Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 09:14 PM EDT

PDB ID	:	4NST / pdb_00004nst
Title	:	Crystal structure of human Cdk12/Cyclin K in complex with ADP-aluminum fluoride
Authors	:	Boesken, C.A.; Farnung, L.; Anand, K.; Geyer, M.
Deposited on	:	2013-11-29
Resolution	:	2.20 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 (i) 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 (i)) were used in the production of this report:

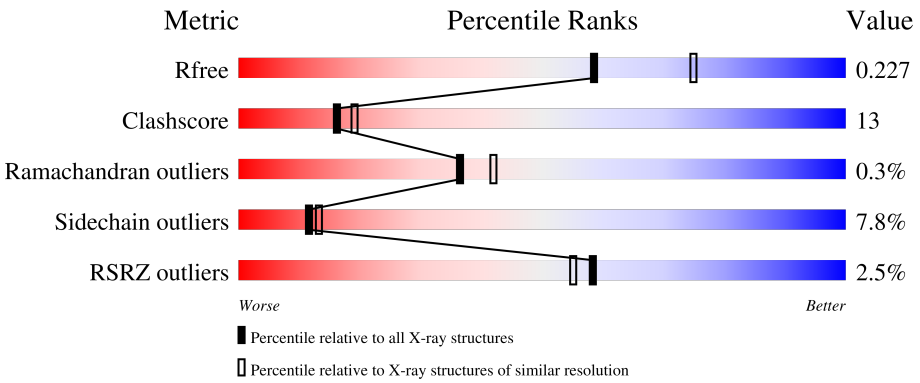
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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 <=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	351	3% 58% 28% 6% 8%
1	C	351	3% 59% 28% • 9%
2	B	268	% 73% 15% • 8%
2	D	268	% 71% 16% • 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	EDO	C	1105	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9618 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 Cyclin-dependent kinase 12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	323	2588	1660	438	472	1	17	0	0	0
1	C	318	2541	1631	426	466	1	17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	713	GLY	-	expression tag	UNP Q9NYV4
C	713	GLY	-	expression tag	UNP Q9NYV4

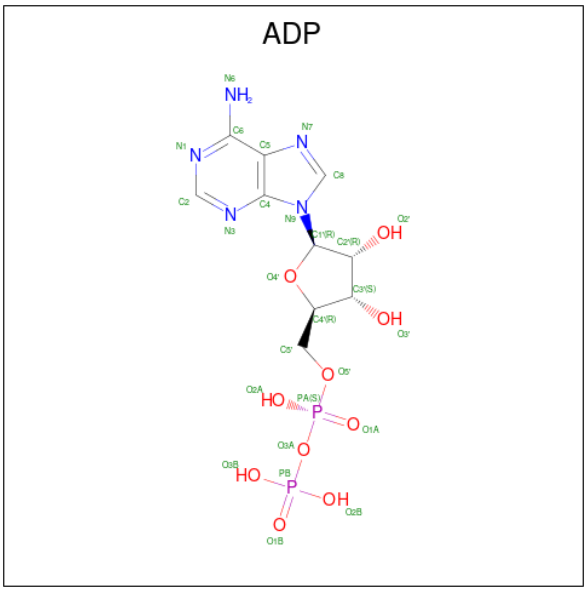
- Molecule 2 is a protein called Cyclin-K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	246	2023	1313	337	361	12	0	0	0
2	D	241	1988	1293	330	353	12	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

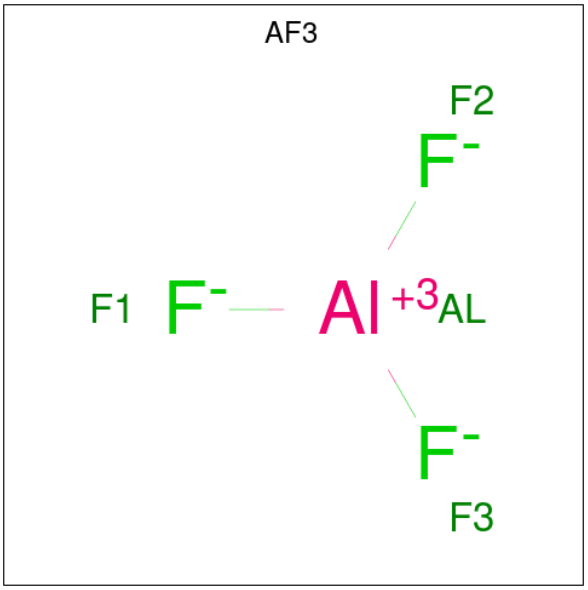
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	GLY	-	expression tag	UNP O75909
D	0	GLY	-	expression tag	UNP O75909

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).

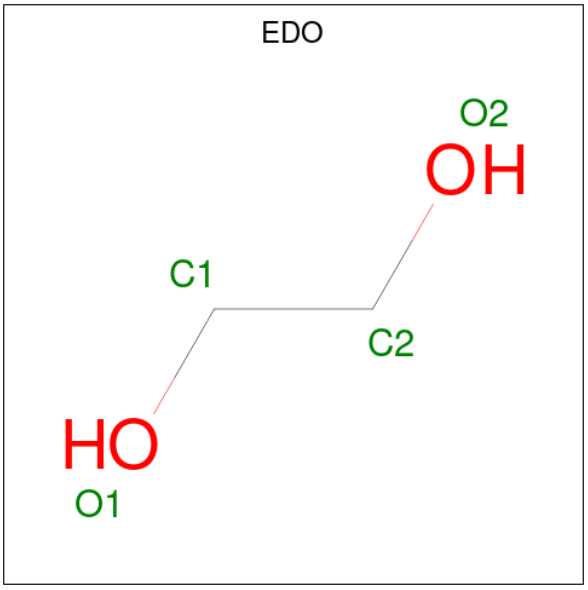


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Al	F		
4	A	1	4	1	3	0	0
			Total	Al	F		
4	C	1	4	1	3	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Mg 3 3	0	0
5	C	2	Total Mg 2 2	0	0
5	D	2	Total Mg 2 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	107	Total O 107 107	0	0
7	B	92	Total O 92 92	0	0

Continued on next page...

Continued from previous page...

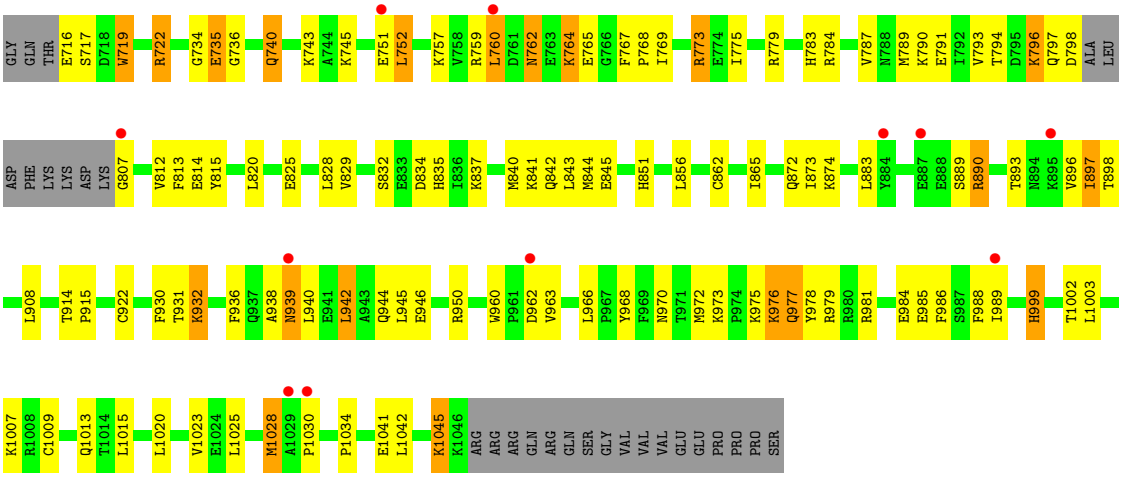
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	C	96	96	96	0	0
			Total	O		
7	D	98	98	98	0	0

3 Residue-property plots (i)

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

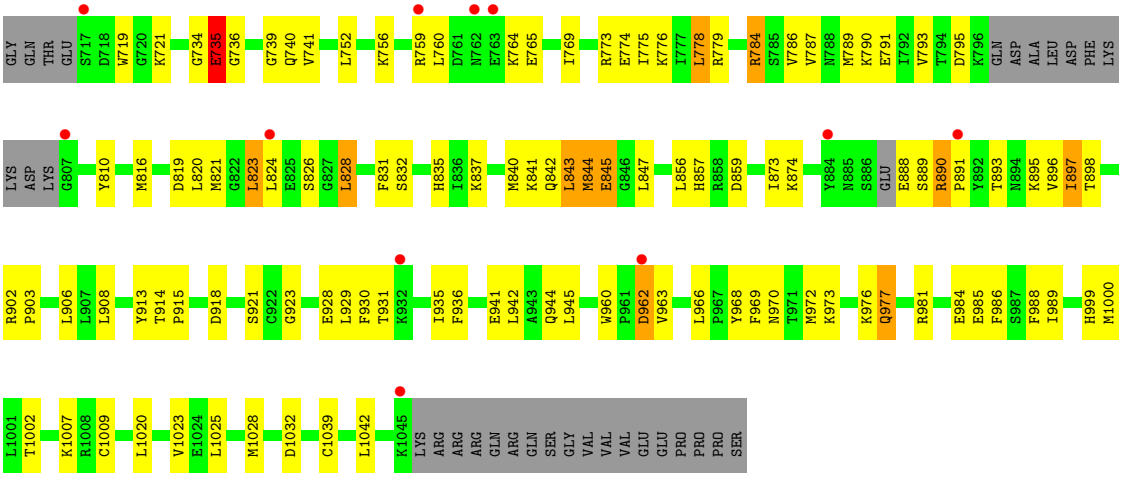
• Molecule 1: Cyclin-dependent kinase 12

Chain A:



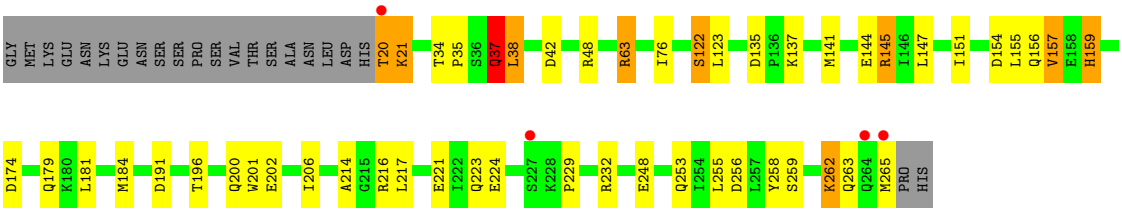
• Molecule 1: Cyclin-dependent kinase 12

Chain C:



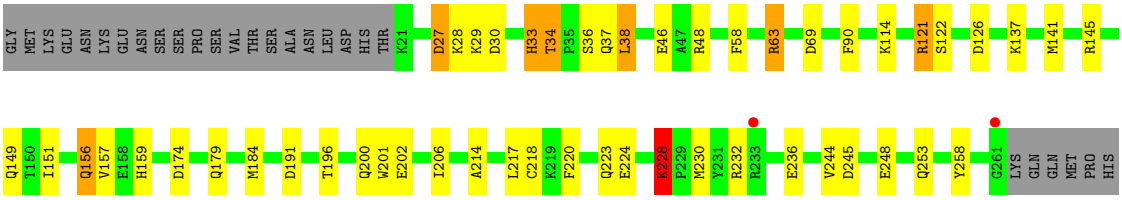
• Molecule 2: Cyclin-K

Chain B:



- Molecule 2: Cyclin-K

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.72Å 78.85Å 91.49Å 104.04° 85.76° 101.46°	Depositor
Resolution (Å)	48.71 – 2.20 48.71 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.71-2.20) 97.3 (48.71-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.91 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.195 , 0.240 0.192 , 0.227	Depositor DCC
R_{free} test set	3264 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9618	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: AF3, ADP, EDO, TPO, 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	A	1.46	23/2636 (0.9%)	1.15	13/3562 (0.4%)
1	C	1.33	15/2588 (0.6%)	1.14	13/3502 (0.4%)
2	B	1.22	8/2078 (0.4%)	1.09	8/2818 (0.3%)
2	D	1.15	5/2043 (0.2%)	1.01	6/2770 (0.2%)
All	All	1.31	51/9345 (0.5%)	1.10	40/12652 (0.3%)

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	857	HIS	CG-ND1	-7.77	1.29	1.38
1	C	859	ASP	C-O	-7.70	1.17	1.24
1	A	999	HIS	CG-ND1	-7.44	1.30	1.38
1	A	783	HIS	CG-ND1	-6.94	1.30	1.38
1	A	865	ILE	C-O	-6.76	1.16	1.24
1	A	851	HIS	CG-ND1	-6.59	1.30	1.38
1	C	734	GLY	C-O	-6.49	1.17	1.24
1	C	856	LEU	C-O	-6.45	1.16	1.24
1	A	851	HIS	CD2-NE2	-6.44	1.30	1.37
2	B	147	LEU	C-O	-6.10	1.17	1.24
1	A	791	GLU	C-O	-6.04	1.17	1.23
1	C	845	GLU	C-O	-5.92	1.17	1.24
2	B	37	GLN	C-O	-5.91	1.17	1.24
1	A	783	HIS	CD2-NE2	-5.89	1.31	1.37
1	A	812	VAL	C-O	-5.89	1.17	1.24
1	A	856	LEU	C-O	-5.86	1.17	1.24
1	C	857	HIS	CD2-NE2	-5.80	1.31	1.37
1	A	1013	GLN	C-O	-5.73	1.17	1.24
2	D	38	LEU	C-O	-5.73	1.17	1.24
1	A	897	ILE	C-O	-5.73	1.17	1.24
2	B	35	PRO	C-O	-5.71	1.17	1.24
1	A	734	GLY	C-O	-5.69	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	790	LYS	C-O	-5.63	1.17	1.24
2	B	181	LEU	C-O	-5.61	1.17	1.24
1	C	844	MET	C-O	-5.59	1.17	1.24
2	B	151	ILE	C-O	-5.59	1.17	1.24
1	C	820	LEU	C-O	-5.56	1.17	1.24
1	A	825	GLU	C-O	-5.56	1.17	1.24
1	A	815	TYR	C-O	-5.53	1.17	1.23
1	A	896	VAL	C-O	-5.44	1.18	1.24
1	C	821	MET	C-O	-5.37	1.18	1.24
1	C	890	ARG	C-O	-5.36	1.19	1.24
1	A	1034	PRO	C-O	-5.35	1.17	1.23
2	D	151	ILE	CA-CB	5.35	1.61	1.54
1	A	1002	THR	C-O	-5.33	1.17	1.24
1	A	793	VAL	C-O	-5.32	1.17	1.23
1	C	903	PRO	CA-C	5.32	1.57	1.52
1	C	1042	LEU	C-O	-5.31	1.18	1.24
2	D	34	THR	C-O	-5.28	1.17	1.23
2	B	135	ASP	C-O	-5.24	1.18	1.24
1	A	999	HIS	CD2-NE2	-5.24	1.32	1.37
1	C	786	VAL	C-O	-5.24	1.18	1.24
1	A	743	LYS	C-O	-5.18	1.17	1.23
1	A	773	ARG	C-O	-5.08	1.18	1.24
1	A	735	GLU	N-CA	-5.08	1.40	1.46
1	A	722	ARG	C-O	-5.04	1.17	1.23
2	D	33	HIS	CG-ND1	-5.03	1.32	1.38
2	B	38	LEU	C-O	-5.03	1.18	1.24
2	B	144	GLU	C-O	-5.03	1.18	1.24
1	C	1002	THR	C-O	-5.01	1.17	1.24
2	D	58	PHE	C-O	-5.01	1.18	1.24

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	976	LYS	CB-CA-C	-8.40	93.67	110.30
1	A	975	LYS	N-CA-C	8.30	123.99	112.45
2	B	123	LEU	N-CA-C	8.16	120.26	111.36
1	C	935	ILE	N-CA-C	7.90	118.69	110.72
1	C	891	PRO	O-C-N	7.79	132.88	123.06
1	C	966	LEU	CA-C-N	7.17	128.81	119.84
1	C	966	LEU	C-N-CA	7.17	128.81	119.84
1	A	790	LYS	N-CA-C	7.08	119.08	111.36
1	C	790	LYS	N-CA-C	6.95	118.64	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	930	PHE	N-CA-C	6.68	118.64	111.36
1	A	930	PHE	N-CA-C	6.50	118.45	111.36
1	C	903	PRO	CA-C-N	6.16	125.64	119.24
1	C	903	PRO	C-N-CA	6.16	125.64	119.24
1	A	1030	PRO	N-CA-C	-5.96	103.44	110.70
2	B	155	LEU	N-CA-C	5.91	117.80	111.36
1	C	735	GLU	N-CA-C	-5.85	100.16	109.76
2	D	36	SER	N-CA-C	5.85	117.74	111.36
1	C	857	HIS	N-CA-C	5.81	117.42	111.14
1	A	719	TRP	N-CA-C	5.71	118.93	110.48
1	A	938	ALA	CA-C-N	5.70	128.38	120.29
1	A	938	ALA	C-N-CA	5.70	128.38	120.29
1	A	939	ASN	N-CA-C	5.69	117.56	111.36
1	A	825	GLU	N-CA-C	5.65	118.38	111.82
2	B	42	ASP	CA-C-N	5.62	125.47	119.28
2	B	42	ASP	C-N-CA	5.62	125.47	119.28
2	D	228	LYS	N-CA-C	5.54	118.18	110.20
1	A	966	LEU	CA-C-N	5.53	126.75	119.84
1	A	966	LEU	C-N-CA	5.53	126.75	119.84
2	D	90	PHE	CA-C-N	5.20	125.44	119.83
2	D	90	PHE	C-N-CA	5.20	125.44	119.83
1	C	928	GLU	N-CA-C	5.13	117.61	111.71
1	A	1003	LEU	N-CA-C	5.13	116.87	111.28
2	B	154	ASP	CA-C-N	5.05	127.45	120.29
2	B	154	ASP	C-N-CA	5.05	127.45	120.29
2	D	159	HIS	CA-C-N	-5.04	114.47	119.56
2	D	159	HIS	C-N-CA	-5.04	114.47	119.56
2	B	159	HIS	CA-C-N	-5.03	114.48	119.56
2	B	159	HIS	C-N-CA	-5.03	114.48	119.56
1	C	891	PRO	CA-C-N	-5.00	112.69	121.70
1	C	891	PRO	C-N-CA	-5.00	112.69	121.70

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	2588	0	2555	83	1
1	C	2541	0	2492	92	0
2	B	2023	0	1972	41	0
2	D	1988	0	1945	36	0
3	A	27	0	12	1	0
3	C	27	0	9	2	0
4	A	4	0	0	0	0
4	C	4	0	0	0	0
5	A	3	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	4	0	6	2	0
6	B	4	0	6	0	0
6	C	4	0	6	7	0
6	D	4	0	6	0	0
7	A	107	0	0	9	0
7	B	92	0	0	4	0
7	C	96	0	0	6	0
7	D	98	0	0	4	0
All	All	9618	0	9009	238	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 13.

All (238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:739:GLY:HA2	1:C:759:ARG:NH1	1.46	1.30
1:A:939:ASN:ND2	1:A:940:LEU:HD12	1.55	1.22
1:A:796:LYS:HD3	1:A:796:LYS:N	1.48	1.21
1:A:740:GLN:OE1	1:A:759:ARG:NH2	1.74	1.19
1:C:888:GLU:HG3	1:C:890:ARG:NH1	1.58	1.18
1:C:739:GLY:CA	1:C:759:ARG:NH1	2.11	1.13
2:B:191:ASP:OD2	2:B:258:TYR:OH	1.71	1.08
1:C:843:LEU:HD13	1:C:844:MET:CE	1.91	1.01
1:A:794:THR:OG1	7:A:1271:HOH:O	1.77	1.01
1:A:796:LYS:HD3	1:A:796:LYS:H	0.87	1.00
1:C:843:LEU:HD13	1:C:844:MET:HE1	1.36	0.99
1:A:796:LYS:H	1:A:796:LYS:CD	1.77	0.98
1:C:888:GLU:HG3	1:C:890:ARG:HH12	1.21	0.97
1:C:888:GLU:CG	1:C:890:ARG:HH12	1.78	0.97
1:C:739:GLY:HA2	1:C:759:ARG:HH11	1.15	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:HIS:CE1	1:A:1009:CYS:HB3	1.99	0.96
2:B:259:SER:O	2:B:262:LYS:HE3	1.66	0.95
1:C:739:GLY:CA	1:C:759:ARG:HH11	1.77	0.95
1:A:939:ASN:HD22	1:A:940:LEU:CD1	1.81	0.93
1:A:939:ASN:HD22	1:A:940:LEU:HD12	1.11	0.93
1:A:765:GLU:OE1	7:A:1241:HOH:O	1.84	0.93
1:A:960:TRP:O	1:A:963:VAL:HG12	1.70	0.92
1:C:740:GLN:H	1:C:759:ARG:HH12	1.17	0.91
2:D:232:ARG:HD2	2:D:236:GLU:OE1	1.73	0.88
1:C:999:HIS:CE1	1:C:1009:CYS:HB3	2.10	0.86
2:B:63:ARG:NH2	2:B:122:SER:OG	2.09	0.86
1:C:823:LEU:HD13	1:C:1039:CYS:HB2	1.57	0.86
1:C:740:GLN:N	1:C:759:ARG:HH12	1.73	0.86
2:D:228:LYS:NZ	7:D:476:HOH:O	1.87	0.86
1:C:960:TRP:O	1:C:963:VAL:HG12	1.77	0.84
2:D:63:ARG:NH2	2:D:122:SER:OG	2.10	0.84
1:C:981:ARG:NH1	1:C:985:GLU:OE1	2.10	0.84
2:B:179:GLN:HE22	1:C:1007:LYS:NZ	1.77	0.82
1:C:843:LEU:HB3	1:C:844:MET:HE2	1.61	0.82
1:A:807:GLY:HA3	2:B:145:ARG:NH2	1.96	0.80
1:C:765:GLU:OE1	7:C:1273:HOH:O	1.98	0.80
2:B:259:SER:O	2:B:262:LYS:CE	2.30	0.79
2:D:121:ARG:HD3	2:D:121:ARG:O	1.83	0.79
1:C:776:LYS:HA	6:C:1105:EDO:H21	1.64	0.77
1:A:834:ASP:O	1:A:1028:MET:HE2	1.85	0.77
1:C:739:GLY:CA	1:C:759:ARG:HH12	1.93	0.77
1:A:862:CYS:HB2	6:A:1106:EDO:H22	1.65	0.76
1:C:776:LYS:CA	6:C:1105:EDO:H21	2.16	0.76
1:A:757:LYS:HD3	1:A:759:ARG:HE	1.51	0.75
1:A:986:PHE:HB3	1:A:989:ILE:HD12	1.69	0.74
2:D:232:ARG:CD	2:D:236:GLU:OE1	2.35	0.74
1:A:814:GLU:OE2	7:A:1236:HOH:O	2.07	0.73
1:C:888:GLU:CD	1:C:890:ARG:HH12	1.97	0.72
1:A:976:LYS:HG2	1:A:977:GLN:N	2.02	0.72
1:C:824:LEU:HD11	1:C:831:PHE:HE2	1.55	0.72
2:B:184:MET:HE1	2:B:217:LEU:HB2	1.72	0.72
2:B:256:ASP:OD2	7:B:492:HOH:O	2.07	0.71
2:B:179:GLN:HE22	1:C:1007:LYS:HZ3	1.39	0.71
1:A:1007:LYS:NZ	2:D:179:GLN:HE22	1.88	0.71
1:A:931:THR:C	1:A:932:LYS:HG2	2.14	0.70
2:D:184:MET:HE1	2:D:217:LEU:HB2	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:986:PHE:HB3	1:C:989:ILE:HD12	1.73	0.69
1:A:840:MET:CE	1:A:844:MET:HE3	2.22	0.69
1:C:970:ASN:HA	1:C:973:LYS:HE3	1.75	0.69
2:B:259:SER:N	2:B:262:LYS:HZ2	1.91	0.68
1:A:769:ILE:O	1:A:773:ARG:HG3	1.94	0.67
2:D:27:ASP:HB3	2:D:30:ASP:H	1.60	0.67
1:A:976:LYS:CG	1:A:977:GLN:N	2.57	0.66
2:D:184:MET:CE	2:D:214:ALA:HA	2.26	0.66
1:C:774:GLU:HG2	1:C:778:LEU:HD22	1.77	0.66
1:A:950:ARG:HD2	7:A:1247:HOH:O	1.97	0.65
2:B:259:SER:O	2:B:262:LYS:NZ	2.29	0.65
1:C:960:TRP:O	1:C:963:VAL:CG1	2.45	0.65
1:A:796:LYS:N	1:A:796:LYS:CD	2.37	0.65
1:A:999:HIS:ND1	1:A:1009:CYS:HB3	2.12	0.64
2:D:223:GLN:HB2	2:D:228:LYS:HE3	1.80	0.64
1:C:888:GLU:CG	1:C:890:ARG:NH1	2.42	0.64
2:B:184:MET:CE	2:B:214:ALA:HA	2.28	0.63
1:A:832:SER:H	1:A:835:HIS:CD2	2.16	0.63
2:B:179:GLN:NE2	1:C:1007:LYS:HZ3	1.97	0.63
1:C:832:SER:H	1:C:835:HIS:CD2	2.17	0.62
1:C:962:ASP:OD2	1:C:962:ASP:N	2.30	0.62
2:D:184:MET:HE3	2:D:214:ALA:HA	1.82	0.62
1:A:775:ILE:O	1:A:779:ARG:HG3	2.00	0.62
1:C:842:GLN:NE2	7:C:1212:HOH:O	2.26	0.61
2:D:200:GLN:HE22	2:D:253:GLN:HE22	1.47	0.61
2:B:20:THR:OG1	2:B:21:LYS:N	2.32	0.61
1:C:897:ILE:HG21	1:C:902:ARG:HA	1.83	0.60
1:C:776:LYS:O	6:C:1105:EDO:H21	2.01	0.60
1:C:999:HIS:ND1	1:C:1009:CYS:HB3	2.16	0.60
1:C:791:GLU:OE2	7:C:1274:HOH:O	2.17	0.60
1:A:862:CYS:HB2	6:A:1106:EDO:C2	2.32	0.60
1:A:840:MET:HE1	1:A:844:MET:HE3	1.84	0.59
1:A:840:MET:HE3	1:A:844:MET:HE3	1.84	0.59
1:A:807:GLY:HA3	2:B:145:ARG:HH21	1.64	0.59
2:B:200:GLN:HE22	2:B:253:GLN:HE22	1.50	0.59
1:C:735:GLU:OE1	1:C:735:GLU:HA	2.04	0.58
1:A:898:THR:HG23	7:A:1222:HOH:O	2.03	0.58
1:C:739:GLY:HA3	1:C:759:ARG:NH1	2.13	0.58
1:A:981:ARG:NH1	1:A:985:GLU:OE1	2.36	0.58
2:D:34:THR:OG1	2:D:37:GLN:HG2	2.04	0.58
1:A:976:LYS:CG	1:A:977:GLN:H	2.17	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:739:GLY:C	1:C:759:ARG:HH12	2.12	0.57
2:D:121:ARG:HD3	2:D:121:ARG:C	2.28	0.57
1:C:936:PHE:CB	1:C:944:GLN:HE22	2.18	0.57
1:A:807:GLY:CA	2:B:145:ARG:NH2	2.66	0.57
6:C:1105:EDO:H22	2:D:156:GLN:HB2	1.87	0.57
1:A:760:LEU:HG	1:A:807:GLY:O	2.05	0.56
1:A:736:GLY:HA2	3:A:1101:ADP:O1B	2.05	0.56
1:A:841:LYS:HE3	1:A:845:GLU:OE2	2.06	0.56
1:A:842:GLN:NE2	1:A:873:ILE:H	2.04	0.56
1:A:970:ASN:HA	1:A:973:LYS:HE3	1.88	0.55
1:C:775:ILE:O	1:C:779:ARG:HG3	2.06	0.55
1:C:769:ILE:O	1:C:773:ARG:HG3	2.07	0.55
1:A:797:GLN:O	1:A:798:ASP:CB	2.54	0.55
2:B:157:VAL:HG12	2:B:159:HIS:CE1	2.41	0.55
1:A:834:ASP:O	1:A:1028:MET:CE	2.55	0.55
1:A:936:PHE:CB	1:A:944:GLN:HE22	2.20	0.55
2:B:37:GLN:HB2	7:B:453:HOH:O	2.07	0.55
1:A:1007:LYS:HZ2	2:D:179:GLN:HE22	1.55	0.54
1:C:736:GLY:HA2	3:C:1101:ADP:O1B	2.07	0.54
1:C:776:LYS:HA	6:C:1105:EDO:C2	2.38	0.54
1:C:784:ARG:NH1	1:C:845:GLU:OE1	2.40	0.54
2:D:27:ASP:HB2	2:D:30:ASP:OD2	2.08	0.54
1:A:889:SER:O	1:A:890:ARG:HD3	2.09	0.53
1:C:843:LEU:CD1	1:C:844:MET:CE	2.78	0.53
1:C:969:PHE:O	1:C:973:LYS:HE3	2.08	0.53
2:B:184:MET:HE2	2:B:214:ALA:HA	1.90	0.53
1:C:936:PHE:HB3	1:C:944:GLN:NE2	2.23	0.53
1:C:896:VAL:O	1:C:897:ILE:HB	2.07	0.53
1:C:914:THR:HB	1:C:915:PRO:HD2	1.90	0.53
1:A:942:LEU:HA	1:A:972:MET:HE3	1.91	0.53
2:D:137:LYS:O	2:D:141:MET:HG2	2.09	0.52
1:A:936:PHE:HB3	1:A:944:GLN:NE2	2.25	0.52
1:A:936:PHE:HB2	1:A:944:GLN:HE22	1.75	0.52
1:A:751:GLU:HG3	1:A:752:LEU:N	2.24	0.52
1:A:986:PHE:HD1	1:A:989:ILE:HD11	1.74	0.52
1:A:945:LEU:HD22	1:A:972:MET:HE2	1.92	0.51
1:C:936:PHE:HB2	1:C:944:GLN:HE22	1.75	0.51
1:C:898:THR:HG23	7:C:1209:HOH:O	2.08	0.51
2:B:179:GLN:NE2	1:C:1007:LYS:NZ	2.52	0.51
1:C:976:LYS:CG	1:C:977:GLN:N	2.74	0.51
1:C:776:LYS:C	6:C:1105:EDO:H21	2.36	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:MET:HB2	1:A:813:PHE:CE1	2.46	0.50
1:C:843:LEU:HB3	1:C:844:MET:CE	2.37	0.50
2:D:156:GLN:HG3	7:D:420:HOH:O	2.11	0.50
2:B:259:SER:OG	2:B:262:LYS:NZ	2.30	0.50
1:A:719:TRP:HZ3	1:A:789:MET:HE3	1.77	0.50
2:D:174:ASP:OD1	2:D:174:ASP:C	2.54	0.50
1:A:716:GLU:HA	1:A:716:GLU:OE1	2.11	0.49
1:C:793:VAL:HG23	1:C:810:TYR:HB2	1.95	0.49
2:B:174:ASP:OD1	2:B:174:ASP:C	2.56	0.49
1:C:824:LEU:CD1	1:C:831:PHE:HE2	2.24	0.49
1:C:986:PHE:HD1	1:C:989:ILE:HD11	1.78	0.48
1:A:784:ARG:HG3	7:A:1229:HOH:O	2.12	0.48
2:D:191:ASP:OD2	2:D:258:TYR:OH	2.20	0.48
1:C:931:THR:HG22	1:C:988:PHE:HZ	1.78	0.48
2:B:184:MET:CE	2:B:217:LEU:HB2	2.42	0.48
2:B:34:THR:OG1	2:B:37:GLN:HG2	2.14	0.48
1:A:844:MET:HE1	1:A:922:CYS:HB3	1.95	0.48
1:C:841:LYS:HG2	1:C:1025:LEU:HD11	1.96	0.48
1:A:976:LYS:HG2	1:A:977:GLN:H	1.71	0.47
1:A:874:LYS:NZ	7:A:1274:HOH:O	2.44	0.47
2:B:137:LYS:O	2:B:141:MET:HG2	2.14	0.47
2:D:218:CYS:HB3	2:D:220:PHE:CE2	2.49	0.47
1:A:986:PHE:HD1	1:A:989:ILE:CD1	2.27	0.47
2:D:196:THR:O	2:D:200:GLN:HG3	2.14	0.47
1:A:936:PHE:CB	1:A:944:GLN:NE2	2.78	0.47
2:B:201:TRP:HB2	2:B:206:ILE:HD11	1.97	0.47
2:D:121:ARG:HH22	2:D:126:ASP:HA	1.79	0.47
2:B:179:GLN:HE22	1:C:1007:LYS:HZ2	1.60	0.46
1:C:719:TRP:HZ3	1:C:789:MET:HE3	1.80	0.46
1:C:784:ARG:HG3	7:C:1276:HOH:O	2.14	0.46
1:A:890:ARG:HD2	1:A:890:ARG:HA	1.58	0.46
1:A:914:THR:HB	1:A:915:PRO:HD2	1.96	0.46
1:C:721:LYS:HD3	2:D:149:GLN:HB3	1.97	0.46
1:C:936:PHE:CB	1:C:944:GLN:NE2	2.78	0.46
1:A:767:PHE:HA	1:A:768:PRO:HD3	1.76	0.46
1:A:842:GLN:HE22	1:A:873:ILE:H	1.63	0.46
1:C:819:ASP:OD2	1:C:819:ASP:C	2.59	0.45
1:C:840:MET:HE3	1:C:844:MET:HE3	1.99	0.45
1:A:1007:LYS:HZ3	2:D:179:GLN:HE22	1.61	0.45
2:D:244:VAL:O	2:D:248:GLU:HG2	2.17	0.45
1:C:986:PHE:HD1	1:C:989:ILE:CD1	2.28	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:37:GLN:NE2	2:D:46:GLU:OE1	2.39	0.45
2:B:184:MET:HE3	2:B:214:ALA:HA	1.98	0.45
1:C:776:LYS:HA	6:C:1105:EDO:C1	2.46	0.45
1:A:844:MET:HE1	1:A:922:CYS:SG	2.57	0.45
2:B:184:MET:HE2	2:B:214:ALA:CA	2.46	0.45
1:C:841:LYS:HG2	1:C:1025:LEU:HD21	1.98	0.45
1:A:764:LYS:HB2	1:A:764:LYS:HE2	1.75	0.44
2:D:184:MET:CE	2:D:217:LEU:HB2	2.44	0.44
2:B:48:ARG:NH2	7:B:456:HOH:O	2.49	0.44
2:B:258:TYR:CD2	2:B:263:GLN:HB3	2.52	0.44
1:C:874:LYS:NZ	7:C:1277:HOH:O	2.46	0.44
2:D:29:LYS:O	2:D:33:HIS:HD2	2.01	0.44
1:C:795:ASP:OD1	1:C:810:TYR:HE2	2.00	0.44
1:A:931:THR:HG22	1:A:988:PHE:HZ	1.83	0.43
1:A:946:GLU:O	1:A:950:ARG:HG3	2.18	0.43
1:C:735:GLU:OE1	1:C:735:GLU:CA	2.64	0.43
1:C:816:MET:O	3:C:1101:ADP:H2	2.00	0.43
1:C:842:GLN:NE2	1:C:873:ILE:H	2.16	0.43
1:A:769:ILE:HG22	7:A:1240:HOH:O	2.17	0.43
2:B:223:GLN:O	2:B:229:PRO:HA	2.19	0.43
1:C:741:VAL:HG22	1:C:756:LYS:HG2	2.00	0.43
2:D:34:THR:O	2:D:38:LEU:HG	2.19	0.43
2:D:201:TRP:HB2	2:D:206:ILE:HD11	2.00	0.43
1:A:968:TYR:HB3	1:A:972:MET:HG3	1.99	0.43
2:D:184:MET:HE2	2:D:214:ALA:HB1	2.01	0.43
1:C:837:LYS:HB3	1:C:1023:VAL:HG21	2.00	0.43
1:C:936:PHE:HB3	1:C:944:GLN:HE22	1.82	0.43
1:C:960:TRP:CG	1:C:963:VAL:HB	2.54	0.42
1:C:906:LEU:HD21	1:C:913:TYR:CD2	2.54	0.42
1:C:826:SER:OG	1:C:828:LEU:HB2	2.19	0.42
2:D:48:ARG:NH2	7:D:462:HOH:O	2.52	0.42
1:A:1041:GLU:HG2	1:A:1045:LYS:HE3	2.00	0.42
1:C:968:TYR:HB3	1:C:972:MET:HG3	2.00	0.42
1:A:745:LYS:NZ	7:A:1266:HOH:O	2.52	0.42
1:A:807:GLY:N	2:B:145:ARG:NH2	2.67	0.42
1:A:842:GLN:HE22	1:A:872:GLN:HA	1.84	0.42
2:B:256:ASP:O	2:B:262:LYS:NZ	2.44	0.42
1:A:946:GLU:OE2	1:A:978:TYR:OH	2.33	0.42
1:A:931:THR:C	1:A:932:LYS:CG	2.87	0.42
2:B:157:VAL:CG1	2:B:159:HIS:CE1	3.03	0.41
2:B:38:LEU:HA	2:B:38:LEU:HD23	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:837:LYS:HB3	1:A:1023:VAL:HG21	2.02	0.41
2:B:216:ARG:HH22	2:B:248:GLU:CD	2.28	0.41
1:C:739:GLY:HA3	1:C:759:ARG:HH11	1.70	0.41
1:A:1007:LYS:NZ	2:D:179:GLN:NE2	2.62	0.41
2:D:69:ASP:HB2	7:D:491:HOH:O	2.20	0.41
1:C:784:ARG:HG3	1:C:784:ARG:H	1.68	0.41
1:C:945:LEU:HD22	1:C:972:MET:HE2	2.02	0.41
2:B:48:ARG:NH1	7:B:455:HOH:O	2.54	0.41
1:C:889:SER:O	1:C:890:ARG:HD3	2.21	0.41
1:A:764:LYS:HE3	1:A:764:LYS:HB3	1.68	0.41
1:C:918:ASP:O	1:C:921:SER:HB2	2.22	0.40
1:A:843:LEU:HG	1:A:844:MET:HE2	2.04	0.40
2:B:196:THR:O	2:B:200:GLN:HG3	2.21	0.40
1:C:776:LYS:HB3	1:C:776:LYS:HE2	1.90	0.40
1:C:923:GLY:N	1:C:1000:MET:HE2	2.36	0.40
1:A:986:PHE:CD1	1:A:989:ILE:CD1	3.05	0.40
2:B:255:LEU:HD23	2:B:255:LEU:HA	1.94	0.40
1:C:896:VAL:O	1:C:897:ILE:CB	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:ASN:ND2	1:A:1015:LEU:O[1_455]	1.37	0.83

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	318/351 (91%)	313 (98%)	4 (1%)	1 (0%)	36 42
1	C	311/351 (89%)	304 (98%)	5 (2%)	2 (1%)	21 23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	244/268 (91%)	244 (100%)	0	0	100	100
2	D	239/268 (89%)	239 (100%)	0	0	100	100
All	All	1112/1238 (90%)	1100 (99%)	9 (1%)	3 (0%)	36	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	897	ILE
1	C	897	ILE
1	C	764	LYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	279/316 (88%)	252 (90%)	27 (10%)	8	8
1	C	274/316 (87%)	253 (92%)	21 (8%)	12	13
2	B	215/241 (89%)	200 (93%)	15 (7%)	14	16
2	D	212/241 (88%)	199 (94%)	13 (6%)	17	20
All	All	980/1114 (88%)	904 (92%)	76 (8%)	11	13

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	717	SER
1	A	722	ARG
1	A	735	GLU
1	A	740	GLN
1	A	752	LEU
1	A	760	LEU
1	A	762	ASN
1	A	764	LYS
1	A	787	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	796	LYS
1	A	820	LEU
1	A	828	LEU
1	A	829	VAL
1	A	883	LEU
1	A	890	ARG
1	A	908	LEU
1	A	932	LYS
1	A	942	LEU
1	A	962	ASP
1	A	977	GLN
1	A	979	ARG
1	A	984	GLU
1	A	1020	LEU
1	A	1025	LEU
1	A	1028	MET
1	A	1042	LEU
1	A	1045	LYS
2	B	20	THR
2	B	21	LYS
2	B	37	GLN
2	B	63	ARG
2	B	76	ILE
2	B	122	SER
2	B	145	ARG
2	B	156	GLN
2	B	157	VAL
2	B	202	GLU
2	B	221	GLU
2	B	224	GLU
2	B	232	ARG
2	B	262	LYS
2	B	265	MET
1	C	735	GLU
1	C	752	LEU
1	C	760	LEU
1	C	778	LEU
1	C	784	ARG
1	C	787	VAL
1	C	823	LEU
1	C	828	LEU
1	C	843	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	847	LEU
1	C	895	LYS
1	C	908	LEU
1	C	929	LEU
1	C	941	GLU
1	C	942	LEU
1	C	962	ASP
1	C	977	GLN
1	C	984	GLU
1	C	1020	LEU
1	C	1028	MET
1	C	1032	ASP
2	D	27	ASP
2	D	28	LYS
2	D	63	ARG
2	D	114	LYS
2	D	121	ARG
2	D	145	ARG
2	D	156	GLN
2	D	157	VAL
2	D	202	GLU
2	D	224	GLU
2	D	228	LYS
2	D	230	MET
2	D	245	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	780	GLN
1	A	797	GLN
1	A	835	HIS
1	A	842	GLN
1	A	937	GLN
1	A	944	GLN
1	A	977	GLN
1	A	1035	HIS
1	A	1037	GLN
2	B	149	GLN
2	B	179	GLN
2	B	200	GLN
2	B	237	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	780	GLN
1	C	835	HIS
1	C	842	GLN
1	C	944	GLN
1	C	1035	HIS
2	D	33	HIS
2	D	67	HIS
2	D	179	GLN
2	D	200	GLN
2	D	237	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)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	TPO	A	893	1	8,10,11	1.61	1 (12%)	10,14,16	1.64	2 (20%)
1	TPO	C	893	1	8,10,11	1.00	0	10,14,16	2.04	3 (30%)

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
1	TPO	A	893	1	-	1/9/11/13	-
1	TPO	C	893	1	-	0/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	893	TPO	P-OG1	2.75	1.64	1.59

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	893	TPO	CG2-CB-CA	-5.14	103.26	113.26
1	A	893	TPO	CG2-CB-CA	-3.60	106.24	113.26
1	A	893	TPO	O3P-P-OG1	2.71	116.43	105.85
1	C	893	TPO	O3P-P-OG1	2.42	115.28	105.85
1	C	893	TPO	P-OG1-CB	-2.09	117.64	123.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	893	TPO	CA-CB-OG1-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	A	1101	5	28,29,29	1.46	5 (17%)	43,45,45	1.96	12 (27%)
6	EDO	A	1106	-	3,3,3	0.35	0	2,2,2	1.08	0
4	AF3	C	1102	-	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	C	1105	-	3,3,3	0.67	0	2,2,2	0.69	0
4	AF3	A	1102	-	0,3,3	-	-	-		
6	EDO	B	301	-	3,3,3	0.67	0	2,2,2	0.08	0
6	EDO	D	303	-	3,3,3	0.30	0	2,2,2	1.07	0
3	ADP	C	1101	5	28,29,29	1.74	8 (28%)	43,45,45	2.80	18 (41%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	1101	5	-	4/16/32/32	0/3/3/3
6	EDO	A	1106	-	-	0/1/1/1	-
6	EDO	C	1105	-	-	0/1/1/1	-
6	EDO	B	301	-	-	1/1/1/1	-
6	EDO	D	303	-	-	1/1/1/1	-
3	ADP	C	1101	5	-	4/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	ADP	C5-C4	4.62	1.47	1.39
3	C	1101	ADP	C5-C4	-3.56	1.32	1.39
3	C	1101	ADP	C2-N1	2.78	1.38	1.33
3	A	1101	ADP	C5-C6	2.63	1.48	1.41
3	A	1101	ADP	PA-O5'	2.49	1.69	1.59
3	C	1101	ADP	O2'-C2'	-2.45	1.36	1.43
3	A	1101	ADP	C8-N7	2.32	1.36	1.31
3	C	1101	ADP	C6-N6	2.29	1.40	1.34
3	C	1101	ADP	PA-O3A	-2.27	1.57	1.59
3	C	1101	ADP	O3'-C3'	-2.24	1.37	1.43
3	C	1101	ADP	O4'-C4'	2.19	1.49	1.45
3	A	1101	ADP	C5-N7	-2.18	1.35	1.39
3	C	1101	ADP	C1'-N9	-2.05	1.40	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	1101	ADP	O3'-C3'-C4'	6.69	130.30	111.08
3	C	1101	ADP	O4'-C1'-N9	6.47	120.52	108.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1101	ADP	C5-C4-N3	-5.53	119.10	126.72
3	C	1101	ADP	O4'-C4'-C5'	5.36	126.51	109.33
3	C	1101	ADP	C2'-C1'-N9	5.29	126.46	113.30
3	C	1101	ADP	N9-C8-N7	-5.12	106.68	113.94
3	C	1101	ADP	N3-C2-N1	-5.08	120.89	128.58
3	A	1101	ADP	N3-C4-N9	4.74	135.22	127.17
3	C	1101	ADP	O2'-C2'-C1'	4.43	125.36	110.10
3	C	1101	ADP	C4-N9-C8	4.18	110.13	105.74
3	C	1101	ADP	O3'-C3'-C2'	3.88	124.25	111.82
3	A	1101	ADP	C2-N3-C4	3.82	121.17	111.83
3	A	1101	ADP	N3-C2-N1	-3.61	123.11	128.58
3	A	1101	ADP	O5'-PA-O1A	-3.28	95.92	108.94
3	A	1101	ADP	C4-N9-C8	3.26	109.16	105.74
3	C	1101	ADP	O4'-C1'-C2'	-3.24	99.68	106.62
3	A	1101	ADP	C4-C5-N7	-3.01	107.14	110.58
3	C	1101	ADP	C5-N7-C8	2.99	108.15	103.45
3	C	1101	ADP	O3A-PA-O1A	2.93	119.52	110.70
3	A	1101	ADP	O3B-PB-O3A	2.89	114.33	104.64
3	C	1101	ADP	C4'-O4'-C1'	-2.75	103.39	109.47
3	C	1101	ADP	N3-C4-N9	2.61	131.61	127.17
3	A	1101	ADP	C2'-C1'-N9	-2.61	106.83	113.30
3	C	1101	ADP	C2-N3-C4	2.43	117.77	111.83
3	A	1101	ADP	C5-N7-C8	2.41	107.23	103.45
3	C	1101	ADP	C5-C4-N3	-2.27	123.60	126.72
3	A	1101	ADP	N9-C8-N7	-2.22	110.79	113.94
3	A	1101	ADP	C6-C5-N7	2.21	136.35	132.09
3	C	1101	ADP	C2'-C3'-C4'	-2.18	98.39	102.61
3	C	1101	ADP	C5'-C4'-C3'	2.13	122.90	115.21

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	ADP	PA-O3A-PB-O3B
3	C	1101	ADP	PA-O3A-PB-O2B
3	C	1101	ADP	PA-O3A-PB-O3B
3	C	1101	ADP	C3'-C4'-C5'-O5'
6	B	301	EDO	O1-C1-C2-O2
3	A	1101	ADP	C5'-O5'-PA-O1A
6	D	303	EDO	O1-C1-C2-O2
3	C	1101	ADP	PA-O3A-PB-O1B
3	A	1101	ADP	PA-O3A-PB-O2B

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	1101	ADP	PB-O3A-PA-O2A

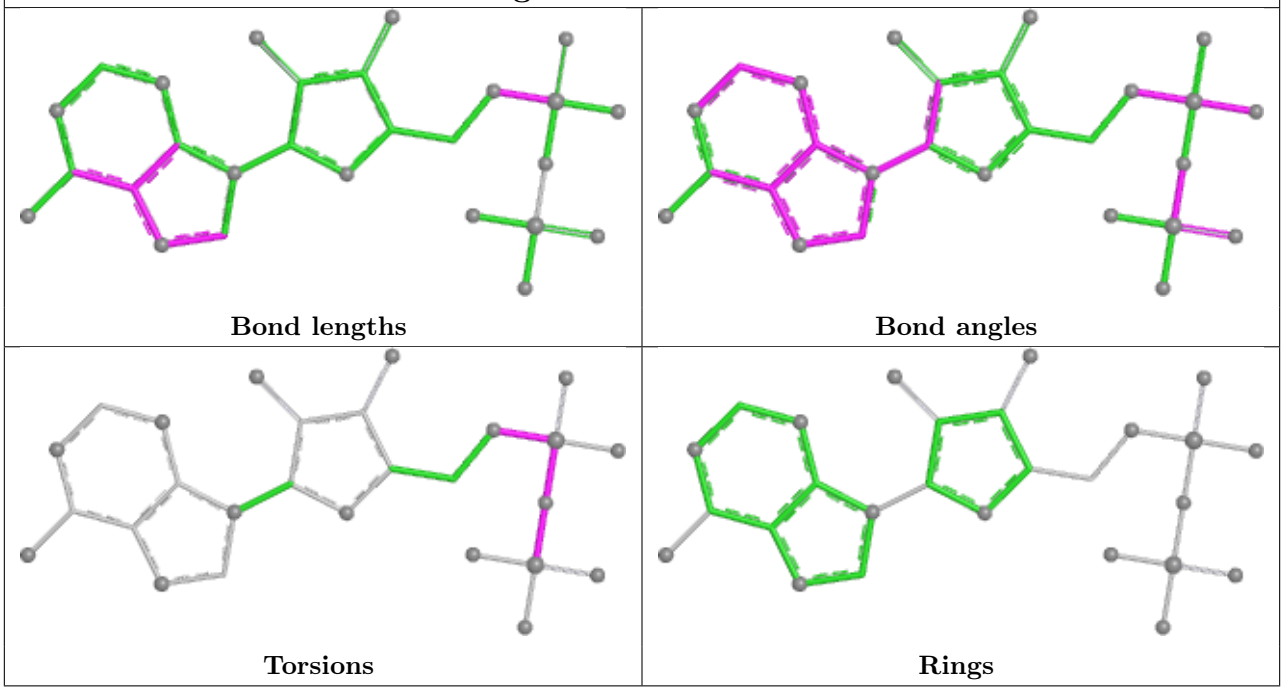
There are no ring outliers.

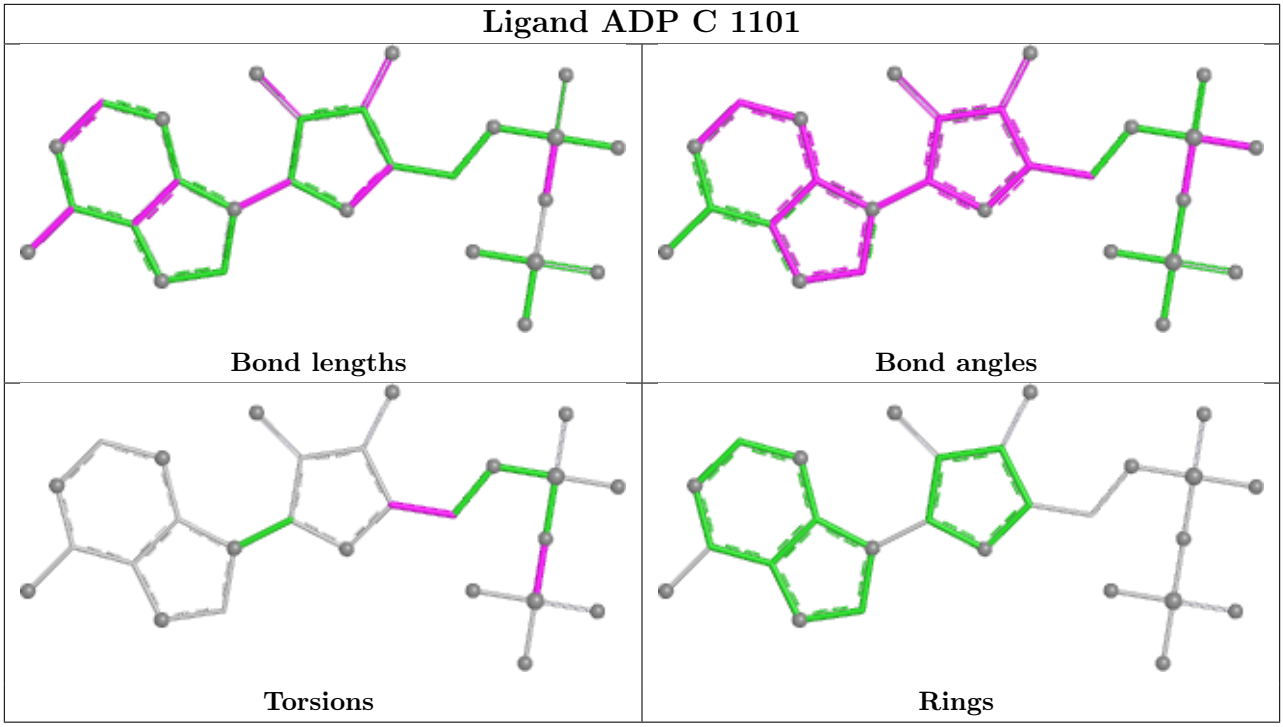
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	ADP	1	0
6	A	1106	EDO	2	0
6	C	1105	EDO	7	0
3	C	1101	ADP	2	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP A 1101





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	322/351 (91%)	0.31	11 (3%)	48	45	23, 41, 74, 98	0
1	C	317/351 (90%)	0.26	11 (3%)	47	44	24, 42, 74, 99	0
2	B	246/268 (91%)	-0.03	4 (1%)	70	67	19, 36, 72, 88	0
2	D	241/268 (89%)	-0.04	2 (0%)	82	80	21, 37, 65, 87	0
All	All	1126/1238 (90%)	0.15	28 (2%)	58	55	19, 40, 72, 99	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	264	GLN	6.3
1	A	807	GLY	4.1
2	B	265	MET	3.8
1	A	884	TYR	3.5
1	A	751	GLU	3.4
2	D	233	ARG	3.0
2	B	227	SER	2.9
2	D	261	GLY	2.9
1	C	759	ARG	2.8
1	C	932	LYS	2.8
1	C	717	SER	2.8
1	C	884	TYR	2.7
1	A	962	ASP	2.7
1	C	1045	LYS	2.6
1	A	1029	ALA	2.6
2	B	20	THR	2.6
1	A	1030	PRO	2.5
1	C	891	PRO	2.5
1	A	989	ILE	2.4
1	C	762	ASN	2.3
1	C	962	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	824	LEU	2.3
1	C	807	GLY	2.3
1	A	895	LYS	2.3
1	C	763	GLU	2.2
1	A	760	LEU	2.1
1	A	939	ASN	2.1
1	A	887	GLU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	TPO	A	893	11/12	0.90	0.11	24,35,43,44	0
1	TPO	C	893	11/12	0.94	0.09	27,34,41,48	0

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(Å^2)	Q<0.9
5	MG	D	302	1/1	0.78	0.28	74,74,74,74	0
6	EDO	A	1106	4/4	0.79	0.20	48,53,59,65	0
6	EDO	B	301	4/4	0.81	0.19	64,71,73,77	0
4	AF3	C	1102	4/4	0.82	0.14	45,69,86,132	0
4	AF3	A	1102	4/4	0.87	0.14	41,68,89,97	0
5	MG	A	1105	1/1	0.88	0.24	70,70,70,70	0
6	EDO	C	1105	4/4	0.89	0.14	39,43,45,52	0
6	EDO	D	303	4/4	0.89	0.16	44,46,57,60	0
3	ADP	A	1101	27/27	0.92	0.16	26,56,63,65	0

Continued on next page...

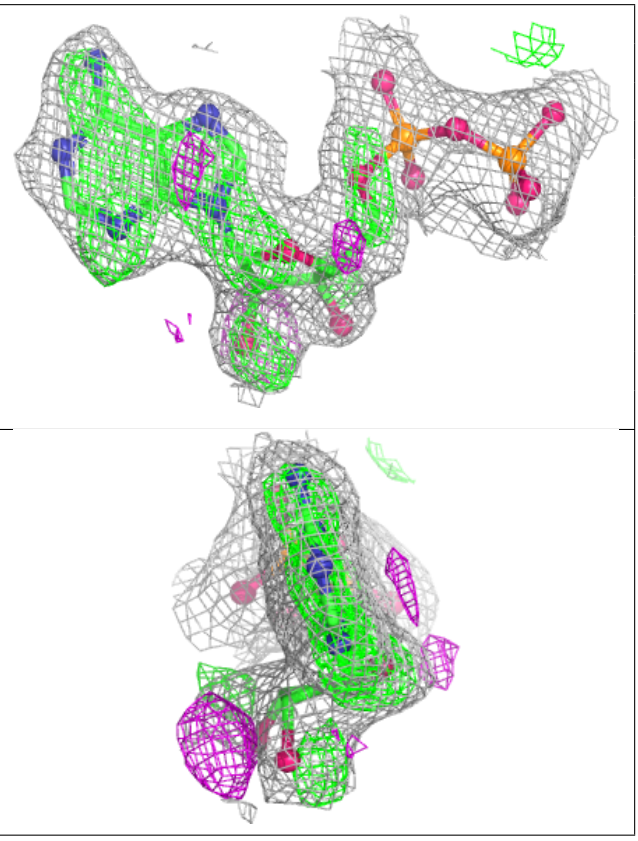
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	D	301	1/1	0.93	0.12	49,49,49,49	0
5	MG	C	1103	1/1	0.95	0.08	32,32,32,32	0
5	MG	C	1104	1/1	0.96	0.07	56,56,56,56	0
5	MG	A	1104	1/1	0.97	0.07	51,51,51,51	0
3	ADP	C	1101	27/27	0.97	0.07	23,32,40,42	0
5	MG	A	1103	1/1	0.98	0.03	27,27,27,27	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.

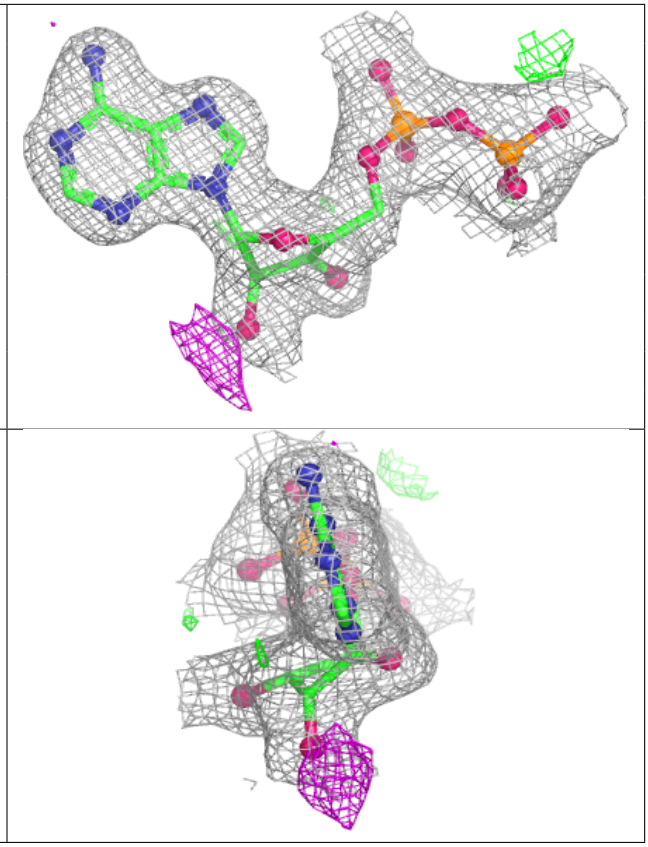
Electron density around ADP A 1101:

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 C 1101:

$2mF_o$-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.