Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 03:06 PM EST

PDB ID	:	1R0Y
Title	:	Cystic fibrosis transmembrane conductance regulator (CFTR) nucleotide-binding domain one (NBD1) with ADP
Authors	:	Lewis, H.A.; Buchanan, S.G.; Burley, S.K.; Conners, K.; Dickey, M.; Dorwart, M.; Fowler, R.; Gao, X.; Guggino, W.B.; Hendrickson, W.A.
Deposited on	:	2003-09-23
Resolution	:	2.55 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 following versions of software and data (see references ⓘ) were used in the production of this report:

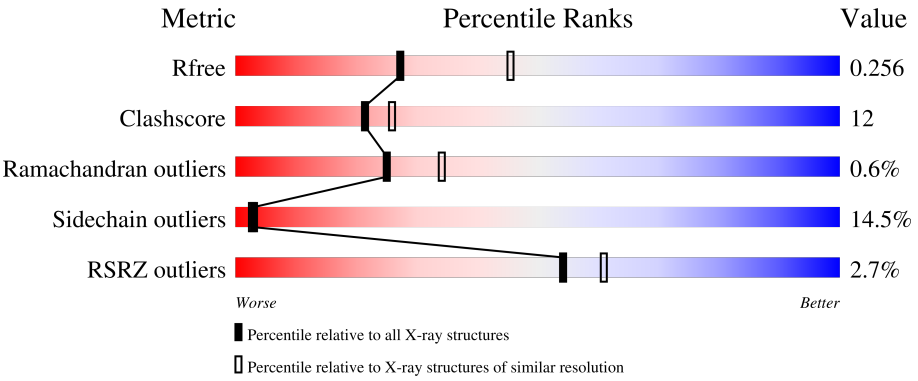
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	286	63% 23% 6% 7%
1	B	286	64% 20% 9% 7%
1	C	286	66% 22% 5% 7%
1	D	286	6% 51% 33% 7% 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8853 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.

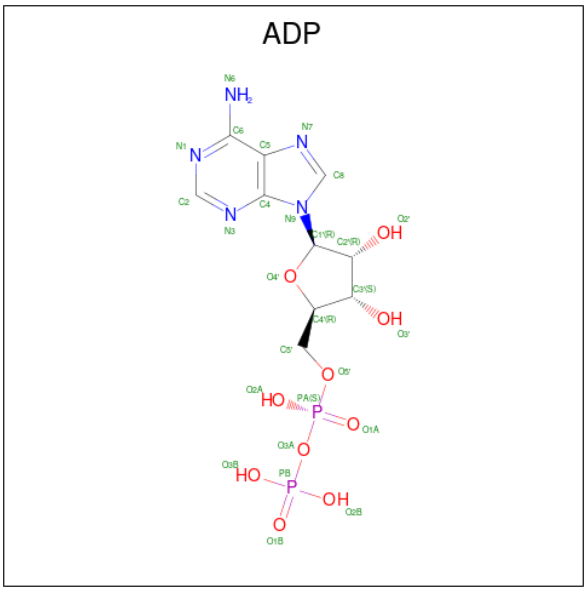
- Molecule 1 is a protein called Cystic fibrosis transmembrane conductance regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2098	1336	347	403	12			
1	B	267	Total	C	N	O	S	0	0	0
			2105	1340	348	405	12			
1	C	267	Total	C	N	O	S	0	0	0
			2105	1340	348	405	12			
1	D	264	Total	C	N	O	S	0	0	0
			2083	1328	344	399	12			

There are 4 discrepancies between the modelled and reference sequences:

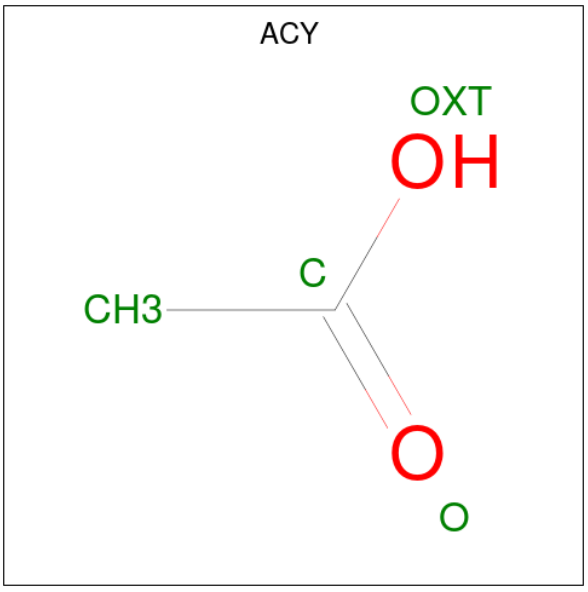
Chain	Residue	Modelled	Actual	Comment	Reference
A	388	SER	-	cloning artifact	UNP P26361
B	388	SER	-	cloning artifact	UNP P26361
C	388	SER	-	cloning artifact	UNP P26361
D	388	SER	-	cloning artifact	UNP P26361

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 4 is water.

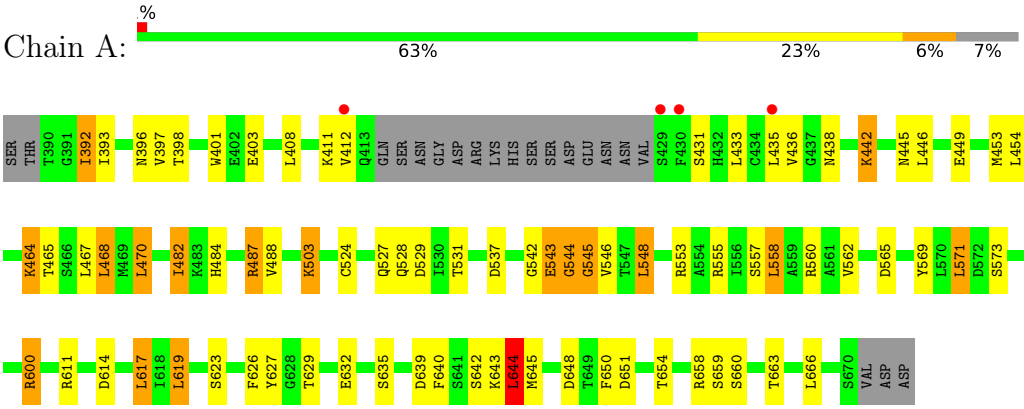
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	98	Total O 98 98	0	0
4	B	86	Total O 86 86	0	0
4	C	79	Total O 79 79	0	0
4	D	67	Total O 67 67	0	0

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.

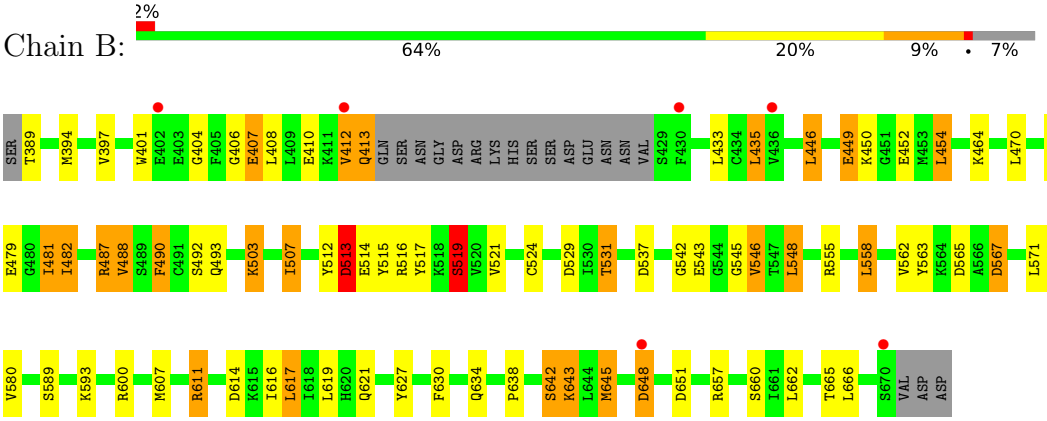
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain A:



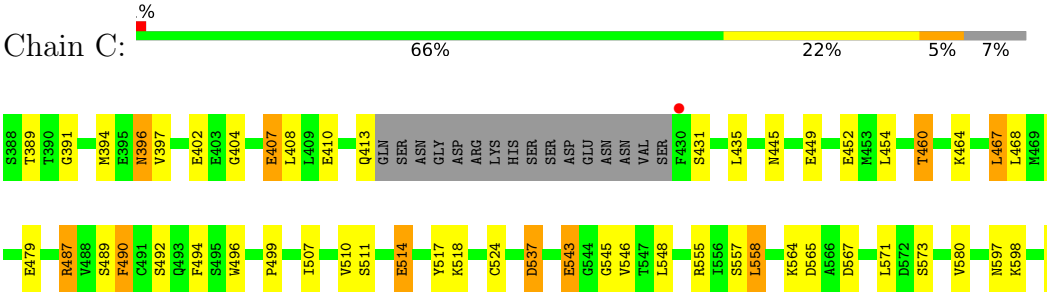
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

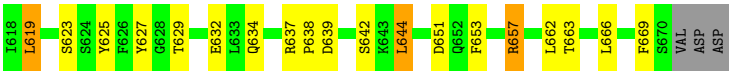
Chain B:



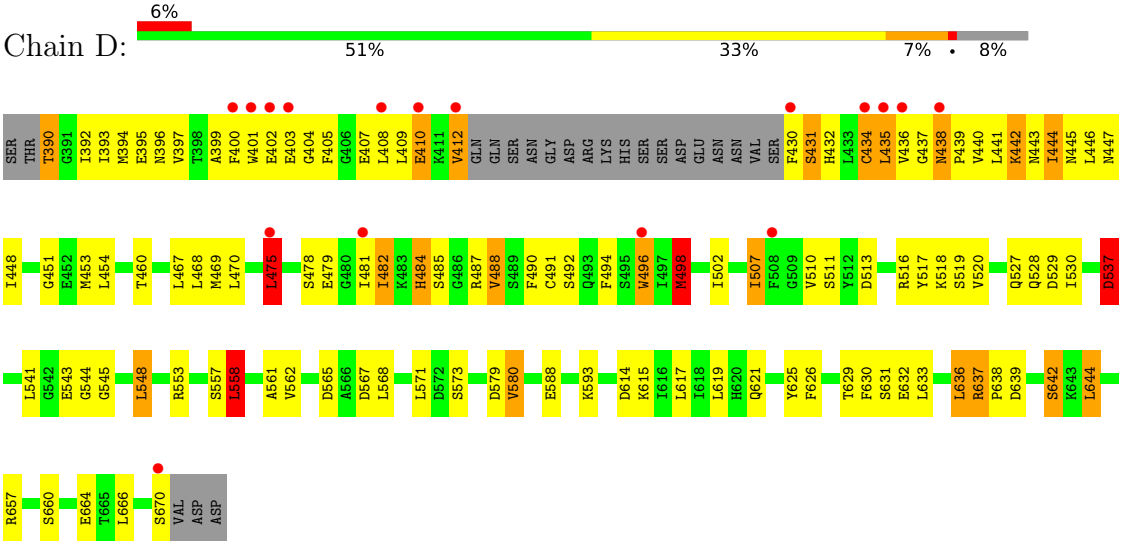
• Molecule 1: Cystic fibrosis transmembrane conductance regulator

Chain C:





• Molecule 1: Cystic fibrosis transmembrane conductance regulator



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α, β, γ	171.87Å 171.87Å 109.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.00 – 2.55 121.53 – 2.39	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.00-2.55) 99.3 (121.53-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.257 0.200 , 0.256	Depositor DCC
R_{free} test set	3303 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	44.5	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8853	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACY, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.17	3/2133 (0.1%)	1.18	18/2868 (0.6%)
1	B	1.17	1/2140 (0.0%)	1.23	20/2878 (0.7%)
1	C	1.18	1/2140 (0.0%)	1.15	9/2878 (0.3%)
1	D	1.10	5/2118 (0.2%)	1.17	13/2848 (0.5%)
All	All	1.16	10/8531 (0.1%)	1.18	60/11472 (0.5%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	498	MET	CG-SD	6.98	1.99	1.81
1	A	627	TYR	CD2-CE2	6.79	1.49	1.39
1	D	537	ASP	CB-CG	-6.23	1.38	1.51
1	D	496	TRP	CB-CG	-5.99	1.39	1.50
1	A	545	GLY	CA-C	5.64	1.60	1.51
1	D	520	VAL	CB-CG2	5.62	1.64	1.52
1	A	569	TYR	CE2-CZ	5.23	1.45	1.38
1	B	490	PHE	CE1-CZ	5.20	1.47	1.37
1	C	490	PHE	CE1-CZ	5.11	1.47	1.37
1	D	453	MET	CG-SD	-5.10	1.67	1.81

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	565	ASP	CB-CG-OD2	9.16	126.54	118.30
1	B	651	ASP	CB-CG-OD1	9.04	126.44	118.30
1	D	579	ASP	CB-CG-OD2	8.94	126.34	118.30
1	D	644	LEU	CA-CB-CG	-8.51	95.73	115.30
1	B	513	ASP	CB-CG-OD2	8.40	125.86	118.30
1	B	537	ASP	CB-CG-OD2	8.40	125.86	118.30
1	B	529	ASP	CB-CG-OD2	8.15	125.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	565	ASP	CB-CG-OD2	8.05	125.55	118.30
1	B	614	ASP	CB-CG-OD2	7.91	125.42	118.30
1	A	565	ASP	CB-CG-OD2	7.72	125.25	118.30
1	A	529	ASP	CB-CG-OD2	7.26	124.83	118.30
1	C	614	ASP	CB-CG-OD2	7.11	124.70	118.30
1	C	558	LEU	CB-CG-CD2	7.05	122.99	111.00
1	D	639	ASP	CB-CG-OD2	6.83	124.45	118.30
1	D	529	ASP	CB-CG-OD2	6.79	124.42	118.30
1	D	558	LEU	CB-CG-CD2	6.71	122.40	111.00
1	B	611	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	A	651	ASP	CB-CG-OD2	6.41	124.07	118.30
1	A	644	LEU	CA-CB-CG	-6.41	100.57	115.30
1	A	648	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	567	ASP	CB-CG-OD2	6.38	124.04	118.30
1	D	580	VAL	CG1-CB-CG2	6.35	121.06	110.90
1	A	600	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	548	LEU	CB-CG-CD1	6.34	121.77	111.00
1	C	644	LEU	CA-CB-CG	-6.31	100.80	115.30
1	B	531	THR	OG1-CB-CG2	-6.27	95.57	110.00
1	A	614	ASP	CB-CG-OD2	6.27	123.94	118.30
1	B	572	ASP	CB-CG-OD2	6.25	123.92	118.30
1	C	639	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	446	LEU	CB-CG-CD2	-6.18	100.49	111.00
1	A	611	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	C	565	ASP	CB-CG-OD2	6.15	123.84	118.30
1	D	513	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	560	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	600	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	A	611	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	454	LEU	CB-CG-CD2	5.94	121.10	111.00
1	A	571	LEU	CA-CB-CG	5.82	128.69	115.30
1	B	648	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	468	LEU	CB-CG-CD1	5.60	120.52	111.00
1	A	470	LEU	CA-CB-CG	5.59	128.17	115.30
1	B	488	VAL	CG1-CB-CG2	5.58	119.82	110.90
1	D	657	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	B	548	LEU	CA-CB-CG	5.50	127.96	115.30
1	C	651	ASP	CB-CG-OD2	5.44	123.19	118.30
1	C	537	ASP	CB-CG-OD1	5.39	123.15	118.30
1	B	503	LYS	CD-CE-NZ	-5.29	99.54	111.70
1	D	475	LEU	CA-CB-CG	5.27	127.43	115.30
1	D	614	ASP	CB-CG-OD2	5.27	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	537	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	516	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	546	VAL	CG1-CB-CG2	5.21	119.23	110.90
1	D	537	ASP	N-CA-CB	-5.16	101.32	110.60
1	A	579	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	465	THR	OG1-CB-CG2	-5.12	98.22	110.00
1	C	391	GLY	N-CA-C	-5.12	100.30	113.10
1	C	617	LEU	CB-CG-CD2	5.09	119.66	111.00
1	B	519	SER	N-CA-CB	-5.04	102.93	110.50
1	A	571	LEU	CB-CG-CD1	5.03	119.56	111.00
1	B	617	LEU	CA-CB-CG	5.02	126.85	115.30

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	2098	0	2096	42	0
1	B	2105	0	2103	47	0
1	C	2105	0	2103	40	0
1	D	2083	0	2083	75	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0
2	C	27	0	12	0	0
2	D	27	0	12	2	0
3	A	8	0	6	0	0
3	B	4	0	3	0	0
3	C	4	0	3	0	0
3	D	8	0	6	1	0
4	A	98	0	0	6	0
4	B	86	0	0	1	0
4	C	79	0	0	5	0
4	D	67	0	0	9	0
All	All	8853	0	8451	203	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 12.

All (203) 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:D:498:MET:SD	1:D:498:MET:CE	2.02	1.48
1:D:395:GLU:HB2	1:D:481:ILE:HB	1.30	1.10
3:D:5:ACY:H1	4:D:281:HOH:O	1.48	1.09
1:B:487:ARG:HG3	1:B:487:ARG:HH21	1.26	0.99
1:D:637:ARG:HG2	1:D:637:ARG:HH21	1.30	0.94
1:D:567:ASP:HB3	4:D:325:HOH:O	1.70	0.91
4:A:73:HOH:O	1:B:621:GLN:HG2	1.75	0.85
1:D:625:TYR:CE1	1:D:637:ARG:HD2	2.12	0.85
1:C:404:GLY:O	1:C:407:GLU:HG2	1.82	0.79
1:A:629:THR:OG1	1:A:632:GLU:HG3	1.82	0.78
1:D:399:ALA:HB1	1:D:475:LEU:HD11	1.67	0.77
1:D:637:ARG:NH2	1:D:637:ARG:HG2	2.01	0.75
1:D:438:ASN:ND2	1:D:438:ASN:H	1.85	0.75
1:D:448:ILE:HD13	1:D:615:LYS:HD3	1.72	0.72
1:B:487:ARG:CG	1:B:487:ARG:HH21	2.02	0.72
1:D:518:LYS:HG2	4:D:333:HOH:O	1.90	0.72
1:B:481:ILE:HD12	1:B:482:ILE:H	1.54	0.71
1:A:640:PHE:CZ	1:A:644:LEU:HD13	2.26	0.71
1:B:516:ARG:HG3	1:B:516:ARG:HH11	1.56	0.71
1:A:527:GLN:HB2	4:A:29:HOH:O	1.93	0.69
1:D:397:VAL:HG11	1:D:470:LEU:HD21	1.75	0.68
1:A:543:GLU:HG3	1:A:544:GLY:N	2.07	0.68
1:C:490:PHE:CE2	1:C:492:SER:HB3	2.29	0.67
1:B:389:THR:HG22	1:C:449:GLU:HG3	1.76	0.67
1:D:629:THR:OG1	1:D:632:GLU:HG3	1.93	0.67
1:D:494:PHE:CE2	1:D:496:TRP:HB3	2.30	0.66
1:D:432:HIS:O	1:D:436:VAL:HB	1.96	0.66
1:B:449:GLU:O	1:B:452:GLU:HB2	1.96	0.66
1:D:401:TRP:CZ2	2:D:10:ADP:H4'	2.30	0.66
1:A:436:VAL:HG12	1:A:438:ASN:HD21	1.61	0.66
1:C:629:THR:OG1	1:C:632:GLU:HG3	1.95	0.66
1:C:580:VAL:CG2	4:C:206:HOH:O	2.45	0.65
1:C:499:PRO:HG3	4:C:266:HOH:O	1.97	0.64
1:D:430:PHE:O	1:D:432:HIS:N	2.32	0.63
1:D:451:GLY:O	4:D:330:HOH:O	2.15	0.63
1:D:632:GLU:O	1:D:636:LEU:HB2	1.99	0.61
1:A:639:ASP:HB2	4:A:88:HOH:O	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:ILE:HG13	1:D:484:HIS:HB3	1.82	0.61
1:B:515:TYR:O	1:B:519:SER:HB2	2.01	0.60
1:D:394:MET:HB2	1:D:446:LEU:HG	1.83	0.60
1:B:476:GLU:H	1:B:476:GLU:CD	2.03	0.60
1:B:487:ARG:HG3	1:B:487:ARG:NH2	2.07	0.60
1:C:396:ASN:N	1:C:445:ASN:OD1	2.29	0.59
1:A:392:ILE:HG13	1:A:393:ILE:N	2.17	0.59
1:D:407:GLU:O	1:D:410:GLU:CB	2.51	0.59
1:C:402:GLU:HG3	1:C:476:GLU:CD	2.23	0.59
1:A:640:PHE:CE1	1:A:644:LEU:HD13	2.36	0.59
1:A:436:VAL:CG1	1:A:438:ASN:HD21	2.17	0.58
1:A:436:VAL:HG12	1:A:438:ASN:ND2	2.18	0.58
1:A:544:GLY:O	1:A:553:ARG:HD3	2.03	0.57
1:B:493:GLN:HG3	1:B:573:SER:HB2	1.86	0.57
1:B:412:VAL:HG12	1:B:413:GLN:HG2	1.86	0.56
1:A:482:ILE:HD11	1:A:484:HIS:HD2	1.70	0.56
1:C:460:THR:HG22	1:C:663:THR:OG1	2.06	0.56
1:C:514:GLU:OE2	1:C:518:LYS:NZ	2.39	0.56
1:B:389:THR:C	1:B:567:ASP:OD1	2.44	0.56
1:B:589:SER:HA	1:B:593:LYS:HE3	1.88	0.56
1:B:638:PRO:O	1:B:642:SER:HB3	2.06	0.55
1:D:467:LEU:CD2	1:D:617:LEU:CD1	2.85	0.55
1:D:434:CYS:O	1:D:437:GLY:N	2.40	0.54
1:A:412:VAL:HG21	1:B:435:LEU:HD21	1.90	0.54
1:A:542:GLY:O	1:A:545:GLY:N	2.39	0.54
1:C:487:ARG:CZ	1:C:567:ASP:OD2	2.56	0.54
1:D:510:VAL:HG12	1:D:511:SER:N	2.22	0.54
1:C:487:ARG:NH2	1:C:567:ASP:OD2	2.41	0.54
1:D:407:GLU:O	1:D:410:GLU:HB2	2.08	0.54
1:D:498:MET:CE	1:D:543:GLU:OE1	2.55	0.54
1:D:439:PRO:HG3	1:D:442:LYS:HD2	1.88	0.54
1:B:476:GLU:HG2	4:B:84:HOH:O	2.07	0.54
1:C:625:TYR:HE2	1:C:669:PHE:O	1.91	0.53
1:D:399:ALA:CB	1:D:475:LEU:HD11	2.37	0.53
1:D:544:GLY:O	1:D:553:ARG:HD3	2.08	0.53
1:B:481:ILE:HD12	1:B:482:ILE:N	2.22	0.53
1:C:580:VAL:HG22	4:C:206:HOH:O	2.07	0.53
1:D:394:MET:HG2	1:D:482:ILE:HG12	1.91	0.53
1:D:467:LEU:HD21	1:D:617:LEU:CD1	2.39	0.52
1:C:625:TYR:CE1	1:C:637:ARG:HD2	2.44	0.52
1:D:400:PHE:HA	1:D:439:PRO:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:630:PHE:O	1:D:633:LEU:HB3	2.10	0.51
1:B:607:MET:CE	1:B:662:LEU:HD21	2.39	0.51
1:A:543:GLU:C	1:A:545:GLY:H	2.14	0.51
1:C:543:GLU:HB3	4:C:266:HOH:O	2.10	0.51
1:A:558:LEU:HD22	1:A:562:VAL:HG23	1.91	0.51
1:D:588:GLU:HG2	1:D:593:LYS:HE2	1.92	0.51
1:C:653:PHE:HB3	1:C:657:ARG:HG2	1.92	0.50
1:C:404:GLY:C	1:C:407:GLU:HG2	2.32	0.50
1:D:636:LEU:O	1:D:637:ARG:NH2	2.44	0.50
1:D:434:CYS:O	1:D:435:LEU:C	2.50	0.50
1:A:643:LYS:HE2	4:A:169:HOH:O	2.12	0.49
1:A:398:THR:HG23	1:A:442:LYS:HA	1.93	0.49
1:A:459:SER:HB3	1:A:663:THR:HA	1.93	0.49
1:B:524:CYS:O	1:B:555:ARG:HD2	2.11	0.49
1:D:664:GLU:HG3	4:D:315:HOH:O	2.11	0.49
1:A:528:GLN:HB2	4:A:85:HOH:O	2.12	0.49
1:D:527:GLN:OE1	1:D:530:ILE:HD11	2.13	0.48
1:A:617:LEU:CD2	1:A:619:LEU:HD13	2.44	0.48
1:C:389:THR:HG21	1:C:597:ASN:O	2.13	0.48
1:D:399:ALA:HB1	1:D:475:LEU:CD1	2.41	0.48
1:A:401:TRP:CE2	1:A:433:LEU:HD13	2.49	0.48
1:D:405:PHE:CZ	1:D:475:LEU:HD22	2.49	0.48
1:D:626:PHE:CE1	1:D:633:LEU:HB2	2.49	0.48
1:A:446:LEU:HD12	1:A:446:LEU:C	2.34	0.48
1:B:487:ARG:CG	1:B:487:ARG:NH2	2.69	0.48
1:C:394:MET:CE	1:C:467:LEU:HD11	2.43	0.48
1:C:617:LEU:HD13	1:C:619:LEU:HD13	1.94	0.48
1:D:517:TYR:OH	1:D:537:ASP:OD1	2.27	0.48
1:B:607:MET:HE1	1:B:662:LEU:HD21	1.95	0.48
1:D:404:GLY:O	1:D:407:GLU:HB2	2.14	0.48
1:B:478:SER:O	1:B:479:GLU:HG3	2.14	0.47
1:A:396:ASN:N	1:A:445:ASN:OD1	2.41	0.47
1:D:434:CYS:HA	4:D:336:HOH:O	2.14	0.47
1:A:453:MET:HG2	1:A:600:ARG:HG3	1.95	0.47
1:C:449:GLU:O	1:C:452:GLU:HB2	2.14	0.47
1:B:645:MET:SD	1:B:645:MET:N	2.87	0.47
1:D:408:LEU:HD21	1:D:469:MET:SD	2.55	0.47
1:B:406:GLY:O	1:B:410:GLU:HG3	2.14	0.46
1:C:543:GLU:CB	4:C:266:HOH:O	2.63	0.46
1:D:405:PHE:CE1	1:D:409:LEU:HD11	2.50	0.46
1:B:507:ILE:HD11	1:B:517:TYR:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:VAL:HA	1:B:479:GLU:O	2.15	0.46
1:B:513:ASP:OD2	1:B:513:ASP:C	2.53	0.46
1:C:467:LEU:O	1:C:467:LEU:HD12	2.16	0.46
1:B:407:GLU:CD	1:B:407:GLU:H	2.18	0.46
1:B:464:LYS:HE2	1:B:464:LYS:HB2	1.68	0.46
1:D:392:ILE:HG13	1:D:484:HIS:CB	2.45	0.46
1:D:407:GLU:O	1:D:410:GLU:HB3	2.15	0.46
1:D:545:GLY:O	1:D:548:LEU:HB2	2.16	0.46
1:A:543:GLU:HG3	1:A:544:GLY:H	1.80	0.45
1:D:390:THR:HA	4:D:328:HOH:O	2.15	0.45
1:D:436:VAL:HG12	1:D:438:ASN:HD21	1.82	0.45
1:D:528:GLN:HB2	4:D:319:HOH:O	2.14	0.45
1:D:558:LEU:HD22	1:D:562:VAL:HG23	1.99	0.45
1:A:456:ILE:HD13	1:A:467:LEU:HD23	1.98	0.45
1:C:517:TYR:OH	1:C:537:ASP:OD2	2.29	0.45
1:A:482:ILE:HD11	1:A:484:HIS:CD2	2.49	0.45
1:A:543:GLU:C	1:A:545:GLY:N	2.69	0.45
1:D:482:ILE:HD13	1:D:482:ILE:C	2.38	0.45
1:A:487:ARG:NH2	1:A:487:ARG:HB2	2.32	0.45
1:B:490:PHE:CE2	1:B:492:SER:HB3	2.52	0.45
1:B:401:TRP:CE2	1:B:433:LEU:HD13	2.53	0.44
1:B:476:GLU:N	1:B:476:GLU:CD	2.70	0.44
1:B:542:GLY:O	1:B:543:GLU:C	2.56	0.44
1:A:581:PHE:O	1:A:585:GLN:HG3	2.17	0.44
1:C:397:VAL:HG11	1:C:470:LEU:HD21	2.00	0.44
1:A:464:LYS:HB2	1:A:464:LYS:HE2	1.63	0.44
1:B:517:TYR:O	1:B:521:VAL:HG23	2.18	0.44
1:D:436:VAL:HG12	1:D:438:ASN:ND2	2.33	0.44
1:D:496:TRP:N	1:D:496:TRP:CD1	2.85	0.44
1:C:617:LEU:CD1	1:C:619:LEU:HD13	2.48	0.44
1:D:393:ILE:HG12	1:D:447:ASN:OD1	2.18	0.44
1:D:507:ILE:O	1:D:507:ILE:HG23	2.17	0.44
1:A:397:VAL:HG11	1:A:470:LEU:HD21	1.99	0.43
1:D:440:VAL:CG1	1:D:441:LEU:N	2.81	0.43
1:B:470:LEU:HD12	1:B:475:LEU:O	2.18	0.43
1:D:507:ILE:O	1:D:507:ILE:CG2	2.66	0.43
1:A:392:ILE:HD12	1:A:484:HIS:HB3	2.00	0.43
1:A:626:PHE:CD1	1:A:626:PHE:C	2.91	0.43
1:C:510:VAL:HG12	1:C:511:SER:N	2.32	0.43
1:C:494:PHE:CE2	1:C:496:TRP:HB3	2.54	0.43
1:C:402:GLU:HG3	1:C:476:GLU:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:489:SER:HB2	1:C:564:LYS:HE2	2.00	0.43
1:C:389:THR:HG21	1:C:598:LYS:HA	2.00	0.43
1:B:404:GLY:HA2	1:B:407:GLU:OE1	2.19	0.43
1:B:516:ARG:CG	1:B:516:ARG:HH11	2.28	0.43
1:B:542:GLY:O	1:B:545:GLY:N	2.37	0.43
1:A:446:LEU:HD12	1:A:446:LEU:O	2.19	0.42
1:B:503:LYS:HE3	1:B:512:TYR:CE1	2.54	0.42
1:A:524:CYS:O	1:A:555:ARG:HD2	2.19	0.42
1:B:558:LEU:HD22	1:B:562:VAL:HG23	2.01	0.42
1:B:579:ASP:N	1:B:579:ASP:OD2	2.49	0.42
1:A:617:LEU:HD22	1:A:619:LEU:HD13	2.02	0.42
1:D:494:PHE:HE2	1:D:496:TRP:HB3	1.78	0.42
1:D:510:VAL:CG1	1:D:511:SER:N	2.83	0.42
1:D:487:ARG:NH2	1:D:567:ASP:OD2	2.53	0.42
1:D:488:VAL:HA	1:D:568:LEU:O	2.20	0.42
1:C:404:GLY:HA2	1:C:407:GLU:CG	2.50	0.42
1:D:436:VAL:CG1	1:D:438:ASN:HD21	2.33	0.42
1:C:397:VAL:HA	1:C:479:GLU:O	2.19	0.42
1:D:638:PRO:O	1:D:642:SER:HB3	2.20	0.42
1:D:491:CYS:HB2	1:D:561:ALA:CB	2.50	0.41
1:A:654:THR:O	1:A:658:ARG:HG3	2.20	0.41
1:C:464:LYS:HE2	1:C:464:LYS:HB2	1.74	0.41
1:A:503:LYS:HB2	1:A:503:LYS:HE3	1.77	0.41
1:D:444:ILE:HD13	1:D:444:ILE:HA	1.64	0.41
1:D:397:VAL:HA	1:D:479:GLU:O	2.21	0.41
1:A:639:ASP:CB	4:A:88:HOH:O	2.66	0.41
1:B:394:MET:HB2	1:B:446:LEU:HG	2.03	0.41
1:B:563:TYR:O	1:B:563:TYR:CD2	2.74	0.41
1:B:643:LYS:HG2	1:B:665:THR:CG2	2.49	0.41
1:C:616:ILE:O	1:C:627:TYR:HA	2.21	0.41
1:D:394:MET:O	1:D:445:ASN:HA	2.20	0.41
1:C:644:LEU:CD2	1:C:662:LEU:HD23	2.51	0.41
1:A:650:PHE:CZ	1:A:658:ARG:HB3	2.55	0.41
1:B:616:ILE:O	1:B:627:TYR:HA	2.21	0.41
1:D:412:VAL:HG21	1:D:469:MET:HE1	2.02	0.41
1:D:490:PHE:CE2	1:D:492:SER:HB3	2.56	0.41
1:B:630:PHE:O	1:B:634:GLN:HG3	2.21	0.41
1:C:524:CYS:O	1:C:555:ARG:HD2	2.20	0.41
1:C:638:PRO:O	1:C:642:SER:HB2	2.20	0.41
1:D:401:TRP:HZ2	2:D:10:ADP:H4'	1.82	0.41
1:D:544:GLY:HA2	4:D:313:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471:ILE:HD13	1:C:471:ILE:HG21	1.85	0.40
1:D:502:ILE:HG12	1:D:541:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	262/286 (92%)	251 (96%)	10 (4%)	1 (0%)	34	46
1	B	263/286 (92%)	250 (95%)	13 (5%)	0	100	100
1	C	263/286 (92%)	251 (95%)	11 (4%)	1 (0%)	34	46
1	D	260/286 (91%)	238 (92%)	18 (7%)	4 (2%)	10	14
All	All	1048/1144 (92%)	990 (94%)	52 (5%)	6 (1%)	25	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	431	SER
1	A	544	GLY
1	C	545	GLY
1	D	434	CYS
1	D	435	LEU
1	D	537	ASP

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	233/252 (92%)	197 (84%)	36 (16%)	2	2
1	B	234/252 (93%)	202 (86%)	32 (14%)	3	3
1	C	234/252 (93%)	206 (88%)	28 (12%)	5	5
1	D	231/252 (92%)	192 (83%)	39 (17%)	2	2
All	All	932/1008 (92%)	797 (86%)	135 (14%)	3	3

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	ILE
1	A	403	GLU
1	A	408	LEU
1	A	411	LYS
1	A	431	SER
1	A	435	LEU
1	A	442	LYS
1	A	449	GLU
1	A	454	LEU
1	A	459	SER
1	A	460	THR
1	A	464	LYS
1	A	468	LEU
1	A	482	ILE
1	A	487	ARG
1	A	488	VAL
1	A	503	LYS
1	A	531	THR
1	A	543	GLU
1	A	546	VAL
1	A	548	LEU
1	A	557	SER
1	A	558	LEU
1	A	571	LEU
1	A	573	SER
1	A	580	VAL
1	A	617	LEU
1	A	619	LEU
1	A	623	SER
1	A	635	SER

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Mol	Chain	Res	Type
1	A	642	SER
1	A	644	LEU
1	A	645	MET
1	A	659	SER
1	A	660	SER
1	A	666	LEU
1	B	407	GLU
1	B	408	LEU
1	B	412	VAL
1	B	413	GLN
1	B	435	LEU
1	B	449	GLU
1	B	450	LYS
1	B	454	LEU
1	B	481	ILE
1	B	482	ILE
1	B	487	ARG
1	B	488	VAL
1	B	507	ILE
1	B	513	ASP
1	B	514	GLU
1	B	519	SER
1	B	531	THR
1	B	546	VAL
1	B	548	LEU
1	B	558	LEU
1	B	571	LEU
1	B	580	VAL
1	B	611	ARG
1	B	617	LEU
1	B	619	LEU
1	B	642	SER
1	B	643	LYS
1	B	645	MET
1	B	648	ASP
1	B	657	ARG
1	B	660	SER
1	B	666	LEU
1	C	396	ASN
1	C	407	GLU
1	C	408	LEU
1	C	410	GLU

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Mol	Chain	Res	Type
1	C	413	GLN
1	C	431	SER
1	C	435	LEU
1	C	454	LEU
1	C	460	THR
1	C	467	LEU
1	C	468	LEU
1	C	476	GLU
1	C	487	ARG
1	C	507	ILE
1	C	514	GLU
1	C	543	GLU
1	C	546	VAL
1	C	548	LEU
1	C	557	SER
1	C	558	LEU
1	C	571	LEU
1	C	573	SER
1	C	617	LEU
1	C	619	LEU
1	C	623	SER
1	C	634	GLN
1	C	657	ARG
1	C	666	LEU
1	D	390	THR
1	D	396	ASN
1	D	402	GLU
1	D	403	GLU
1	D	410	GLU
1	D	412	VAL
1	D	431	SER
1	D	438	ASN
1	D	442	LYS
1	D	443	ASN
1	D	444	ILE
1	D	454	LEU
1	D	460	THR
1	D	468	LEU
1	D	475	LEU
1	D	478	SER
1	D	482	ILE
1	D	484	HIS

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Mol	Chain	Res	Type
1	D	485	SER
1	D	488	VAL
1	D	498	MET
1	D	507	ILE
1	D	519	SER
1	D	548	LEU
1	D	557	SER
1	D	558	LEU
1	D	571	LEU
1	D	573	SER
1	D	580	VAL
1	D	619	LEU
1	D	621	GLN
1	D	631	SER
1	D	636	LEU
1	D	637	ARG
1	D	642	SER
1	D	644	LEU
1	D	660	SER
1	D	666	LEU
1	D	670	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	HIS
1	A	438	ASN
1	A	443	ASN
1	A	484	HIS
1	A	538	ASN
1	B	396	ASN
1	B	413	GLN
1	B	443	ASN
1	B	538	ASN
1	C	621	GLN
1	D	438	ASN

5.3.3 RNA

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)

10 ligands 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	$\#\|Z\| > 2$
2	ADP	D	10	-	24,29,29	1.26	2 (8%)	29,45,45	1.72	4 (13%)
2	ADP	B	8	-	24,29,29	1.17	1 (4%)	29,45,45	1.85	5 (17%)
3	ACY	A	6	-	1,3,3	0.81	0	0,3,3	0.00	-
3	ACY	D	4	-	1,3,3	1.57	0	0,3,3	0.00	-
2	ADP	C	9	-	24,29,29	1.26	3 (12%)	29,45,45	1.54	4 (13%)
3	ACY	C	3	-	1,3,3	0.90	0	0,3,3	0.00	-
3	ACY	A	1	-	1,3,3	1.80	0	0,3,3	0.00	-
3	ACY	D	5	-	1,3,3	0.91	0	0,3,3	0.00	-
2	ADP	A	7	-	24,29,29	1.23	2 (8%)	29,45,45	1.69	4 (13%)
3	ACY	B	2	-	1,3,3	2.26	1 (100%)	0,3,3	0.00	-

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
2	ADP	A	7	-	-	4/12/32/32	0/3/3/3
2	ADP	B	8	-	-	3/12/32/32	0/3/3/3
2	ADP	D	10	-	-	4/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	C	9	-	-	3/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10	ADP	C2-N3	4.51	1.39	1.32
2	B	8	ADP	C2-N3	4.48	1.39	1.32
2	C	9	ADP	C2-N3	4.39	1.39	1.32
2	A	7	ADP	C2-N3	4.27	1.39	1.32
2	D	10	ADP	C2-N1	2.74	1.39	1.33
2	A	7	ADP	C2-N1	2.62	1.38	1.33
2	C	9	ADP	C2-N1	2.41	1.38	1.33
3	B	2	ACY	CH3-C	2.26	1.51	1.48
2	C	9	ADP	O4'-C1'	2.11	1.44	1.41

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	8	ADP	N3-C2-N1	-6.45	118.60	128.68
2	D	10	ADP	N3-C2-N1	-6.00	119.30	128.68
2	A	7	ADP	N3-C2-N1	-5.48	120.11	128.68
2	C	9	ADP	N3-C2-N1	-5.00	120.86	128.68
2	B	8	ADP	PA-O3A-PB	-3.79	119.81	132.83
2	D	10	ADP	PA-O3A-PB	-3.78	119.87	132.83
2	A	7	ADP	O3B-PB-O3A	3.60	116.70	104.64
2	B	8	ADP	O2B-PB-O3A	3.26	115.58	104.64
2	A	7	ADP	C3'-C2'-C1'	3.03	105.54	100.98
2	A	7	ADP	O3'-C3'-C4'	-2.95	102.53	111.05
2	D	10	ADP	O3B-PB-O3A	2.74	113.83	104.64
2	D	10	ADP	C3'-C2'-C1'	2.47	104.70	100.98
2	C	9	ADP	C4-C5-N7	-2.45	106.85	109.40
2	B	8	ADP	O2'-C2'-C1'	2.37	119.60	110.85
2	C	9	ADP	O4'-C1'-C2'	-2.13	103.82	106.93
2	B	8	ADP	C1'-N9-C4	-2.07	123.00	126.64
2	C	9	ADP	PA-O3A-PB	-2.06	125.74	132.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	9	ADP	O4'-C4'-C5'-O5'

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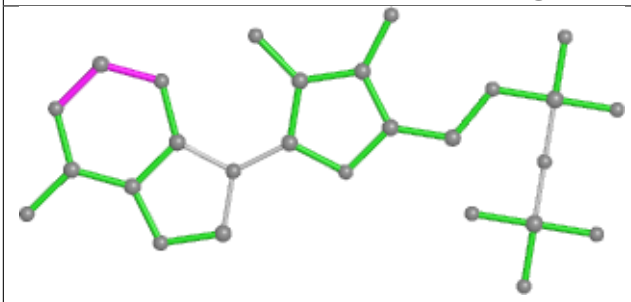
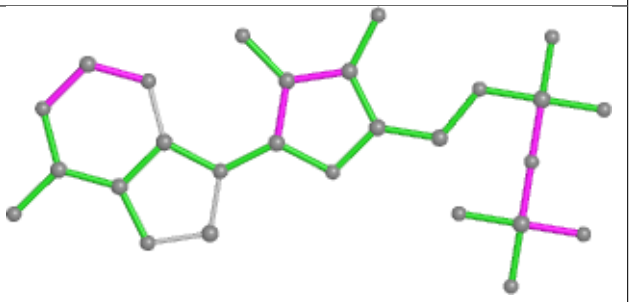
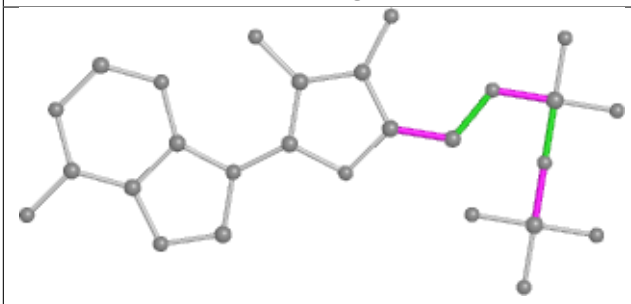
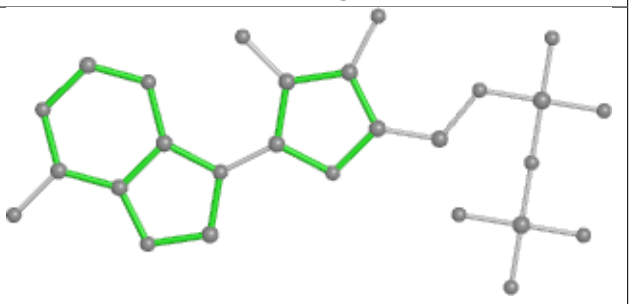
Mol	Chain	Res	Type	Atoms
2	A	7	ADP	PA-O3A-PB-O1B
2	D	10	ADP	PA-O3A-PB-O1B
2	B	8	ADP	C5'-O5'-PA-O3A
2	A	7	ADP	C5'-O5'-PA-O3A
2	B	8	ADP	C5'-O5'-PA-O1A
2	A	7	ADP	C5'-O5'-PA-O1A
2	A	7	ADP	C5'-O5'-PA-O2A
2	C	9	ADP	C3'-C4'-C5'-O5'
2	C	9	ADP	PA-O3A-PB-O1B
2	D	10	ADP	O4'-C4'-C5'-O5'
2	D	10	ADP	C3'-C4'-C5'-O5'
2	D	10	ADP	C5'-O5'-PA-O1A
2	B	8	ADP	C5'-O5'-PA-O2A

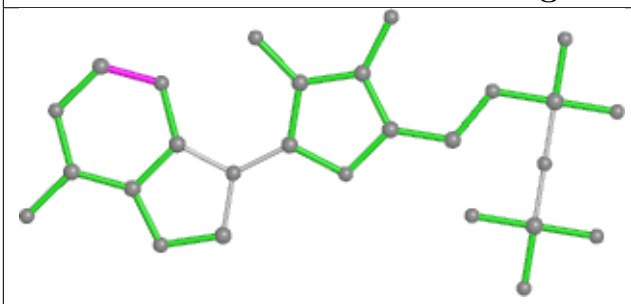
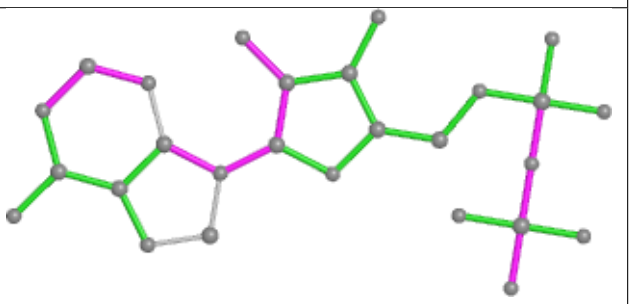
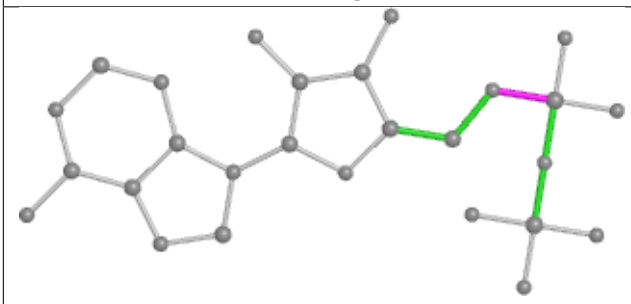
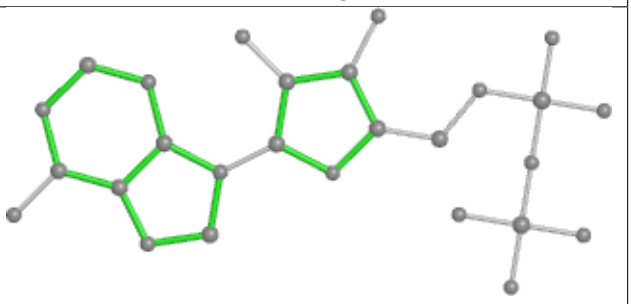
There are no ring outliers.

2 monomers are involved in 3 short contacts:

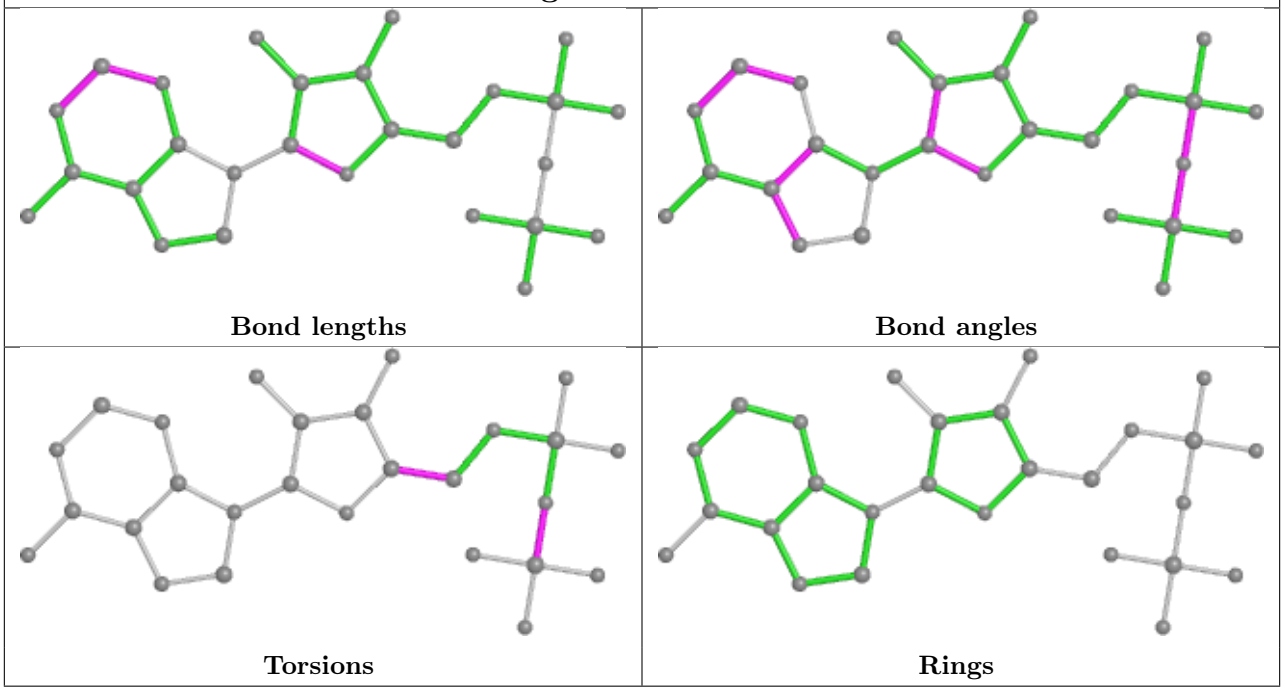
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	10	ADP	2	0
3	D	5	ACY	1	0

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 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.

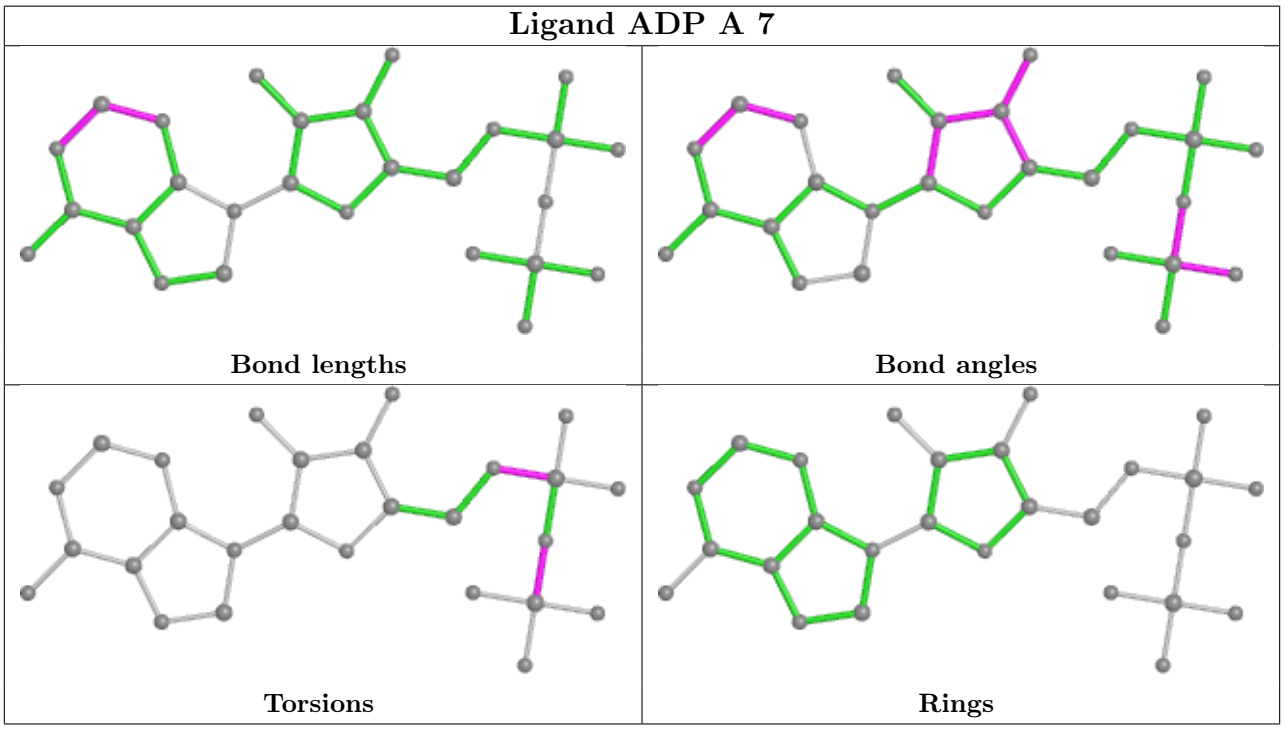
Ligand ADP D 10	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP B 8	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 9



Ligand ADP A 7



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	266/286 (93%)	-0.02	4 (1%)	73	79	19, 39, 65, 76	0
1	B	267/286 (93%)	0.01	6 (2%)	62	68	23, 38, 61, 83	0
1	C	267/286 (93%)	-0.00	2 (0%)	87	90	19, 36, 63, 74	0
1	D	264/286 (92%)	0.16	17 (6%)	19	22	21, 43, 80, 94	0
All	All	1064/1144 (93%)	0.04	29 (2%)	54	61	19, 39, 67, 94	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	401	TRP	5.9
1	A	429	SER	3.6
1	D	434	CYS	3.6
1	D	436	VAL	3.4
1	D	481	ILE	3.1
1	A	430	PHE	3.0
1	D	408	LEU	2.9
1	D	412	VAL	2.8
1	D	496	TRP	2.8
1	D	435	LEU	2.8
1	D	670	SER	2.7
1	D	410	GLU	2.7
1	D	475	LEU	2.5
1	D	403	GLU	2.5
1	B	430	PHE	2.5
1	D	400	PHE	2.4
1	D	438	ASN	2.4
1	B	670	SER	2.3
1	C	476	GLU	2.3
1	B	412	VAL	2.3
1	B	648	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	436	VAL	2.2
1	A	435	LEU	2.2
1	B	402	GLU	2.2
1	D	508	PHE	2.1
1	A	412	VAL	2.1
1	D	430	PHE	2.1
1	C	430	PHE	2.1
1	D	402	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

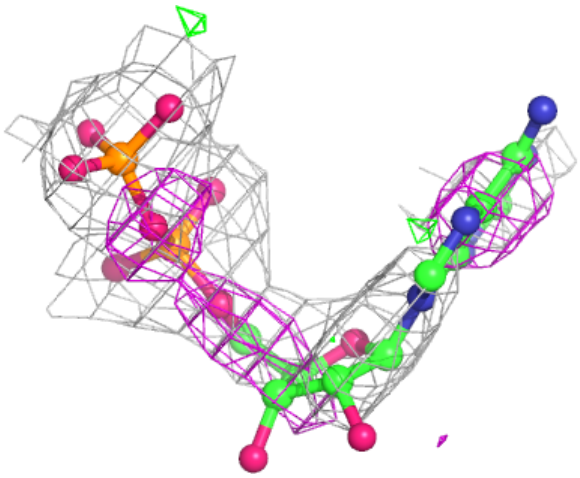
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

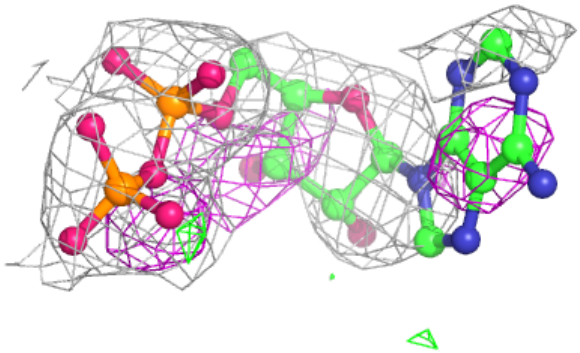
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	D	10	27/27	0.85	0.30	63,94,105,106	0
2	ADP	C	9	27/27	0.90	0.30	51,68,75,76	0
3	ACY	D	5	4/4	0.92	0.14	35,36,37,37	0
2	ADP	A	7	27/27	0.92	0.27	49,74,84,85	0
2	ADP	B	8	27/27	0.94	0.22	40,51,61,63	0
3	ACY	A	6	4/4	0.97	0.16	40,40,40,41	0
3	ACY	D	4	4/4	0.98	0.17	39,40,41,41	0
3	ACY	A	1	4/4	0.98	0.19	27,28,28,29	0
3	ACY	B	2	4/4	0.98	0.20	41,41,42,43	0
3	ACY	C	3	4/4	0.99	0.18	27,30,30,34	0

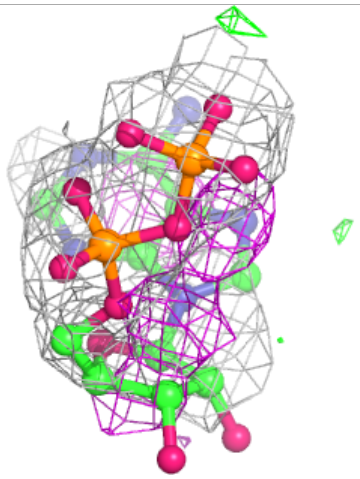
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP D 10:

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

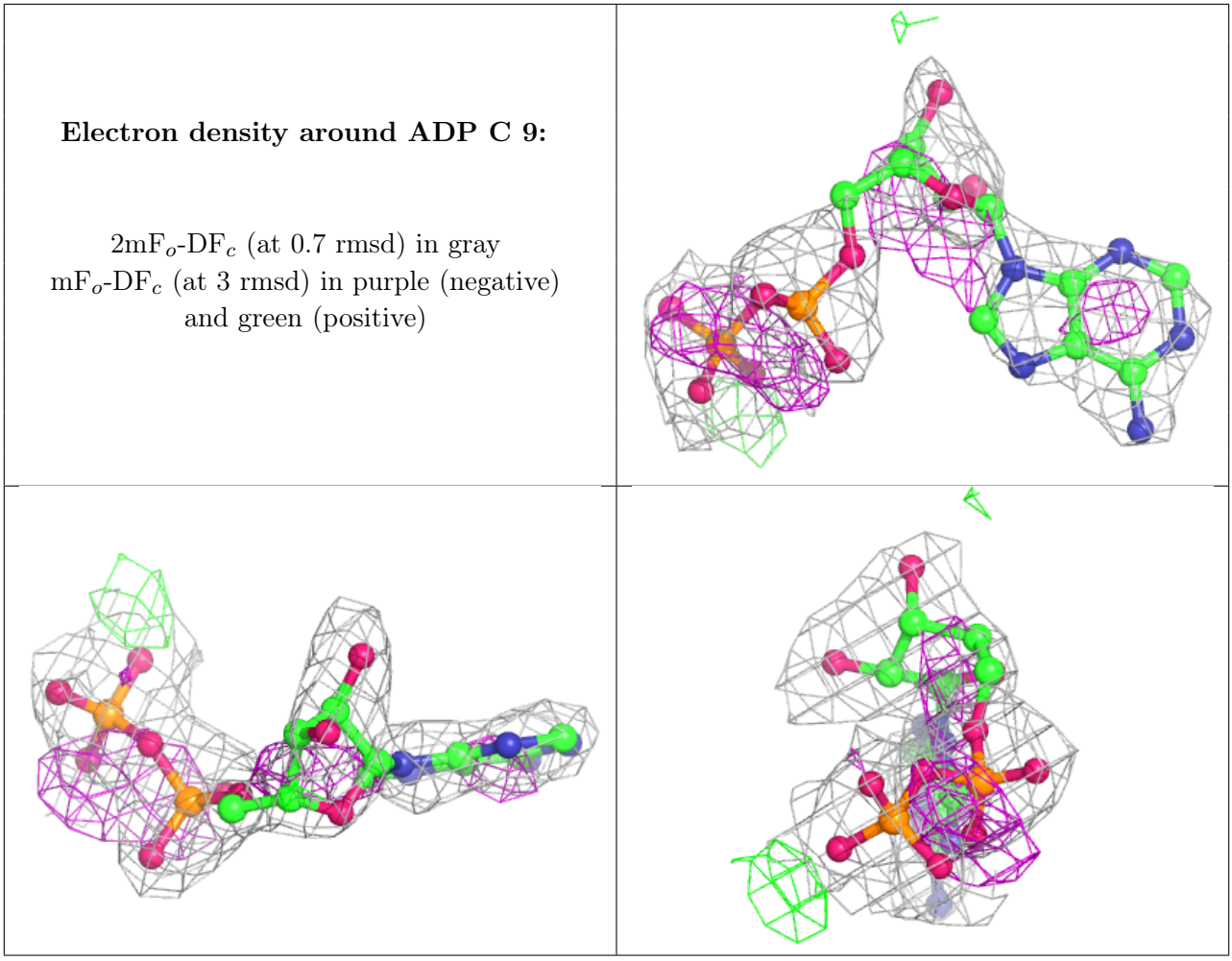






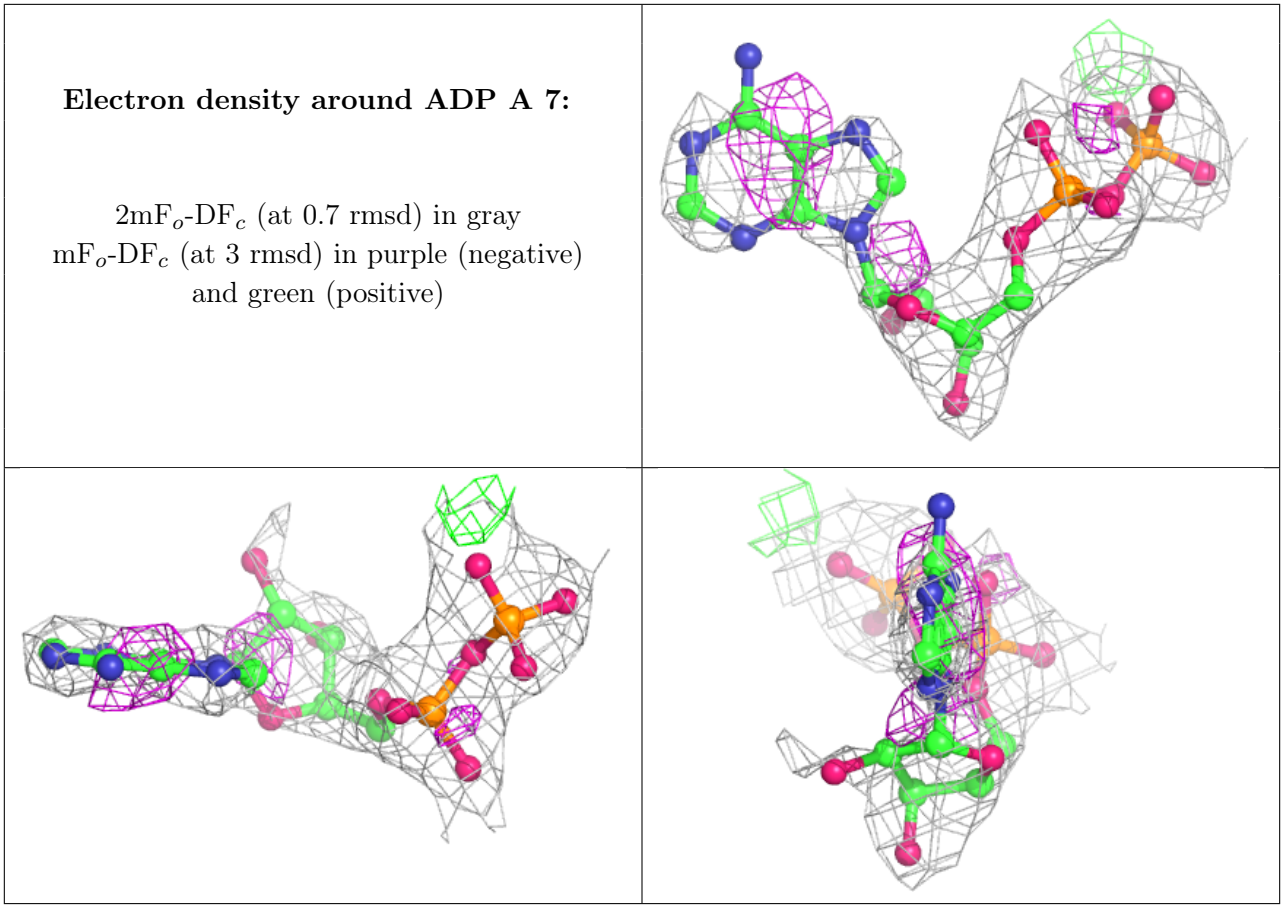
Electron density around ADP C 9:

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



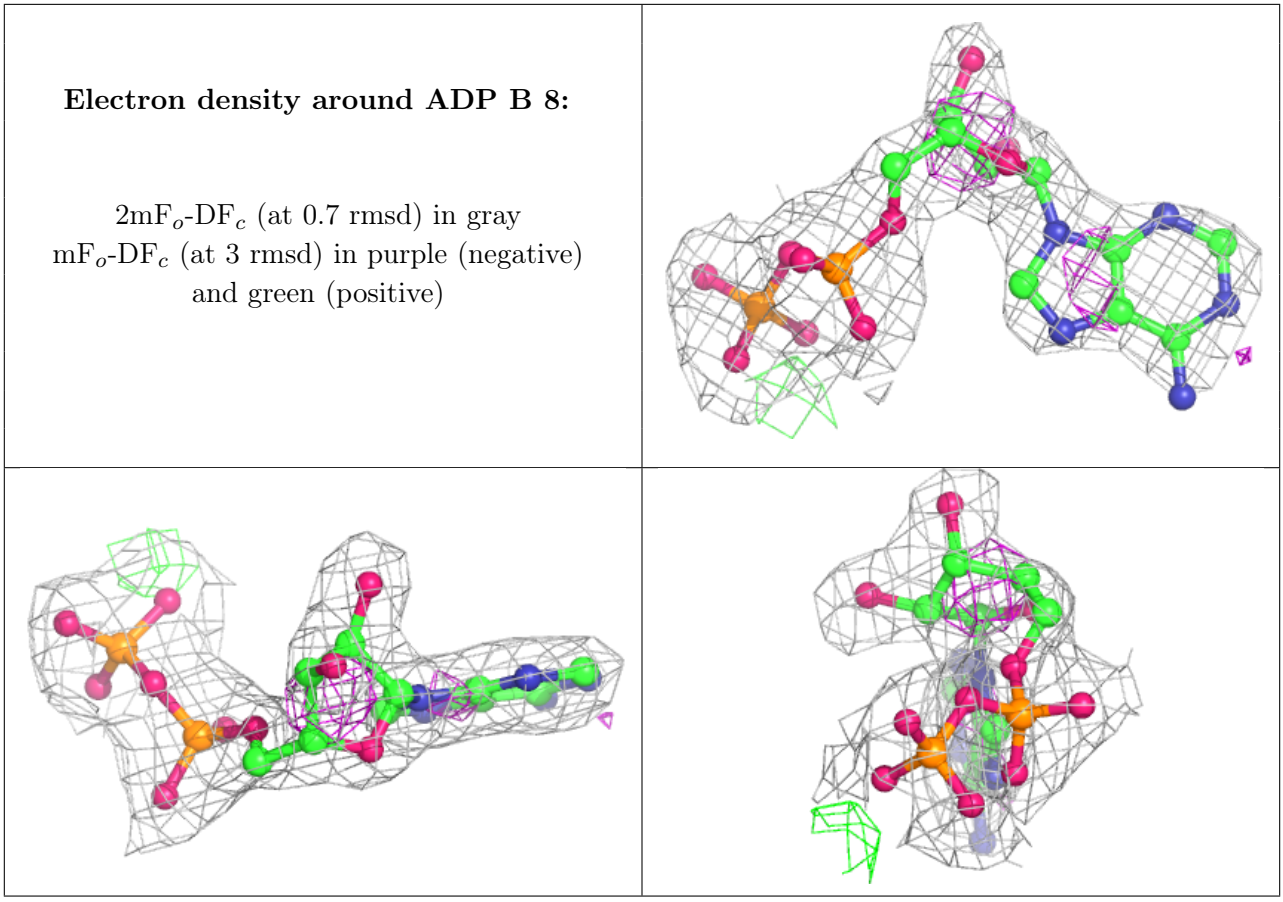
Electron density around ADP A 7:

$2mF_o$-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 8:

$2mF_o$-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.