



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:56 PM UTC

PDB ID : 1R0Y / pdb_00001r0y
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

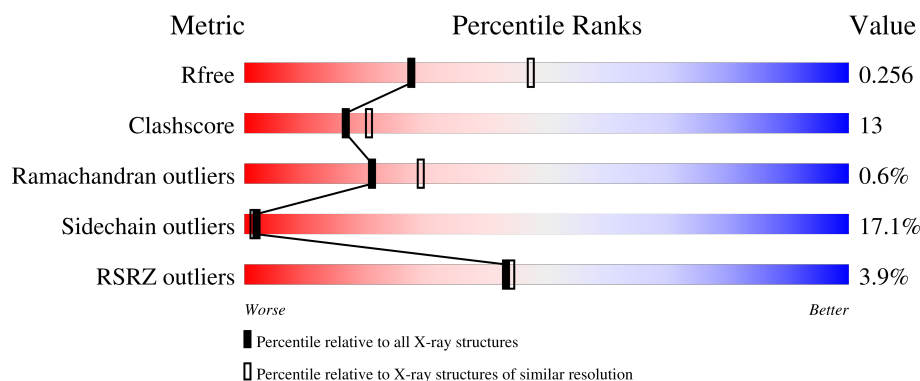
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	286	2% 60% 26% 7% 7%
1	B	286	3% 61% 24% 7% 7%
1	C	286	2% 61% 26% 7% 7%
1	D	286	7% 50% 33% 8% 8%

2 Entry composition

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.

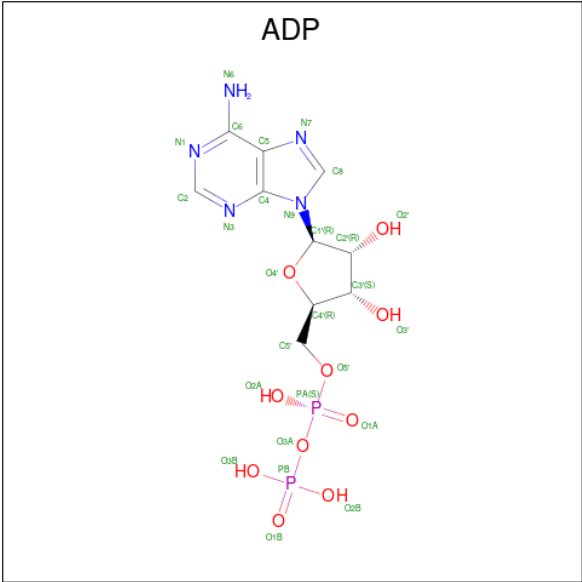
- Molecule 1 is a protein called Cystic fibrosis transmembrane conductance regulator.

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:

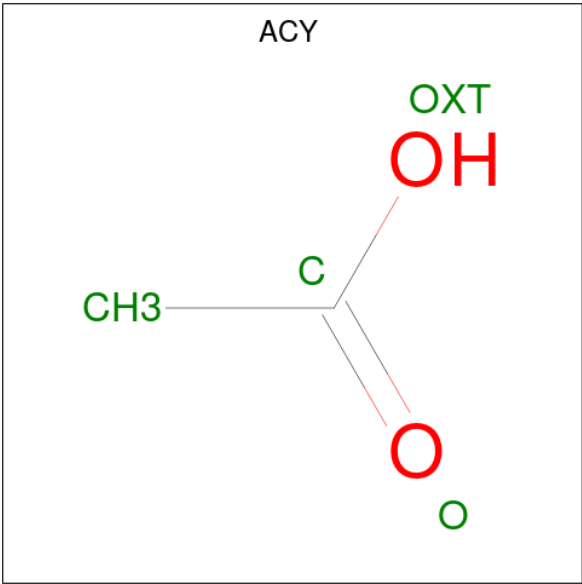
Chain	Residue	Modelled	Actual	Comment	Reference
A	388	SER	-	cloning artifact	UNP P26361
B	388	SER	-	cloning artifact	UNP P26361
C	388	SER	-	cloning artifact	UNP P26361
D	388	SER	-	cloning artifact	UNP P26361

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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 (CCD ID: ACY) (formula: C₂H₄O₂).



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

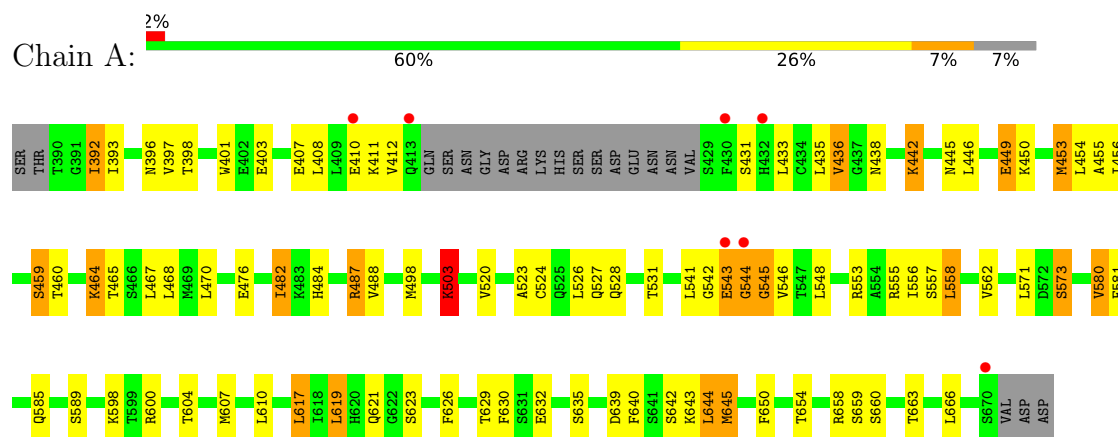
- Molecule 4 is water.

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

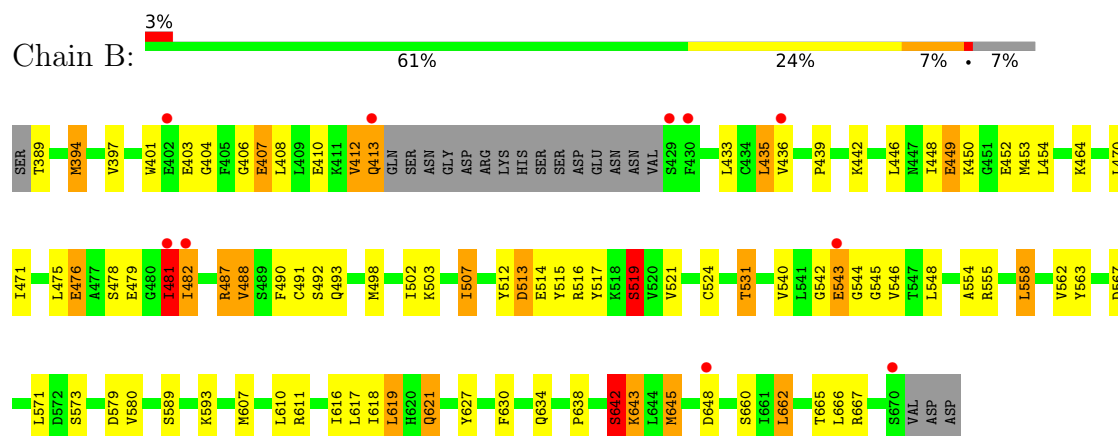
3 Residue-property plots [i](#)

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.

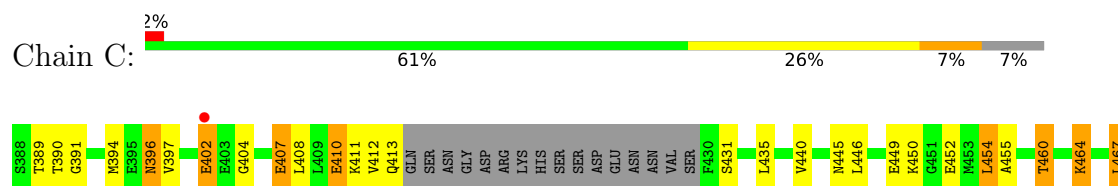
- Molecule 1: Cystic fibrosis transmembrane conductance regulator

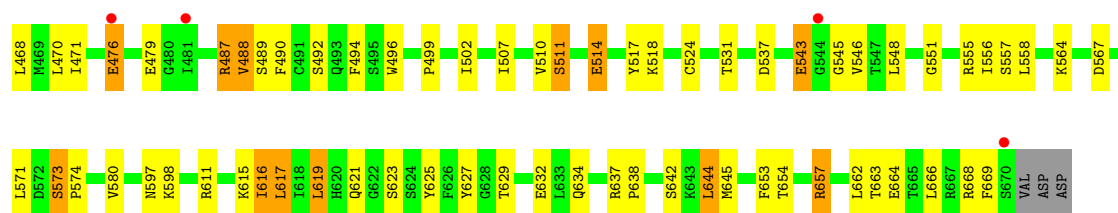


- Molecule 1: Cystic fibrosis transmembrane conductance regulator

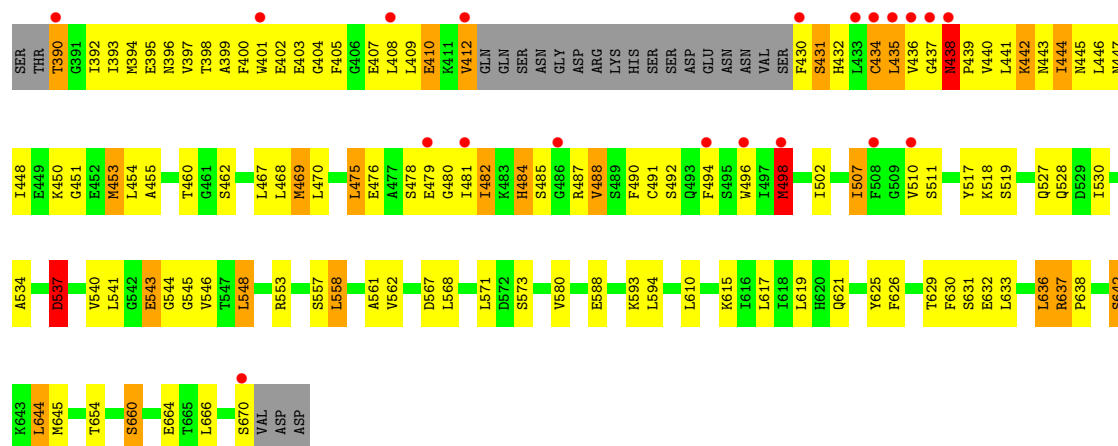


- Molecule 1: Cystic fibrosis transmembrane conductance regulator





● Molecule 1: Cystic fibrosis transmembrane conductance regulator



4 Data and refinement statistics

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 36.00 – 2.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.00-2.55) 99.2 (36.00-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ 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)	0.35 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.40	13/2133 (0.6%)	1.38	8/2868 (0.3%)
1	B	1.42	14/2140 (0.7%)	1.46	13/2878 (0.5%)
1	C	1.44	5/2140 (0.2%)	1.40	12/2878 (0.4%)
1	D	1.35	9/2118 (0.4%)	1.37	9/2848 (0.3%)
All	All	1.40	41/8531 (0.5%)	1.40	42/11472 (0.4%)

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	498	MET	SD-CE	9.05	2.02	1.79
1	C	573	SER	C-O	-8.26	1.19	1.23
1	C	616	ILE	CA-CB	-8.14	1.44	1.54
1	B	498	MET	SD-CE	7.46	1.98	1.79
1	D	498	MET	CG-SD	7.42	1.99	1.80
1	C	573	SER	CA-C	-7.05	1.49	1.53
1	A	503	LYS	CA-C	6.95	1.61	1.52
1	D	540	VAL	CA-CB	6.84	1.62	1.54
1	A	545	GLY	CA-C	6.38	1.60	1.51
1	B	453	MET	C-O	6.10	1.30	1.24
1	A	556	ILE	CA-CB	-6.07	1.46	1.54
1	B	619	LEU	CA-C	5.96	1.60	1.52
1	D	534	ALA	CA-CB	-5.96	1.44	1.53
1	B	448	ILE	CA-CB	5.94	1.61	1.53
1	D	469	MET	SD-CE	-5.92	1.64	1.79
1	C	488	VAL	CA-CB	5.91	1.62	1.54
1	A	607	MET	SD-CE	5.88	1.94	1.79
1	B	519	SER	N-CA	-5.74	1.39	1.46
1	B	436	VAL	CA-CB	5.72	1.61	1.54
1	B	540	VAL	CA-CB	5.56	1.61	1.54
1	D	455	ALA	CA-CB	-5.49	1.45	1.53
1	A	541	LEU	CA-C	5.44	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	436	VAL	CA-C	5.41	1.59	1.52
1	B	471	ILE	C-O	-5.37	1.17	1.24
1	B	394	MET	CA-C	-5.36	1.46	1.52
1	D	537	ASP	CB-CG	-5.35	1.38	1.52
1	A	520	VAL	CA-CB	5.33	1.60	1.54
1	A	545	GLY	N-CA	5.29	1.53	1.45
1	D	645	MET	SD-CE	5.26	1.92	1.79
1	C	455	ALA	CA-CB	-5.21	1.46	1.53
1	A	523	ALA	CA-C	5.20	1.59	1.52
1	A	604	THR	CA-CB	5.18	1.62	1.53
1	B	491	CYS	C-O	5.18	1.29	1.23
1	A	598	LYS	CA-C	-5.15	1.46	1.52
1	D	453	MET	CG-SD	-5.15	1.67	1.80
1	A	453	MET	SD-CE	5.07	1.92	1.79
1	B	554	ALA	CA-CB	5.06	1.61	1.53
1	A	498	MET	SD-CE	5.05	1.92	1.79
1	A	455	ALA	CA-CB	-5.04	1.46	1.53
1	B	618	ILE	CA-CB	-5.04	1.48	1.54
1	B	498	MET	CG-SD	5.00	1.93	1.80

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	481	ILE	N-CA-C	8.96	121.39	108.48
1	C	391	GLY	N-CA-C	-8.04	100.30	112.60
1	C	502	ILE	N-CA-C	-7.69	103.31	110.53
1	B	662	LEU	N-CA-C	-7.58	103.09	111.36
1	A	589	SER	N-CA-C	7.50	120.92	111.69
1	D	480	GLY	N-CA-C	7.44	119.02	111.95
1	B	531	THR	OG1-CB-CG2	-6.86	95.57	109.30
1	D	660	SER	N-CA-C	-6.71	103.43	111.69
1	B	667	ARG	N-CA-C	-6.51	104.26	111.36
1	B	642	SER	N-CA-C	-6.38	104.25	111.14
1	C	440	VAL	N-CA-C	-6.32	104.10	113.39
1	C	551	GLY	N-CA-C	-6.31	104.70	112.77
1	C	654	THR	N-CA-C	-6.22	102.32	110.53
1	C	668	ARG	N-CA-C	6.17	117.67	111.07
1	A	573	SER	CB-CA-C	-6.12	104.96	110.71
1	B	502	ILE	N-CA-C	-5.92	104.96	110.53
1	D	644	LEU	CA-CB-CG	-5.88	95.73	116.30
1	D	438	ASN	N-CA-C	5.87	122.78	109.81
1	B	436	VAL	N-CA-C	5.76	117.18	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	574	PRO	N-CA-C	-5.69	106.74	113.86
1	D	462	SER	N-CA-C	5.65	119.92	113.19
1	A	465	THR	OG1-CB-CG2	-5.54	98.22	109.30
1	B	488	VAL	N-CA-CB	5.47	117.55	110.99
1	C	410	GLU	N-CA-C	-5.45	105.03	110.97
1	D	537	ASP	N-CA-CB	-5.43	101.32	110.49
1	C	556	ILE	N-CA-C	-5.41	105.25	110.72
1	A	580	VAL	N-CA-CB	-5.39	101.00	110.77
1	B	610	LEU	N-CA-C	-5.39	105.06	111.69
1	A	610	LEU	N-CA-C	-5.36	105.52	111.36
1	A	556	ILE	N-CA-C	-5.35	105.31	110.72
1	A	604	THR	N-CA-C	5.30	116.89	108.79
1	C	573	SER	CB-CA-C	-5.29	105.74	110.71
1	D	610	LEU	N-CA-C	-5.28	105.19	111.69
1	B	543	GLU	N-CA-C	-5.27	102.73	110.42
1	A	526	LEU	N-CA-C	-5.25	106.88	113.28
1	C	531	THR	OG1-CB-CG2	-5.18	98.93	109.30
1	D	443	ASN	N-CA-C	5.17	118.33	111.30
1	B	439	PRO	CA-C-O	-5.12	115.75	121.23
1	C	390	THR	N-CA-C	-5.10	101.61	109.52
1	B	488	VAL	CB-CA-C	5.10	117.78	110.84
1	D	654	THR	N-CA-C	-5.07	103.80	110.43
1	B	519	SER	N-CA-C	5.05	116.48	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	45	0
1	B	2105	0	2103	48	0
1	C	2105	0	2103	47	0
1	D	2083	0	2083	79	0
2	A	27	0	12	0	0
2	B	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	218	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 13.

All (218) 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:HH21	1:B:487:ARG:HG3	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:HG2	1:D:637:ARG:NH2	2.01	0.75
1:D:438:ASN:H	1:D:438:ASN:ND2	1.85	0.75
1:D:448:ILE:HD13	1:D:615:LYS:HD3	1.72	0.72
1:B:487:ARG:HH21	1:B:487:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:496:TRP:H	1:D:496:TRP:CD1	2.13	0.66
1:C:580:VAL:CG2	4:C:206:HOH:O	2.45	0.65
1:B:476:GLU:CD	1:B:476:GLU:H	2.03	0.65
1:C:499:PRO:HG3	4:C:266:HOH:O	1.97	0.64
1:B:607:MET:HE1	1:B:662:LEU:HD21	1.79	0.64
1:C:402:GLU:HG3	1:C:476:GLU:CD	2.23	0.63
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:C:394:MET:HE1	1:C:467:LEU:CD1	2.29	0.63
1:C:394:MET:HE1	1:C:467:LEU:HD11	1.80	0.62
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
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:B:389:THR:C	1:B:567:ASP:OD1	2.44	0.60
1:D:394:MET:HB2	1:D:446:LEU:HG	1.83	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:A:640:PHE:CE1	1:A:644:LEU:HD13	2.36	0.59
1:A:436:VAL:HG12	1:A:438:ASN:ND2	2.18	0.58
1:A:436:VAL:CG1	1:A:438:ASN:HD21	2.17	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:A:482:ILE:HD11	1:A:484:HIS:HD2	1.70	0.56
1:B:412:VAL:HG12	1:B:413:GLN:HG2	1.86	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:A:543:GLU:C	1:A:545:GLY:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:GLY:C	1:C:407:GLU:HG2	2.32	0.55
1:D:434:CYS:O	1:D:435:LEU:C	2.50	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:A:446:LEU:HD12	1:A:446:LEU:C	2.34	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:B:407:GLU:CD	1:B:407:GLU:H	2.18	0.52
1:D:400:PHE:HA	1:D:439:PRO:HA	1.91	0.51
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:B:513:ASP:C	1:B:513:ASP:OD2	2.53	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:D:636:LEU:O	1:D:637:ARG:NH2	2.44	0.50
1:A:543:GLU:C	1:A:545:GLY:N	2.69	0.49
1:A:643:LYS:HE2	4:A:169:HOH:O	2.12	0.49
1:D:482:ILE:HD13	1:D:482:ILE:C	2.38	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:D:412:VAL:HG11	1:D:469:MET:HE3	1.92	0.49
1:B:476:GLU:CD	1:B:476:GLU:N	2.70	0.49
1:B:524:CYS:O	1:B:555:ARG:HD2	2.11	0.49
1:B:542:GLY:O	1:B:543:GLU:C	2.56	0.49
1:D:664:GLU:HG3	4:D:315:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:611:ARG:NH2	1:C:645:MET:HE2	2.28	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:626:PHE:CD1	1:A:626:PHE:C	2.91	0.48
1:B:487:ARG:CG	1:B:487:ARG:NH2	2.69	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: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:C:394:MET:CE	1:C:467:LEU:HD11	2.43	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
1:B:397:VAL:HA	1:B:479:GLU:O	2.15	0.46
1:C:467:LEU:HD12	1:C:467:LEU:O	2.16	0.46
1:B:464:LYS:HB2	1:B:464:LYS:HE2	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:A:482:ILE:HD11	1:A:484:HIS:CD2	2.49	0.45
1:C:517:TYR:OH	1:C:537:ASP:OD2	2.29	0.45
1:A:487:ARG:HB2	1:A:487:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:407:GLU:CD	1:C:407:GLU:H	2.25	0.44
1:D:593:LYS:O	1:D:594:LEU:C	2.59	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:CD1	1:D:496:TRP:N	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:A:397:VAL:HG11	1:A:470:LEU:HD21	1.99	0.43
1:A:449:GLU:O	1:A:450:LYS:C	2.60	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:D:507:ILE:O	1:D:507:ILE:HG23	2.17	0.43
1:C:510:VAL:HG12	1:C:511:SER:N	2.32	0.43
1:A:617:LEU:CD2	1:A:617:LEU:C	2.91	0.43
1:C:494:PHE:CE2	1:C:496:TRP:HB3	2.54	0.43
1:C:389:THR:HG21	1:C:598:LYS:HA	2.00	0.43
1:C:402:GLU:HG3	1:C:476:GLU:CG	2.49	0.43
1:C:489:SER:HB2	1:C:564:LYS:HE2	2.00	0.43
1:B:404:GLY:HA2	1:B:407:GLU:OE1	2.19	0.43
1:B:516:ARG:HH11	1:B:516:ARG:CG	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:OD2	1:B:579:ASP:N	2.49	0.42
1:C:514:GLU:CD	1:C:518:LYS:NZ	2.77	0.42
1:A:617:LEU:HD22	1:A:619:LEU:HD13	2.02	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:PHE:CE1	1:A:645:MET:HE3	2.55	0.42
1:C:397:VAL:HA	1:C:479:GLU:O	2.19	0.42
1:D:408:LEU:HD23	1:D:408:LEU:C	2.44	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:B:544:GLY:O	1:B:545:GLY:C	2.63	0.41
1:C:454:LEU:HD23	1:C:615:LYS:C	2.45	0.41
1:D:397:VAL:HA	1:D:479:GLU:O	2.21	0.41
1:D:444:ILE:HD13	1:D:444:ILE:HA	1.64	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: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:C:467:LEU:HD12	1:C:467:LEU:C	2.45	0.41
1:C:644:LEU:CD2	1:C:662:LEU:HD23	2.51	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
1:C:471:ILE:HG21	1:C:471:ILE:HD13	1.85	0.40
1:D:482:ILE:C	1:D:482:ILE:CD1	2.95	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%)	30	39
1	B	263/286 (92%)	250 (95%)	13 (5%)	0	100	100
1	C	263/286 (92%)	251 (95%)	11 (4%)	1 (0%)	30	39
1	D	260/286 (91%)	238 (92%)	18 (7%)	4 (2%)	8	10
All	All	1048/1144 (92%)	990 (94%)	52 (5%)	6 (1%)	21	29

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 ⓘ

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%)	192 (82%)	41 (18%)	2	1
1	B	234/252 (93%)	199 (85%)	35 (15%)	3	2
1	C	234/252 (93%)	195 (83%)	39 (17%)	2	2
1	D	231/252 (92%)	187 (81%)	44 (19%)	1	1
All	All	932/1008 (92%)	773 (83%)	159 (17%)	2	1

All (159) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	392	ILE
1	A	403	GLU

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Mol	Chain	Res	Type
1	A	407	GLU
1	A	408	LEU
1	A	410	GLU
1	A	411	LYS
1	A	431	SER
1	A	435	LEU
1	A	436	VAL
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	476	GLU
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	621	GLN
1	A	623	SER
1	A	635	SER
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	403	GLU
1	B	407	GLU
1	B	408	LEU

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Mol	Chain	Res	Type
1	B	412	VAL
1	B	413	GLN
1	B	435	LEU
1	B	442	LYS
1	B	449	GLU
1	B	450	LYS
1	B	454	LEU
1	B	476	GLU
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	621	GLN
1	B	642	SER
1	B	643	LYS
1	B	645	MET
1	B	648	ASP
1	B	660	SER
1	B	666	LEU
1	C	396	ASN
1	C	402	GLU
1	C	407	GLU
1	C	408	LEU
1	C	410	GLU
1	C	411	LYS
1	C	412	VAL
1	C	413	GLN
1	C	431	SER
1	C	435	LEU

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Mol	Chain	Res	Type
1	C	446	LEU
1	C	450	LYS
1	C	454	LEU
1	C	460	THR
1	C	464	LYS
1	C	467	LEU
1	C	468	LEU
1	C	476	GLU
1	C	487	ARG
1	C	488	VAL
1	C	507	ILE
1	C	511	SER
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	621	GLN
1	C	623	SER
1	C	634	GLN
1	C	644	LEU
1	C	657	ARG
1	C	664	GLU
1	C	666	LEU
1	D	390	THR
1	D	396	ASN
1	D	398	THR
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	444	ILE
1	D	450	LYS
1	D	453	MET

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Mol	Chain	Res	Type
1	D	454	LEU
1	D	460	THR
1	D	468	LEU
1	D	475	LEU
1	D	476	GLU
1	D	478	SER
1	D	482	ILE
1	D	484	HIS
1	D	485	SER
1	D	488	VAL
1	D	498	MET
1	D	507	ILE
1	D	519	SER
1	D	543	GLU
1	D	546	VAL
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 (17) 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	493	GLN
1	A	538	ASN
1	A	585	GLN

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Mol	Chain	Res	Type
1	A	652	GLN
1	B	396	ASN
1	B	413	GLN
1	B	443	ASN
1	B	484	HIS
1	B	493	GLN
1	B	538	ASN
1	C	585	GLN
1	D	438	ASN
1	D	585	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
3	ACY	D	5	-	3,3,3	0.33	0	3,3,3	1.66	1 (33%)
2	ADP	B	8	-	28,29,29	1.01	2 (7%)	43,45,45	2.04	11 (25%)
3	ACY	C	3	-	3,3,3	0.65	0	3,3,3	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACY	B	2	-	3,3,3	0.72	0	3,3,3	1.36	0
2	ADP	D	10	-	28,29,29	1.17	3 (10%)	43,45,45	1.99	9 (20%)
3	ACY	A	6	-	3,3,3	0.88	0	3,3,3	0.96	0
3	ACY	D	4	-	3,3,3	0.71	0	3,3,3	1.06	0
2	ADP	C	9	-	28,29,29	1.16	3 (10%)	43,45,45	1.84	8 (18%)
3	ACY	A	1	-	3,3,3	1.03	0	3,3,3	1.24	0
2	ADP	A	7	-	28,29,29	1.30	4 (14%)	43,45,45	2.03	10 (23%)

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	B	8	-	-	2/16/32/32	0/3/3/3
2	ADP	A	7	-	-	4/16/32/32	0/3/3/3
2	ADP	D	10	-	-	8/16/32/32	0/3/3/3
2	ADP	C	9	-	-	3/16/32/32	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	7	ADP	PA-O3A	3.51	1.63	1.59
2	D	10	ADP	C2-N3	3.06	1.39	1.33
2	B	8	ADP	C2-N3	3.03	1.39	1.33
2	C	9	ADP	C2-N3	2.95	1.39	1.33
2	D	10	ADP	C2-N1	2.85	1.39	1.33
2	A	7	ADP	C2-N3	2.84	1.39	1.33
2	A	7	ADP	C2-N1	2.73	1.38	1.33
2	C	9	ADP	C2-N1	2.51	1.38	1.33
2	D	10	ADP	C8-N7	2.46	1.36	1.31
2	C	9	ADP	C8-N7	2.45	1.36	1.31
2	B	8	ADP	C8-N7	2.17	1.35	1.31
2	A	7	ADP	C8-N7	2.01	1.35	1.31

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	8	ADP	N3-C2-N1	-6.60	118.60	128.58
2	D	10	ADP	N3-C2-N1	-6.13	119.30	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	7	ADP	N3-C2-N1	-5.60	120.11	128.58
2	A	7	ADP	C5-C4-N3	-5.43	119.24	126.72
2	C	9	ADP	N3-C2-N1	-5.10	120.86	128.58
2	C	9	ADP	C5-C4-N3	-4.97	119.88	126.72
2	D	10	ADP	C5-C4-N3	-4.90	119.97	126.72
2	B	8	ADP	N9-C8-N7	-4.44	107.64	113.94
2	D	10	ADP	C2-N3-C4	3.98	121.56	111.83
2	D	10	ADP	N9-C8-N7	-3.90	108.41	113.94
2	A	7	ADP	C2-N3-C4	3.89	121.32	111.83
2	B	8	ADP	C5-C4-N3	-3.87	121.38	126.72
2	B	8	ADP	C2-N3-C4	3.77	121.04	111.83
2	A	7	ADP	N3-C4-N9	3.67	133.40	127.17
2	D	10	ADP	C5-N7-C8	3.65	109.19	103.45
2	A	7	ADP	O3B-PB-O3A	3.60	116.70	104.64
2	C	9	ADP	C2-N3-C4	3.58	120.57	111.83
2	B	8	ADP	C5-N7-C8	3.51	108.96	103.45
2	D	10	ADP	N3-C4-N9	3.31	132.80	127.17
2	C	9	ADP	C5-N7-C8	3.30	108.64	103.45
2	A	7	ADP	C5-N7-C8	3.29	108.62	103.45
2	B	8	ADP	O2B-PB-O3A	3.26	115.58	104.64
2	C	9	ADP	C4-C5-N7	-3.26	106.85	110.58
2	A	7	ADP	N9-C8-N7	-3.23	109.35	113.94
2	C	9	ADP	N9-C8-N7	-3.14	109.48	113.94
2	A	7	ADP	O3'-C3'-C4'	-2.98	102.53	111.08
2	B	8	ADP	O4'-C1'-N9	-2.78	102.75	108.09
2	B	8	ADP	O2'-C2'-C1'	2.76	119.60	110.10
2	D	10	ADP	O3B-PB-O3A	2.74	113.83	104.64
2	D	10	ADP	C4-C5-N7	-2.70	107.49	110.58
2	C	9	ADP	N3-C4-N9	2.64	131.66	127.17
2	B	8	ADP	C4-N9-C8	2.59	108.45	105.74
2	B	8	ADP	N3-C4-N9	2.53	131.46	127.17
2	B	8	ADP	C4-C5-N7	-2.44	107.79	110.58
2	C	9	ADP	C5-C4-N9	2.43	108.45	105.81
2	A	7	ADP	C4-C5-N7	-2.42	107.82	110.58
2	D	10	ADP	O2A-PA-O3A	2.32	113.55	107.27
3	D	5	ACY	O-C-CH3	-2.27	113.21	122.53
2	A	7	ADP	C3'-C2'-C1'	2.15	105.54	101.46

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	9	ADP	O4'-C4'-C5'-O5'
2	A	7	ADP	PA-O3A-PB-O1B
2	D	10	ADP	PA-O3A-PB-O1B
2	D	10	ADP	C2'-C1'-N9-C8
2	A	7	ADP	C5'-O5'-PA-O1A
2	A	7	ADP	C5'-O5'-PA-O2A
2	A	7	ADP	C5'-O5'-PA-O3A
2	B	8	ADP	C5'-O5'-PA-O1A
2	B	8	ADP	C5'-O5'-PA-O3A
2	D	10	ADP	C5'-O5'-PA-O1A
2	C	9	ADP	PA-O3A-PB-O1B
2	D	10	ADP	C2'-C1'-N9-C4
2	C	9	ADP	C3'-C4'-C5'-O5'
2	D	10	ADP	O4'-C1'-N9-C8
2	D	10	ADP	O4'-C1'-N9-C4
2	D	10	ADP	C3'-C4'-C5'-O5'
2	D	10	ADP	O4'-C4'-C5'-O5'

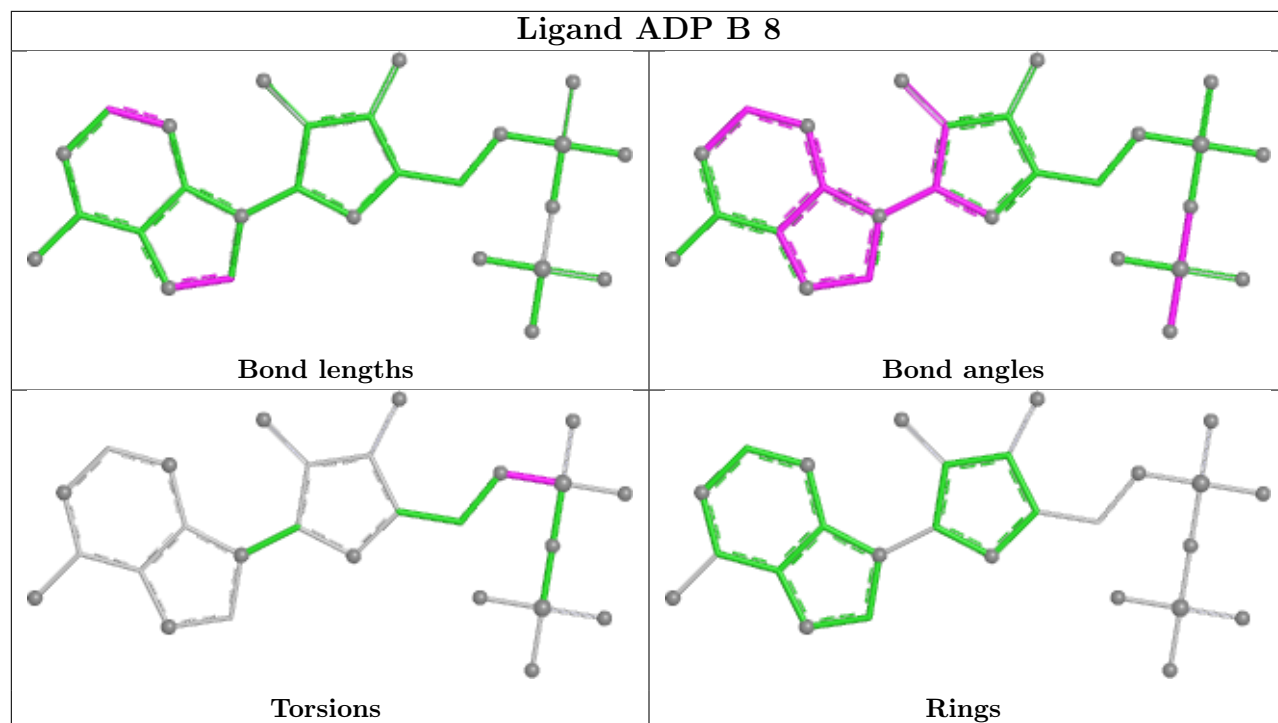
There are no ring outliers.

2 monomers are involved in 3 short contacts:

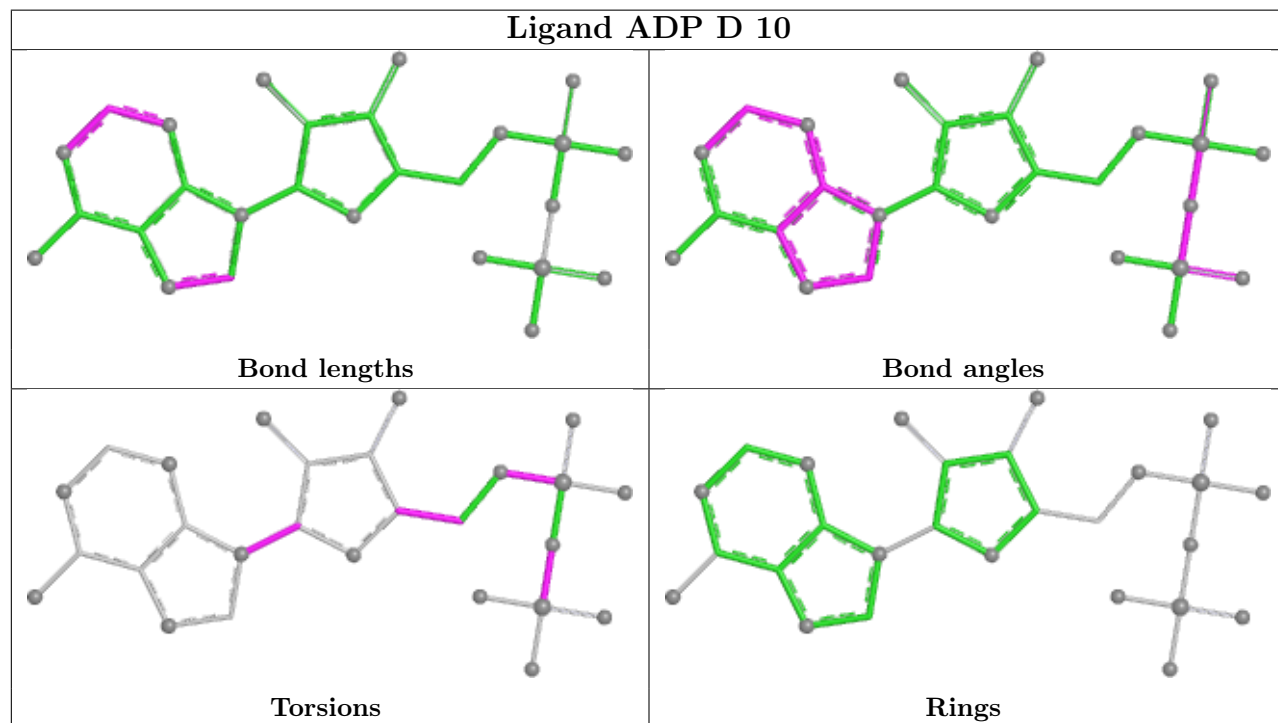
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	5	ACY	1	0
2	D	10	ADP	2	0

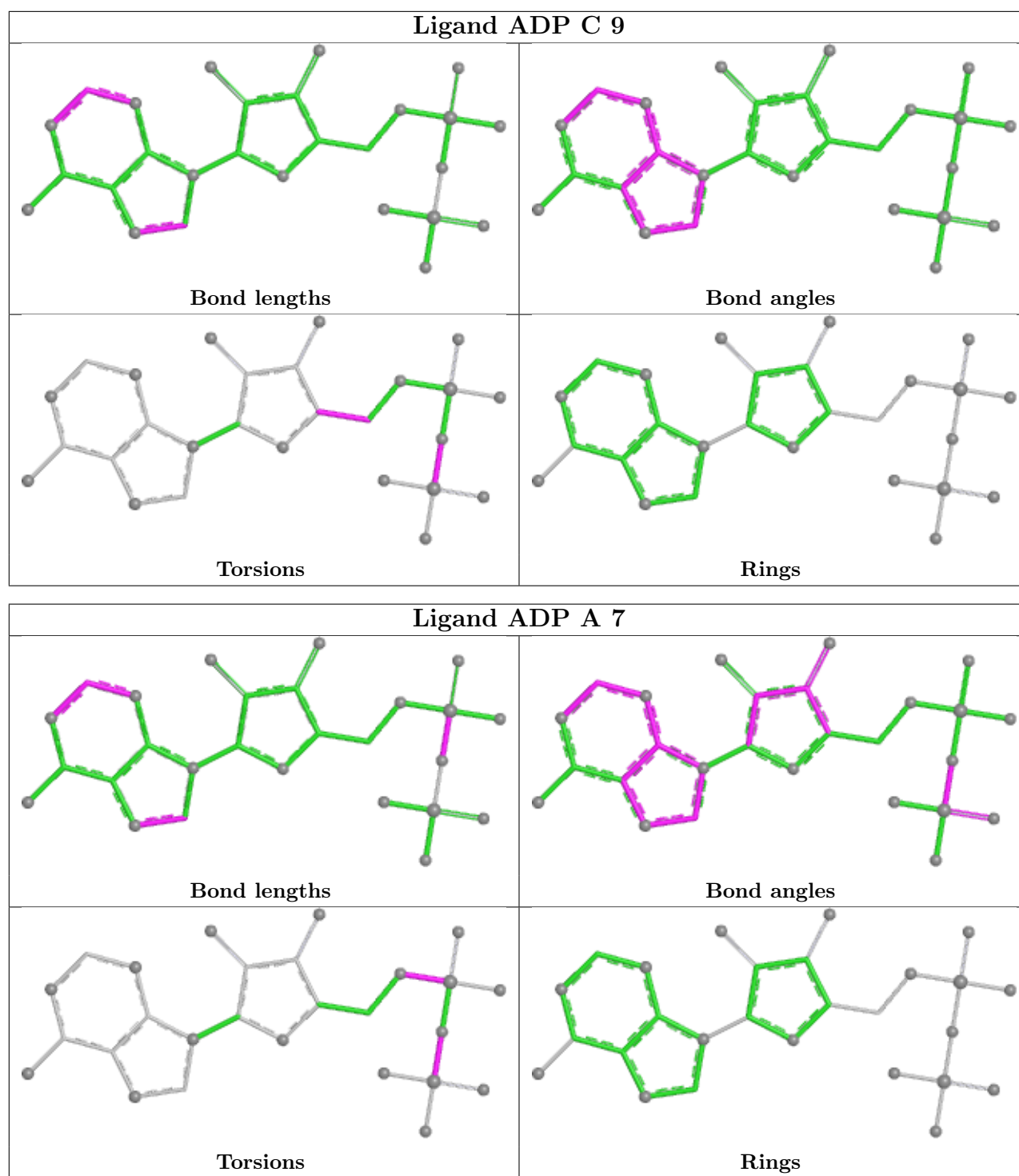
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand ADP B 8



Ligand ADP D 10





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	266/286 (93%)	-0.09	7 (2%) 57 58	19, 39, 65, 76	0
1	B	267/286 (93%)	-0.03	10 (3%) 45 46	23, 38, 61, 83	0
1	C	267/286 (93%)	-0.08	5 (1%) 66 66	19, 36, 63, 74	0
1	D	264/286 (92%)	0.26	20 (7%) 20 19	21, 43, 80, 94	0
All	All	1064/1144 (93%)	0.02	42 (3%) 43 44	19, 39, 67, 94	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	670	SER	4.6
1	D	430	PHE	4.3
1	D	412	VAL	4.2
1	D	435	LEU	4.2
1	D	401	TRP	3.7
1	B	436	VAL	3.6
1	D	434	CYS	3.5
1	C	476	GLU	3.4
1	C	670	SER	3.4
1	A	413	GLN	3.0
1	D	436	VAL	3.0
1	D	496	TRP	3.0
1	B	648	ASP	2.9
1	B	430	PHE	2.9
1	A	543	GLU	2.7
1	A	544	GLY	2.7
1	A	430	PHE	2.6
1	A	670	SER	2.6
1	C	544	GLY	2.6
1	C	402	GLU	2.5
1	B	670	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	479	GLU	2.4
1	D	481	ILE	2.4
1	C	481	ILE	2.4
1	B	413	GLN	2.4
1	D	438	ASN	2.4
1	D	498	MET	2.3
1	D	494	PHE	2.2
1	D	508	PHE	2.2
1	A	410	GLU	2.2
1	D	390	THR	2.2
1	B	481	ILE	2.2
1	B	429	SER	2.2
1	D	433	LEU	2.1
1	B	482	ILE	2.1
1	B	543	GLU	2.1
1	D	437	GLY	2.1
1	D	486	GLY	2.1
1	B	402	GLU	2.1
1	D	510	VAL	2.0
1	D	408	LEU	2.0
1	A	432	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	D	10	27/27	0.81	0.17	63,94,105,106	0
2	ADP	C	9	27/27	0.88	0.13	51,68,75,76	0

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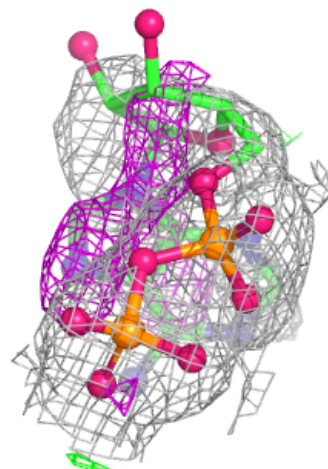
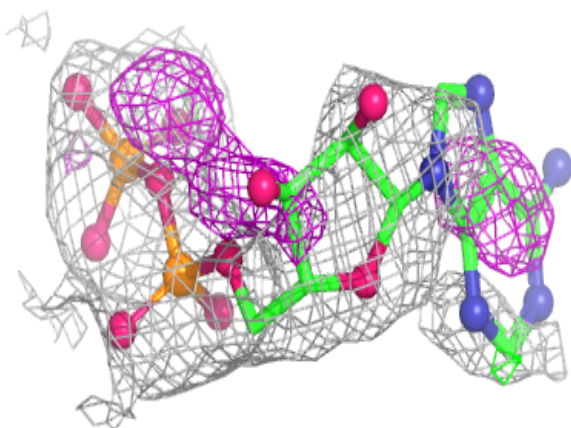
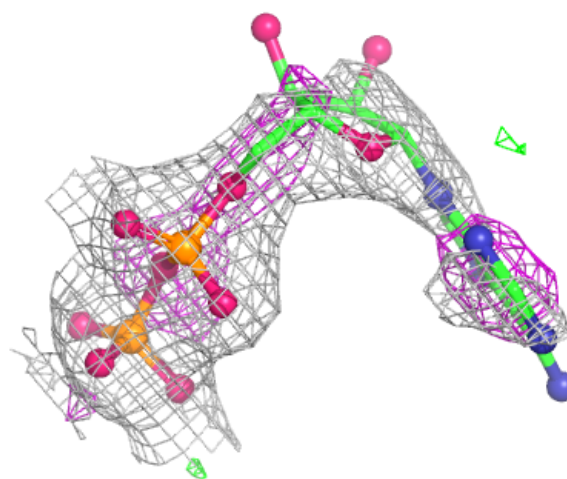
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	A	7	27/27	0.91	0.12	49,74,84,85	0
3	ACY	D	5	4/4	0.91	0.11	35,36,37,37	0
3	ACY	A	6	4/4	0.94	0.11	40,40,40,41	0
2	ADP	B	8	27/27	0.94	0.10	40,51,61,63	0
3	ACY	A	1	4/4	0.95	0.07	27,28,28,29	0
3	ACY	D	4	4/4	0.96	0.07	39,40,41,41	0
3	ACY	C	3	4/4	0.97	0.06	27,30,30,34	0
3	ACY	B	2	4/4	0.98	0.08	41,41,42,43	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.

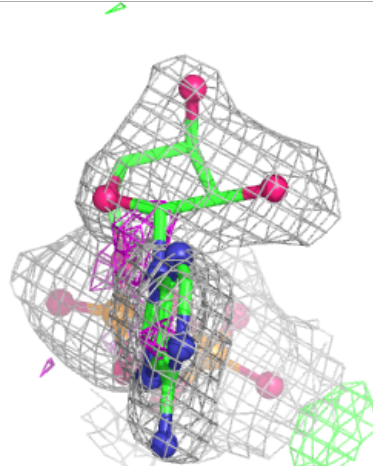
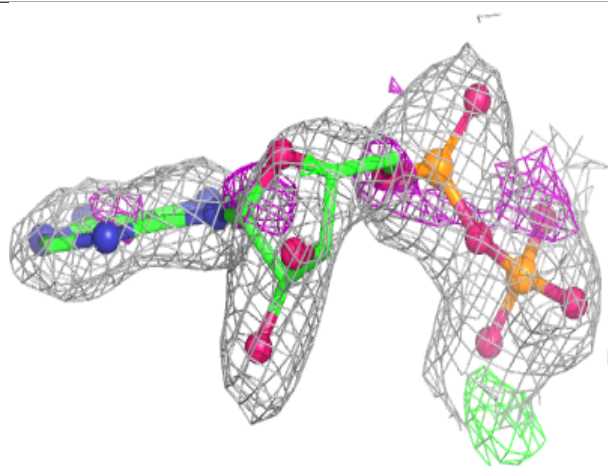
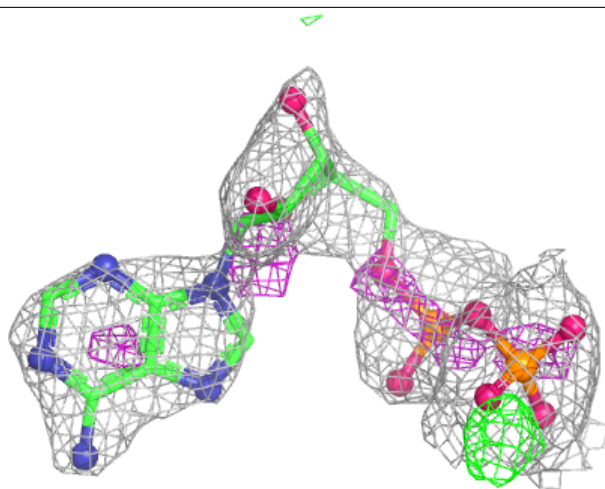
Electron density around ADP D 10:

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



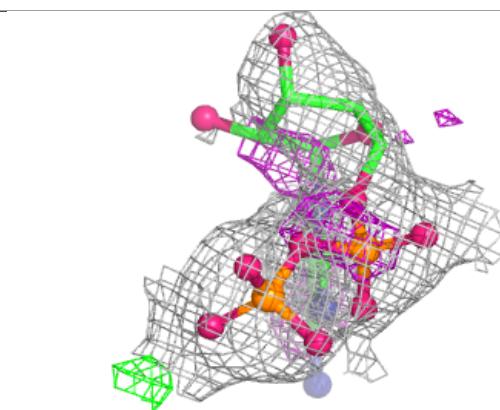
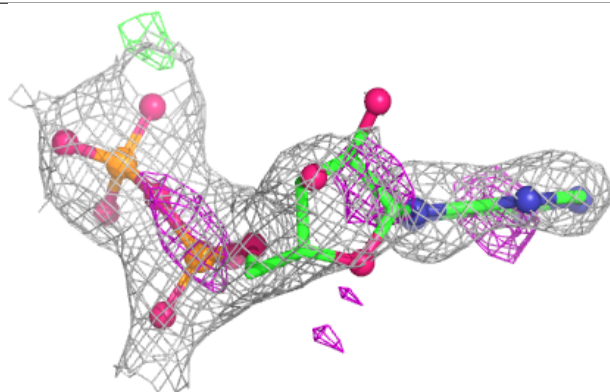
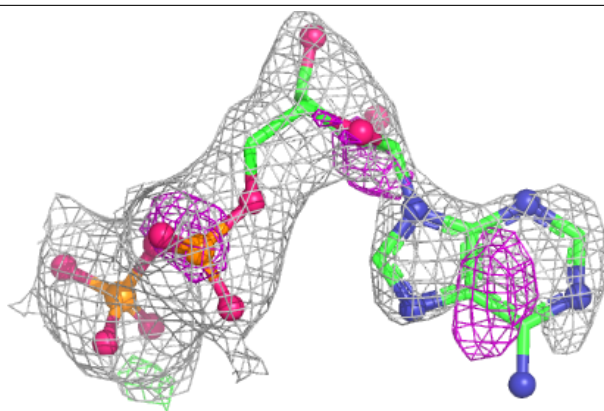
Electron density around ADP C 9:

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

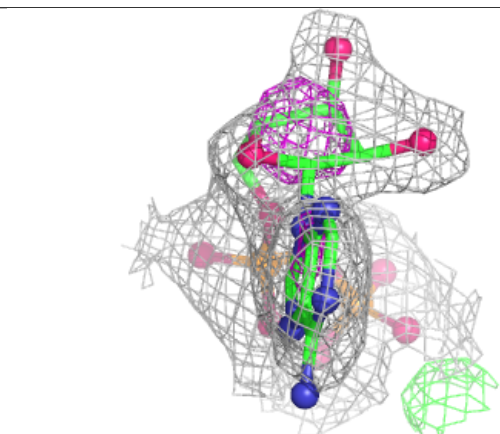
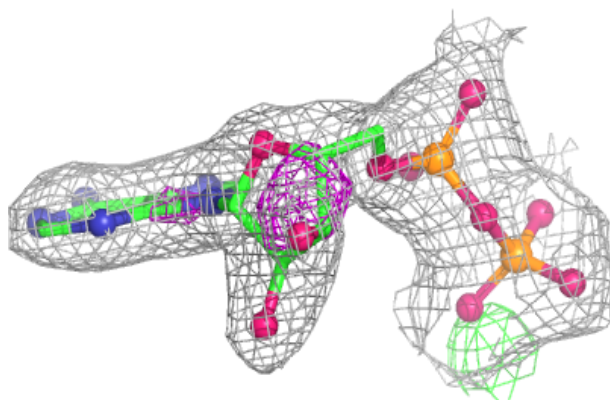
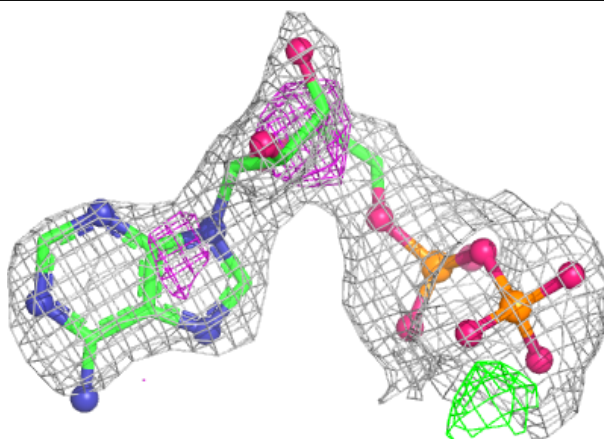


Electron density around ADP A 7:

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.