A7G6
D	988	SER	-	linker	UNP P0A7G6
D	989	THR	-	linker	UNP P0A7G6
D	990	GLY	-	linker	UNP P0A7G6
D	991	SER	-	linker	UNP P0A7G6
D	992	GLY	-	linker	UNP P0A7G6
D	993	THR	-	linker	UNP P0A7G6
D	994	THR	-	linker	UNP P0A7G6
D	995	GLY	-	linker	UNP P0A7G6
D	996	SER	-	linker	UNP P0A7G6
D	997	THR	-	linker	UNP P0A7G6
D	998	GLY	-	linker	UNP P0A7G6
D	999	SER	-	linker	UNP P0A7G6
D	1000	MET	-	linker	UNP P0A7G6
D	1986	THR	-	linker	UNP P0A7G6
D	1987	GLY	-	linker	UNP P0A7G6
D	1988	SER	-	linker	UNP P0A7G6
D	1989	THR	-	linker	UNP P0A7G6
D	1990	GLY	-	linker	UNP P0A7G6
D	1991	SER	-	linker	UNP P0A7G6
D	1992	MET	-	linker	UNP P0A7G6

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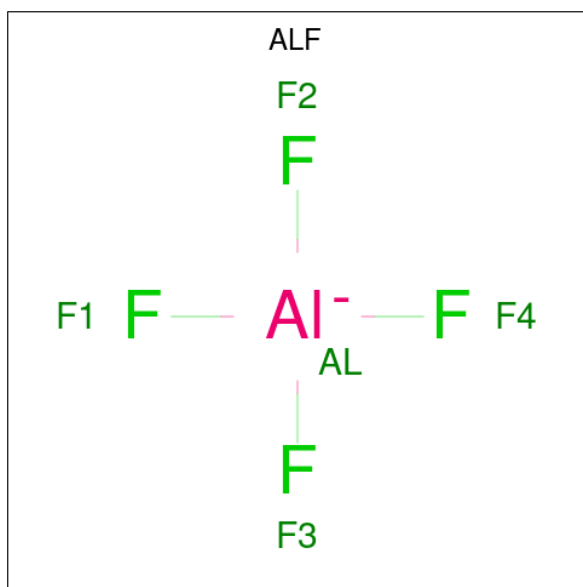
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1993	GLY	-	linker	UNP P0A7G6
D	1994	HIS	-	linker	UNP P0A7G6
D	1995	THR	-	linker	UNP P0A7G6
D	1996	THR	-	linker	UNP P0A7G6
D	1997	GLY	-	linker	UNP P0A7G6
D	1998	SER	-	linker	UNP P0A7G6
D	1999	MET	-	linker	UNP P0A7G6
D	2000	SER	-	linker	UNP P0A7G6
D	2985	THR	-	linker	UNP P0A7G6
D	2986	GLY	-	linker	UNP P0A7G6
D	2987	SER	-	linker	UNP P0A7G6
D	2988	THR	-	linker	UNP P0A7G6
D	2989	GLY	-	linker	UNP P0A7G6
D	2990	SER	-	linker	UNP P0A7G6
D	2991	ALA	-	linker	UNP P0A7G6
D	2992	SER	-	linker	UNP P0A7G6
D	2993	GLY	-	linker	UNP P0A7G6
D	2994	SER	-	linker	UNP P0A7G6
D	2995	SER	-	linker	UNP P0A7G6
D	2996	THR	-	linker	UNP P0A7G6
D	2997	GLY	-	linker	UNP P0A7G6
D	2998	SER	-	linker	UNP P0A7G6
D	2999	MET	-	linker	UNP P0A7G6
D	3000	SER	-	linker	UNP P0A7G6
D	3986	THR	-	linker	UNP P0A7G6
D	3987	GLY	-	linker	UNP P0A7G6
D	3988	SER	-	linker	UNP P0A7G6
D	3989	THR	-	linker	UNP P0A7G6
D	3990	GLY	-	linker	UNP P0A7G6
D	3991	SER	-	linker	UNP P0A7G6
D	3992	MET	-	linker	UNP P0A7G6
D	3993	SER	-	linker	UNP P0A7G6
D	3994	GLY	-	linker	UNP P0A7G6
D	3995	ARG	-	linker	UNP P0A7G6
D	3996	THR	-	linker	UNP P0A7G6
D	3997	GLY	-	linker	UNP P0A7G6
D	3998	SER	-	linker	UNP P0A7G6
D	3999	MET	-	linker	UNP P0A7G6
D	4000	SER	-	linker	UNP P0A7G6

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

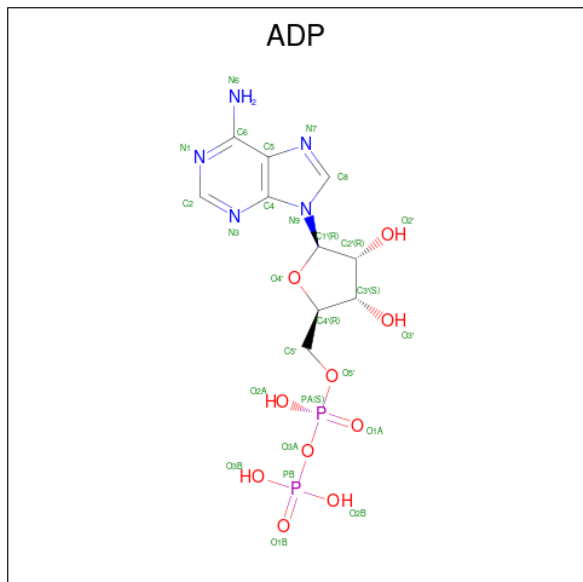
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total Mg 5 5	0	0
4	D	5	Total Mg 5 5	0	0

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Al F 5 1 4	0	0
5	A	1	Total Al F 5 1 4	0	0
5	A	1	Total Al F 5 1 4	0	0
5	A	1	Total Al F 5 1 4	0	0
5	A	1	Total Al F 5 1 4	0	0
5	D	1	Total Al F 5 1 4	0	0
5	D	1	Total Al F 5 1 4	0	0
5	D	1	Total Al F 5 1 4	0	0
5	D	1	Total Al F 5 1 4	0	0
5	D	1	Total Al F 5 1 4	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



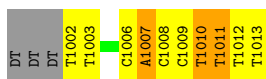
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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. 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. 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.

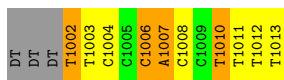
- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3')

Chain B: 



- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3')

Chain E: 



- Molecule 2: DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3')

Chain C: 




- Molecule 2: DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3')

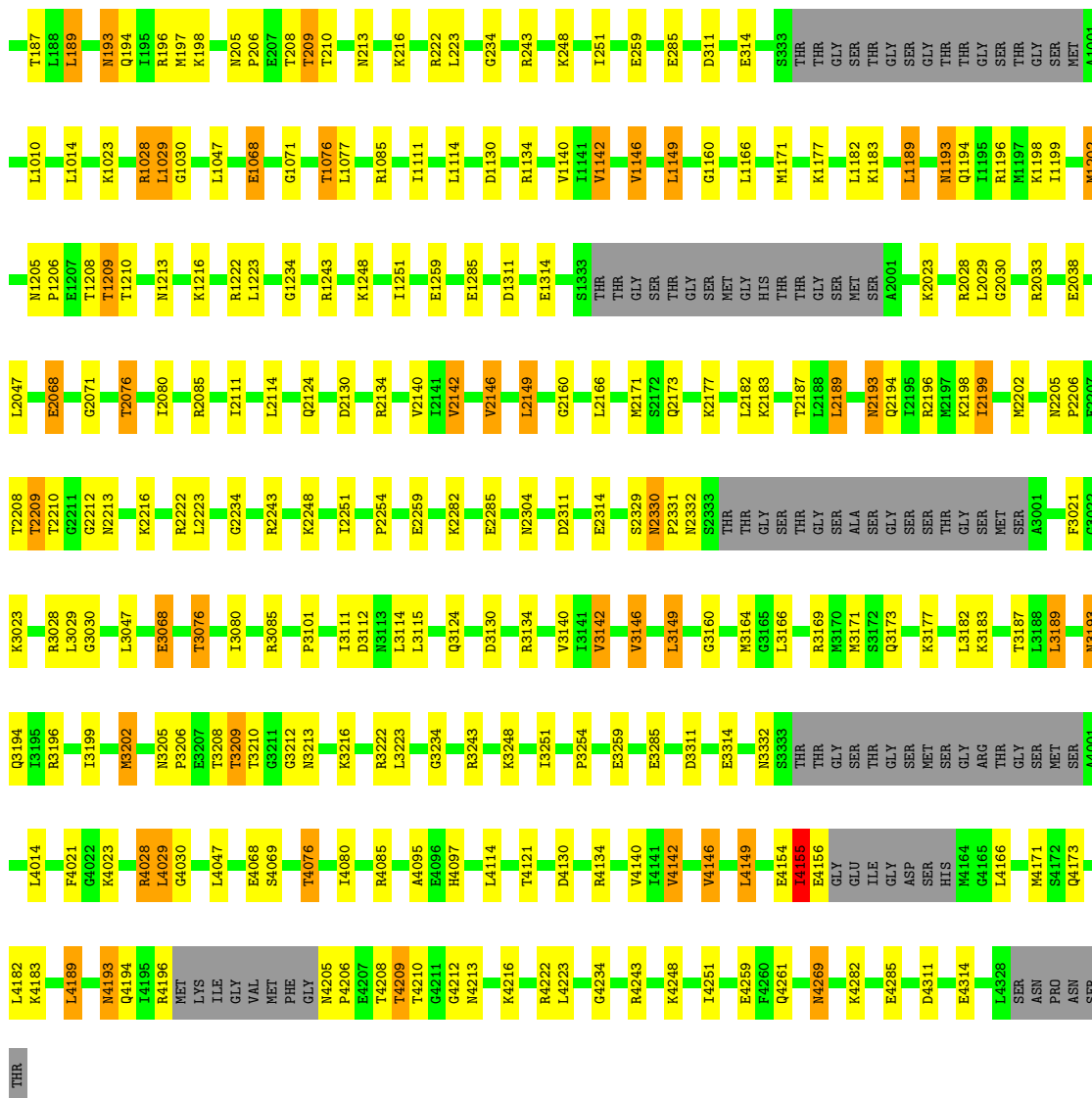
Chain F: 



- Molecule 3: Protein recA

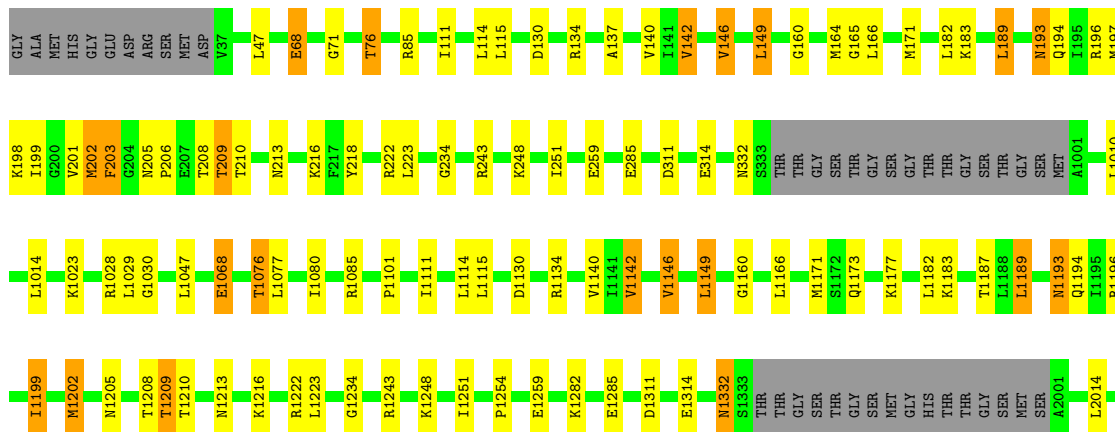
Chain A: 





• Molecule 3: Protein recA

Chain D: 78% 13% 6%



L4182	L4183	T4187	L4188	L4189	M4193	Q4194	I4195	R4196	M4197	K4198	ILE	GLY	VAL	MET	PHE	GLY	N4205	P4206	E4207	T4208	T4209	T4210	G4211	G4212	N4213	K4216	K4217	K4218	K4219	G4220	L4221	L4222	L4223	G4234	R4243	K4248	I4251	P4254	E4259	E4285	D4311	E4314	L4328	SER	ASN	PRO	ASN	SER	THR																																						
GLY	SER	MET	A4001	F4021	G4022	K4023	R4028	L4029	L4047	E4068	S4069	T4076	T4080	R4085	E4086	G4087	L4114	L4126	D4130	R4134	V4140	L4141	V4142	V4146	L4149	E4154	ILE	GLU	GLY	ILE	GLY	ASP	SER	HIS	M4164	G4165	L4166	M4171	K4177	M3202	N3205	P3206	E3207	T3208	T3209	T3210	G3211	N3213	K3216	R3222	L3223	G3234	R3243	K3248	I3251	E3259	F3260	Q3261	L3262	L3263	M3269	K3282	E3285	D3311	E3314	L3328	S3329	M3330	P3331	N3332	S3333	THR	THR	GLY	THR	GLY	THR	GLY	N3193	Q3194	T3195	R3196	M3197	K3198	I3199		
F3021	G3022	K3023	R3028	P3206	L3029	G3030	L3047	E3068	T3076	T3080	R3085	I3111	L3114	Q3124	D3130	R3134	V3140	I3141	V3142	V3146	L3149	I3155	I3159	L3166	M3171	S3172	Q3173	L3182	K3183	T3187	L3188	L3189	N3193	Q3194	T3195	R3196	M3197	K3198	I3199	M3202	N3205	P3206	E3207	T3208	T3209	T3210	G3211	N3213	K3216	R3222	L3223	G3234	R3243	I3251	F3260	Q3261	L3262	L3263	M3269	K3282	E3285	D3311	E3314	L3328	S3329	M3330	P3331	N3332	S3333	THR	THR	GLY	THR	GLY	THR	GLY	N3193	Q3194	T3195	R3196	M3197	K3198	I3199				
K2023	R2028	L2029	G2030	T2039	L2047	E2068	T2076	L2077	L2080	R2085	P2101	L2111	L2114	Q2124	D2130	R2134	V2140	T2141	V2142	V2146	L2149	G2160	L2166	R2169	M2170	M2171	S2172	Q2173	L2182	K2183	T2187	L2188	L2189	M2193	T2194	L2195	R2196	M2197	K2198	L2199	M2202	N2205	P2206	E2207	T2208	T2209	T2210	G2211	G2212	N2213	K2216	R2222	L2223	G2234	R2243	K2248	I2251	E2259	E2285	N2304	D2311	E2314	M2332	S2333	THR	THR	GLY	SER	THR	THR	GLY	SER	ALA	SER	GLY	SER	SER	THR	THR	GLY	SER	MET	SER	MET	SER	ARG	A3001

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.00Å 300.50Å 80.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.15 39.75 – 2.98	Depositor EDS
% Data completeness (in resolution range)	89.9 (40.00-3.15) 86.7 (39.75-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.217 , 0.243 0.273 , 0.307	Depositor DCC
R_{free} test set	1459 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtrriage
Anisotropy	0.133	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 19.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	25312	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: ALF, ADP, MG

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	B	1.15	0/260	1.79	7/397 (1.8%)
1	E	1.13	0/260	1.97	12/397 (3.0%)
2	C	3.88	1/146 (0.7%)	2.40	4/225 (1.8%)
2	F	6.25	1/146 (0.7%)	2.40	5/225 (2.2%)
3	A	0.39	0/12264	0.54	0/16503
3	D	0.39	0/12264	0.54	0/16501
All	All	0.70	2/25340 (0.0%)	0.67	28/34248 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2007	DG	P-O5'	-75.00	0.84	1.59
2	C	2007	DG	P-O5'	-45.55	1.14	1.59

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2007	DG	P-O5'-C5'	25.73	162.07	120.90
2	C	2007	DG	O5'-P-OP2	-20.43	86.18	110.70
2	C	2007	DG	O5'-P-OP1	18.46	132.85	110.70
1	E	1006	DC	O4'-C4'-C3'	-8.95	100.63	106.00
2	F	2008	DG	O4'-C1'-N9	-8.52	102.04	108.00
1	B	1006	DC	O4'-C4'-C3'	-8.51	100.89	106.00
1	E	1006	DC	C1'-O4'-C4'	-8.17	101.93	110.10
2	C	2008	DG	O4'-C1'-N9	-8.07	102.35	108.00
1	B	1006	DC	C1'-O4'-C4'	-7.84	102.26	110.10
2	F	2007	DG	O5'-P-OP2	7.55	119.76	110.70
1	E	1010	DT	O4'-C1'-N1	6.91	112.84	108.00
1	B	1010	DT	N3-C2-O2	-6.80	118.22	122.30
1	E	1002	DT	P-O3'-C3'	6.64	127.67	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1010	DT	O4'-C1'-N1	6.28	112.39	108.00
1	E	1002	DT	O4'-C1'-N1	6.28	112.39	108.00
1	E	1007	DA	O4'-C4'-C3'	-5.70	102.22	104.50
2	F	2007	DG	O4'-C1'-C2'	-5.69	101.35	105.90
2	F	2009	DT	C1'-O4'-C4'	-5.49	104.61	110.10
1	B	1007	DA	O4'-C1'-N9	5.43	111.80	108.00
1	B	1011	DT	C1'-O4'-C4'	-5.35	104.75	110.10
1	E	1004	DC	O4'-C1'-N1	-5.31	104.28	108.00
2	C	2007	DG	O4'-C1'-C2'	-5.22	101.72	105.90
1	E	1007	DA	C1'-O4'-C4'	-5.15	104.95	110.10
1	E	1007	DA	O4'-C1'-N9	5.15	111.61	108.00
1	E	1007	DA	C4'-C3'-C2'	5.14	107.72	103.10
1	E	1006	DC	O4'-C1'-N1	5.13	111.59	108.00
1	B	1008	DC	C1'-O4'-C4'	-5.11	105.00	110.10
1	E	1008	DC	C1'-O4'-C4'	-5.05	105.05	110.10

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	B	236	0	139	9	0
1	E	236	0	139	19	0
2	C	130	0	69	0	0
2	F	130	0	69	0	0
3	A	12125	0	12451	176	0
3	D	12125	0	12456	190	1
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	25	0	0	0	0
5	D	25	0	0	2	0
6	A	135	0	60	6	0
6	D	135	0	60	4	0
All	All	25312	0	25443	364	1

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 (364) 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)
3:A:68:GLU:HG2	3:A:1216:LYS:HB3	1.39	1.02
3:D:68:GLU:HG2	3:D:1216:LYS:HB3	1.47	0.97
3:D:160:GLY:H	3:D:1173:GLN:HE22	1.14	0.94
3:A:2068:GLU:HG2	3:A:3216:LYS:HB3	1.54	0.87
3:D:1194:GLN:HE21	3:D:1196:ARG:HH12	1.23	0.86
3:D:4194:GLN:HE21	3:D:4196:ARG:HH12	1.23	0.86
3:D:2194:GLN:HE21	3:D:2196:ARG:HH12	1.24	0.85
3:A:194:GLN:HE21	3:A:196:ARG:HH12	1.25	0.85
3:A:3194:GLN:HE21	3:A:3196:ARG:HH12	1.25	0.85
3:D:1193:ASN:HD22	3:D:1194:GLN:H	1.25	0.84
3:A:3206:PRO:HG3	3:D:3202:MET:HB3	1.58	0.84
3:D:2193:ASN:HD22	3:D:2194:GLN:H	1.26	0.84
3:D:3068:GLU:HG2	3:D:4216:LYS:HB3	1.56	0.84
3:A:4282:LYS:HG3	3:D:1282:LYS:HG3	1.59	0.83
3:A:1194:GLN:HE21	3:A:1196:ARG:HH12	1.24	0.83
3:A:3193:ASN:HD22	3:A:3194:GLN:H	1.26	0.83
3:A:4194:GLN:HE21	3:A:4196:ARG:HH12	1.26	0.82
3:D:1068:GLU:HG2	3:D:2216:LYS:HB3	1.61	0.82
3:D:194:GLN:HE21	3:D:196:ARG:HH12	1.25	0.82
3:A:2193:ASN:HD22	3:A:2194:GLN:H	1.27	0.81
3:A:2194:GLN:HE21	3:A:2196:ARG:HH12	1.24	0.81
3:D:3194:GLN:HE21	3:D:3196:ARG:HH12	1.26	0.81
3:A:193:ASN:HD22	3:A:194:GLN:H	1.28	0.80
3:A:1193:ASN:HD22	3:A:1194:GLN:H	1.28	0.80
3:D:160:GLY:H	3:D:1173:GLN:NE2	1.81	0.79
3:D:4193:ASN:HD22	3:D:4194:GLN:H	1.29	0.79
3:D:3193:ASN:HD22	3:D:3194:GLN:H	1.29	0.79
1:E:1002:DT:H2'	1:E:1003:DT:C6	2.19	0.78
3:D:2068:GLU:HG2	3:D:3216:LYS:HB3	1.66	0.77
3:A:1068:GLU:HG2	3:A:2216:LYS:HB3	1.66	0.77
3:D:193:ASN:HD22	3:D:194:GLN:H	1.32	0.77
1:E:1002:DT:P	3:D:165:GLY:HA2	2.25	0.77
3:A:71:GLY:HA2	6:A:502:ADP:H5'1	1.66	0.76
3:A:111:ILE:HG22	3:A:1030:GLY:CA	2.14	0.76
3:A:4193:ASN:HD22	3:A:4194:GLN:H	1.32	0.75
3:A:3068:GLU:HG2	3:A:4216:LYS:HB3	1.66	0.75
3:D:111:ILE:HG22	3:D:1030:GLY:CA	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:68:GLU:HG2	3:A:1216:LYS:CB	2.17	0.72
3:A:3146:VAL:HA	3:A:3149:LEU:HD22	1.77	0.67
3:D:201:VAL:HA	3:D:203:PHE:CZ	2.29	0.67
3:D:1193:ASN:HD22	3:D:1194:GLN:N	1.91	0.67
3:D:2193:ASN:HD22	3:D:2194:GLN:N	1.92	0.66
3:D:4146:VAL:HA	3:D:4149:LEU:HD22	1.77	0.66
3:D:201:VAL:HA	3:D:203:PHE:CE1	2.30	0.66
3:D:3146:VAL:HA	3:D:3149:LEU:HD22	1.78	0.66
3:A:2193:ASN:HD22	3:A:2194:GLN:N	1.94	0.65
3:D:2160:GLY:H	3:D:3173:GLN:HE22	1.41	0.65
3:D:3076:THR:HG21	3:D:3142:VAL:HG21	1.78	0.65
3:A:2068:GLU:HG2	3:A:3216:LYS:CB	2.26	0.65
3:D:146:VAL:HA	3:D:149:LEU:HD22	1.78	0.65
3:D:2160:GLY:H	3:D:3173:GLN:NE2	1.95	0.65
3:A:193:ASN:HD22	3:A:194:GLN:N	1.94	0.65
3:A:2329:SER:O	3:A:2330:ASN:HB2	1.94	0.65
3:A:4146:VAL:HA	3:A:4149:LEU:HD22	1.78	0.65
3:D:3068:GLU:HG2	3:D:4216:LYS:CB	2.27	0.65
3:D:4193:ASN:HD22	3:D:4194:GLN:N	1.95	0.65
3:A:112:ASP:O	3:A:1028:ARG:HG2	1.97	0.64
3:A:1193:ASN:HD22	3:A:1194:GLN:N	1.95	0.64
3:A:3193:ASN:HD22	3:A:3194:GLN:N	1.94	0.64
3:A:146:VAL:HA	3:A:149:LEU:HD22	1.79	0.64
3:A:1146:VAL:HA	3:A:1149:LEU:HD22	1.78	0.64
3:D:1111:ILE:HG22	3:D:2030:GLY:CA	2.26	0.64
3:D:3193:ASN:OD1	3:D:3209:THR:HG23	1.98	0.64
3:A:2146:VAL:HA	3:A:2149:LEU:HD22	1.80	0.64
3:D:68:GLU:HG2	3:D:1216:LYS:CB	2.26	0.64
3:A:3193:ASN:OD1	3:A:3209:THR:HG23	1.99	0.63
3:A:111:ILE:HG22	3:A:1030:GLY:N	2.13	0.63
3:A:1071:GLY:HA2	6:A:1502:ADP:H5'1	1.79	0.63
3:A:76:THR:HG21	3:A:142:VAL:HG21	1.80	0.63
3:D:193:ASN:OD1	3:D:209:THR:HG23	1.98	0.63
1:E:1013:DT:C7	3:D:3197:MET:HG3	2.29	0.63
3:A:115:LEU:HD21	3:A:1014:LEU:HD21	1.81	0.63
3:D:2146:VAL:HA	3:D:2149:LEU:HD22	1.80	0.63
1:B:1007:DA:H5'	3:A:2212:GLY:HA2	1.80	0.63
1:E:1013:DT:H71	3:D:3197:MET:HG3	1.81	0.62
3:A:1076:THR:HG21	3:A:1142:VAL:HG21	1.81	0.62
3:D:3193:ASN:HD22	3:D:3194:GLN:N	1.96	0.62
3:A:4193:ASN:HD22	3:A:4194:GLN:N	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2193:ASN:OD1	3:D:2209:THR:HG23	2.00	0.62
3:A:193:ASN:OD1	3:A:209:THR:HG23	2.00	0.62
3:D:4076:THR:HG21	3:D:4142:VAL:HG21	1.82	0.62
3:D:1146:VAL:HA	3:D:1149:LEU:HD22	1.80	0.62
3:D:4193:ASN:OD1	3:D:4209:THR:HG23	1.99	0.62
3:A:4076:THR:HG21	3:A:4142:VAL:HG21	1.82	0.61
3:A:4193:ASN:OD1	3:A:4209:THR:HG23	2.00	0.61
3:D:2124:GLN:HG3	3:D:3021:PHE:CD1	2.36	0.61
3:A:2160:GLY:H	3:A:3173:GLN:NE2	1.98	0.61
3:A:3076:THR:HG21	3:A:3142:VAL:HG21	1.82	0.61
3:D:1193:ASN:OD1	3:D:1209:THR:HG23	2.00	0.61
3:A:2330:ASN:H	3:A:2331:PRO:HD3	1.65	0.60
3:A:1193:ASN:OD1	3:A:1209:THR:HG23	2.02	0.60
3:D:111:ILE:HG22	3:D:1030:GLY:HA2	1.83	0.60
1:E:1003:DT:O2	3:D:199:ILE:HG22	2.00	0.60
3:D:76:THR:HG21	3:D:142:VAL:HG21	1.84	0.60
3:A:2193:ASN:OD1	3:A:2209:THR:HG23	2.01	0.60
3:A:3111:ILE:HG22	3:A:4030:GLY:CA	2.32	0.60
3:D:1076:THR:HG21	3:D:1142:VAL:HG21	1.82	0.60
1:B:1002:DT:H2'	1:B:1003:DT:C6	2.38	0.59
3:A:150:THR:HB	3:A:155:ILE:HD11	1.83	0.59
3:A:4121:THR:HG22	3:A:4155:ILE:HD12	1.85	0.59
3:D:193:ASN:HD22	3:D:194:GLN:N	1.98	0.59
1:E:1010:DT:H5'	3:D:3212:GLY:HA2	1.84	0.59
3:A:2160:GLY:H	3:A:3173:GLN:HE22	1.50	0.59
3:D:2076:THR:HG21	3:D:2142:VAL:HG21	1.84	0.59
3:A:2076:THR:HG21	3:A:2142:VAL:HG21	1.85	0.59
3:D:2111:ILE:HG22	3:D:3030:GLY:CA	2.33	0.58
3:D:3328:LEU:HB2	3:D:3331:PRO:HG3	1.84	0.58
3:D:3111:ILE:HG23	3:D:4029:LEU:HD13	1.86	0.58
3:D:4198:LYS:HG2	3:D:4206:PRO:O	2.03	0.58
1:E:1007:DA:H5'	3:D:2212:GLY:HA2	1.86	0.58
3:D:202:MET:O	3:D:202:MET:HG2	2.03	0.57
3:A:4213:ASN:OD1	3:A:4216:LYS:HE2	2.04	0.57
3:D:3243:ARG:NH1	3:D:3259:GLU:OE2	2.37	0.57
3:D:213:ASN:OD1	3:D:216:LYS:HE2	2.05	0.57
3:D:1243:ARG:NH1	3:D:1259:GLU:OE2	2.38	0.57
3:D:2243:ARG:NH1	3:D:2259:GLU:OE2	2.38	0.57
3:D:1194:GLN:NE2	3:D:1196:ARG:HH12	1.99	0.57
3:A:1243:ARG:NH1	3:A:1259:GLU:OE2	2.38	0.56
1:E:1013:DT:H5'	3:D:4212:GLY:HA2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2329:SER:O	3:A:2330:ASN:CB	2.53	0.56
3:A:198:LYS:HG2	3:A:206:PRO:O	2.05	0.56
3:A:2213:ASN:OD1	3:A:2216:LYS:HE2	2.05	0.56
3:D:1160:GLY:H	3:D:2173:GLN:NE2	2.03	0.56
3:D:3213:ASN:OD1	3:D:3216:LYS:HE2	2.05	0.56
3:D:2213:ASN:OD1	3:D:2216:LYS:HE2	2.05	0.56
3:D:3222:ARG:HG3	3:D:3248:LYS:HB3	1.87	0.56
3:A:2149:LEU:HD23	3:A:2171:MET:HE1	1.87	0.56
3:D:1213:ASN:OD1	3:D:1216:LYS:HE2	2.05	0.56
3:A:4243:ARG:NH1	3:A:4259:GLU:OE2	2.39	0.56
3:D:3076:THR:CG2	3:D:3142:VAL:HG21	2.35	0.56
3:D:4213:ASN:OD1	3:D:4216:LYS:HE2	2.05	0.56
3:A:2194:GLN:NE2	3:A:2196:ARG:HH12	2.01	0.55
3:A:3222:ARG:HG3	3:A:3248:LYS:HB3	1.88	0.55
3:A:2304:ASN:ND2	3:D:2304:ASN:OD1	2.27	0.55
3:A:76:THR:CG2	3:A:142:VAL:HG21	2.37	0.55
3:A:3243:ARG:NH1	3:A:3259:GLU:OE2	2.39	0.55
3:D:2222:ARG:HG3	3:D:2248:LYS:HB3	1.89	0.55
1:E:1013:DT:H5''	3:D:4213:ASN:ND2	2.21	0.55
3:A:3076:THR:CG2	3:A:3142:VAL:HG21	2.36	0.55
3:A:3213:ASN:OD1	3:A:3216:LYS:HE2	2.07	0.55
3:D:1076:THR:CG2	3:D:1142:VAL:HG21	2.37	0.55
3:A:243:ARG:NH1	3:A:259:GLU:OE2	2.40	0.54
3:A:149:LEU:HD23	3:A:171:MET:HE1	1.90	0.54
3:A:1111:ILE:HG22	3:A:2030:GLY:CA	2.37	0.54
3:D:4243:ARG:NH1	3:D:4259:GLU:OE2	2.41	0.54
1:E:1010:DT:C2	3:D:2199:ILE:HD12	2.43	0.54
3:A:4076:THR:CG2	3:A:4142:VAL:HG21	2.38	0.54
3:A:4261:GLN:HB2	3:A:4269:ASN:HB3	1.89	0.54
3:D:1160:GLY:H	3:D:2173:GLN:HE22	1.56	0.54
3:D:4194:GLN:NE2	3:D:4196:ARG:HH12	2.00	0.54
3:A:1076:THR:CG2	3:A:1142:VAL:HG21	2.37	0.54
3:D:149:LEU:HD23	3:D:171:MET:HE1	1.89	0.54
3:D:4076:THR:CG2	3:D:4142:VAL:HG21	2.38	0.54
3:A:213:ASN:OD1	3:A:216:LYS:HE2	2.08	0.54
3:D:222:ARG:HG3	3:D:248:LYS:HB3	1.91	0.53
3:D:243:ARG:NH1	3:D:259:GLU:OE2	2.41	0.53
3:D:1068:GLU:HG2	3:D:2216:LYS:CB	2.37	0.53
3:A:2243:ARG:NH1	3:A:2259:GLU:OE2	2.40	0.53
3:A:111:ILE:HG22	3:A:1030:GLY:HA2	1.89	0.53
3:A:1160:GLY:H	3:A:2173:GLN:NE2	2.06	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4206:PRO:HG3	3:D:2202:MET:HB3	1.90	0.53
3:D:4222:ARG:HG3	3:D:4248:LYS:HB3	1.89	0.53
3:A:1222:ARG:HG3	3:A:1248:LYS:HB3	1.90	0.53
3:A:222:ARG:HG3	3:A:248:LYS:HB3	1.90	0.53
3:A:1213:ASN:OD1	3:A:1216:LYS:HE2	2.07	0.53
3:D:2076:THR:CG2	3:D:2142:VAL:HG21	2.38	0.53
3:A:194:GLN:NE2	3:A:196:ARG:HH12	2.01	0.53
3:A:4222:ARG:HG3	3:A:4248:LYS:HB3	1.90	0.52
3:D:1222:ARG:HG3	3:D:1248:LYS:HB3	1.91	0.52
3:A:3206:PRO:HG3	3:D:3202:MET:CB	2.34	0.52
3:A:4069:SER:HB3	6:A:4502:ADP:H3'	1.91	0.52
3:D:194:GLN:NE2	3:D:196:ARG:HH12	2.03	0.52
3:D:2149:LEU:HD23	3:D:2171:MET:HE1	1.90	0.52
1:E:1013:DT:H73	3:D:3198:LYS:O	2.09	0.52
3:A:2222:ARG:HG3	3:A:2248:LYS:HB3	1.90	0.52
3:D:76:THR:CG2	3:D:142:VAL:HG21	2.39	0.52
3:D:1254:PRO:HG3	6:D:502:ADP:O2'	2.10	0.52
3:A:3124:GLN:HG3	3:A:4021:PHE:CD1	2.45	0.52
3:D:2194:GLN:NE2	3:D:2196:ARG:HH12	2.00	0.52
3:D:198:LYS:HG2	3:D:206:PRO:O	2.09	0.51
1:E:1007:DA:C6	3:D:1199:ILE:HG13	2.45	0.51
3:D:1194:GLN:HE22	3:D:1196:ARG:HH22	1.56	0.51
3:A:2076:THR:CG2	3:A:2142:VAL:HG21	2.39	0.51
3:A:2194:GLN:HE22	3:A:2196:ARG:HH22	1.59	0.50
3:A:3194:GLN:NE2	3:A:3196:ARG:HH12	2.01	0.50
1:E:1003:DT:H2'	3:D:197:MET:O	2.11	0.50
3:D:111:ILE:HG22	3:D:1030:GLY:N	2.27	0.50
3:A:101:PRO:HB3	3:A:1029:LEU:HD22	1.93	0.50
3:D:4194:GLN:HE22	3:D:4196:ARG:HH22	1.58	0.50
3:D:4069:SER:HA	6:D:4502:ADP:O3A	2.12	0.50
1:B:1009:DC:O2	3:A:3169:ARG:NH1	2.44	0.50
3:D:201:VAL:HG23	3:D:203:PHE:CD1	2.46	0.50
3:A:3160:GLY:H	3:A:4173:GLN:NE2	2.10	0.49
3:A:3194:GLN:HE22	3:A:3196:ARG:HH22	1.60	0.49
3:D:194:GLN:HE22	3:D:196:ARG:HH22	1.58	0.49
3:D:2068:GLU:HG2	3:D:3216:LYS:CB	2.40	0.49
3:A:194:GLN:HE22	3:A:196:ARG:HH22	1.59	0.49
3:A:1194:GLN:NE2	3:A:1196:ARG:HH12	2.00	0.49
3:D:2194:GLN:HE22	3:D:2196:ARG:HH22	1.58	0.49
1:B:1010:DT:H2'	1:B:1011:DT:C6	2.47	0.49
3:D:1182:LEU:HD11	3:D:1189:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1194:GLN:HE21	3:D:1196:ARG:NH1	2.03	0.49
3:A:3111:ILE:HG22	3:A:4030:GLY:N	2.27	0.49
3:D:2101:PRO:HB3	3:D:3029:LEU:HD22	1.95	0.49
3:A:2124:GLN:HG3	3:A:3021:PHE:CD1	2.48	0.49
3:D:3261:GLN:HB2	3:D:3269:ASN:HB3	1.95	0.48
3:D:3194:GLN:HE22	3:D:3196:ARG:HH22	1.61	0.48
3:A:1194:GLN:HE22	3:A:1196:ARG:HH22	1.59	0.48
3:A:1160:GLY:H	3:A:2173:GLN:HE22	1.62	0.48
3:A:182:LEU:HD11	3:A:189:LEU:HD12	1.96	0.48
3:A:3254:PRO:HG3	6:A:2502:ADP:O2'	2.13	0.48
3:A:1182:LEU:HD11	3:A:1189:LEU:HD12	1.95	0.48
3:D:1115:LEU:HD21	3:D:2014:LEU:HD21	1.95	0.48
3:D:1194:GLN:NE2	3:D:1196:ARG:HH22	2.12	0.48
3:D:137:ALA:HB1	3:D:1010:LEU:HB2	1.95	0.48
3:D:182:LEU:HD11	3:D:189:LEU:HD12	1.96	0.47
3:A:3160:GLY:H	3:A:4173:GLN:HE22	1.61	0.47
3:A:4194:GLN:NE2	3:A:4196:ARG:HH12	2.04	0.47
3:A:1149:LEU:HD23	3:A:1171:MET:HE1	1.96	0.47
3:A:4282:LYS:HG3	3:D:1282:LYS:CG	2.40	0.47
3:D:115:LEU:HD21	3:D:1014:LEU:HD21	1.97	0.47
3:D:2194:GLN:NE2	3:D:2196:ARG:HH22	2.13	0.47
3:D:4194:GLN:NE2	3:D:4196:ARG:HH22	2.13	0.47
3:A:111:ILE:CG2	3:A:1030:GLY:HA2	2.44	0.47
3:A:4194:GLN:HE22	3:A:4196:ARG:HH22	1.61	0.47
3:D:194:GLN:NE2	3:D:196:ARG:HH22	2.11	0.47
3:A:2038:GLU:HA	3:A:2332:ASN:HD21	1.80	0.47
3:D:1149:LEU:HD23	3:D:1171:MET:HE1	1.95	0.47
3:D:2182:LEU:HD11	3:D:2189:LEU:HD12	1.96	0.47
3:A:4182:LEU:HD11	3:A:4189:LEU:HD12	1.95	0.47
3:D:2111:ILE:HG22	3:D:3030:GLY:N	2.30	0.47
3:D:3149:LEU:HD23	3:D:3171:MET:HE1	1.96	0.47
3:D:2130:ASP:OD2	3:D:2134:ARG:NH1	2.47	0.47
1:B:1011:DT:H2'	1:B:1012:DT:C6	2.50	0.46
3:A:3068:GLU:HG2	3:A:4216:LYS:CB	2.40	0.46
3:D:1068:GLU:HA	5:D:1501:ALF:F1	2.05	0.46
3:D:3182:LEU:HD11	3:D:3189:LEU:HD12	1.97	0.46
1:E:1011:DT:H2'	1:E:1012:DT:C6	2.50	0.46
3:A:3149:LEU:HD23	3:A:3171:MET:HE1	1.96	0.46
3:A:2194:GLN:HE21	3:A:2196:ARG:NH1	2.04	0.46
3:D:3194:GLN:NE2	3:D:3196:ARG:HH12	2.02	0.46
3:D:4182:LEU:HD11	3:D:4189:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3112:ASP:O	3:A:4028:ARG:HG2	2.16	0.46
3:A:3111:ILE:HG23	3:A:4029:LEU:HD13	1.98	0.46
1:E:1006:DC:H5'	3:D:2169:ARG:HA	1.97	0.46
3:A:3111:ILE:HG22	3:A:4030:GLY:HA2	1.98	0.46
1:B:1010:DT:C2	3:A:2199:ILE:HD12	2.51	0.45
3:A:194:GLN:NE2	3:A:196:ARG:HH22	2.13	0.45
3:A:2194:GLN:NE2	3:A:2196:ARG:HH22	2.14	0.45
3:A:3080:ILE:HD11	3:A:3142:VAL:CG1	2.46	0.45
3:D:1111:ILE:HG22	3:D:2030:GLY:HA2	1.96	0.45
3:A:111:ILE:HG23	3:A:1029:LEU:HB3	1.98	0.45
3:D:1111:ILE:HG22	3:D:2030:GLY:N	2.31	0.45
1:E:1013:DT:H72	3:D:3197:MET:HG3	1.99	0.45
3:A:159:ILE:HG12	3:A:1177:LYS:HD3	1.98	0.45
3:D:111:ILE:CG2	3:D:1030:GLY:HA2	2.47	0.45
1:B:1013:DT:H5'	3:A:4212:GLY:HA2	1.97	0.45
3:D:3263:LEU:HG	3:D:3269:ASN:HB2	1.99	0.45
3:A:2111:ILE:HG22	3:A:3030:GLY:CA	2.46	0.45
3:A:2182:LEU:HD11	3:A:2189:LEU:HD12	1.99	0.45
3:A:2130:ASP:OD2	3:A:2134:ARG:NH1	2.50	0.45
3:D:4149:LEU:HD23	3:D:4171:MET:HE1	1.99	0.45
3:D:4177:LYS:HB3	3:D:4177:LYS:HE2	1.82	0.45
3:D:149:LEU:HD23	3:D:171:MET:CE	2.47	0.45
1:E:1013:DT:H71	3:D:3197:MET:CG	2.45	0.44
3:A:1194:GLN:NE2	3:A:1196:ARG:HH22	2.14	0.44
3:A:4154:GLU:C	3:A:4156:GLU:H	2.19	0.44
3:A:4194:GLN:NE2	3:A:4196:ARG:HH22	2.14	0.44
3:A:2149:LEU:HD23	3:A:2171:MET:CE	2.47	0.44
3:D:130:ASP:OD2	3:D:134:ARG:NH1	2.50	0.44
3:A:1130:ASP:OD2	3:A:1134:ARG:NH1	2.51	0.44
3:A:3182:LEU:HD11	3:A:3189:LEU:HD12	1.99	0.44
1:E:1007:DA:C5'	3:D:2212:GLY:HA2	2.47	0.44
3:D:2149:LEU:HD23	3:D:2171:MET:CE	2.48	0.44
3:D:194:GLN:HE21	3:D:196:ARG:NH1	2.05	0.43
3:D:1080:ILE:HD11	3:D:1142:VAL:CG1	2.48	0.43
3:D:1130:ASP:OD2	3:D:1134:ARG:NH1	2.51	0.43
3:A:1111:ILE:HG22	3:A:2030:GLY:HA2	2.01	0.43
3:D:4254:PRO:HG3	6:D:3502:ADP:O2'	2.18	0.43
3:A:130:ASP:OD2	3:A:134:ARG:NH1	2.51	0.43
3:A:2177:LYS:HB3	3:A:2177:LYS:HE2	1.83	0.43
3:A:3101:PRO:HB3	3:A:4029:LEU:HD22	1.99	0.43
3:D:3130:ASP:OD2	3:D:3134:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3202:MET:H	3:D:3202:MET:HG2	1.66	0.43
3:A:2243:ARG:HG3	3:A:2259:GLU:HG2	2.00	0.43
3:A:3130:ASP:OD2	3:A:3134:ARG:NH1	2.51	0.43
3:D:1149:LEU:HD23	3:D:1171:MET:CE	2.48	0.43
3:D:3080:ILE:HD11	3:D:3142:VAL:CG1	2.48	0.43
3:D:2194:GLN:HE21	3:D:2196:ARG:NH1	2.04	0.43
3:D:3194:GLN:NE2	3:D:3196:ARG:HH22	2.16	0.43
3:D:4149:LEU:HD23	3:D:4171:MET:CE	2.48	0.43
3:A:1149:LEU:HD23	3:A:1171:MET:CE	2.48	0.43
3:A:3194:GLN:NE2	3:A:3196:ARG:HH22	2.15	0.43
3:A:4149:LEU:HD23	3:A:4171:MET:CE	2.49	0.43
3:A:3182:LEU:HD23	3:A:3187:THR:HB	2.00	0.43
3:D:2039:THR:HG23	3:D:2332:ASN:HD21	1.84	0.43
3:D:2111:ILE:HG22	3:D:3030:GLY:HA2	2.01	0.43
3:D:4194:GLN:HE21	3:D:4196:ARG:NH1	2.03	0.43
3:A:4080:ILE:HD11	3:A:4142:VAL:CG1	2.49	0.43
3:A:137:ALA:HB1	3:A:1010:LEU:HB2	2.00	0.42
3:D:2243:ARG:HG3	3:D:2259:GLU:HG2	2.01	0.42
3:A:1198:LYS:HG2	3:A:1206:PRO:O	2.19	0.42
3:D:3124:GLN:HG3	3:D:4021:PHE:CD1	2.54	0.42
3:D:1076:THR:HG22	3:D:1077:LEU:N	2.34	0.42
3:D:3198:LYS:HG2	3:D:3206:PRO:O	2.20	0.42
3:A:3202:MET:H	3:A:3202:MET:HG2	1.65	0.42
3:D:3159:ILE:HD13	3:D:4126:LEU:HB3	2.02	0.42
1:E:1013:DT:C7	3:D:3198:LYS:O	2.67	0.42
3:A:2071:GLY:HA2	6:A:2502:ADP:H5'1	2.02	0.42
3:D:2080:ILE:HD11	3:D:2142:VAL:CG1	2.48	0.42
3:D:4130:ASP:OD2	3:D:4134:ARG:NH1	2.52	0.42
3:A:4095:ALA:O	3:A:4097:HIS:HD2	2.03	0.42
3:A:4130:ASP:OD2	3:A:4134:ARG:NH1	2.53	0.42
3:A:1243:ARG:HG3	3:A:1259:GLU:HG2	2.02	0.42
3:D:1243:ARG:HG3	3:D:1259:GLU:HG2	2.01	0.42
3:A:2182:LEU:HD23	3:A:2187:THR:HB	2.02	0.42
3:A:149:LEU:HD23	3:A:171:MET:CE	2.48	0.42
3:A:1068:GLU:HG2	3:A:2216:LYS:CB	2.43	0.42
3:D:2080:ILE:HD11	3:D:2142:VAL:HG13	2.02	0.42
3:D:3194:GLN:HE21	3:D:3196:ARG:NH1	2.06	0.42
3:A:2198:LYS:HG2	3:A:2206:PRO:O	2.20	0.41
3:A:3177:LYS:HB3	3:A:3177:LYS:HE2	1.82	0.41
3:A:80:ILE:HD11	3:A:142:VAL:CG1	2.50	0.41
3:D:4023:LYS:H	3:D:4023:LYS:HG2	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3149:LEU:HD23	3:A:3171:MET:CE	2.50	0.41
3:D:71:GLY:HA2	6:D:502:ADP:H5'1	2.03	0.41
3:D:3149:LEU:HD23	3:D:3171:MET:CE	2.50	0.41
1:B:1003:DT:H2'	3:A:197:MET:O	2.20	0.41
3:A:3080:ILE:HD11	3:A:3142:VAL:HG13	2.02	0.41
3:A:243:ARG:HG3	3:A:259:GLU:HG2	2.02	0.41
3:A:1202:MET:H	3:A:1202:MET:HG2	1.64	0.41
3:D:2182:LEU:HD23	3:D:2187:THR:HB	2.01	0.41
3:D:4243:ARG:HG3	3:D:4259:GLU:HG2	2.03	0.41
3:A:177:LYS:HB3	3:A:177:LYS:HE2	1.85	0.41
3:D:3080:ILE:HD11	3:D:3142:VAL:HG13	2.02	0.41
3:A:182:LEU:HD23	3:A:187:THR:HB	2.03	0.41
3:A:2080:ILE:HD11	3:A:2142:VAL:CG1	2.50	0.41
3:D:1080:ILE:HD11	3:D:1142:VAL:HG13	2.02	0.41
3:D:1177:LYS:HB3	3:D:1177:LYS:HE2	1.84	0.41
3:D:1202:MET:H	3:D:1202:MET:HG2	1.65	0.41
3:D:3243:ARG:HG3	3:D:3259:GLU:HG2	2.02	0.41
3:D:4080:ILE:HD11	3:D:4142:VAL:CG1	2.50	0.41
3:A:2254:PRO:HG3	6:A:1502:ADP:O2'	2.21	0.41
3:A:2330:ASN:N	3:A:2331:PRO:HD3	2.35	0.41
3:D:1182:LEU:HD23	3:D:1187:THR:HB	2.03	0.41
3:D:2076:THR:HG22	3:D:2077:LEU:N	2.36	0.41
3:D:3068:GLU:HA	5:D:3501:ALF:F1	2.11	0.41
3:D:3155:ILE:HA	3:D:4177:LYS:HE3	2.03	0.41
3:A:3243:ARG:HG3	3:A:3259:GLU:HG2	2.04	0.40
3:A:4080:ILE:HD11	3:A:4142:VAL:HG13	2.03	0.40
3:A:1076:THR:HG22	3:A:1077:LEU:N	2.36	0.40
3:A:3115:LEU:HD21	3:A:4014:LEU:HD21	2.02	0.40
3:D:4182:LEU:HD23	3:D:4187:THR:HB	2.03	0.40
3:A:2033:ARG:NE	3:A:2033:ARG:HA	2.37	0.40
3:A:2282:LYS:HG3	3:D:3282:LYS:HG3	2.01	0.40
3:D:201:VAL:HG23	3:D:203:PHE:CE1	2.57	0.40
3:D:2146:VAL:O	3:D:2149:LEU:HB2	2.22	0.40
3:D:3182:LEU:HD23	3:D:3187:THR:HB	2.03	0.40
3:A:2199:ILE:HD11	3:A:3164:MET:HE3	2.03	0.40
3:A:4149:LEU:HD23	3:A:4171:MET:HE1	2.01	0.40
3:A:4243:ARG:HG3	3:A:4259:GLU:HG2	2.02	0.40
3:D:1101:PRO:HB3	3:D:2029:LEU:HD22	2.04	0.40
1:B:1010:DT:H5'	3:A:3212:GLY:HA2	2.04	0.40
3:D:2198:LYS:HG2	3:D:2206:PRO:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:218:TYR:OH	3:D:4087:GLY:O[4_456]	2.19	0.01

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	
3	A	1595/1706 (94%)	1549 (97%)	33 (2%)	13 (1%)	19	55
3	D	1595/1706 (94%)	1539 (96%)	43 (3%)	13 (1%)	19	55
All	All	3190/3412 (94%)	3088 (97%)	76 (2%)	26 (1%)	19	55

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1023	LYS
3	A	2023	LYS
3	A	2330	ASN
3	A	3023	LYS
3	A	4023	LYS
3	D	1023	LYS
3	D	2023	LYS
3	D	3023	LYS
3	D	4023	LYS
3	D	1332	ASN
3	D	3269	ASN
3	D	332	ASN
3	D	2332	ASN
3	A	234	GLY
3	A	1234	GLY
3	A	2234	GLY
3	A	3234	GLY
3	A	3332	ASN

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Mol	Chain	Res	Type
3	A	4234	GLY
3	A	4269	ASN
3	D	234	GLY
3	D	1234	GLY
3	D	2234	GLY
3	D	3234	GLY
3	D	4234	GLY
3	A	4155	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	1267/1339 (95%)	1142 (90%)	125 (10%)	8 28
3	D	1267/1339 (95%)	1136 (90%)	131 (10%)	7 26
All	All	2534/2678 (95%)	2278 (90%)	256 (10%)	7 27

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	47	LEU
3	A	68	GLU
3	A	76	THR
3	A	85	ARG
3	A	114	LEU
3	A	140	VAL
3	A	142	VAL
3	A	146	VAL
3	A	149	LEU
3	A	166	LEU
3	A	183	LYS
3	A	189	LEU
3	A	193	ASN
3	A	205	ASN
3	A	208	THR

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Mol	Chain	Res	Type
3	A	209	THR
3	A	210	THR
3	A	223	LEU
3	A	251	ILE
3	A	285	GLU
3	A	311	ASP
3	A	314	GLU
3	A	1028	ARG
3	A	1029	LEU
3	A	1047	LEU
3	A	1068	GLU
3	A	1076	THR
3	A	1085	ARG
3	A	1114	LEU
3	A	1140	VAL
3	A	1142	VAL
3	A	1146	VAL
3	A	1149	LEU
3	A	1166	LEU
3	A	1183	LYS
3	A	1189	LEU
3	A	1193	ASN
3	A	1199	ILE
3	A	1202	MET
3	A	1205	ASN
3	A	1208	THR
3	A	1209	THR
3	A	1210	THR
3	A	1223	LEU
3	A	1251	ILE
3	A	1285	GLU
3	A	1311	ASP
3	A	1314	GLU
3	A	2028	ARG
3	A	2029	LEU
3	A	2047	LEU
3	A	2068	GLU
3	A	2076	THR
3	A	2085	ARG
3	A	2114	LEU
3	A	2140	VAL
3	A	2142	VAL

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Mol	Chain	Res	Type
3	A	2146	VAL
3	A	2149	LEU
3	A	2166	LEU
3	A	2183	LYS
3	A	2189	LEU
3	A	2193	ASN
3	A	2199	ILE
3	A	2202	MET
3	A	2205	ASN
3	A	2208	THR
3	A	2209	THR
3	A	2210	THR
3	A	2223	LEU
3	A	2251	ILE
3	A	2285	GLU
3	A	2311	ASP
3	A	2314	GLU
3	A	3028	ARG
3	A	3029	LEU
3	A	3047	LEU
3	A	3068	GLU
3	A	3076	THR
3	A	3085	ARG
3	A	3114	LEU
3	A	3140	VAL
3	A	3142	VAL
3	A	3146	VAL
3	A	3149	LEU
3	A	3166	LEU
3	A	3183	LYS
3	A	3189	LEU
3	A	3193	ASN
3	A	3199	ILE
3	A	3202	MET
3	A	3205	ASN
3	A	3208	THR
3	A	3209	THR
3	A	3210	THR
3	A	3223	LEU
3	A	3251	ILE
3	A	3285	GLU
3	A	3311	ASP

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Mol	Chain	Res	Type
3	A	3314	GLU
3	A	4028	ARG
3	A	4029	LEU
3	A	4047	LEU
3	A	4068	GLU
3	A	4076	THR
3	A	4085	ARG
3	A	4114	LEU
3	A	4140	VAL
3	A	4142	VAL
3	A	4146	VAL
3	A	4149	LEU
3	A	4155	ILE
3	A	4166	LEU
3	A	4183	LYS
3	A	4189	LEU
3	A	4193	ASN
3	A	4205	ASN
3	A	4208	THR
3	A	4209	THR
3	A	4210	THR
3	A	4223	LEU
3	A	4251	ILE
3	A	4285	GLU
3	A	4311	ASP
3	A	4314	GLU
3	D	47	LEU
3	D	68	GLU
3	D	76	THR
3	D	85	ARG
3	D	114	LEU
3	D	140	VAL
3	D	142	VAL
3	D	146	VAL
3	D	149	LEU
3	D	164	MET
3	D	166	LEU
3	D	183	LYS
3	D	189	LEU
3	D	193	ASN
3	D	202	MET
3	D	203	PHE

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Mol	Chain	Res	Type
3	D	205	ASN
3	D	208	THR
3	D	209	THR
3	D	210	THR
3	D	223	LEU
3	D	251	ILE
3	D	285	GLU
3	D	311	ASP
3	D	314	GLU
3	D	1028	ARG
3	D	1029	LEU
3	D	1047	LEU
3	D	1068	GLU
3	D	1076	THR
3	D	1085	ARG
3	D	1114	LEU
3	D	1140	VAL
3	D	1142	VAL
3	D	1146	VAL
3	D	1149	LEU
3	D	1166	LEU
3	D	1183	LYS
3	D	1189	LEU
3	D	1193	ASN
3	D	1199	ILE
3	D	1202	MET
3	D	1205	ASN
3	D	1208	THR
3	D	1209	THR
3	D	1210	THR
3	D	1223	LEU
3	D	1251	ILE
3	D	1285	GLU
3	D	1311	ASP
3	D	1314	GLU
3	D	1332	ASN
3	D	2028	ARG
3	D	2029	LEU
3	D	2047	LEU
3	D	2068	GLU
3	D	2076	THR
3	D	2085	ARG

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Mol	Chain	Res	Type
3	D	2114	LEU
3	D	2140	VAL
3	D	2142	VAL
3	D	2146	VAL
3	D	2149	LEU
3	D	2166	LEU
3	D	2183	LYS
3	D	2189	LEU
3	D	2193	ASN
3	D	2199	ILE
3	D	2202	MET
3	D	2205	ASN
3	D	2208	THR
3	D	2209	THR
3	D	2210	THR
3	D	2223	LEU
3	D	2251	ILE
3	D	2285	GLU
3	D	2311	ASP
3	D	2314	GLU
3	D	2332	ASN
3	D	3028	ARG
3	D	3029	LEU
3	D	3047	LEU
3	D	3068	GLU
3	D	3076	THR
3	D	3085	ARG
3	D	3114	LEU
3	D	3140	VAL
3	D	3142	VAL
3	D	3146	VAL
3	D	3149	LEU
3	D	3166	LEU
3	D	3183	LYS
3	D	3189	LEU
3	D	3193	ASN
3	D	3199	ILE
3	D	3202	MET
3	D	3205	ASN
3	D	3208	THR
3	D	3209	THR
3	D	3210	THR

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Mol	Chain	Res	Type
3	D	3223	LEU
3	D	3251	ILE
3	D	3285	GLU
3	D	3311	ASP
3	D	3314	GLU
3	D	3329	SER
3	D	4028	ARG
3	D	4029	LEU
3	D	4047	LEU
3	D	4068	GLU
3	D	4076	THR
3	D	4085	ARG
3	D	4114	LEU
3	D	4140	VAL
3	D	4142	VAL
3	D	4146	VAL
3	D	4149	LEU
3	D	4164	MET
3	D	4166	LEU
3	D	4183	LYS
3	D	4189	LEU
3	D	4193	ASN
3	D	4205	ASN
3	D	4208	THR
3	D	4209	THR
3	D	4210	THR
3	D	4223	LEU
3	D	4251	ILE
3	D	4285	GLU
3	D	4311	ASP
3	D	4314	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	97	HIS
3	A	181	ASN
3	A	193	ASN
3	A	194	GLN
3	A	205	ASN
3	A	300	GLN
3	A	304	ASN

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Mol	Chain	Res	Type
3	A	1097	HIS
3	A	1173	GLN
3	A	1181	ASN
3	A	1193	ASN
3	A	1194	GLN
3	A	1205	ASN
3	A	1300	GLN
3	A	1304	ASN
3	A	2097	HIS
3	A	2173	GLN
3	A	2181	ASN
3	A	2193	ASN
3	A	2194	GLN
3	A	2300	GLN
3	A	2304	ASN
3	A	2332	ASN
3	A	3097	HIS
3	A	3173	GLN
3	A	3181	ASN
3	A	3193	ASN
3	A	3194	GLN
3	A	3205	ASN
3	A	3300	GLN
3	A	3304	ASN
3	A	4097	HIS
3	A	4173	GLN
3	A	4181	ASN
3	A	4193	ASN
3	A	4194	GLN
3	A	4205	ASN
3	A	4300	GLN
3	A	4304	ASN
3	D	97	HIS
3	D	181	ASN
3	D	193	ASN
3	D	194	GLN
3	D	205	ASN
3	D	300	GLN
3	D	304	ASN
3	D	332	ASN
3	D	1097	HIS
3	D	1173	GLN

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Mol	Chain	Res	Type
3	D	1181	ASN
3	D	1193	ASN
3	D	1194	GLN
3	D	1205	ASN
3	D	1300	GLN
3	D	1304	ASN
3	D	1332	ASN
3	D	2097	HIS
3	D	2173	GLN
3	D	2181	ASN
3	D	2193	ASN
3	D	2194	GLN
3	D	2205	ASN
3	D	2300	GLN
3	D	2304	ASN
3	D	3097	HIS
3	D	3173	GLN
3	D	3181	ASN
3	D	3193	ASN
3	D	3194	GLN
3	D	3205	ASN
3	D	3300	GLN
3	D	3304	ASN
3	D	4097	HIS
3	D	4173	GLN
3	D	4181	ASN
3	D	4184	GLN
3	D	4193	ASN
3	D	4194	GLN
3	D	4205	ASN
3	D	4300	GLN
3	D	4304	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 10 are monoatomic - leaving 20 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
6	ADP	A	3502	4	24,29,29	0.91	1 (4%)	29,45,45	1.28	3 (10%)
6	ADP	D	3502	4	24,29,29	0.98	1 (4%)	29,45,45	1.25	4 (13%)
5	ALF	D	1501	-	0,4,4	-	-	-	-	-
5	ALF	A	501	-	0,4,4	-	-	-	-	-
6	ADP	D	1502	4	24,29,29	0.84	1 (4%)	29,45,45	1.38	5 (17%)
5	ALF	D	2501	-	0,4,4	-	-	-	-	-
6	ADP	A	4502	4	24,29,29	1.10	3 (12%)	29,45,45	1.28	5 (17%)
5	ALF	A	2501	-	0,4,4	-	-	-	-	-
6	ADP	D	2502	4	24,29,29	0.98	1 (4%)	29,45,45	1.39	3 (10%)
6	ADP	A	502	4	24,29,29	1.05	2 (8%)	29,45,45	1.48	3 (10%)
6	ADP	D	502	4	24,29,29	0.91	1 (4%)	29,45,45	1.36	5 (17%)
6	ADP	D	4502	4	24,29,29	1.04	1 (4%)	29,45,45	1.43	5 (17%)
6	ADP	A	2502	4	24,29,29	0.94	1 (4%)	29,45,45	1.39	4 (13%)
5	ALF	D	4501	-	0,4,4	-	-	-	-	-
6	ADP	A	1502	4	24,29,29	0.96	1 (4%)	29,45,45	1.57	7 (24%)
5	ALF	D	3501	-	0,4,4	-	-	-	-	-
5	ALF	A	1501	-	0,4,4	-	-	-	-	-
5	ALF	A	4501	-	0,4,4	-	-	-	-	-
5	ALF	D	501	-	0,4,4	-	-	-	-	-
5	ALF	A	3501	-	0,4,4	-	-	-	-	-

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
6	ADP	D	2502	4	-	3/12/32/32	0/3/3/3
6	ADP	A	3502	4	-	3/12/32/32	0/3/3/3
6	ADP	D	3502	4	-	2/12/32/32	0/3/3/3
6	ADP	A	1502	4	-	3/12/32/32	0/3/3/3
6	ADP	A	502	4	-	5/12/32/32	0/3/3/3
6	ADP	D	502	4	-	3/12/32/32	0/3/3/3
6	ADP	A	4502	4	-	5/12/32/32	0/3/3/3
6	ADP	D	4502	4	-	4/12/32/32	0/3/3/3
6	ADP	A	2502	4	-	4/12/32/32	0/3/3/3
6	ADP	D	1502	4	-	3/12/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2502	ADP	C5-C4	2.93	1.48	1.40
6	D	4502	ADP	C5-C4	2.93	1.48	1.40
6	A	502	ADP	C5-C4	2.75	1.48	1.40
6	A	4502	ADP	C5-C4	2.67	1.48	1.40
6	D	3502	ADP	C5-C4	2.55	1.47	1.40
6	A	2502	ADP	C5-C4	2.49	1.47	1.40
6	D	502	ADP	C5-C4	2.45	1.47	1.40
6	A	3502	ADP	C5-C4	2.38	1.47	1.40
6	A	1502	ADP	C5-C4	2.35	1.47	1.40
6	A	4502	ADP	O4'-C1'	2.28	1.44	1.41
6	A	502	ADP	C2-N3	2.23	1.35	1.32
6	D	1502	ADP	C5-C4	2.11	1.46	1.40
6	A	4502	ADP	C2-N3	2.04	1.35	1.32

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1502	ADP	N3-C2-N1	-4.06	122.33	128.68
6	A	502	ADP	PA-O3A-PB	-3.78	119.84	132.83
6	D	2502	ADP	N3-C2-N1	-3.77	122.78	128.68
6	A	3502	ADP	N3-C2-N1	-3.70	122.89	128.68
6	D	4502	ADP	N3-C2-N1	-3.48	123.24	128.68
6	A	4502	ADP	N3-C2-N1	-3.47	123.26	128.68
6	D	1502	ADP	N3-C2-N1	-3.27	123.57	128.68
6	A	502	ADP	N3-C2-N1	-3.22	123.65	128.68
6	A	2502	ADP	PA-O3A-PB	-3.08	122.26	132.83
6	D	2502	ADP	C2-N1-C6	3.07	124.01	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3502	ADP	N3-C2-N1	-2.96	124.05	128.68
6	A	2502	ADP	N3-C2-N1	-2.90	124.15	128.68
6	A	1502	ADP	N6-C6-N1	2.72	124.22	118.57
6	D	4502	ADP	C2-N1-C6	2.71	123.39	118.75
6	A	1502	ADP	PA-O3A-PB	-2.67	123.67	132.83
6	A	2502	ADP	C3'-C2'-C1'	2.64	104.96	100.98
6	A	502	ADP	C3'-C2'-C1'	2.53	104.79	100.98
6	D	4502	ADP	C3'-C2'-C1'	2.51	104.75	100.98
6	A	3502	ADP	C2-N1-C6	2.48	123.00	118.75
6	D	502	ADP	N3-C2-N1	-2.46	124.83	128.68
6	A	1502	ADP	O2B-PB-O3A	-2.41	96.57	104.64
6	D	1502	ADP	N6-C6-N1	2.39	123.54	118.57
6	D	4502	ADP	O3B-PB-O2B	2.38	116.73	107.64
6	D	502	ADP	C3'-C2'-C1'	2.38	104.56	100.98
6	D	502	ADP	C4-C5-N7	-2.38	106.92	109.40
6	D	1502	ADP	C3'-C2'-C1'	2.25	104.37	100.98
6	D	502	ADP	O2B-PB-O3A	-2.22	97.19	104.64
6	D	502	ADP	PA-O3A-PB	-2.22	125.22	132.83
6	A	1502	ADP	C3'-C2'-C1'	2.22	104.31	100.98
6	A	4502	ADP	N6-C6-N1	2.22	123.17	118.57
6	A	4502	ADP	C2-N1-C6	2.20	122.52	118.75
6	A	2502	ADP	N6-C6-N1	2.16	123.07	118.57
6	A	4502	ADP	O2B-PB-O1B	2.15	119.11	110.68
6	D	4502	ADP	PA-O3A-PB	-2.15	125.44	132.83
6	D	1502	ADP	O2B-PB-O1B	2.15	119.09	110.68
6	A	1502	ADP	C2-N1-C6	2.14	122.42	118.75
6	D	2502	ADP	PA-O3A-PB	-2.13	125.52	132.83
6	D	3502	ADP	O2B-PB-O3A	-2.13	97.51	104.64
6	D	3502	ADP	PA-O3A-PB	-2.11	125.59	132.83
6	A	1502	ADP	O3B-PB-O2B	2.10	115.68	107.64
6	A	4502	ADP	C4-C5-N7	-2.10	107.21	109.40
6	A	3502	ADP	O2B-PB-O3A	-2.03	97.82	104.64
6	D	3502	ADP	N6-C6-N1	2.01	122.75	118.57
6	D	1502	ADP	O4'-C1'-C2'	-2.01	103.99	106.93

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	502	ADP	O4'-C4'-C5'-O5'
6	A	502	ADP	PA-O3A-PB-O1B
6	A	1502	ADP	PA-O3A-PB-O1B

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Mol	Chain	Res	Type	Atoms
6	A	2502	ADP	PA-O3A-PB-O1B
6	A	3502	ADP	PA-O3A-PB-O1B
6	D	502	ADP	PA-O3A-PB-O1B
6	D	2502	ADP	PA-O3A-PB-O1B
6	D	3502	ADP	PA-O3A-PB-O3B
6	A	4502	ADP	O4'-C4'-C5'-O5'
6	D	4502	ADP	O4'-C4'-C5'-O5'
6	A	4502	ADP	PA-O3A-PB-O1B
6	D	3502	ADP	PA-O3A-PB-O1B
6	D	4502	ADP	PA-O3A-PB-O1B
6	A	502	ADP	C3'-C4'-C5'-O5'
6	A	4502	ADP	C3'-C4'-C5'-O5'
6	A	502	ADP	PA-O3A-PB-O2B
6	A	502	ADP	PA-O3A-PB-O3B
6	A	1502	ADP	PA-O3A-PB-O2B
6	A	1502	ADP	PA-O3A-PB-O3B
6	A	2502	ADP	PA-O3A-PB-O2B
6	A	2502	ADP	PA-O3A-PB-O3B
6	A	3502	ADP	PA-O3A-PB-O2B
6	A	3502	ADP	PA-O3A-PB-O3B
6	A	4502	ADP	PA-O3A-PB-O2B
6	A	4502	ADP	PA-O3A-PB-O3B
6	D	502	ADP	PA-O3A-PB-O2B
6	D	502	ADP	PA-O3A-PB-O3B
6	D	1502	ADP	PA-O3A-PB-O2B
6	D	1502	ADP	PA-O3A-PB-O3B
6	D	2502	ADP	PA-O3A-PB-O2B
6	D	2502	ADP	PA-O3A-PB-O3B
6	D	4502	ADP	PA-O3A-PB-O3B
6	D	4502	ADP	C3'-C4'-C5'-O5'
6	A	2502	ADP	O4'-C4'-C5'-O5'
6	D	1502	ADP	PA-O3A-PB-O1B

There are no ring outliers.

9 monomers are involved in 12 short contacts:

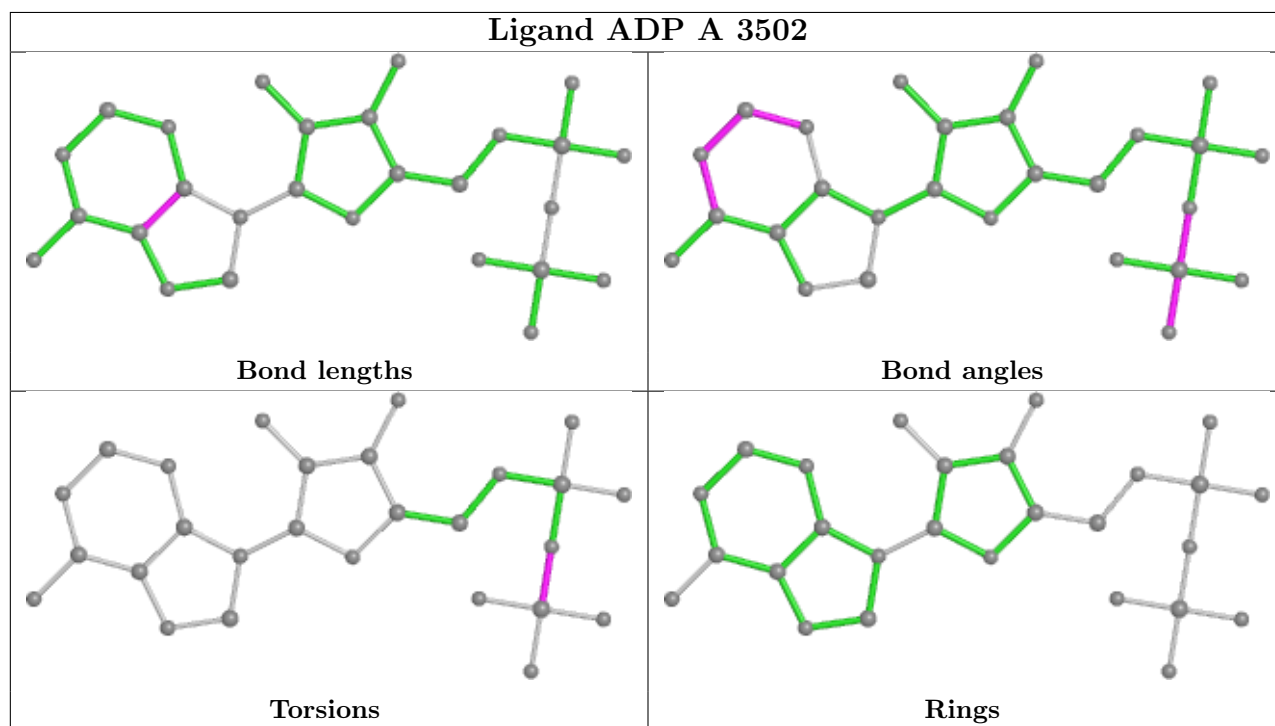
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	3502	ADP	1	0
5	D	1501	ALF	1	0
6	A	4502	ADP	1	0
6	A	502	ADP	1	0
6	D	502	ADP	2	0

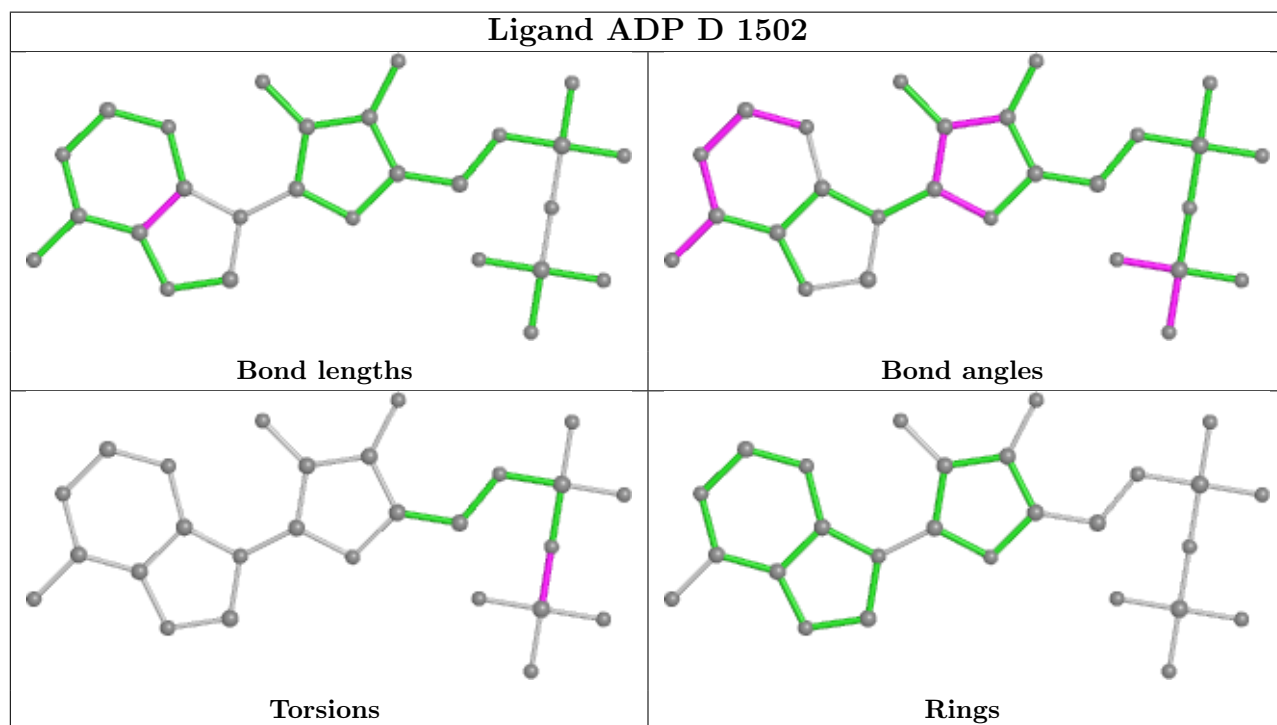
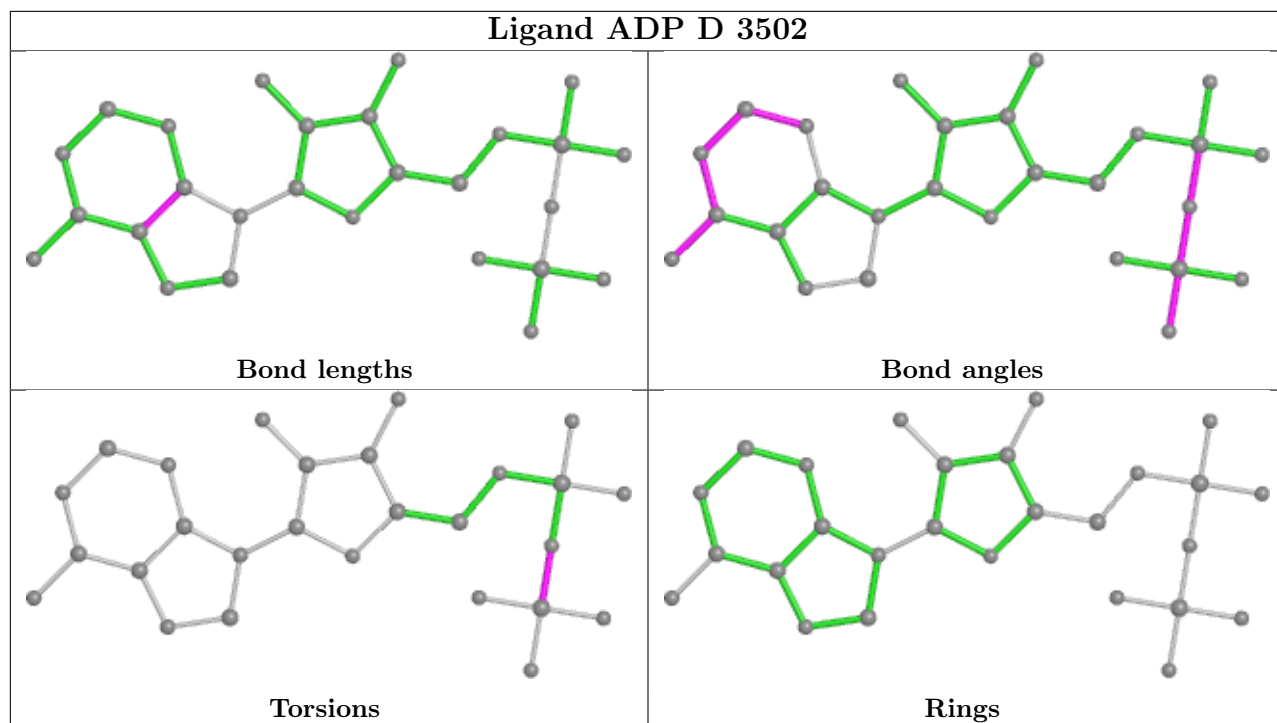
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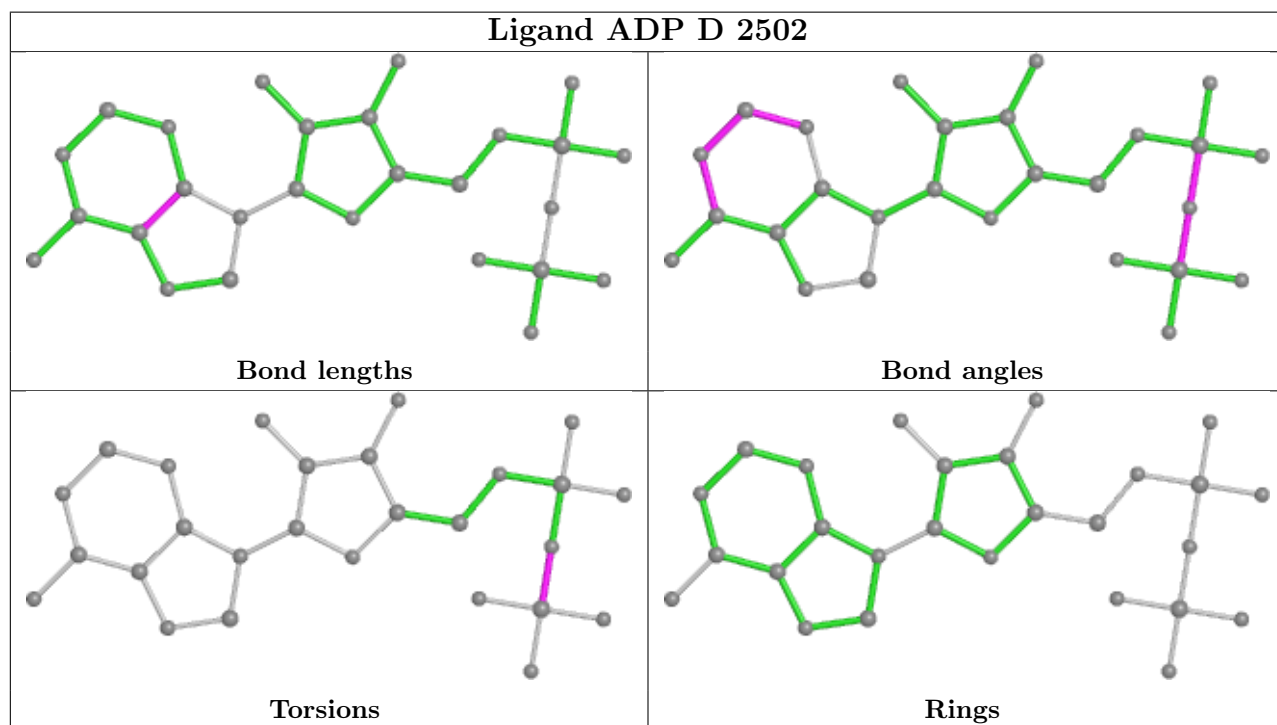
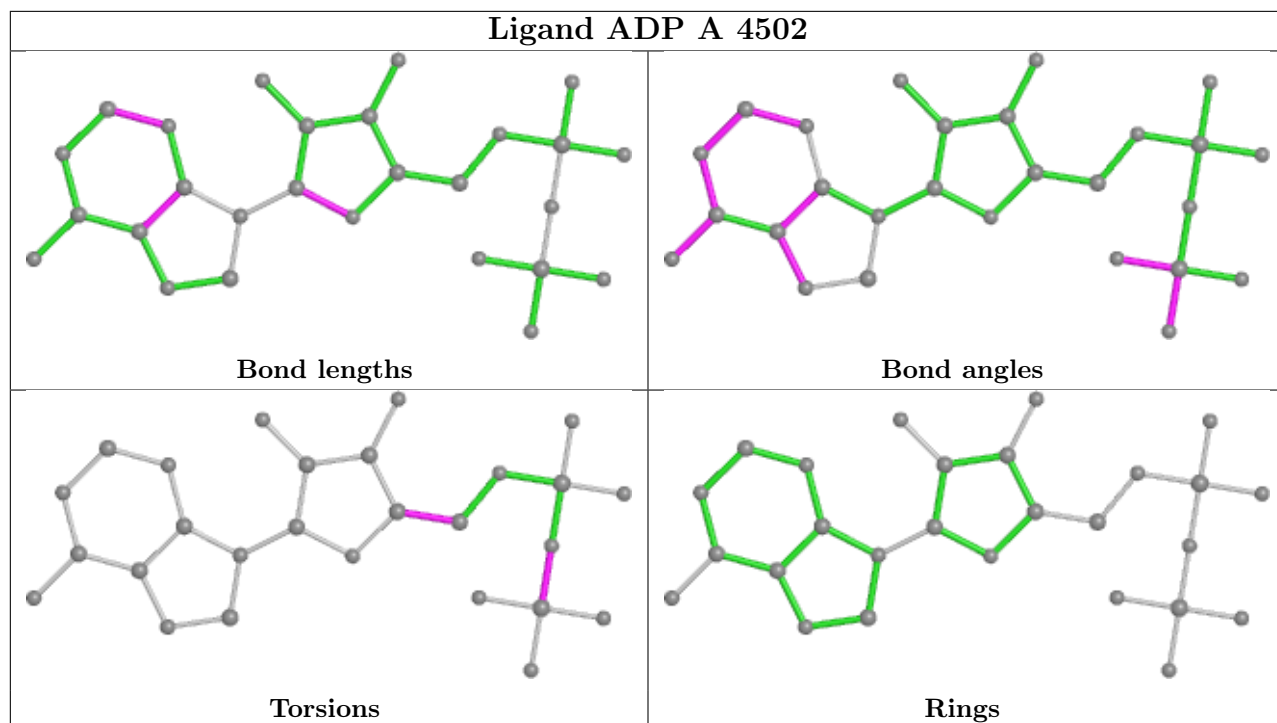
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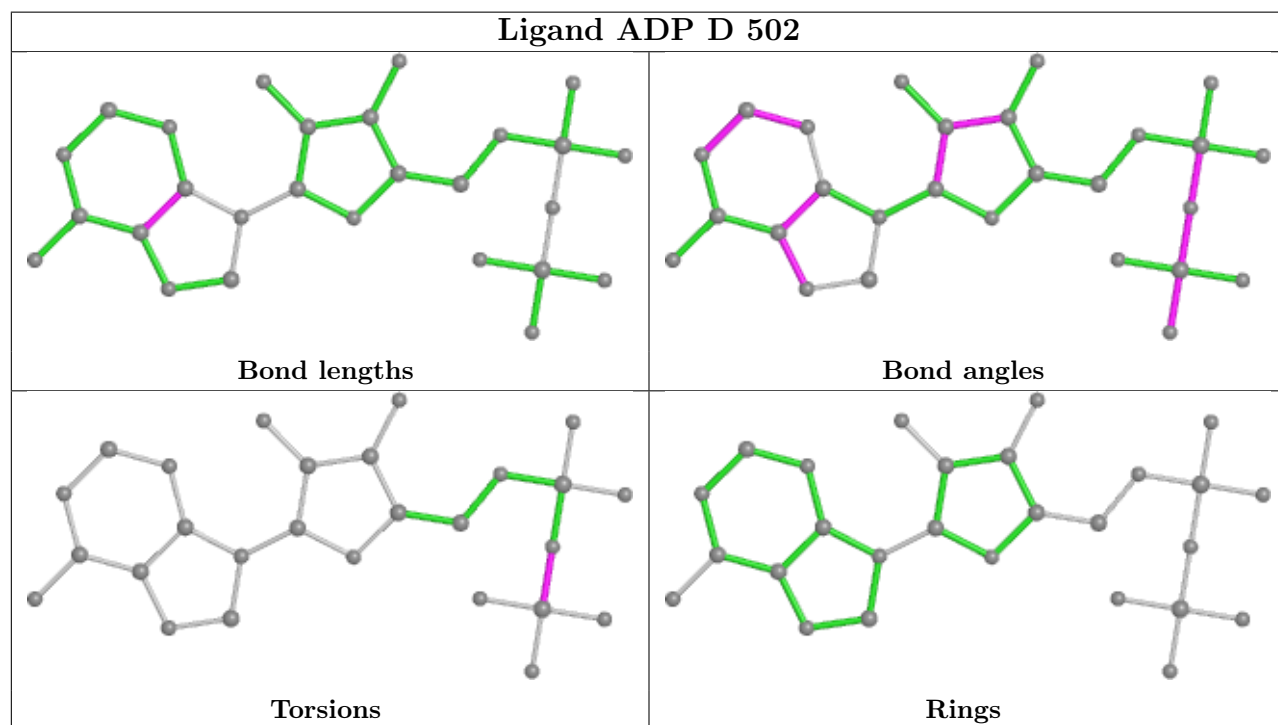
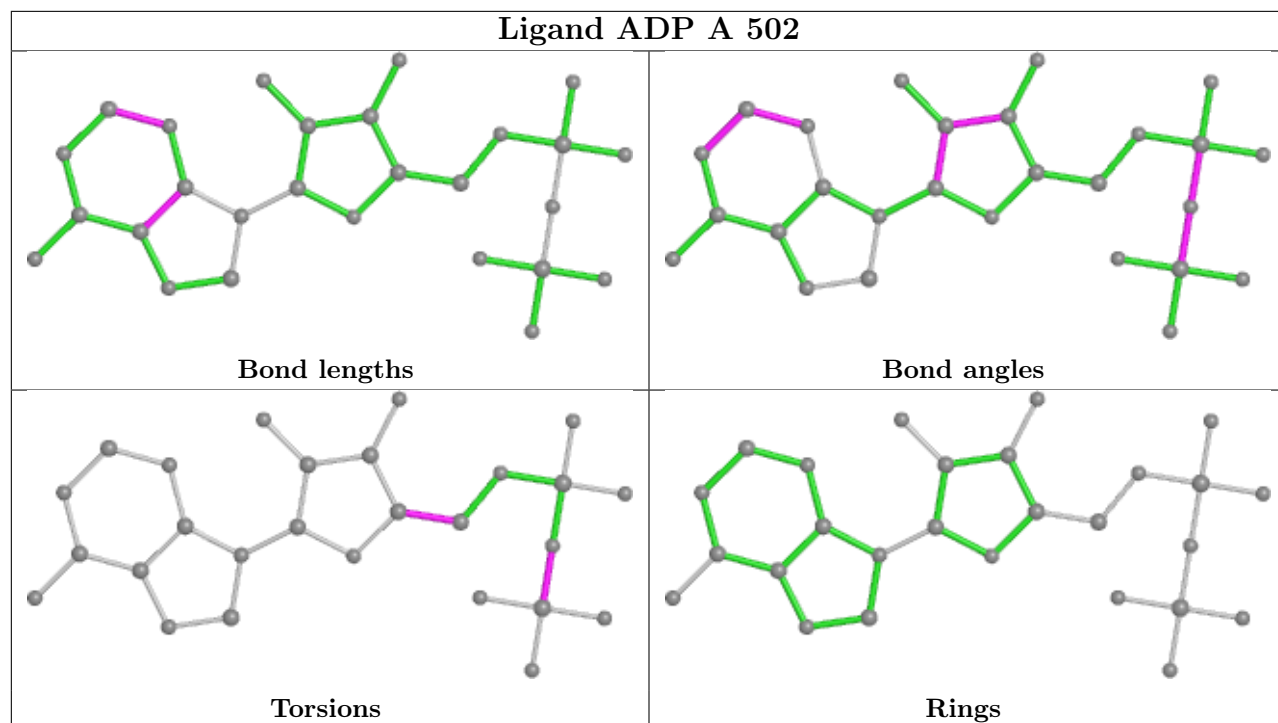
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	4502	ADP	1	0
6	A	2502	ADP	2	0
6	A	1502	ADP	2	0
5	D	3501	ALF	1	0

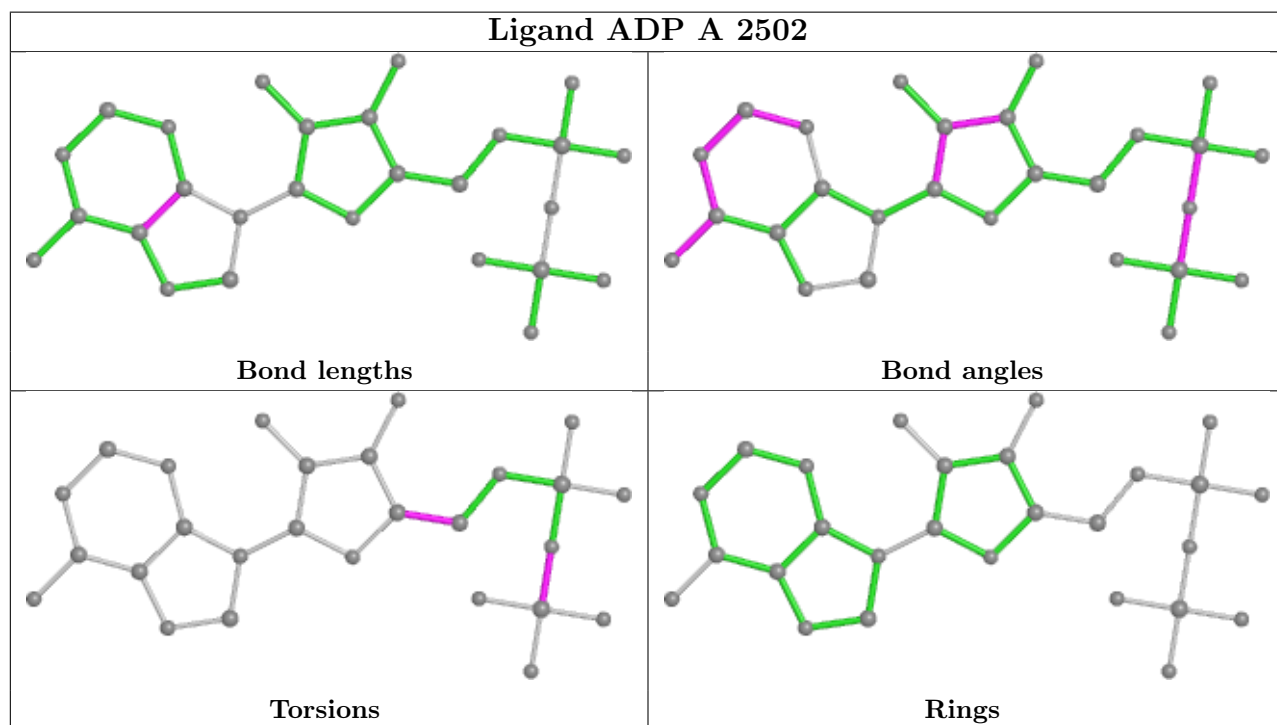
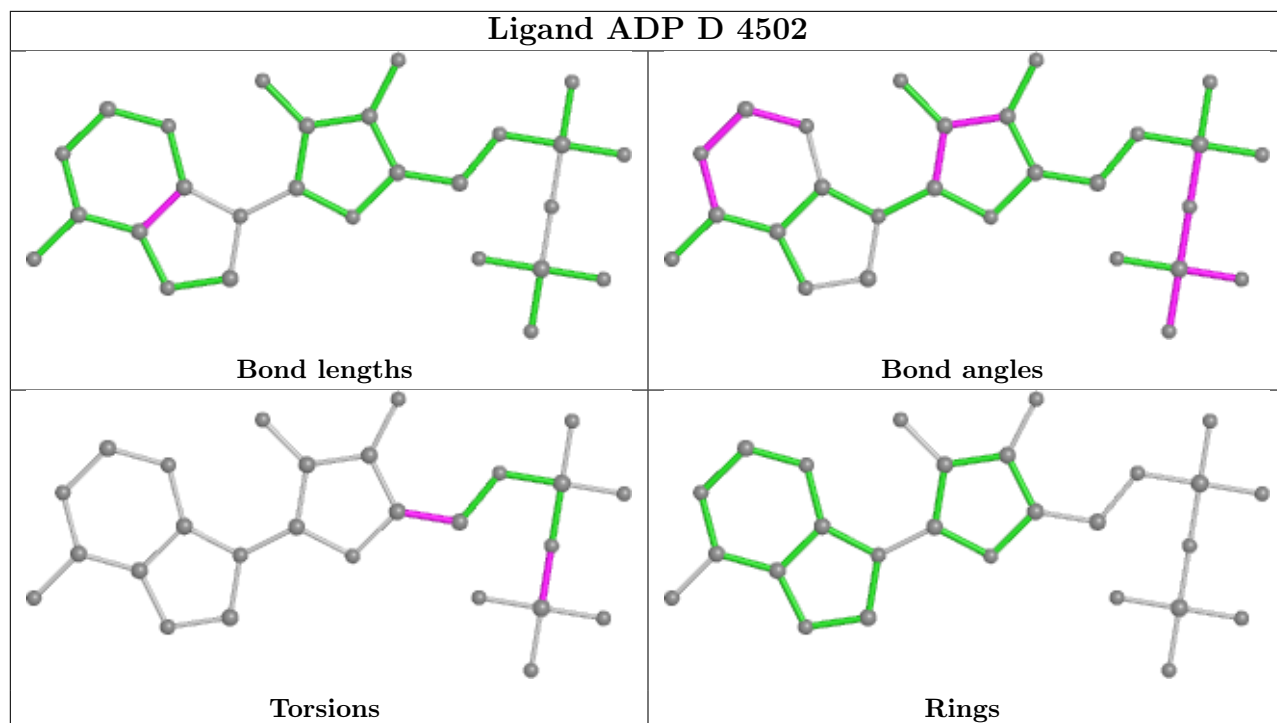
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

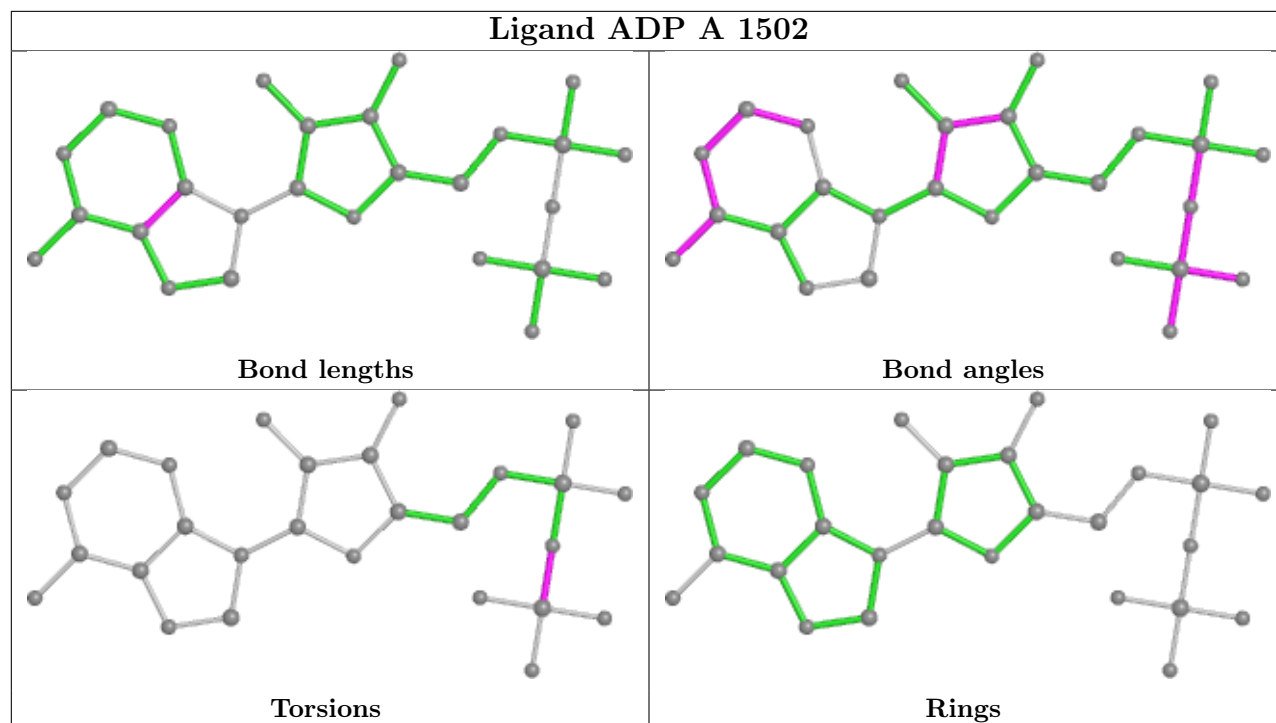












5.7 Other polymers [i](#)

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](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

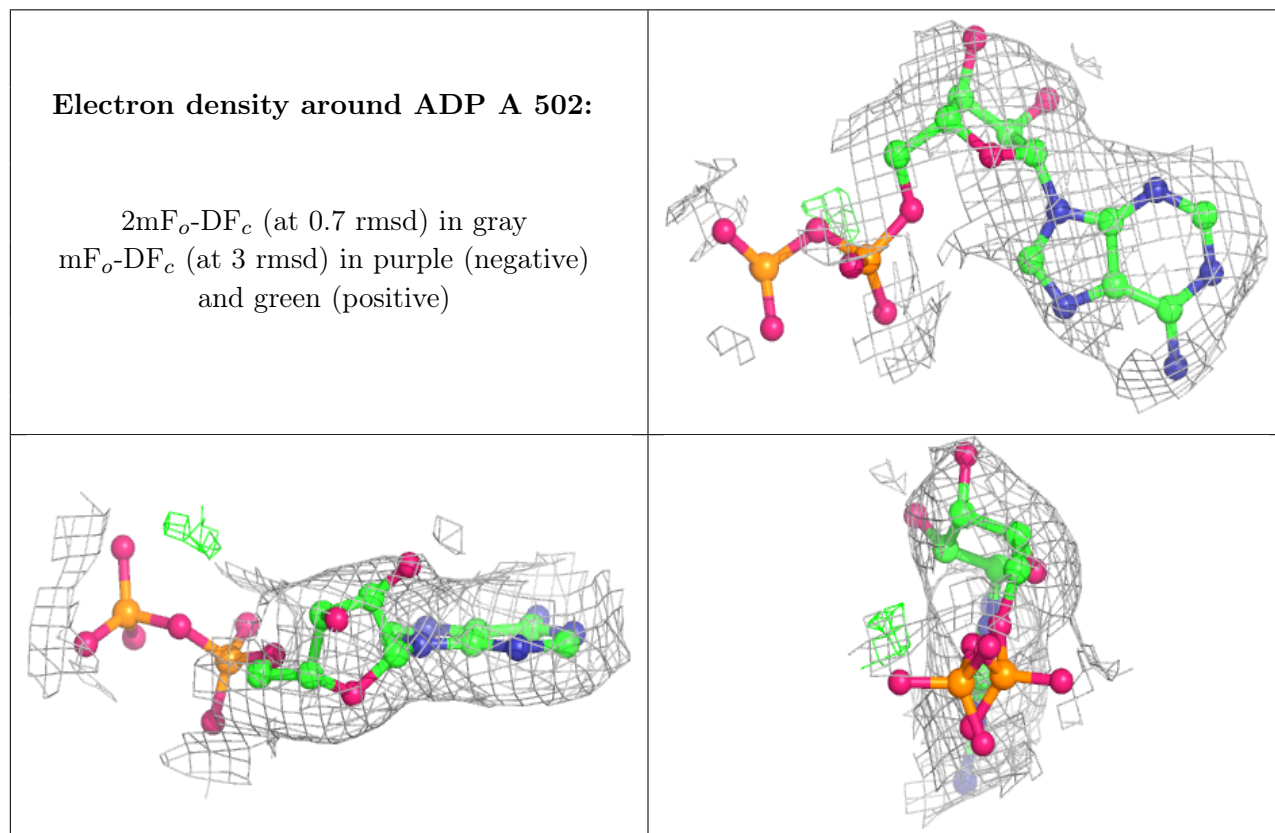
6.3 Carbohydrates [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands [i](#)

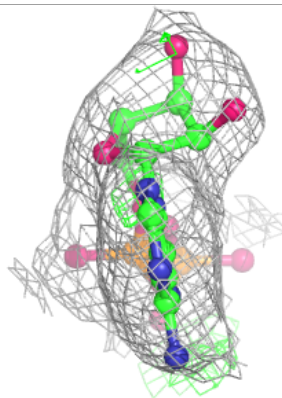
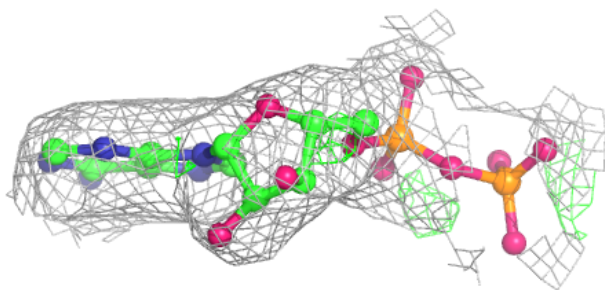
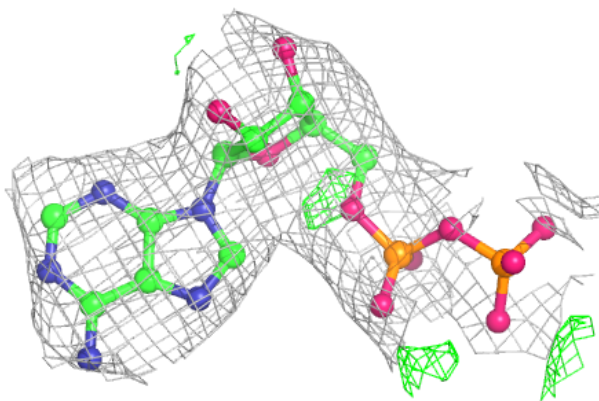
Unable to reproduce the depositors R factor - this section is therefore empty.

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.

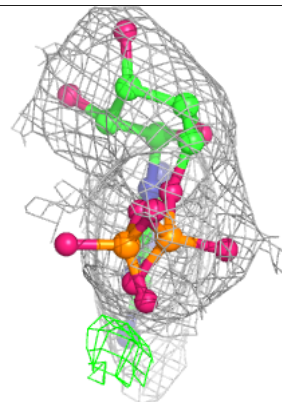
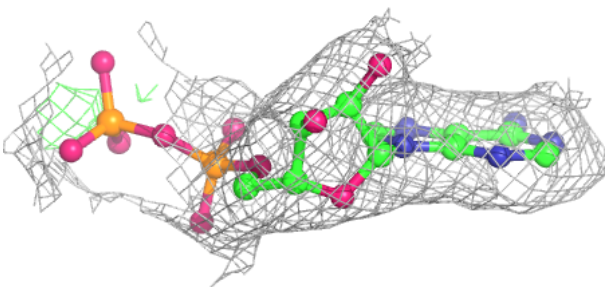
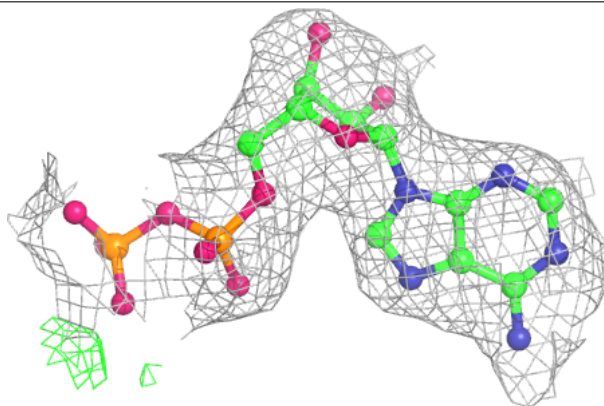


Electron density around ADP A 1502:

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

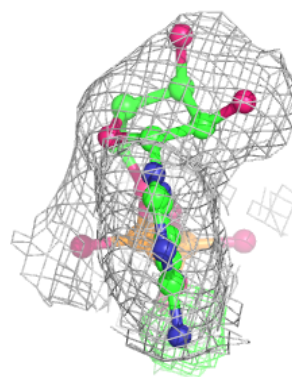
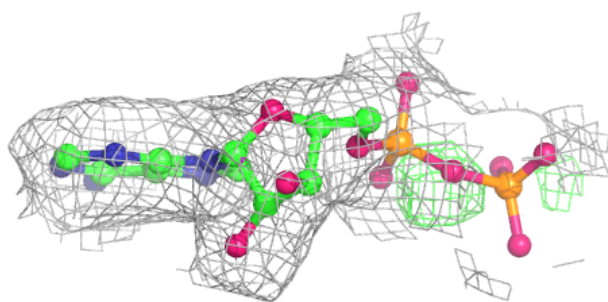
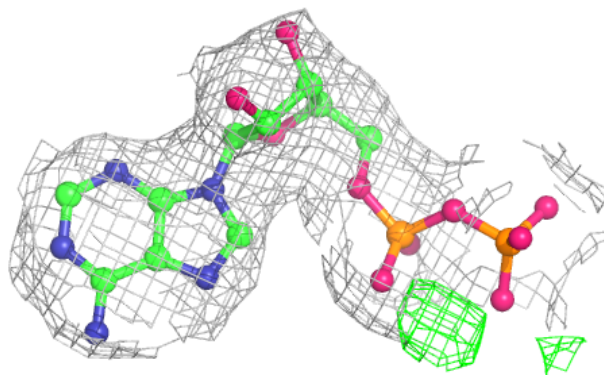
**Electron density around ADP A 2502:**

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



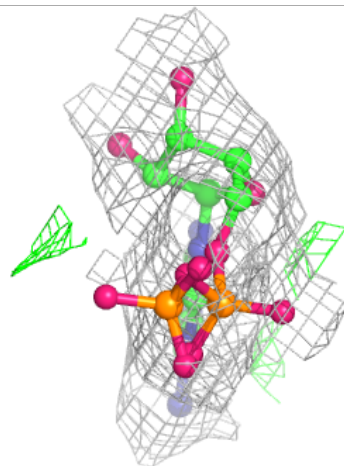
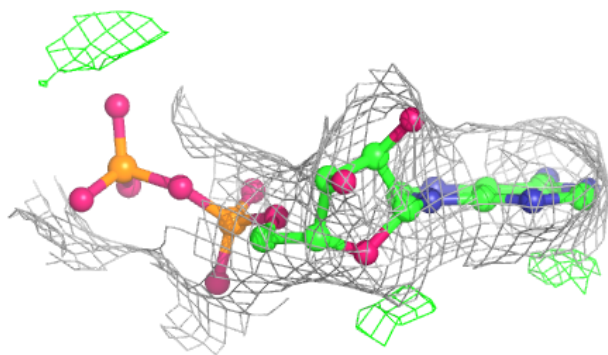
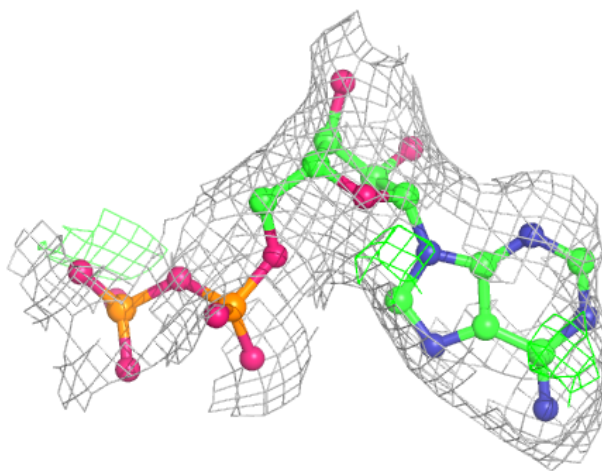
Electron density around ADP A 3502:

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



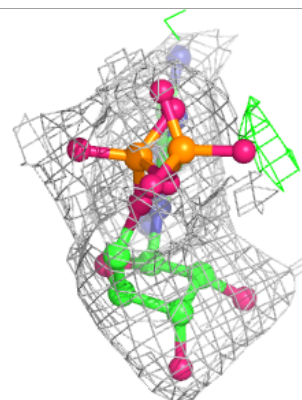
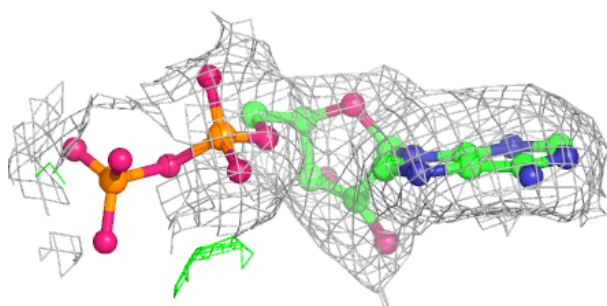
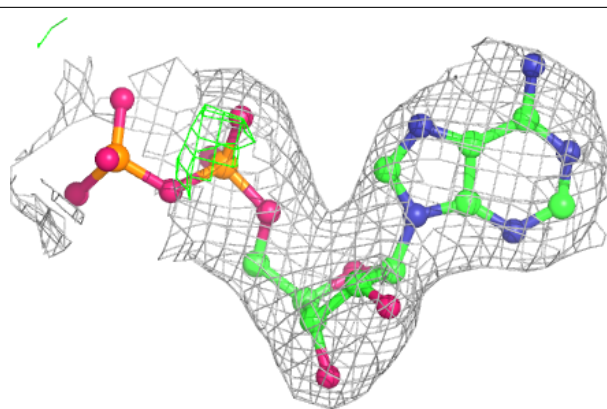
Electron density around ADP A 4502:

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

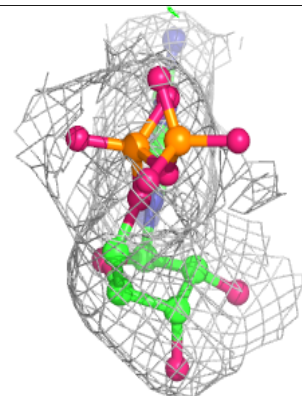
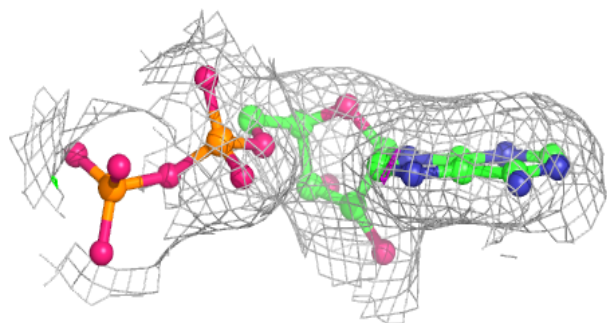
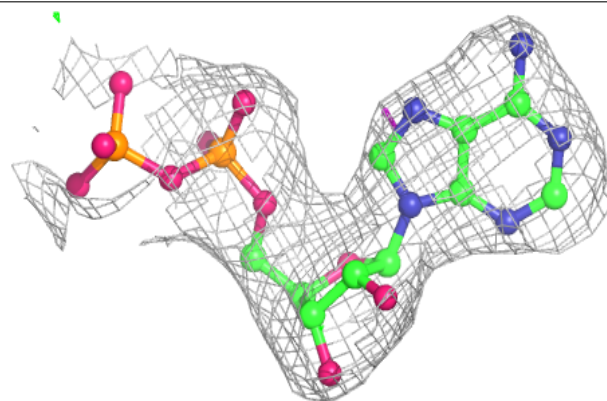


Electron density around ADP D 502:

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

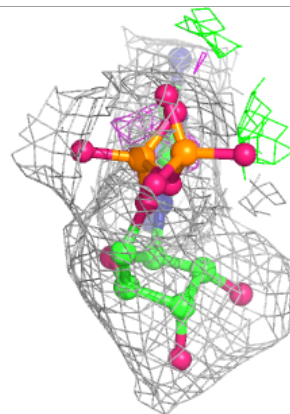
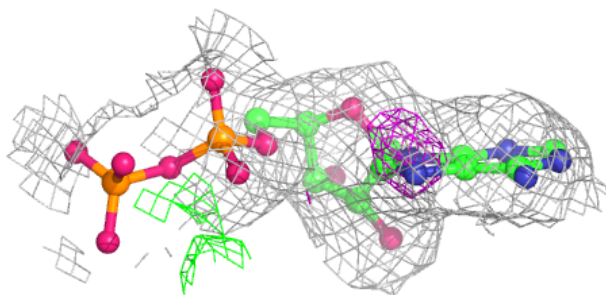
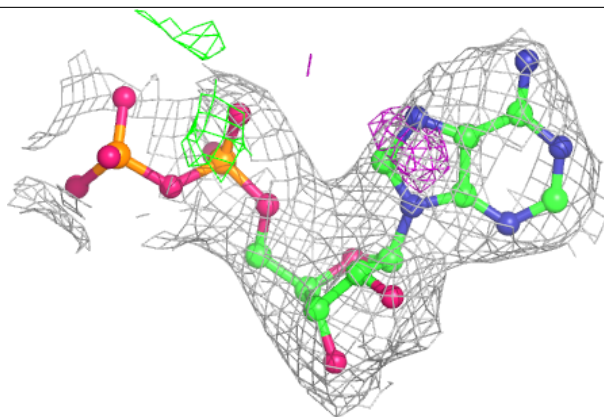
**Electron density around ADP D 1502:**

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

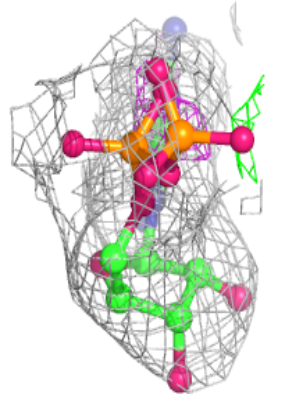
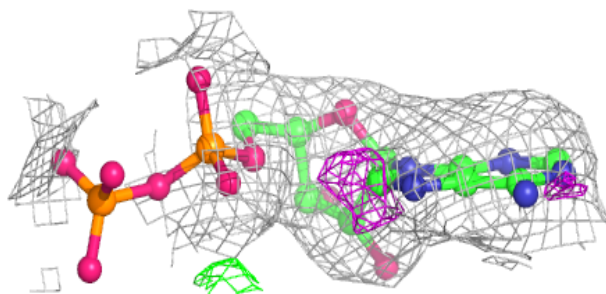
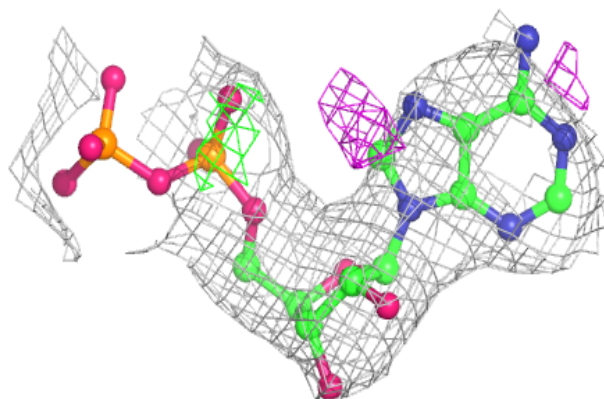


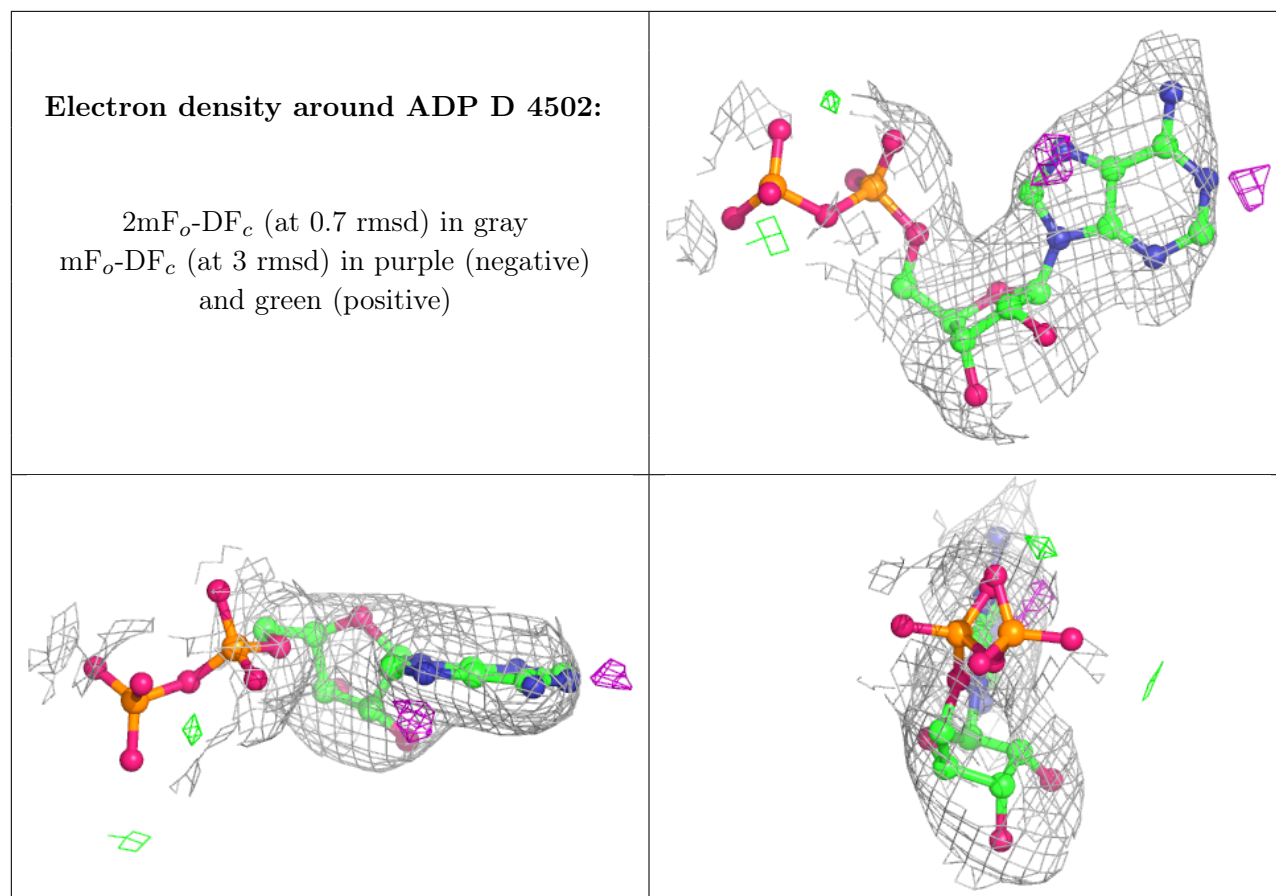
Electron density around ADP D 2502:

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

**Electron density around ADP D 3502:**

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





6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.