Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2021 – 12:45 AM EDT

PDB ID	:	1XCP
Title	:	Crystal Structure of the Nitrogenase Fe protein Phe135Trp with MgADP bound
Authors	:	Jeong, M.S.; Jang, S.B.
Deposited on	:	2004-09-02
Resolution	:	3.20 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 following versions of software and data (see references (i)) were used in the production of this report:

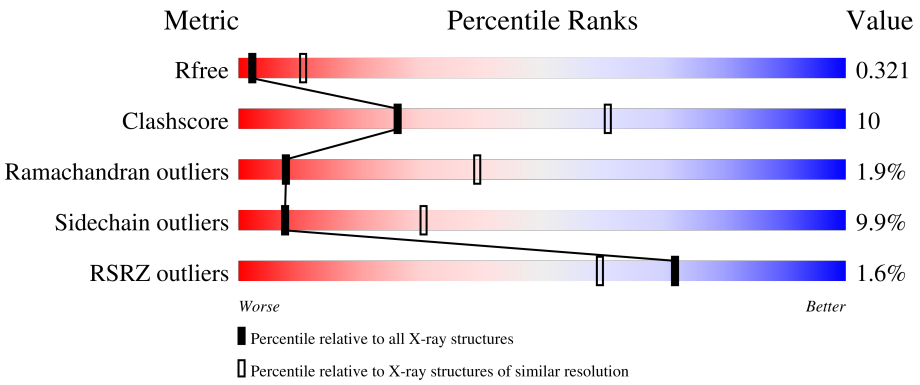
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	289	2% 65% 34%
1	B	289	% 65% 33%
1	C	289	2% 63% 33%
1	D	289	% 65% 31%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8888 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 Nitrogenase iron protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	289	2190	1366	370	433	21	0	0	0
1	B	289	2190	1366	370	433	21	0	0	0
1	C	289	2190	1366	370	433	21	0	0	0
1	D	289	2190	1366	370	433	21	0	0	0

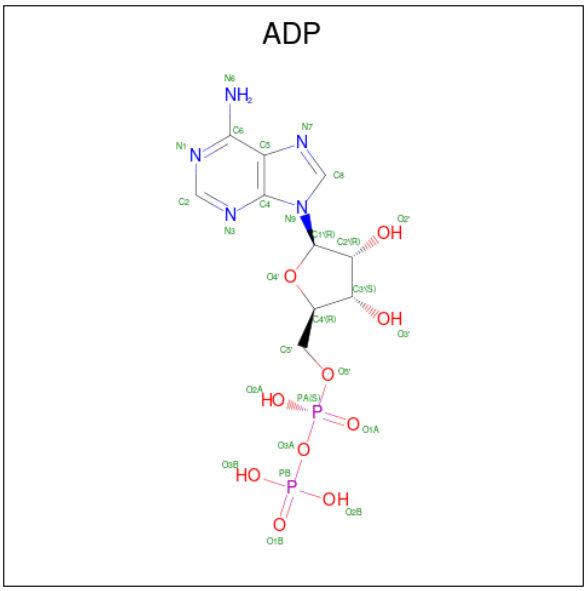
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	TRP	PHE	engineered mutation	UNP P00459
B	135	TRP	PHE	engineered mutation	UNP P00459
C	135	TRP	PHE	engineered mutation	UNP P00459
D	135	TRP	PHE	engineered mutation	UNP P00459

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

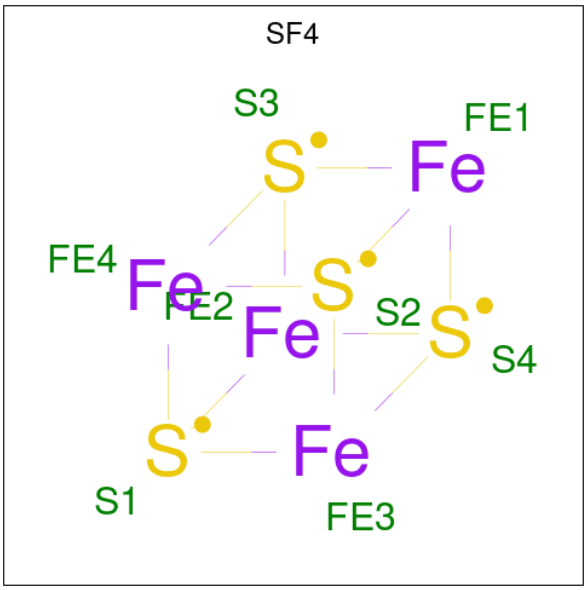
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0

- Molecule 3 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		
3	A	1	27	10	5	10	2	0	0
3	B	1	27	10	5	10	2	0	0
3	C	1	27	10	5	10	2	0	0
3	D	1	27	10	5	10	2	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
4	B	1	8	4	4	0	0
			Total	Fe	S		
4	C	1	8	4	4	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: Nitrogenase iron protein 1

Chain A: 2% 65% 34%

A1 M2 C5 A6 I7 Y8 G9 K10 I13 G14 K15 S16 T19 Q20 N21 L22 A25 L26 K32 I35 D39 P40 K41 T45 R46 L47 I48 I49 H50 M58 A64 D69 E73 D74 V75 L76 V83 K84 C85 P91 E92 G96 C97 A98 G99

R100 I103 I106 L109 E110 E111 E112 Y115 E116 D117 D120 F123 Y124 D125 V126 L127 G128 D129 V130 V131 G134 W135 A136 N142 K143 A144 Q145 E146 I147 Y148 I149 V150 C151 M155 M158 I164 S165 K166 V169 K170 L182 I183 C184 N185 S186 R187 N188

T189 D190 R191 E192 D193 I196 L199 Q206 N215 Q218 R219 R223 R224 M225 T226 V227 I228 E229 R241 A244 R245 L253 V254 I255 L268 E277 D278 E279 S280 I281 V282 G283 K284 T285 A286 E287 E288 V289

• Molecule 1: Nitrogenase iron protein 1

Chain B: % 65% 33%

A1 M2 C5 Y8 G9 K10 I13 G14 Q20 N21 L22 A25 L26 K32 I35 D39 P40 K41 T45 R46 L47 I48 L49 H50 Q64 M58 A64 E73 D74 V75 L76 Y80 V83 K84 C85 V86 P91 E92 G96 C97 A98 G99 R100

I103 I106 L109 E110 E111 E112 D117 D120 F123 Y124 D125 V126 L127 G128 D129 V130 V131 G134 W135 A136 R140 E141 N142 K143 A144 Q145 E146 I147 Y148 I149 V150 C151 M155 M158 N163 I164 S165 K166 V169 K170 Y171 L182 I183 C184 R187 N188

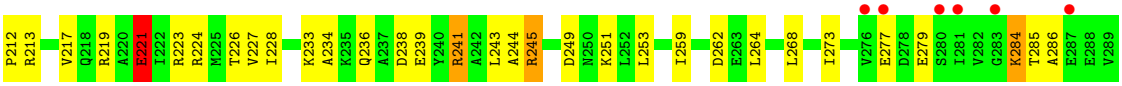
T189 D190 R191 E192 D193 I196 L199 Q206 N215 Q218 R219 R223 R224 M225 T226 V227 I228 E229 R241 A244 R245 L253 V254 I255 L268 E277 D278 E279 S280 I281 V282 G283 K284 T285 A286 E287 E288 V289

• Molecule 1: Nitrogenase iron protein 1

Chain C: 2% 63% 33%

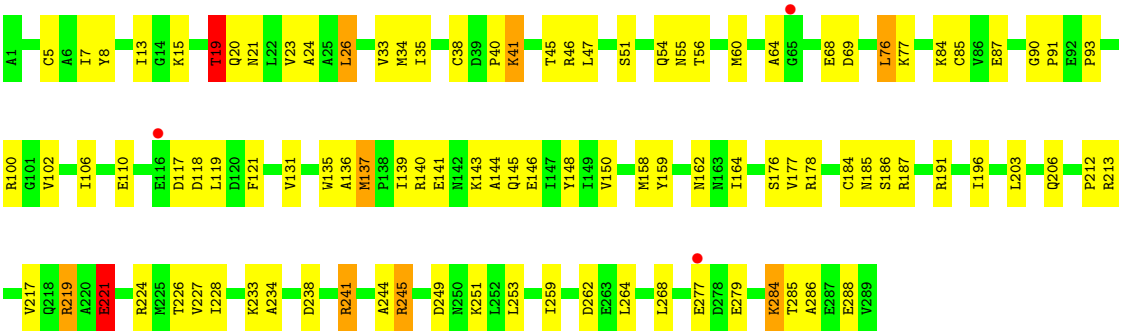
A1 C5 A6 I7 Y8 I13 G14 K15 T19 Q20 N21 L22 V23 A24 A25 L26 V33 M34 I35 C38 D39 P40 K41 T45 R46 L47 S51 Q54 N55 T56 E59 M60 A64 E68 D69 L76 K77 K84 C85 V86 E87 G90 P91 E92 P93

A98 G99 R100 G101 V102 I106 L109 E110 E116 D117 D118 L119 D120 F121 V131 W135 A136 M137 P138 I139 R140 E141 N142 K143 A144 Q145 E146 I147 Y148 I149 V150 M158 Y159 N162 N163 I164 S176 V177 R178 C184 N185 S186 R191 I196 L203 Q206



• Molecule 1: Nitrogenase iron protein 1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.95Å 91.26Å 125.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 19.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-3.20) 89.2 (19.95-3.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 3.22Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.226 , 0.322 0.239 , 0.321	Depositor DCC
R_{free} test set	899 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å^2)	63.2	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 59.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8888	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.02% 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: MG, ADP, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.66	0/2215	1.58	18/2984 (0.6%)
1	B	0.65	0/2215	1.55	19/2984 (0.6%)
1	C	0.65	0/2215	1.56	21/2984 (0.7%)
1	D	0.64	0/2215	1.56	24/2984 (0.8%)
All	All	0.65	0/8860	1.56	82/11936 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	245	ARG	NE-CZ-NH1	23.32	131.96	120.30
1	C	245	ARG	NE-CZ-NH2	-22.18	109.21	120.30
1	D	245	ARG	NE-CZ-NH1	-22.09	109.25	120.30
1	C	100	ARG	NE-CZ-NH2	-21.89	109.35	120.30
1	A	245	ARG	NE-CZ-NH2	-21.76	109.42	120.30
1	A	100	ARG	NE-CZ-NH1	21.51	131.06	120.30
1	C	100	ARG	NE-CZ-NH1	21.46	131.03	120.30
1	D	100	ARG	NE-CZ-NH2	20.73	130.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	100	ARG	NE-CZ-NH2	20.38	130.49	120.30
1	A	100	ARG	NE-CZ-NH2	-20.29	110.15	120.30
1	C	245	ARG	NE-CZ-NH1	20.27	130.44	120.30
1	B	100	ARG	NE-CZ-NH1	-20.23	110.19	120.30
1	D	245	ARG	NE-CZ-NH2	20.07	130.33	120.30
1	B	245	ARG	NE-CZ-NH2	19.72	130.16	120.30
1	D	100	ARG	NE-CZ-NH1	-19.51	110.55	120.30
1	B	245	ARG	NE-CZ-NH1	-18.79	110.91	120.30
1	C	100	ARG	CD-NE-CZ	17.62	148.27	123.60
1	A	245	ARG	CD-NE-CZ	17.52	148.12	123.60
1	B	245	ARG	CD-NE-CZ	17.12	147.57	123.60
1	D	100	ARG	CD-NE-CZ	16.81	147.14	123.60
1	C	245	ARG	CD-NE-CZ	16.67	146.93	123.60
1	D	245	ARG	CD-NE-CZ	16.25	146.35	123.60
1	A	100	ARG	CD-NE-CZ	15.79	145.70	123.60
1	B	100	ARG	CD-NE-CZ	15.16	144.82	123.60
1	B	135	TRP	CD1-CG-CD2	8.16	112.83	106.30
1	D	135	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	A	135	TRP	CD1-CG-CD2	7.98	112.69	106.30
1	A	135	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	D	135	TRP	CE2-CD2-CG	-7.59	101.22	107.30
1	B	135	TRP	CE2-CD2-CG	-7.50	101.30	107.30
1	C	135	TRP	CE2-CD2-CG	-7.42	101.36	107.30
1	C	135	TRP	CD1-CG-CD2	7.41	112.23	106.30
1	D	241	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	135	TRP	CG-CD2-CE3	6.44	139.70	133.90
1	D	224	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	135	TRP	CG-CD2-CE3	6.42	139.68	133.90
1	D	135	TRP	CG-CD2-CE3	6.38	139.64	133.90
1	B	191	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	A	46	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	C	241	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	191	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	D	178	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	A	76	LEU	CA-CB-CG	6.06	129.23	115.30
1	B	219	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	C	135	TRP	CG-CD2-CE3	6.00	139.30	133.90
1	C	223	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	D	224	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	A	199	LEU	CA-CB-CG	5.93	128.95	115.30
1	C	224	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	B	76	LEU	CA-CB-CG	5.86	128.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	46	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	B	199	LEU	CA-CB-CG	5.80	128.65	115.30
1	D	159	TYR	CB-CG-CD1	-5.76	117.54	121.00
1	D	19	THR	CA-CB-CG2	5.72	120.41	112.40
1	A	191	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	A	22	LEU	CA-CB-CG	5.67	128.34	115.30
1	D	277	GLU	N-CA-C	5.65	126.27	111.00
1	C	277	GLU	N-CA-C	5.58	126.07	111.00
1	D	191	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	C	224	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	D	187	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	22	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	129	ASP	N-CA-C	-5.45	96.29	111.00
1	B	129	ASP	N-CA-C	-5.41	96.40	111.00
1	A	135	TRP	CB-CG-CD1	-5.40	119.98	127.00
1	D	140	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	115	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	D	135	TRP	CB-CG-CD1	-5.36	120.03	127.00
1	B	135	TRP	CB-CG-CD1	-5.33	120.07	127.00
1	A	219	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	D	286	ALA	N-CA-C	5.21	125.06	111.00
1	C	221	GLU	CA-CB-CG	5.19	124.82	113.40
1	D	219	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	135	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	C	159	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	B	191	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	C	286	ALA	N-CA-C	5.12	124.83	111.00
1	D	135	TRP	CG-CD1-NE1	-5.12	104.98	110.10
1	C	186	SER	CA-C-N	-5.10	105.98	117.20
1	D	221	GLU	CA-CB-CG	5.09	124.61	113.40
1	C	19	THR	CA-CB-CG2	5.09	119.52	112.40
1	C	178	ARG	NE-CZ-NH1	5.03	122.82	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	92	GLU	Peptide
1	B	92	GLU	Peptide
1	C	90	GLY	Peptide
1	D	90	GLY	Peptide

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	2190	0	2198	48	0
1	B	2190	0	2198	47	0
1	C	2190	0	2197	50	0
1	D	2190	0	2197	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	3	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	1	0
4	B	8	0	0	0	0
4	C	8	0	0	1	0
All	All	8888	0	8838	185	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (185) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ILE:HD13	1:A:151:CYS:HA	1.63	0.79
1:B:13:ILE:HD13	1:B:151:CYS:HA	1.65	0.78
1:C:186:SER:HB3	1:C:212:PRO:HA	1.68	0.75
1:D:186:SER:HB3	1:D:212:PRO:HA	1.68	0.74
1:C:33:VAL:HG12	1:C:121:PHE:HB2	1.68	0.73
1:D:33:VAL:HG12	1:D:121:PHE:HB2	1.69	0.73
1:D:38:CYS:SG	1:D:102:VAL:HG21	2.34	0.66
1:B:21:ASN:ND2	1:B:227:VAL:HG12	2.11	0.66
1:C:38:CYS:SG	1:C:102:VAL:HG21	2.36	0.66
1:D:284:LYS:HA	1:D:284:LYS:HE2	1.78	0.65
1:D:184:CYS:HB2	1:D:196:ILE:HG21	1.79	0.65
1:A:21:ASN:ND2	1:A:227:VAL:HG12	2.12	0.64
1:D:106:ILE:HD13	1:D:143:LYS:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:LYS:HA	1:C:284:LYS:HE2	1.79	0.63
1:C:106:ILE:HD13	1:C:143:LYS:HG2	1.80	0.63
1:B:106:ILE:HA	1:B:109:LEU:HD12	1.81	0.63
1:A:106:ILE:HA	1:A:109:LEU:HD12	1.82	0.62
1:B:278:ASP:HB3	1:B:281:ILE:HG12	1.84	0.60
1:D:20:GLN:HE22	1:D:47:LEU:H	1.48	0.60
1:D:186:SER:O	1:D:213:ARG:HG3	2.02	0.59
1:A:284:LYS:O	1:B:223:ARG:HD3	2.02	0.59
1:A:278:ASP:HB3	1:A:281:ILE:HG12	1.85	0.59
1:C:184:CYS:HB2	1:C:196:ILE:HG21	1.83	0.59
1:C:139:ILE:HA	1:C:177:VAL:HG11	1.85	0.59
1:D:15:LYS:O	1:D:19:THR:HB	2.03	0.59
1:C:20:GLN:HE22	1:C:47:LEU:H	1.51	0.58
1:D:34:MET:HA	1:D:84:LYS:O	2.03	0.58
1:A:5:CYS:HB3	1:A:146:GLU:HB2	1.85	0.58
1:C:21:ASN:HD21	1:C:227:VAL:H	1.53	0.57
1:D:139:ILE:HA	1:D:177:VAL:HG11	1.86	0.57
1:C:131:VAL:HG12	1:C:136:ALA:HB2	1.87	0.57
1:D:186:SER:CB	1:D:212:PRO:HA	2.33	0.57
1:D:131:VAL:HG12	1:D:136:ALA:HB2	1.86	0.56
1:C:46:ARG:HG3	1:C:51:SER:O	2.05	0.56
1:D:41:LYS:HD3	1:D:41:LYS:H	1.71	0.56
1:C:34:MET:HA	1:C:84:LYS:O	2.05	0.56
1:D:46:ARG:HG3	1:D:51:SER:O	2.06	0.56
1:C:15:LYS:O	1:C:19:THR:HB	2.06	0.56
1:C:98:ALA:HB3	4:C:2290:SF4:S1	2.46	0.56
1:C:186:SER:O	1:C:213:ARG:HG3	2.06	0.56
1:C:186:SER:CB	1:C:212:PRO:HA	2.35	0.55
1:B:5:CYS:HB3	1:B:146:GLU:HB2	1.88	0.55
1:A:21:ASN:HD21	1:A:227:VAL:H	1.54	0.55
1:C:41:LYS:HD3	1:C:41:LYS:H	1.72	0.54
1:D:21:ASN:HD21	1:D:227:VAL:H	1.55	0.54
1:A:184:CYS:HB2	1:A:196:ILE:HG21	1.90	0.54
1:B:215:ASN:HA	1:B:218:GLN:NE2	2.22	0.54
1:D:8:TYR:HB3	1:D:164:ILE:HD13	1.89	0.54
1:B:21:ASN:HD21	1:B:227:VAL:H	1.55	0.54
1:B:187:ARG:O	1:B:188:ASN:HB2	2.08	0.54
1:D:144:ALA:O	1:D:177:VAL:HG12	2.08	0.53
1:A:215:ASN:HA	1:A:218:GLN:NE2	2.23	0.53
1:C:141:GLU:O	1:C:143:LYS:HD2	2.08	0.53
1:B:279:GLU:O	1:B:282:VAL:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ARG:O	1:A:188:ASN:HB2	2.09	0.53
1:B:187:ARG:HB2	1:B:192:GLU:OE1	2.09	0.53
1:D:45:THR:HG22	1:D:85:CYS:HB2	1.90	0.52
1:B:146:GLU:HG2	1:B:253:LEU:HD21	1.91	0.52
1:C:8:TYR:HB3	1:C:164:ILE:HD13	1.91	0.52
1:C:162:ASN:HD21	1:C:259:ILE:H	1.58	0.52
1:A:229:GLU:O	1:B:285:THR:HG22	2.09	0.52
1:D:141:GLU:O	1:D:143:LYS:HD2	2.09	0.52
1:D:162:ASN:HD21	1:D:259:ILE:H	1.58	0.52
1:C:45:THR:HG22	1:C:85:CYS:HB2	1.92	0.51
1:A:223:ARG:HD3	1:B:284:LYS:O	2.11	0.51
1:A:279:GLU:O	1:A:282:VAL:HG12	2.11	0.50
1:D:213:ARG:HA	3:D:2292:ADP:N1	2.26	0.50
1:D:238:ASP:HA	1:D:241:ARG:HG2	1.93	0.50
1:A:45:THR:HB	1:A:85:CYS:HB3	1.94	0.50
1:A:187:ARG:HB2	1:A:192:GLU:OE1	2.10	0.50
1:C:144:ALA:O	1:C:177:VAL:HG12	2.12	0.50
1:A:144:ALA:HB1	1:A:147:ILE:HD11	1.93	0.50
1:D:26:LEU:HD13	1:D:244:ALA:HB1	1.94	0.50
1:A:146:GLU:HG2	1:A:253:LEU:HD21	1.93	0.49
1:B:184:CYS:HB2	1:B:196:ILE:HG21	1.94	0.49
1:A:149:ILE:HB	1:A:182:LEU:HD23	1.95	0.49
1:C:26:LEU:HD13	1:C:244:ALA:HB1	1.93	0.49
1:A:20:GLN:HE22	1:A:47:LEU:N	2.11	0.49
1:B:45:THR:HB	1:B:85:CYS:HB3	1.95	0.49
1:A:5:CYS:O	1:A:123:PHE:HA	2.13	0.48
1:A:124:TYR:O	1:A:126:VAL:HG12	2.13	0.48
1:C:23:VAL:HG11	1:C:35:ILE:HD11	1.95	0.48
1:D:145:GLN:HG3	1:D:176:SER:HB2	1.95	0.48
1:B:20:GLN:HE22	1:B:47:LEU:N	2.11	0.48
1:B:124:TYR:O	1:B:126:VAL:HG12	2.13	0.48
1:B:144:ALA:HB1	1:B:147:ILE:HD11	1.96	0.48
1:B:5:CYS:O	1:B:123:PHE:HA	2.13	0.48
1:A:185:ASN:HD21	3:A:1291:ADP:N6	2.11	0.48
1:C:145:GLN:HG3	1:C:176:SER:HB2	1.96	0.48
1:C:238:ASP:HA	1:C:241:ARG:HG2	1.94	0.48
1:B:149:ILE:HB	1:B:182:LEU:HD23	1.96	0.48
1:A:131:VAL:HG12	1:A:136:ALA:HB2	1.96	0.47
1:B:32:LYS:NZ	1:B:84:LYS:HE2	2.29	0.47
1:D:13:ILE:HD12	1:D:150:VAL:O	2.15	0.47
1:A:97:CYS:SG	1:A:98:ALA:N	2.86	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ILE:O	1:A:106:ILE:HG13	2.14	0.47
1:D:5:CYS:SG	1:D:146:GLU:HG3	2.54	0.47
1:C:158:MET:SD	1:C:268:LEU:HD21	2.54	0.47
1:A:8:TYR:HB3	1:A:164:ILE:HD13	1.96	0.47
1:B:10:LYS:HB3	1:B:13:ILE:HD11	1.97	0.47
1:D:158:MET:SD	1:D:268:LEU:HD21	2.55	0.47
1:A:25:ALA:HB1	1:A:241:ARG:HA	1.97	0.47
1:C:24:ALA:CB	1:C:226:THR:HG21	2.45	0.47
1:A:10:LYS:HB3	1:A:13:ILE:HD11	1.97	0.47
1:C:23:VAL:HG13	1:C:33:VAL:HG21	1.98	0.46
1:D:23:VAL:HG11	1:D:35:ILE:HD11	1.97	0.46
1:D:184:CYS:SG	1:D:196:ILE:HG13	2.55	0.46
1:A:32:LYS:NZ	1:A:84:LYS:HE2	2.30	0.46
1:B:103:ILE:O	1:B:106:ILE:HG13	2.15	0.46
1:D:24:ALA:CB	1:D:226:THR:HG21	2.45	0.46
1:C:217:VAL:O	1:C:221:GLU:HG2	2.16	0.46
1:B:99:GLY:HA3	1:B:134:GLY:O	2.16	0.46
1:A:2:MET:HA	1:A:120:ASP:O	2.16	0.46
1:A:21:ASN:HD21	1:A:227:VAL:N	2.12	0.46
1:A:48:ILE:HG21	1:A:83:VAL:HG23	1.98	0.46
1:B:25:ALA:HB1	1:B:241:ARG:HA	1.97	0.46
1:B:131:VAL:HG12	1:B:136:ALA:HB2	1.98	0.45
1:B:21:ASN:HD21	1:B:227:VAL:N	2.14	0.45
1:C:54:GLN:HG2	1:C:55:ASN:N	2.32	0.45
1:C:13:ILE:HD12	1:C:150:VAL:O	2.16	0.45
1:B:48:ILE:HG21	1:B:83:VAL:HG23	1.98	0.45
1:D:20:GLN:NE2	1:D:47:LEU:H	2.14	0.45
1:C:184:CYS:SG	1:C:196:ILE:HG13	2.56	0.45
1:D:217:VAL:O	1:D:221:GLU:HG2	2.16	0.45
1:B:39:ASP:HB3	1:B:41:LYS:NZ	2.31	0.45
1:C:5:CYS:SG	1:C:146:GLU:HG3	2.56	0.45
1:A:16:SER:HB2	3:A:1291:ADP:O1A	2.17	0.44
1:B:206:GLN:H	1:B:206:GLN:HE21	1.65	0.44
1:B:8:TYR:HB3	1:B:164:ILE:HD13	1.98	0.44
1:A:99:GLY:HA3	1:A:134:GLY:O	2.18	0.44
1:C:56:THR:HG22	1:C:87:GLU:HB3	1.99	0.44
1:D:117:ASP:HB2	1:D:119:LEU:HD13	2.00	0.44
1:D:245:ARG:HD2	1:D:245:ARG:HA	1.83	0.44
1:B:2:MET:HA	1:B:120:ASP:O	2.17	0.44
1:C:7:ILE:HD13	1:C:148:TYR:HB2	2.00	0.44
1:A:158:MET:SD	1:A:268:LEU:HD21	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:CYS:SG	1:B:98:ALA:N	2.90	0.43
1:A:47:LEU:O	1:A:225:MET:HA	2.18	0.43
1:B:158:MET:SD	1:B:268:LEU:HD21	2.58	0.43
1:A:26:LEU:HD13	1:A:244:ALA:HB1	2.01	0.43
1:A:39:ASP:HB3	1:A:41:LYS:NZ	2.33	0.43
1:D:56:THR:HG22	1:D:87:GLU:HB3	2.01	0.43
1:C:76:LEU:HD11	1:C:84:LYS:HB3	2.01	0.43
1:A:206:GLN:HE21	1:A:206:GLN:H	1.67	0.43
1:C:226:THR:HG22	1:C:228:ILE:H	1.84	0.43
1:D:7:ILE:HD13	1:D:148:TYR:HB2	2.00	0.43
1:D:54:GLN:HG2	1:D:55:ASN:N	2.33	0.43
1:B:97:CYS:SG	1:B:134:GLY:HA3	2.59	0.42
1:D:226:THR:HG22	1:D:228:ILE:H	1.84	0.42
1:A:35:ILE:HD11	1:A:83:VAL:HB	2.02	0.42
1:C:106:ILE:O	1:C:110:GLU:HG2	2.18	0.42
1:B:80:TYR:O	1:B:83:VAL:HG22	2.20	0.42
1:C:117:ASP:HB2	1:C:119:LEU:HD13	2.02	0.42
1:B:54:GLN:HE22	1:B:86:VAL:HA	1.85	0.42
1:D:106:ILE:O	1:D:110:GLU:HG2	2.19	0.42
1:B:35:ILE:HD11	1:B:83:VAL:HB	2.01	0.42
1:D:84:LYS:CE	1:D:119:LEU:HD11	2.50	0.42
1:A:16:SER:O	1:A:20:GLN:HG3	2.20	0.42
1:C:22:LEU:HD13	1:C:243:LEU:HG	2.02	0.42
1:C:268:LEU:HD22	1:C:273:ILE:HG21	2.03	0.41
1:A:97:CYS:SG	1:A:134:GLY:HA3	2.61	0.41
1:A:285:THR:HG22	1:B:229:GLU:O	2.20	0.41
1:A:15:LYS:HB2	3:A:1291:ADP:O1B	2.21	0.41
1:B:140:ARG:HA	1:B:171:TYR:CE1	2.55	0.41
1:C:20:GLN:NE2	1:C:47:LEU:H	2.17	0.41
1:A:223:ARG:HA	1:B:282:VAL:HA	2.03	0.41
1:B:47:LEU:O	1:B:225:MET:HA	2.20	0.41
1:C:146:GLU:HB3	1:C:253:LEU:HD21	2.02	0.41
1:A:97:CYS:SG	1:A:99:GLY:N	2.94	0.41
1:B:21:ASN:HD21	1:B:227:VAL:HG12	1.84	0.41
1:C:206:GLN:HE21	1:C:206:GLN:H	1.68	0.41
1:D:23:VAL:HG13	1:D:33:VAL:HG21	2.02	0.41
1:D:146:GLU:HB3	1:D:253:LEU:HD21	2.02	0.41
1:A:166:LYS:O	1:A:169:VAL:HB	2.20	0.41
1:B:26:LEU:HD13	1:B:244:ALA:HB1	2.02	0.41
1:C:84:LYS:CE	1:C:119:LEU:HD11	2.51	0.40
1:C:236:GLN:O	1:C:239:GLU:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLU:HB3	1:D:253:LEU:CD2	2.51	0.40
1:B:166:LYS:O	1:B:169:VAL:HB	2.20	0.40
1:C:56:THR:OG1	1:C:59:GLU:HG2	2.22	0.40
1:A:7:ILE:HG21	1:A:19:THR:OG1	2.21	0.40
1:D:76:LEU:HD11	1:D:84:LYS:HB3	2.02	0.40
1:B:215:ASN:HA	1:B:218:GLN:HE21	1.85	0.40
1:C:106:ILE:HA	1:C:109:LEU:HD12	2.03	0.40
1:C:146:GLU:HB3	1:C:253:LEU:CD2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	287/289 (99%)	258 (90%)	25 (9%)	4 (1%)	11	46
1	B	287/289 (99%)	258 (90%)	25 (9%)	4 (1%)	11	46
1	C	287/289 (99%)	258 (90%)	22 (8%)	7 (2%)	6	34
1	D	287/289 (99%)	258 (90%)	22 (8%)	7 (2%)	6	34
All	All	1148/1156 (99%)	1032 (90%)	94 (8%)	22 (2%)	8	39

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	ASP
1	B	190	ASP
1	C	118	ASP
1	C	137	MET
1	D	118	ASP
1	D	137	MET
1	A	14	GLY

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Mol	Chain	Res	Type
1	A	64	ALA
1	B	14	GLY
1	B	64	ALA
1	C	234	ALA
1	C	285	THR
1	D	285	THR
1	C	64	ALA
1	D	64	ALA
1	D	234	ALA
1	C	91	PRO
1	D	91	PRO
1	D	93	PRO
1	C	93	PRO
1	A	128	GLY
1	B	128	GLY

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	233/233 (100%)	211 (91%)	22 (9%)	8 33
1	B	233/233 (100%)	209 (90%)	24 (10%)	7 29
1	C	233/233 (100%)	210 (90%)	23 (10%)	8 30
1	D	233/233 (100%)	210 (90%)	23 (10%)	8 30
All	All	932/932 (100%)	840 (90%)	92 (10%)	8 30

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	CYS
1	A	50	HIS
1	A	58	MET
1	A	75	VAL
1	A	91	PRO
1	A	110	GLU

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Mol	Chain	Res	Type
1	A	112	GLU
1	A	117	ASP
1	A	127	LEU
1	A	129	ASP
1	A	142	ASN
1	A	155	MET
1	A	170	LYS
1	A	187	ARG
1	A	189	THR
1	A	193	ASP
1	A	206	GLN
1	A	255	ILE
1	A	277	GLU
1	A	279	GLU
1	A	287	GLU
1	A	289	VAL
1	B	5	CYS
1	B	50	HIS
1	B	58	MET
1	B	75	VAL
1	B	91	PRO
1	B	110	GLU
1	B	112	GLU
1	B	117	ASP
1	B	127	LEU
1	B	129	ASP
1	B	142	ASN
1	B	155	MET
1	B	163	ASN
1	B	170	LYS
1	B	187	ARG
1	B	189	THR
1	B	193	ASP
1	B	206	GLN
1	B	245	ARG
1	B	255	ILE
1	B	277	GLU
1	B	279	GLU
1	B	287	GLU
1	B	289	VAL
1	C	19	THR
1	C	26	LEU

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Mol	Chain	Res	Type
1	C	40	PRO
1	C	41	LYS
1	C	60	MET
1	C	68	GLU
1	C	69	ASP
1	C	76	LEU
1	C	77	LYS
1	C	137	MET
1	C	185	ASN
1	C	203	LEU
1	C	206	GLN
1	C	219	ARG
1	C	221	GLU
1	C	233	LYS
1	C	245	ARG
1	C	249	ASP
1	C	251	LYS
1	C	262	ASP
1	C	264	LEU
1	C	279	GLU
1	C	284	LYS
1	D	19	THR
1	D	26	LEU
1	D	40	PRO
1	D	41	LYS
1	D	60	MET
1	D	68	GLU
1	D	69	ASP
1	D	76	LEU
1	D	77	LYS
1	D	137	MET
1	D	185	ASN
1	D	203	LEU
1	D	206	GLN
1	D	219	ARG
1	D	221	GLU
1	D	233	LYS
1	D	249	ASP
1	D	251	LYS
1	D	262	ASP
1	D	264	LEU
1	D	279	GLU

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Mol	Chain	Res	Type
1	D	284	LYS
1	D	288	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	21	ASN
1	A	145	GLN
1	A	162	ASN
1	A	163	ASN
1	A	173	ASN
1	A	185	ASN
1	A	206	GLN
1	A	218	GLN
1	B	20	GLN
1	B	21	ASN
1	B	145	GLN
1	B	162	ASN
1	B	163	ASN
1	B	173	ASN
1	B	185	ASN
1	B	206	GLN
1	B	218	GLN
1	C	20	GLN
1	C	21	ASN
1	C	54	GLN
1	C	107	ASN
1	C	162	ASN
1	C	173	ASN
1	C	206	GLN
1	C	218	GLN
1	D	20	GLN
1	D	21	ASN
1	D	54	GLN
1	D	162	ASN
1	D	163	ASN
1	D	206	GLN
1	D	218	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	D	2292	2	24,29,29	1.66	4 (16%)	29,45,45	1.65	8 (27%)
4	SF4	C	2290	1	0,12,12	-	-	-		
3	ADP	C	2291	2	24,29,29	1.60	3 (12%)	29,45,45	1.76	8 (27%)
3	ADP	A	1291	2	24,29,29	2.02	3 (12%)	29,45,45	1.84	7 (24%)
3	ADP	B	1292	2	24,29,29	1.65	3 (12%)	29,45,45	1.67	6 (20%)
4	SF4	B	1290	1	0,12,12	-	-	-		

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	D	2292	2	-	0/12/32/32	0/3/3/3
4	SF4	C	2290	1	-	-	0/6/5/5
3	ADP	C	2291	2	-	1/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	1291	2	-	1/12/32/32	0/3/3/3
3	ADP	B	1292	2	-	2/12/32/32	0/3/3/3
4	SF4	B	1290	1	-	-	0/6/5/5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1291	ADP	PB-O1B	7.75	1.75	1.50
3	B	1292	ADP	PB-O3B	5.81	1.77	1.54
3	D	2292	ADP	PB-O3B	5.62	1.76	1.54
3	C	2291	ADP	PB-O3B	5.58	1.76	1.54
3	A	1291	ADP	O4'-C1'	3.78	1.46	1.41
3	D	2292	ADP	O4'-C1'	3.77	1.46	1.41
3	B	1292	ADP	O4'-C1'	3.51	1.46	1.41
3	C	2291	ADP	O4'-C1'	3.33	1.45	1.41
3	C	2291	ADP	C2'-C3'	-2.36	1.46	1.53
3	D	2292	ADP	C2'-C3'	-2.34	1.46	1.53
3	D	2292	ADP	C8-N7	-2.21	1.30	1.34
3	B	1292	ADP	C8-N7	-2.18	1.30	1.34
3	A	1291	ADP	C2'-C3'	-2.02	1.47	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1291	ADP	C3'-C2'-C1'	-4.71	93.89	100.98
3	B	1292	ADP	C3'-C2'-C1'	-4.67	93.95	100.98
3	C	2291	ADP	C3'-C2'-C1'	-4.15	94.73	100.98
3	D	2292	ADP	C3'-C2'-C1'	-3.83	95.21	100.98
3	C	2291	ADP	O2B-PB-O3A	3.68	116.97	104.64
3	A	1291	ADP	O2B-PB-O1B	-3.67	96.32	110.68
3	B	1292	ADP	O2B-PB-O3A	3.35	115.86	104.64
3	A	1291	ADP	O2B-PB-O3A	3.27	115.62	104.64
3	A	1291	ADP	O3B-PB-O3A	3.21	115.42	104.64
3	C	2291	ADP	O4'-C4'-C3'	-3.06	99.06	105.11
3	B	1292	ADP	C2'-C3'-C4'	-2.98	96.85	102.64
3	B	1292	ADP	O3B-PB-O2B	-2.91	96.51	107.64
3	A	1291	ADP	C2'-C3'-C4'	-2.84	97.12	102.64
3	D	2292	ADP	O2B-PB-O3A	2.73	113.78	104.64
3	D	2292	ADP	C2'-C3'-C4'	-2.59	97.61	102.64
3	D	2292	ADP	O3B-PB-O1B	-2.54	100.75	110.68
3	C	2291	ADP	C5-C6-N6	2.53	124.19	120.35
3	C	2291	ADP	C2'-C3'-C4'	-2.50	97.79	102.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	2291	ADP	C1'-N9-C4	-2.47	122.31	126.64
3	D	2292	ADP	C1'-N9-C4	-2.43	122.36	126.64
3	D	2292	ADP	PA-O3A-PB	-2.39	124.63	132.83
3	D	2292	ADP	O4'-C4'-C3'	-2.31	100.53	105.11
3	D	2292	ADP	C5-C6-N6	2.31	123.86	120.35
3	C	2291	ADP	PA-O3A-PB	-2.20	125.27	132.83
3	A	1291	ADP	O3B-PB-O1B	-2.16	102.21	110.68
3	A	1291	ADP	O3B-PB-O2B	2.13	115.79	107.64
3	B	1292	ADP	O4'-C4'-C3'	-2.06	101.04	105.11
3	C	2291	ADP	O5'-PA-O1A	-2.05	101.06	109.07
3	B	1292	ADP	O3B-PB-O1B	-2.01	102.80	110.68

There are no chirality outliers.

All (4) torsion outliers are listed below:

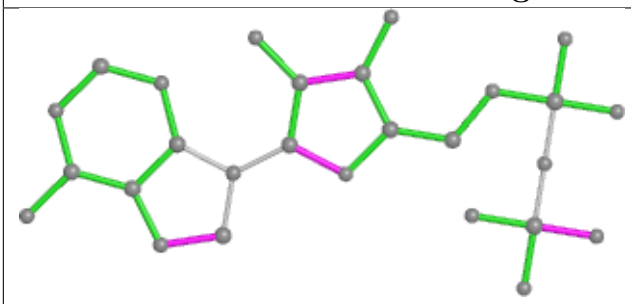
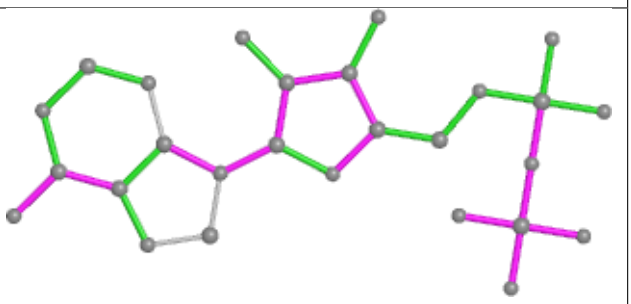
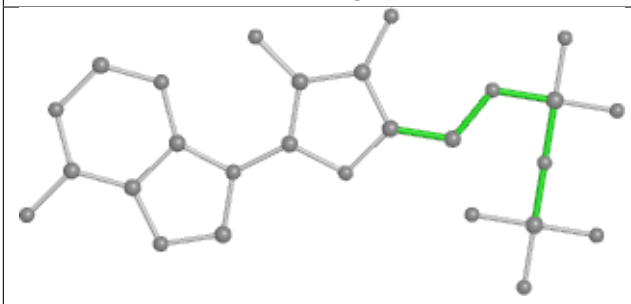
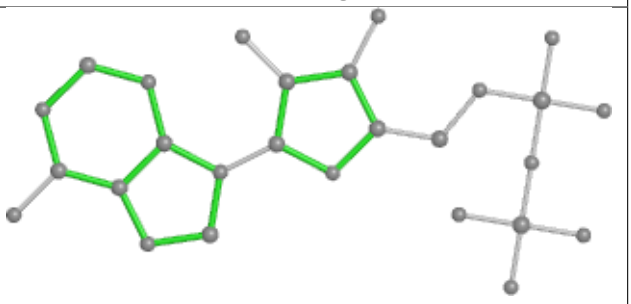
Mol	Chain	Res	Type	Atoms
3	B	1292	ADP	PA-O3A-PB-O3B
3	C	2291	ADP	PA-O3A-PB-O2B
3	A	1291	ADP	PA-O3A-PB-O2B
3	B	1292	ADP	PA-O3A-PB-O2B

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2292	ADP	1	0
4	C	2290	SF4	1	0
3	A	1291	ADP	3	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 D 2292	
 Bond lengths	 Bond angles
 Torsions	 Rings

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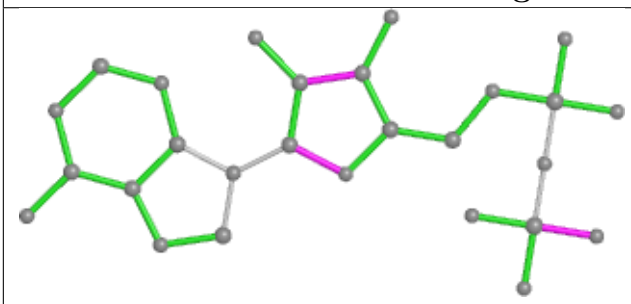
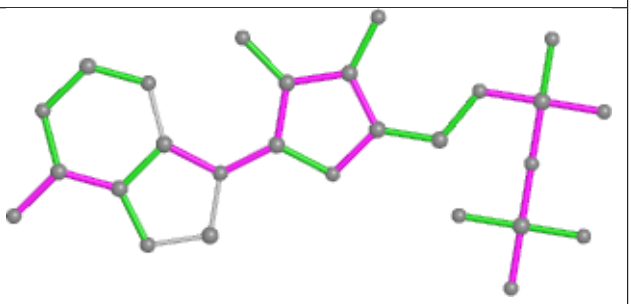
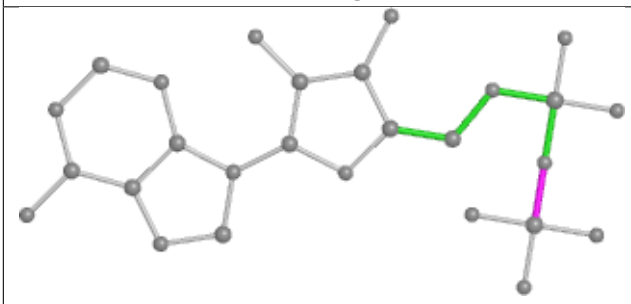
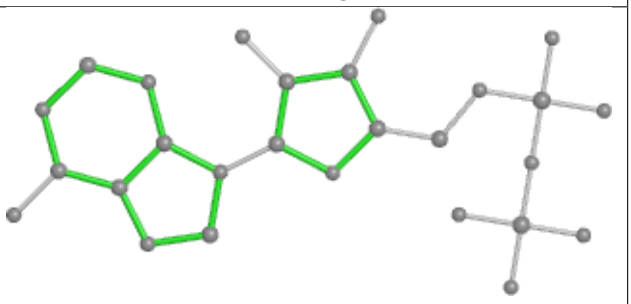
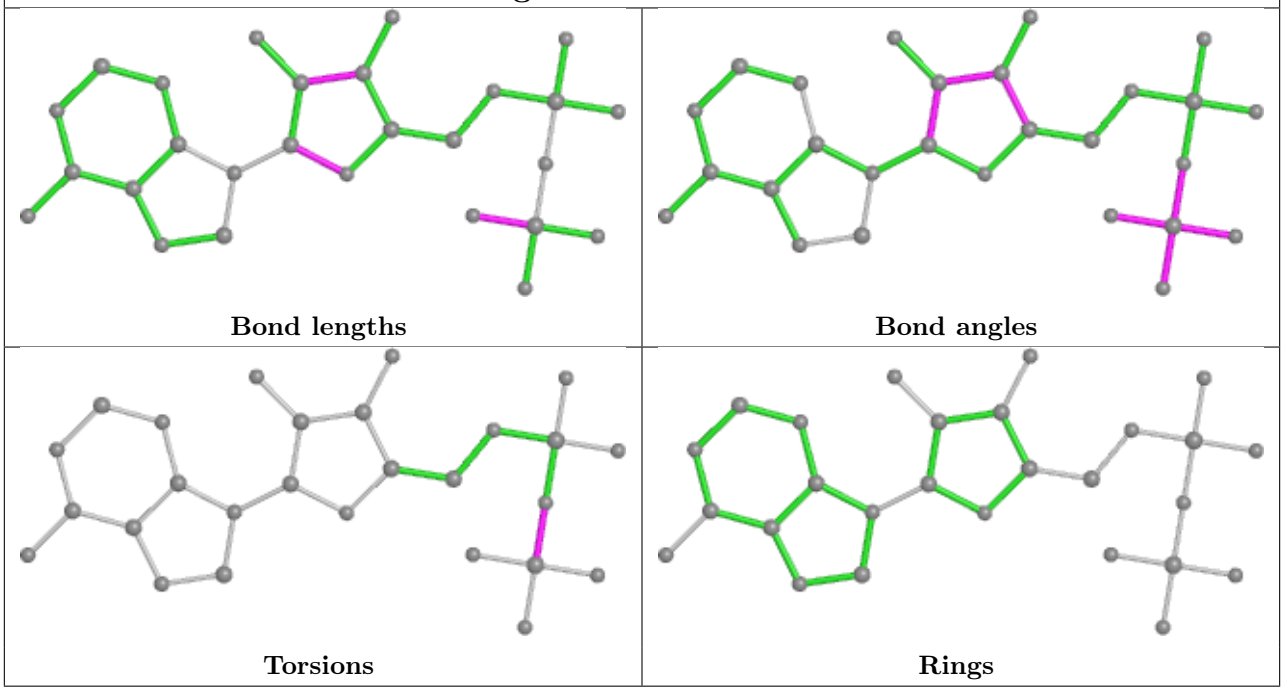
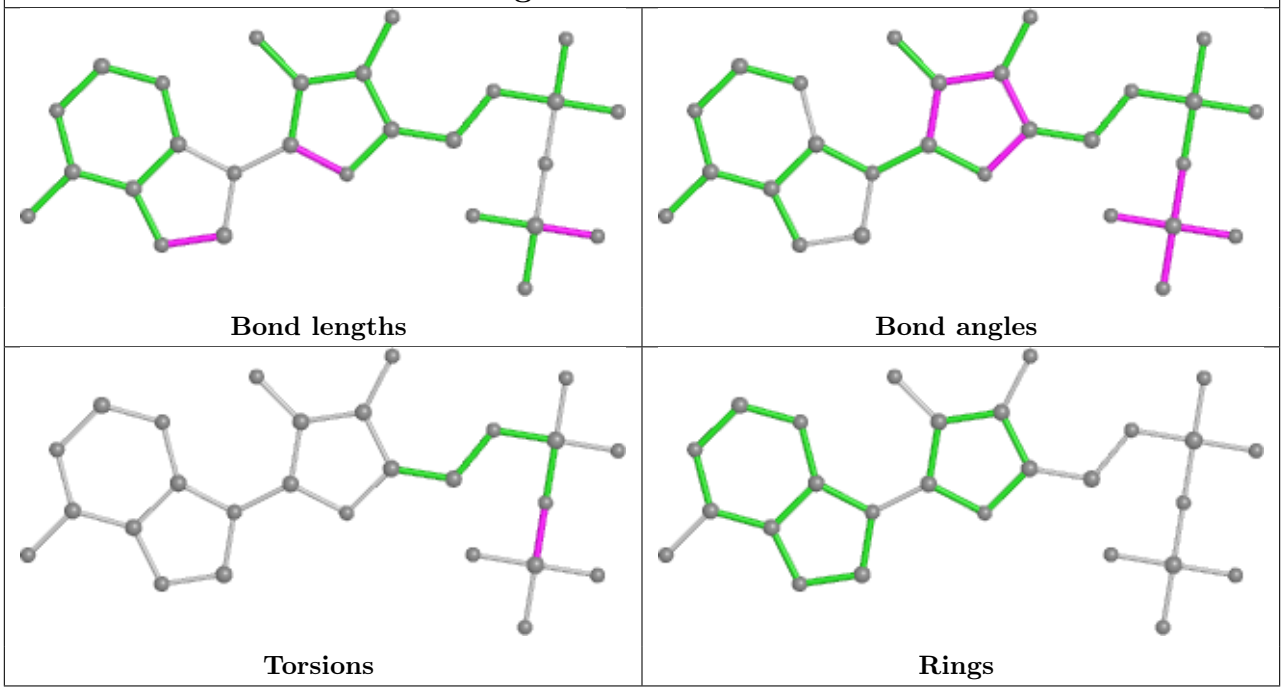
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 1291



Ligand ADP B 1292



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	289/289 (100%)	0.11	5 (1%)	70	57	39, 85, 100, 100	0
1	B	289/289 (100%)	0.13	4 (1%)	75	63	39, 85, 100, 100	0
1	C	289/289 (100%)	-0.18	7 (2%)	59	44	21, 65, 99, 100	0
1	D	289/289 (100%)	-0.19	3 (1%)	82	72	20, 66, 99, 100	0
All	All	1156/1156 (100%)	-0.03	19 (1%)	72	59	20, 75, 100, 100	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	VAL	3.6
1	B	1	ALA	3.3
1	A	96	GLY	3.3
1	D	65	GLY	3.1
1	A	69	ASP	2.9
1	C	287	GLU	2.9
1	B	74	ASP	2.8
1	C	116	GLU	2.8
1	B	96	GLY	2.7
1	A	1	ALA	2.7
1	D	277	GLU	2.6
1	C	277	GLU	2.6
1	C	280	SER	2.6
1	D	116	GLU	2.4
1	A	73	GLU	2.3
1	C	283	GLY	2.2
1	A	226	THR	2.2
1	B	73	GLU	2.1
1	C	281	ILE	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

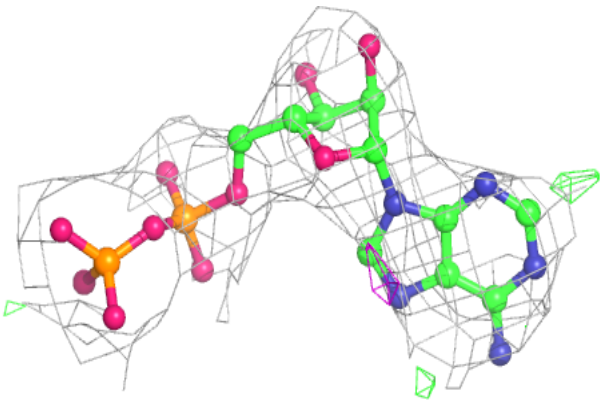
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

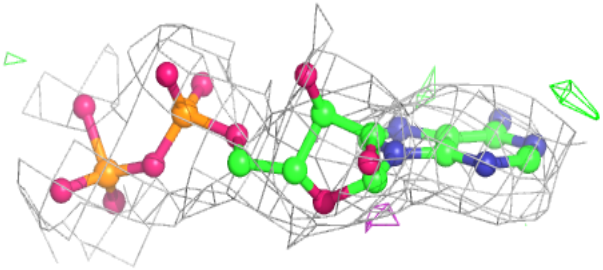
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	A	1293	1/1	0.92	0.08	19,19,19,19	0
2	MG	C	2293	1/1	0.92	0.07	7,7,7,7	0
2	MG	B	1294	1/1	0.93	0.12	41,41,41,41	0
3	ADP	A	1291	27/27	0.95	0.16	48,64,71,73	0
3	ADP	B	1292	27/27	0.95	0.14	50,63,70,71	0
2	MG	D	2294	1/1	0.96	0.05	2,2,2,2	0
3	ADP	C	2291	27/27	0.96	0.14	41,51,57,60	0
3	ADP	D	2292	27/27	0.96	0.17	38,46,58,61	0
4	SF4	B	1290	8/8	0.96	0.08	50,60,63,64	0
4	SF4	C	2290	8/8	0.99	0.06	41,49,52,53	0

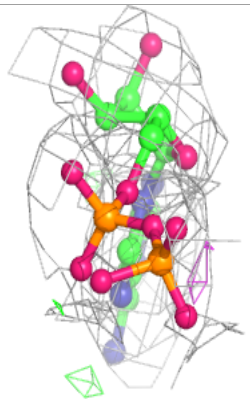
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 1291:

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

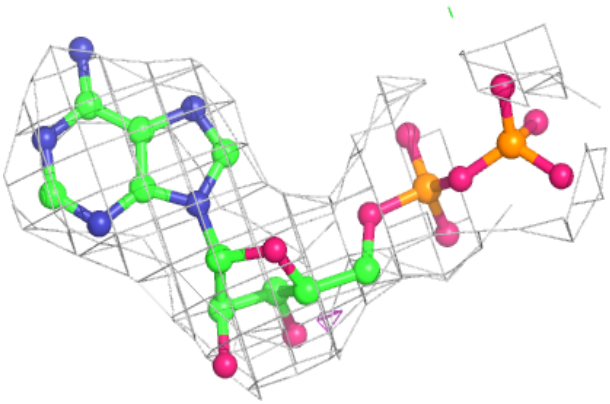


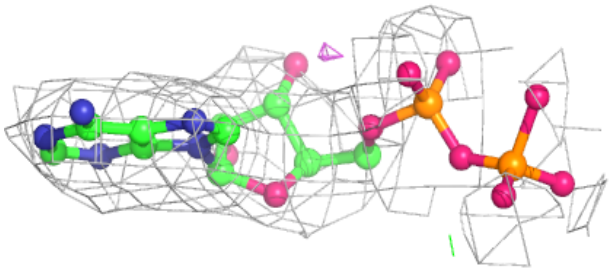


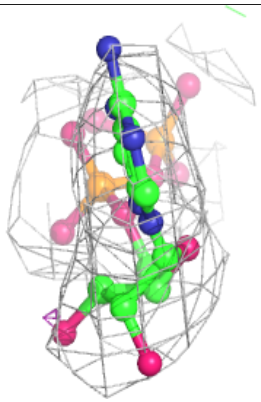


Electron density around ADP B 1292:

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

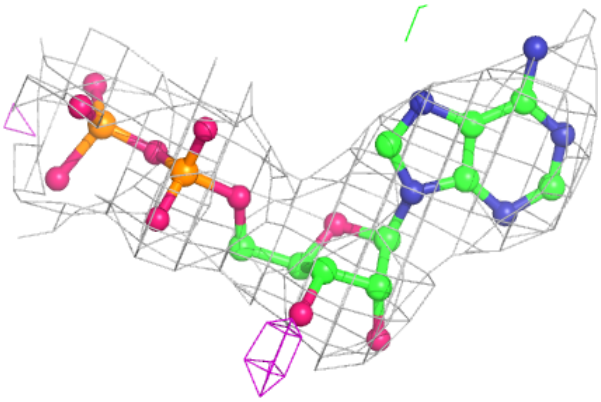


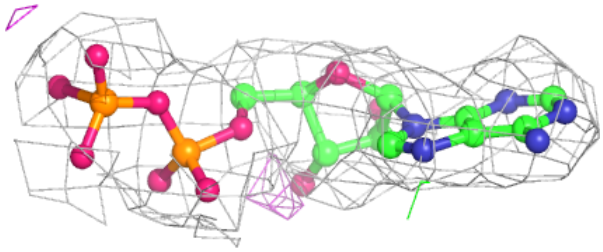


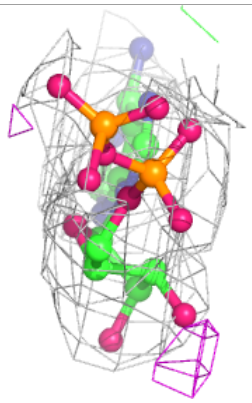


Electron density around ADP C 2291:

$2mF_o$-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 2292:

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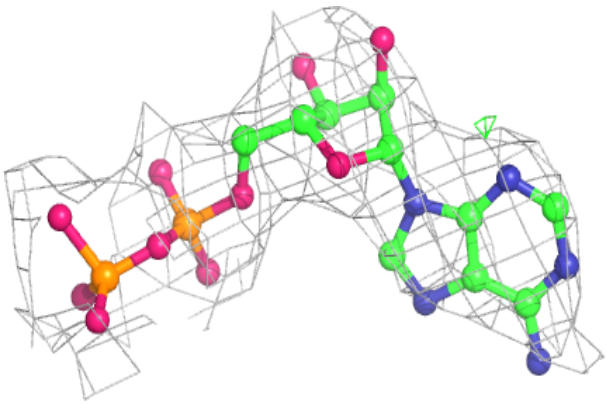
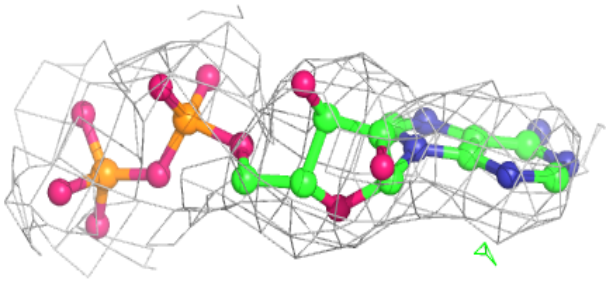
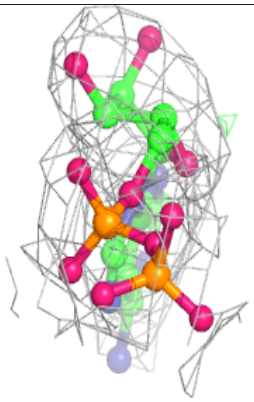
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.