



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:36 PM UTC

PDB ID : 4M9X / pdb_00004m9x
Title : Crystal structure of CED-4 bound CED-3 fragment
Authors : Huang, W.J.; Jinag, T.Y.; Choi, W.Y.; Wang, J.W.; Shi, Y.G.
Deposited on : 2013-08-15
Resolution : 3.34 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

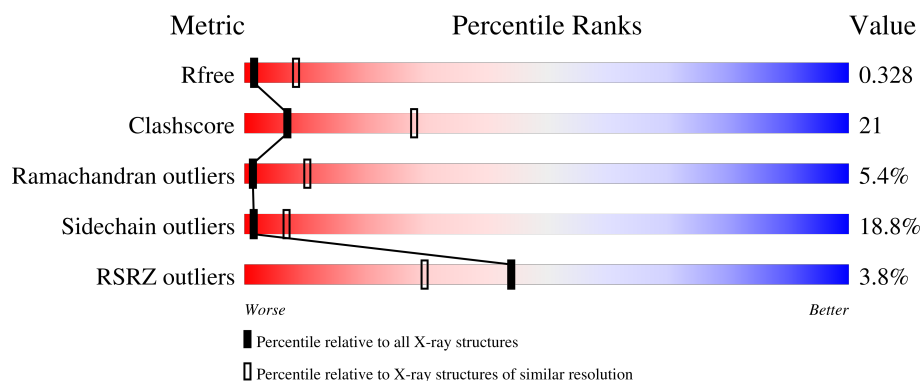
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.34 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	1434 (3.38-3.30)
Clashscore	190562	1479 (3.38-3.30)
Ramachandran outliers	187476	1456 (3.38-3.30)
Sidechain outliers	187428	1455 (3.38-3.30)
RSRZ outliers	180081	1434 (3.38-3.30)

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	549	3% 46% 35% 11% 7%
1	B	549	4% 43% 36% 13% 7%
2	C	8	25% 50% 25% 12% 12%
2	D	8	25% 38% 38%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8349 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 Cell death protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	0	0
			4088	2606	685	767	30			
1	B	511	Total	C	N	O	S	0	0	0
			4094	2607	688	768	31			

- Molecule 2 is a protein called CED-3 fragment.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	7	Total	C	N	O	0	0	0
			57	41	8	8			
2	D	5	Total	C	N	O	0	0	0
			46	34	6	6			

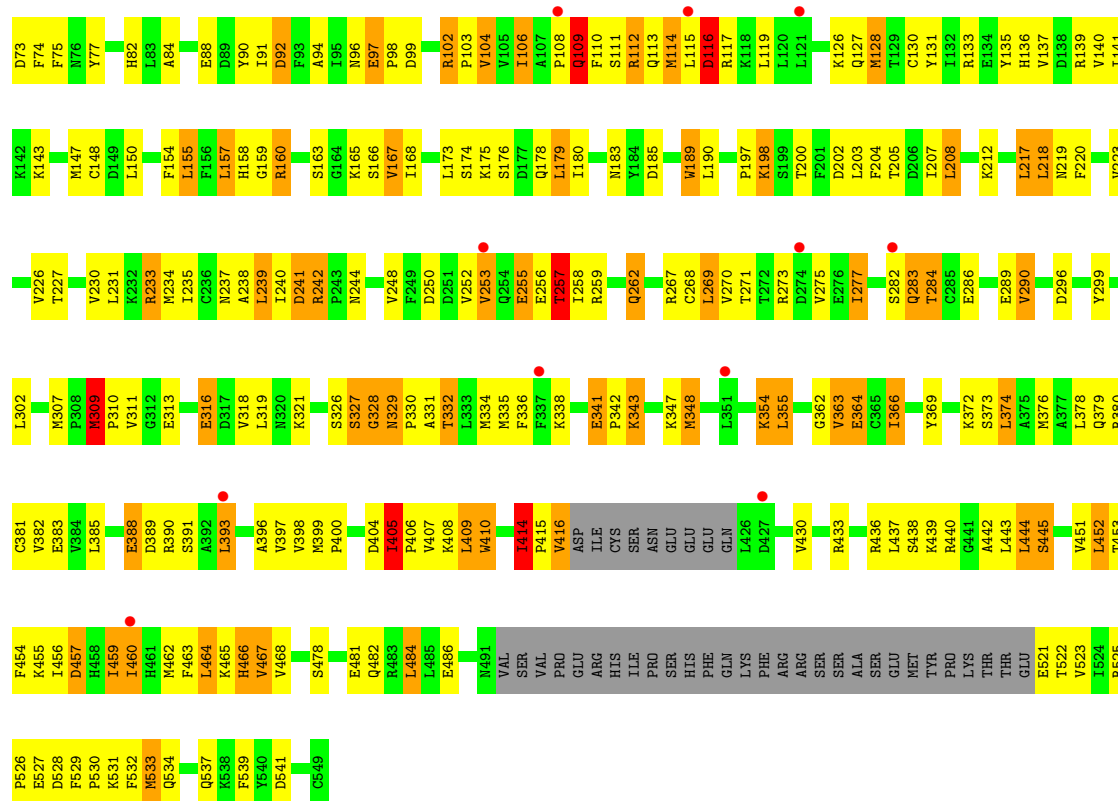
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



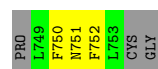
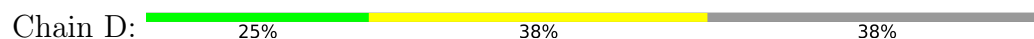
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0



● Molecule 2: CED-3 fragment



● Molecule 2: CED-3 fragment



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	182.80Å 182.80Å 202.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.64 – 3.34 41.64 – 3.34	Depositor EDS
% Data completeness (in resolution range)	66.4 (41.64-3.34) 66.3 (41.64-3.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.272 , 0.333 0.267 , 0.328	Depositor DCC
R_{free} test set	858 reflections (3.42%)	wwPDB-VP
Wilson B-factor (Å ²)	97.3	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 225.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	8349	wwPDB-VP
Average B, all atoms (Å ²)	252.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/4163	1.07	25/5625 (0.4%)
1	B	0.43	0/4169	1.09	29/5633 (0.5%)
2	C	0.38	0/59	0.75	0/78
2	D	0.33	0/47	0.60	0/62
All	All	0.44	0/8438	1.08	54/11398 (0.5%)

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

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	484	LEU	N-CA-C	-10.37	99.94	111.14
1	A	540	TYR	N-CA-C	-7.90	104.25	114.04
1	B	414	ILE	CA-C-N	7.86	128.92	120.11
1	B	414	ILE	C-N-CA	7.86	128.92	120.11
1	B	329	ASN	CA-C-N	7.69	129.46	119.84
1	B	329	ASN	C-N-CA	7.69	129.46	119.84
1	A	242	ARG	CA-C-N	7.60	127.52	119.85
1	A	242	ARG	C-N-CA	7.60	127.52	119.85
1	B	405	ILE	CA-C-N	7.58	128.03	119.92
1	B	405	ILE	C-N-CA	7.58	128.03	119.92
1	A	414	ILE	CA-C-N	7.08	128.03	120.11
1	A	414	ILE	C-N-CA	7.08	128.03	120.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	MET	CA-C-N	6.74	127.11	119.83
1	B	307	MET	C-N-CA	6.74	127.11	119.83
1	A	541	ASP	N-CA-C	-6.68	104.39	112.54
1	A	217	LEU	N-CA-C	-6.61	105.51	113.97
1	A	329	ASN	CA-C-N	6.57	128.05	119.84
1	A	329	ASN	C-N-CA	6.57	128.05	119.84
1	B	464	LEU	N-CA-C	6.46	118.32	111.28
1	A	405	ILE	CA-C-N	6.39	126.75	119.92
1	A	405	ILE	C-N-CA	6.39	126.75	119.92
1	B	92	ASP	N-CA-C	-6.19	104.07	111.69
1	A	165	LYS	N-CA-C	6.17	117.67	111.07
1	B	268	CYS	N-CA-C	6.00	118.68	108.90
1	A	307	MET	CA-C-N	5.85	126.15	119.83
1	A	307	MET	C-N-CA	5.85	126.15	119.83
1	A	113	GLN	N-CA-C	-5.82	106.80	114.31
1	B	30	LEU	N-CA-C	-5.81	106.32	113.41
1	B	309	MET	CA-C-N	5.81	126.62	120.11
1	B	309	MET	C-N-CA	5.81	126.62	120.11
1	B	60	ILE	N-CA-C	5.72	117.14	110.62
1	A	30	LEU	N-CA-C	5.72	120.39	113.41
1	B	283	GLN	N-CA-C	5.71	115.93	107.88
1	B	217	LEU	N-CA-C	-5.67	106.71	113.97
1	B	114	MET	N-CA-C	5.63	117.10	111.07
1	A	71	LEU	N-CA-C	-5.61	107.68	114.75
1	A	525	ARG	CA-C-N	5.47	125.45	120.03
1	A	525	ARG	C-N-CA	5.47	125.45	120.03
1	B	242	ARG	CA-C-N	5.41	125.36	119.78
1	B	242	ARG	C-N-CA	5.41	125.36	119.78
1	B	393	LEU	N-CA-C	-5.39	105.40	111.28
1	B	7	CYS	N-CA-C	-5.33	105.92	112.90
1	A	80	GLN	N-CA-C	-5.31	105.03	112.25
1	A	212	LYS	N-CA-C	5.20	117.76	110.23
1	A	331	ALA	N-CA-C	5.19	116.62	111.07
1	B	400	PRO	CA-C-N	-5.17	114.66	120.14
1	B	400	PRO	C-N-CA	-5.17	114.66	120.14
1	A	69	GLY	CA-C-N	5.13	126.26	119.84
1	A	69	GLY	C-N-CA	5.13	126.26	119.84
1	B	40	HIS	N-CA-C	-5.10	105.61	111.07
1	A	34	ASN	N-CA-C	5.10	116.87	110.91
1	B	439	LYS	N-CA-C	5.05	118.21	111.75
1	B	331	ALA	N-CA-C	5.04	116.47	111.07
1	B	343	LYS	N-CA-CB	-5.02	109.08	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	485	LEU	Peptide

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	4088	0	4107	167	0
1	B	4094	0	4116	182	0
2	C	57	0	54	1	0
2	D	46	0	45	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	1	0
4	B	31	0	12	3	0
All	All	8349	0	8346	349	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 21.

All (349) 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:B:230:VAL:HG12	1:B:234:MET:HE2	1.53	0.90
1:B:20:ASP:OD2	1:B:82:HIS:NE2	2.12	0.83
1:A:484:LEU:HD11	1:A:533:MET:HG2	1.61	0.81
1:A:262:GLN:HE21	1:A:283:GLN:HB2	1.46	0.80
1:A:63:ARG:HE	1:A:240:ILE:HD11	1.46	0.80
1:B:366:ILE:HD12	1:B:366:ILE:H	1.49	0.77
1:A:75:PHE:HB2	1:A:84:ALA:HB2	1.66	0.76
1:A:47:MET:HB2	1:A:53:ARG:HG3	1.68	0.75
1:A:366:ILE:HD12	1:A:366:ILE:H	1.49	0.75
1:B:200:THR:HG21	1:B:256:GLU:HB3	1.74	0.70
1:B:102:ARG:HG3	1:B:103:PRO:HD2	1.73	0.69
1:A:364:GLU:HB2	1:A:373:SER:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:PRO:HA	1:B:453:THR:HG22	1.74	0.68
1:B:190:LEU:HD12	1:B:207:ILE:HG13	1.76	0.68
1:A:96:ASN:O	1:A:98:PRO:HD3	1.95	0.67
1:B:24:ARG:HH22	1:B:53:ARG:HH11	1.42	0.67
1:B:165:LYS:HG2	1:B:290:VAL:HG21	1.76	0.67
1:B:72:ILE:HG21	1:B:88:GLU:HG3	1.76	0.67
1:B:335:MET:HE3	1:B:364:GLU:HA	1.75	0.66
2:C:750:PHE:O	2:C:752:PHE:N	2.28	0.66
1:B:372:LYS:H	1:B:376:MET:HE2	1.60	0.66
1:A:8:ARG:HG2	1:A:8:ARG:HH11	1.60	0.66
1:B:75:PHE:HB2	1:B:84:ALA:HB2	1.77	0.66
1:B:478:SER:O	1:B:482:GLN:HG2	1.95	0.66
1:A:414:ILE:HG21	1:A:430:VAL:HG13	1.78	0.65
1:B:135:TYR:O	1:B:139:ARG:HG3	1.95	0.65
1:A:443:LEU:HD23	1:A:460:ILE:HD11	1.79	0.65
1:A:58:LEU:O	1:A:62:ARG:HG3	1.97	0.65
1:B:112:ARG:HA	1:B:116:ASP:HB2	1.79	0.64
1:A:406:PRO:HA	1:A:453:THR:HG22	1.80	0.64
1:B:341:GLU:HB2	1:B:342:PRO:HD3	1.79	0.64
1:A:212:LYS:HA	1:A:212:LYS:HE2	1.80	0.64
1:B:231:LEU:HA	1:B:234:MET:HE3	1.80	0.63
1:A:67:GLU:HG2	1:A:69:GLY:H	1.64	0.63
1:A:341:GLU:HB2	1:A:342:PRO:HD3	1.80	0.62
1:B:342:PRO:O	1:B:343:LYS:HB3	1.99	0.62
1:A:190:LEU:HD12	1:A:207:ILE:HG13	1.80	0.62
1:A:335:MET:HE3	1:A:364:GLU:HA	1.81	0.62
1:A:452:LEU:HD23	1:A:452:LEU:H	1.65	0.62
1:B:443:LEU:HD23	1:B:460:ILE:HD11	1.80	0.62
1:A:204:PHE:HA	1:A:207:ILE:HD12	1.81	0.62
1:B:255:GLU:O	1:B:259:ARG:HG3	2.00	0.61
1:B:108:PRO:O	1:B:109:GLN:HB2	2.00	0.61
1:B:8:ARG:HH11	1:B:8:ARG:HG2	1.63	0.61
1:A:205:THR:HA	1:A:231:LEU:HD11	1.83	0.60
1:B:154:PHE:HE1	1:B:262:GLN:HG3	1.65	0.60
1:A:255:GLU:O	1:A:259:ARG:HG3	2.00	0.60
1:B:409:LEU:HD12	1:B:533:MET:HE2	1.83	0.60
1:A:309:MET:HG3	1:A:310:PRO:HD2	1.84	0.60
1:A:155:LEU:HB3	1:A:269:LEU:HD23	1.83	0.60
1:B:464:LEU:O	1:B:468:VAL:HG22	2.02	0.60
1:A:457:ASP:OD1	1:A:457:ASP:N	2.35	0.59
1:B:309:MET:HG3	1:B:310:PRO:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ARG:HG3	1:B:103:PRO:CD	2.33	0.59
1:A:262:GLN:NE2	1:A:283:GLN:HB2	2.18	0.59
1:A:397:VAL:HG21	1:A:468:VAL:HG21	1.85	0.59
1:A:464:LEU:O	1:A:468:VAL:HG22	2.03	0.58
1:B:364:GLU:HB2	1:B:373:SER:HB3	1.85	0.58
1:A:72:ILE:HG21	1:A:88:GLU:HG3	1.84	0.58
1:A:327:SER:HB2	1:A:459:ILE:HG13	1.84	0.58
1:B:166:SER:HA	1:B:271:THR:HG21	1.86	0.58
1:B:397:VAL:HG21	1:B:468:VAL:HG21	1.85	0.58
1:B:457:ASP:N	1:B:457:ASP:OD1	2.36	0.58
1:B:50:ARG:HA	1:B:53:ARG:HE	1.69	0.57
1:B:59:ARG:HH11	1:B:63:ARG:HH22	1.52	0.57
1:B:109:GLN:C	1:B:111:SER:H	2.12	0.57
1:A:44:ILE:O	1:A:53:ARG:HG2	2.05	0.57
1:A:91:ILE:O	1:A:95:ILE:HG13	2.04	0.57
1:A:342:PRO:O	1:A:343:LYS:HB3	2.05	0.57
1:B:437:LEU:HB3	1:B:444:LEU:HD22	1.86	0.57
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.70	0.56
1:A:247:PHE:HE2	1:A:266:LEU:HD22	1.70	0.56
1:A:463:PHE:O	1:A:467:VAL:HB	2.05	0.56
1:B:23:PRO:HG2	1:B:53:ARG:C	2.31	0.56
1:A:477:ILE:HG21	1:A:544:LYS:HE3	1.88	0.56
1:B:157:LEU:HD11	1:B:168:ILE:HG22	1.87	0.56
1:B:327:SER:HB2	1:B:459:ILE:HG13	1.88	0.56
1:B:150:LEU:O	1:B:267:ARG:NH1	2.39	0.56
1:A:150:LEU:O	1:A:267:ARG:NH1	2.38	0.56
1:A:143:LYS:O	1:A:147:MET:HG3	2.05	0.56
1:B:197:PRO:HD2	1:B:198:LYS:HE2	1.86	0.56
1:B:40:HIS:HD2	1:B:60:ILE:HG23	1.71	0.56
1:A:410:TRP:HD1	1:A:414:ILE:HD13	1.70	0.55
1:B:165:LYS:N	4:B:602:ATP:O2B	2.38	0.55
1:A:532:PHE:HB2	1:A:534:GLN:HG2	1.87	0.55
1:A:248:VAL:HG22	1:A:269:LEU:HB3	1.88	0.55
1:B:414:ILE:HG21	1:B:430:VAL:HG13	1.88	0.55
1:A:332:THR:HG23	1:A:374:LEU:HB2	1.88	0.55
1:A:159:GLY:N	1:A:165:LYS:HD3	2.21	0.55
1:B:521:GLU:C	1:B:523:VAL:H	2.14	0.55
1:A:521:GLU:C	1:A:523:VAL:H	2.15	0.54
1:B:128:MET:HG3	1:B:167:VAL:HG22	1.88	0.54
1:A:393:LEU:HB2	1:A:437:LEU:HD11	1.90	0.54
1:B:452:LEU:HD23	1:B:452:LEU:H	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:MET:HB2	1:B:53:ARG:HG3	1.88	0.54
1:A:415:PRO:O	1:A:416:VAL:HG23	2.06	0.54
1:B:204:PHE:HA	1:B:207:ILE:HD12	1.89	0.54
1:B:47:MET:HE3	1:B:52:GLU:HG2	1.90	0.53
1:B:529:PHE:N	1:B:530:PRO:HD3	2.23	0.53
1:A:137:VAL:O	1:A:141:ILE:HG13	2.09	0.53
1:A:233:ARG:HG3	1:A:233:ARG:HH11	1.73	0.53
1:B:92:ASP:OD1	1:B:96:ASN:ND2	2.41	0.53
1:A:283:GLN:HG2	1:A:284:THR:H	1.72	0.53
1:A:354:LYS:HD3	1:A:362:GLY:O	2.08	0.53
1:B:35:ILE:HD12	1:B:70:PRO:HG2	1.91	0.53
1:A:391:SER:OG	1:A:415:PRO:HG2	2.08	0.53
1:A:326:SER:O	1:A:328:GLY:N	2.42	0.53
1:B:44:ILE:O	1:B:53:ARG:HG2	2.09	0.53
1:B:155:LEU:HB3	1:B:269:LEU:HD23	1.91	0.53
1:B:4:GLU:O	1:B:8:ARG:HB2	2.09	0.52
1:A:465:LYS:HD3	1:A:466:HIS:CE1	2.44	0.52
1:A:437:LEU:HB3	1:A:444:LEU:HD22	1.90	0.52
1:B:111:SER:O	1:B:115:LEU:HB3	2.09	0.52
1:B:143:LYS:O	1:B:147:MET:HG3	2.10	0.52
1:A:272:THR:HG21	1:A:277:ILE:HD11	1.92	0.52
1:B:257:THR:HG22	1:B:258:ILE:N	2.24	0.52
1:A:135:TYR:CZ	1:A:139:ARG:HD2	2.45	0.52
1:B:257:THR:HG22	1:B:258:ILE:HD12	1.91	0.52
1:B:4:GLU:HG3	1:B:5:ILE:N	2.24	0.52
1:B:237:ASN:C	1:B:239:LEU:H	2.18	0.52
1:B:299:TYR:HA	1:B:302:LEU:HD12	1.92	0.52
1:B:527:GLU:N	1:B:527:GLU:OE1	2.42	0.52
1:A:67:GLU:HG2	1:A:69:GLY:N	2.25	0.51
1:A:136:HIS:O	1:A:140:VAL:HG23	2.10	0.51
1:B:8:ARG:HD3	1:B:90:TYR:OH	2.10	0.51
1:B:253:VAL:HG11	1:B:380:ARG:HD3	1.90	0.51
1:B:318:VAL:O	1:B:321:LYS:HB3	2.10	0.51
1:A:257:THR:HG22	1:A:258:ILE:N	2.25	0.51
1:B:269:LEU:HD22	1:B:270:VAL:H	1.76	0.51
1:A:313:GLU:O	1:A:316:GLU:HG3	2.10	0.51
1:B:24:ARG:HH22	1:B:53:ARG:NH1	2.07	0.51
1:A:368:PRO:HG3	1:B:282:SER:HB3	1.92	0.51
1:B:173:LEU:HD23	1:B:179:LEU:HD23	1.93	0.51
1:B:88:GLU:HA	1:B:91:ILE:HG22	1.92	0.51
1:B:302:LEU:HD13	1:B:319:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ILE:HG13	1:A:241:ASP:OD1	2.11	0.51
1:A:529:PHE:N	1:A:530:PRO:HD3	2.26	0.50
1:B:341:GLU:CB	1:B:342:PRO:HD3	2.42	0.50
1:A:90:TYR:HE2	1:A:106:ILE:HD11	1.75	0.50
1:A:447:LYS:HE2	1:A:450:PRO:HD2	1.93	0.50
1:A:111:SER:C	1:A:113:GLN:H	2.20	0.50
1:B:532:PHE:C	1:B:534:GLN:H	2.19	0.50
1:A:252:VAL:HG11	1:A:258:ILE:HD13	1.93	0.50
1:A:102:ARG:HG2	1:A:182:ILE:HG22	1.94	0.50
1:B:5:ILE:HD13	1:B:94:ALA:HB1	1.93	0.50
1:B:415:PRO:O	1:B:416:VAL:HG23	2.12	0.49
1:A:235:ILE:O	1:A:239:LEU:HB2	2.12	0.49
1:B:336:PHE:HE1	1:B:348:MET:HG2	1.77	0.49
1:B:463:PHE:O	1:B:467:VAL:HB	2.12	0.49
1:A:188:VAL:HB	1:A:247:PHE:CD1	2.47	0.49
1:A:197:PRO:HD2	1:A:198:LYS:HE2	1.94	0.49
2:D:751:ASN:O	2:D:751:ASN:ND2	2.45	0.49
1:B:109:GLN:C	1:B:111:SER:N	2.69	0.49
1:A:200:THR:HG21	1:A:256:GLU:HB3	1.94	0.49
1:B:56:ASN:O	1:B:60:ILE:HB	2.13	0.49
1:B:1:MET:HA	1:B:62:ARG:O	2.13	0.49
1:B:255:GLU:HB3	1:B:277:ILE:HG22	1.95	0.49
1:B:273:ARG:NE	4:B:602:ATP:O3G	2.46	0.49
1:B:32:GLY:C	1:B:34:ASN:H	2.21	0.49
1:B:379:GLN:O	1:B:383:GLU:HG3	2.12	0.48
1:B:481:GLU:O	1:B:484:LEU:HG	2.12	0.48
1:B:23:PRO:HG2	1:B:53:ARG:O	2.14	0.48
1:A:343:LYS:O	1:A:343:LYS:HG2	2.13	0.48
1:A:165:LYS:HG2	1:A:290:VAL:HG21	1.96	0.48
1:B:158:HIS:CE1	1:B:289:GLU:HB2	2.49	0.48
1:A:465:LYS:HD3	1:A:466:HIS:HE1	1.79	0.48
1:A:527:GLU:C	1:A:530:PRO:HD3	2.39	0.48
1:B:115:LEU:O	1:B:119:LEU:HB2	2.14	0.48
1:B:159:GLY:N	1:B:165:LYS:HD3	2.28	0.48
1:B:158:HIS:HE1	1:B:289:GLU:HB2	1.79	0.48
1:B:233:ARG:HH11	1:B:233:ARG:CG	2.27	0.48
1:B:49:THR:HG22	1:B:50:ARG:N	2.29	0.48
1:A:341:GLU:CB	1:A:342:PRO:HD3	2.44	0.47
1:A:269:LEU:HD22	1:A:270:VAL:H	1.79	0.47
1:A:385:LEU:HD22	1:A:389:ASP:HB3	1.96	0.47
1:A:116:ASP:OD1	1:A:116:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:529:PHE:HB3	1:B:532:PHE:CZ	2.49	0.47
1:A:444:LEU:HD12	1:A:444:LEU:HA	1.74	0.47
1:B:158:HIS:CD2	1:B:275:VAL:HG13	2.50	0.47
1:A:30:LEU:HD21	1:A:70:PRO:O	2.14	0.47
1:A:90:TYR:CE2	1:A:106:ILE:HD11	2.49	0.47
1:A:255:GLU:HB3	1:A:277:ILE:HG22	1.96	0.47
1:A:160:ARG:HG2	1:A:161:ALA:H	1.80	0.47
1:A:163:SER:C	1:A:330:PRO:HG2	2.40	0.47
1:A:443:LEU:HA	1:A:460:ILE:HG12	1.97	0.47
1:B:35:ILE:CD1	1:B:70:PRO:HG2	2.45	0.47
1:A:253:VAL:HG11	1:A:380:ARG:HD3	1.96	0.47
1:A:160:ARG:NH1	1:A:442:ALA:O	2.48	0.47
1:A:527:GLU:OE1	1:A:527:GLU:N	2.47	0.47
1:B:385:LEU:HD11	1:B:393:LEU:HD12	1.96	0.47
1:B:326:SER:O	1:B:328:GLY:N	2.47	0.47
1:A:478:SER:O	1:A:482:GLN:HG2	2.15	0.46
1:B:248:VAL:HG22	1:B:269:LEU:HB3	1.97	0.46
1:A:92:ASP:C	1:A:94:ALA:H	2.23	0.46
1:A:436:ARG:O	1:A:440:ARG:HG3	2.15	0.46
1:B:484:LEU:HD13	1:B:531:LYS:O	2.15	0.46
1:B:537:GLN:O	1:B:541:ASP:N	2.44	0.46
1:A:397:VAL:HG22	1:A:464:LEU:HB3	1.97	0.46
1:B:30:LEU:HB3	1:B:36:PHE:CD1	2.50	0.46
1:B:133:ARG:O	1:B:137:VAL:HG23	2.16	0.46
1:B:332:THR:HG23	1:B:374:LEU:HB2	1.97	0.46
1:A:25:ASP:HB3	1:A:78:ASN:HD21	1.80	0.46
1:A:274:ASP:OD2	1:A:440:ARG:NH1	2.49	0.46
1:A:157:LEU:HD11	1:A:168:ILE:HG22	1.98	0.46
1:A:178:GLN:O	1:A:182:ILE:HB	2.16	0.46
1:B:460:ILE:HD12	1:B:460:ILE:HA	1.79	0.46
1:B:527:GLU:C	1:B:530:PRO:HD3	2.40	0.46
1:B:136:HIS:O	1:B:140:VAL:HG23	2.16	0.46
1:A:233:ARG:HH11	1:A:233:ARG:CG	2.29	0.46
1:A:233:ARG:HA	1:A:236:CYS:SG	2.55	0.46
1:B:189:TRP:CE3	1:B:248:VAL:HG11	2.51	0.46
1:B:385:LEU:O	1:B:390:ARG:NH2	2.49	0.46
1:A:142:LYS:O	1:A:146:GLU:HG3	2.15	0.46
1:B:21:PHE:CG	1:B:22:GLU:N	2.84	0.46
1:A:347:LYS:HA	1:A:350:GLN:HB2	1.97	0.45
1:A:240:ILE:C	1:A:242:ARG:H	2.25	0.45
1:A:115:LEU:HD21	1:A:180:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ASN:ND2	1:B:36:PHE:O	2.48	0.45
1:B:313:GLU:O	1:B:316:GLU:HG3	2.15	0.45
1:B:444:LEU:HD12	1:B:444:LEU:HA	1.74	0.45
1:A:21:PHE:CG	1:A:22:GLU:N	2.85	0.45
1:A:189:TRP:CD1	1:A:189:TRP:C	2.94	0.45
1:A:17:LEU:HD23	1:A:21:PHE:CD2	2.51	0.45
1:B:379:GLN:NE2	2:D:752:PHE:O	2.50	0.45
1:A:156:PHE:HB2	1:A:287:PHE:CD2	2.52	0.45
1:B:250:ASP:HA	1:B:271:THR:OG1	2.16	0.45
1:B:343:LYS:HB3	1:B:343:LYS:HE3	1.74	0.45
1:B:459:ILE:HG13	1:B:459:ILE:H	1.46	0.45
1:A:40:HIS:O	1:A:44:ILE:HG13	2.17	0.45
1:B:72:ILE:C	1:B:74:PHE:H	2.25	0.44
1:B:40:HIS:O	1:B:44:ILE:HG13	2.17	0.44
1:B:88:GLU:O	1:B:91:ILE:HG22	2.18	0.44
1:A:160:ARG:HB3	1:A:163:SER:HB3	1.99	0.44
1:A:189:TRP:CE3	1:A:248:VAL:HG11	2.52	0.44
1:B:135:TYR:CE1	1:B:139:ARG:HD2	2.52	0.44
1:B:436:ARG:O	1:B:440:ARG:HG3	2.16	0.44
1:B:189:TRP:CD1	1:B:189:TRP:C	2.95	0.44
1:B:235:ILE:O	1:B:239:LEU:HB2	2.16	0.44
1:A:8:ARG:HD3	1:A:90:TYR:OH	2.18	0.44
1:A:160:ARG:NH2	1:A:457:ASP:OD2	2.50	0.44
1:A:379:GLN:O	1:A:383:GLU:HG3	2.17	0.44
1:B:481:GLU:HA	1:B:484:LEU:CD2	2.48	0.44
1:B:334:MET:HE2	1:B:338:LYS:CD	2.48	0.44
1:A:237:ASN:C	1:A:239:LEU:H	2.25	0.44
1:A:397:VAL:C	1:A:399:MET:H	2.25	0.44
1:A:525:ARG:HD3	1:A:535:LEU:HD13	1.99	0.44
1:B:355:LEU:HD21	1:B:363:VAL:HB	1.99	0.44
1:A:36:PHE:HD2	1:A:40:HIS:HB3	1.83	0.43
1:A:390:ARG:HE	1:A:390:ARG:HB2	1.59	0.43
1:B:391:SER:OG	1:B:415:PRO:HG2	2.17	0.43
1:A:332:THR:O	1:A:336:PHE:HB2	2.18	0.43
1:B:354:LYS:HD3	1:B:362:GLY:O	2.18	0.43
1:A:250:ASP:HA	1:A:271:THR:OG1	2.18	0.43
1:B:69:GLY:C	1:B:71:LEU:H	2.24	0.43
1:B:527:GLU:HA	1:B:530:PRO:HG3	2.01	0.43
1:A:47:MET:HB2	1:A:53:ARG:CG	2.44	0.43
1:A:167:VAL:HG11	4:A:602:ATP:C5	2.54	0.43
1:A:466:HIS:ND1	1:A:466:HIS:N	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ASN:HA	1:B:330:PRO:HD2	1.74	0.43
1:B:397:VAL:HG22	1:B:464:LEU:HB3	2.00	0.43
1:B:525:ARG:HA	1:B:526:PRO:HD3	1.89	0.43
1:A:69:GLY:C	1:A:71:LEU:H	2.27	0.43
1:B:49:THR:HG22	1:B:51:LEU:H	1.83	0.43
1:B:163:SER:C	1:B:330:PRO:HG2	2.43	0.43
1:B:406:PRO:CA	1:B:453:THR:HG22	2.47	0.43
1:B:481:GLU:HA	1:B:484:LEU:HG	2.01	0.43
1:A:7:CYS:SG	1:A:62:ARG:HD3	2.58	0.43
1:A:527:GLU:HA	1:A:530:PRO:HG3	2.00	0.43
1:B:167:VAL:HG11	4:B:602:ATP:C6	2.54	0.43
1:A:102:ARG:HG2	1:A:182:ILE:CG2	2.48	0.43
1:A:187:ILE:HD13	1:A:246:LEU:HB3	2.01	0.43
1:A:252:VAL:HG11	1:A:258:ILE:CD1	2.49	0.43
1:A:462:MET:HE3	1:A:462:MET:HB2	1.79	0.43
1:A:26:ALA:HB2	1:A:74:PHE:CE1	2.53	0.42
1:A:115:LEU:CD2	1:A:180:ILE:HB	2.49	0.42
1:A:349:ALA:HA	1:A:352:ASN:HB2	2.01	0.42
1:A:444:LEU:HB3	1:A:445:SER:H	1.57	0.42
1:B:237:ASN:O	1:B:240:ILE:HG23	2.19	0.42
1:B:390:ARG:HE	1:B:390:ARG:HB2	1.58	0.42
1:B:405:ILE:HA	1:B:406:PRO:HD3	1.78	0.42
1:B:438:SER:O	1:B:442:ALA:HA	2.19	0.42
1:A:111:SER:O	1:A:113:GLN:N	2.52	0.42
1:B:240:ILE:HG13	1:B:241:ASP:OD1	2.19	0.42
1:B:445:SER:HB3	1:B:455:LYS:O	2.19	0.42
1:A:13:ALA:HB2	1:A:86:PHE:CE1	2.54	0.42
1:B:408:LYS:HD2	1:B:408:LYS:HA	1.76	0.42
1:A:24:ARG:HH21	1:A:53:ARG:NH1	2.17	0.42
1:A:141:ILE:HD11	1:A:175:LYS:HB3	2.01	0.42
1:B:374:LEU:HD13	1:B:378:LEU:HG	2.01	0.42
1:A:133:ARG:O	1:A:137:VAL:HG23	2.19	0.42
1:A:314:LYS:HA	1:A:317:ASP:HB2	2.01	0.42
1:B:18:ILE:O	1:B:50:ARG:NH2	2.53	0.42
1:A:437:LEU:HD22	1:A:437:LEU:HA	1.84	0.42
1:B:388:GLU:HB3	1:B:433:ARG:HH21	1.85	0.42
1:A:167:VAL:O	1:A:171:GLN:HG3	2.20	0.42
1:B:160:ARG:NH1	1:B:442:ALA:O	2.53	0.42
1:A:131:TYR:CD1	1:A:131:TYR:C	2.98	0.42
1:A:336:PHE:HE2	1:A:348:MET:SD	2.43	0.42
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:H	1:A:46:LYS:HG3	1.56	0.42
1:A:255:GLU:CB	1:A:277:ILE:HG22	2.49	0.41
1:A:347:LYS:O	1:A:347:LYS:HD3	2.19	0.41
1:A:408:LYS:HD2	1:A:408:LYS:HA	1.77	0.41
1:B:252:VAL:HG22	1:B:257:THR:HG21	2.01	0.41
1:B:407:VAL:HG23	1:B:452:LEU:O	2.20	0.41
1:B:410:TRP:CZ3	1:B:454:PHE:HB2	2.55	0.41
1:A:406:PRO:CA	1:A:453:THR:HG22	2.49	0.41
1:B:30:LEU:HD13	1:B:36:PHE:CE1	2.56	0.41
1:B:110:PHE:HA	1:B:113:GLN:HB2	2.01	0.41
1:B:218:LEU:HG	1:B:219:ASN:N	2.36	0.41
1:B:237:ASN:C	1:B:239:LEU:N	2.76	0.41
1:B:240:ILE:HG13	1:B:241:ASP:N	2.35	0.41
1:A:219:ASN:O	1:A:220:PHE:C	2.63	0.41
1:A:240:ILE:HG13	1:A:241:ASP:N	2.35	0.41
1:B:97:GLU:HA	1:B:98:PRO:HD3	1.93	0.41
1:B:137:VAL:O	1:B:141:ILE:HG13	2.21	0.41
1:B:240:ILE:C	1:B:242:ARG:H	2.28	0.41
1:B:135:TYR:CZ	1:B:139:ARG:HD2	2.56	0.41
1:B:239:LEU:HD22	1:B:242:ARG:HB2	2.02	0.41
1:B:521:GLU:O	1:B:523:VAL:N	2.52	0.41
1:A:326:SER:O	1:A:327:SER:C	2.63	0.41
1:B:410:TRP:HD1	1:B:414:ILE:HD13	1.84	0.41
1:A:23:PRO:HG2	1:A:53:ARG:C	2.46	0.41
1:A:296:ASP:O	1:A:299:TYR:HB2	2.20	0.41
1:B:466:HIS:ND1	1:B:466:HIS:N	2.68	0.41
1:A:135:TYR:O	1:A:139:ARG:HG3	2.20	0.41
1:A:243:PRO:O	1:A:244:ASN:C	2.63	0.41
1:A:405:ILE:HA	1:A:406:PRO:HD3	1.82	0.41
1:A:533:MET:HE3	1:A:533:MET:O	2.21	0.41
1:B:24:ARG:NH2	1:B:53:ARG:HH11	2.15	0.41
1:B:92:ASP:C	1:B:94:ALA:H	2.28	0.41
1:B:178:GLN:HB3	1:B:183:ASN:OD1	2.20	0.41
1:B:233:ARG:NH1	1:B:237:ASN:HD21	2.19	0.41
1:B:347:LYS:O	1:B:347:LYS:HD3	2.20	0.41
1:B:385:LEU:HD22	1:B:389:ASP:HB3	2.02	0.41
1:A:165:LYS:H	1:A:165:LYS:HG3	1.69	0.41
1:A:188:VAL:HB	1:A:247:PHE:HD1	1.85	0.41
1:A:430:VAL:O	1:A:434:LEU:HG	2.20	0.41
1:A:72:ILE:C	1:A:74:PHE:H	2.29	0.40
1:B:190:LEU:HD23	1:B:190:LEU:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LYS:HE2	1:B:212:LYS:HA	2.01	0.40
1:A:484:LEU:CD1	1:A:533:MET:HG2	2.42	0.40
1:A:410:TRP:CD1	1:A:414:ILE:HD13	2.51	0.40
1:B:269:LEU:HD22	1:B:270:VAL:N	2.37	0.40
1:A:525:ARG:HA	1:A:526:PRO:HD3	1.67	0.40
1:B:252:VAL:CG2	1:B:257:THR:HG21	2.52	0.40
1:B:397:VAL:C	1:B:399:MET:H	2.30	0.40
1:B:202:ASP:O	1:B:205:THR:HB	2.22	0.40
1:B:204:PHE:O	1:B:235:ILE:HD11	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	504/549 (92%)	406 (81%)	73 (14%)	25 (5%)	1	11
1	B	505/549 (92%)	407 (81%)	71 (14%)	27 (5%)	1	10
2	C	5/8 (62%)	2 (40%)	1 (20%)	2 (40%)	0	0
2	D	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0
All	All	1017/1114 (91%)	816 (80%)	146 (14%)	55 (5%)	1	10

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	A	327	SER
1	A	341	GLU
1	A	398	VAL
1	A	445	SER
2	C	751	ASN

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Mol	Chain	Res	Type
1	B	109	GLN
1	B	127	GLN
1	B	327	SER
1	B	341	GLU
1	B	398	VAL
1	B	445	SER
1	A	112	ARG
1	A	208	LEU
1	A	244	ASN
1	A	396	ALA
1	A	465	LYS
1	A	522	THR
1	B	244	ASN
1	B	396	ALA
1	B	465	LYS
1	B	522	THR
1	A	2	LEU
1	A	73	ASP
1	A	160	ARG
1	A	238	ALA
1	A	284	THR
2	C	750	PHE
1	B	2	LEU
1	B	73	ASP
1	B	104	VAL
1	B	160	ARG
1	B	176	SER
1	B	208	LEU
1	B	238	ALA
1	B	284	THR
1	A	485	LEU
2	D	750	PHE
1	A	33	LYS
1	A	237	ASN
1	B	35	ILE
1	B	116	ASP
1	B	257	THR
1	B	328	GLY
1	B	354	LYS
1	A	484	LEU
1	B	102	ARG
1	A	311	VAL

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Mol	Chain	Res	Type
1	B	311	VAL
1	A	70	PRO
1	A	108	PRO
1	B	70	PRO
1	B	106	ILE
1	A	35	ILE
1	A	416	VAL

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	462/501 (92%)	380 (82%)	82 (18%)	2	8
1	B	464/501 (93%)	371 (80%)	93 (20%)	1	5
2	C	6/7 (86%)	5 (83%)	1 (17%)	2	11
2	D	5/7 (71%)	5 (100%)	0	100	100
All	All	937/1016 (92%)	761 (81%)	176 (19%)	1	7

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	8	ARG
1	A	15	THR
1	A	17	LEU
1	A	43	LEU
1	A	46	LYS
1	A	51	LEU
1	A	52	GLU
1	A	67	GLU
1	A	68	LEU
1	A	77	TYR
1	A	82	HIS
1	A	95	ILE
1	A	100	LEU

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Mol	Chain	Res	Type
1	A	113	GLN
1	A	115	LEU
1	A	116	ASP
1	A	126	LYS
1	A	128	MET
1	A	130	CYS
1	A	131	TYR
1	A	155	LEU
1	A	157	LEU
1	A	167	VAL
1	A	174	SER
1	A	179	LEU
1	A	180	ILE
1	A	185	ASP
1	A	198	LYS
1	A	203	LEU
1	A	205	THR
1	A	217	LEU
1	A	218	LEU
1	A	220	PHE
1	A	223	VAL
1	A	224	GLU
1	A	226	VAL
1	A	227	THR
1	A	233	ARG
1	A	239	LEU
1	A	241	ASP
1	A	253	VAL
1	A	255	GLU
1	A	257	THR
1	A	262	GLN
1	A	264	LEU
1	A	269	LEU
1	A	277	ILE
1	A	284	THR
1	A	286	GLU
1	A	290	VAL
1	A	296	ASP
1	A	309	MET
1	A	316	GLU
1	A	332	THR
1	A	348	MET

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Mol	Chain	Res	Type
1	A	355	LEU
1	A	363	VAL
1	A	364	GLU
1	A	366	ILE
1	A	369	TYR
1	A	374	LEU
1	A	381	CYS
1	A	404	ASP
1	A	405	ILE
1	A	409	LEU
1	A	410	TRP
1	A	414	ILE
1	A	416	VAL
1	A	437	LEU
1	A	444	LEU
1	A	451	VAL
1	A	452	LEU
1	A	456	ILE
1	A	457	ASP
1	A	459	ILE
1	A	460	ILE
1	A	466	HIS
1	A	467	VAL
1	A	485	LEU
1	A	525	ARG
1	A	533	MET
2	C	750	PHE
1	B	1	MET
1	B	4	GLU
1	B	8	ARG
1	B	15	THR
1	B	17	LEU
1	B	35	ILE
1	B	43	LEU
1	B	46	LYS
1	B	51	LEU
1	B	52	GLU
1	B	64	GLN
1	B	67	GLU
1	B	68	LEU
1	B	77	TYR
1	B	97	GLU

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Mol	Chain	Res	Type
1	B	99	ASP
1	B	104	VAL
1	B	106	ILE
1	B	109	GLN
1	B	112	ARG
1	B	114	MET
1	B	116	ASP
1	B	117	ARG
1	B	126	LYS
1	B	128	MET
1	B	130	CYS
1	B	131	TYR
1	B	148	CYS
1	B	155	LEU
1	B	157	LEU
1	B	167	VAL
1	B	174	SER
1	B	175	LYS
1	B	179	LEU
1	B	180	ILE
1	B	185	ASP
1	B	189	TRP
1	B	198	LYS
1	B	203	LEU
1	B	208	LEU
1	B	217	LEU
1	B	218	LEU
1	B	220	PHE
1	B	223	VAL
1	B	226	VAL
1	B	227	THR
1	B	233	ARG
1	B	239	LEU
1	B	241	ASP
1	B	253	VAL
1	B	255	GLU
1	B	257	THR
1	B	262	GLN
1	B	269	LEU
1	B	277	ILE
1	B	283	GLN
1	B	284	THR

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Mol	Chain	Res	Type
1	B	286	GLU
1	B	290	VAL
1	B	296	ASP
1	B	309	MET
1	B	316	GLU
1	B	332	THR
1	B	348	MET
1	B	355	LEU
1	B	363	VAL
1	B	364	GLU
1	B	366	ILE
1	B	369	TYR
1	B	374	LEU
1	B	381	CYS
1	B	382	VAL
1	B	388	GLU
1	B	404	ASP
1	B	405	ILE
1	B	409	LEU
1	B	410	TRP
1	B	414	ILE
1	B	416	VAL
1	B	444	LEU
1	B	451	VAL
1	B	452	LEU
1	B	456	ILE
1	B	457	ASP
1	B	459	ILE
1	B	460	ILE
1	B	462	MET
1	B	466	HIS
1	B	467	VAL
1	B	486	GLU
1	B	528	ASP
1	B	533	MET
1	B	539	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	136	HIS

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Mol	Chain	Res	Type
1	A	183	ASN
1	A	237	ASN
1	A	536	HIS
1	B	136	HIS
1	B	171	GLN
1	B	237	ASN
1	B	329	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
4	ATP	A	602	3	32,33,33	1.42	4 (12%)	48,52,52	1.71	8 (16%)
4	ATP	B	602	3	32,33,33	1.42	4 (12%)	48,52,52	1.80	10 (20%)

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
4	ATP	A	602	3	-	0/22/38/38	0/3/3/3
4	ATP	B	602	3	-	3/22/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	ATP	C5-C4	4.98	1.48	1.39
4	A	602	ATP	C5-C4	4.86	1.47	1.39
4	B	602	ATP	C5-C6	2.82	1.48	1.41
4	A	602	ATP	C5-C6	2.75	1.48	1.41
4	B	602	ATP	C8-N7	2.30	1.36	1.31
4	A	602	ATP	C8-N7	2.26	1.36	1.31
4	A	602	ATP	C5-N7	-2.19	1.35	1.39
4	B	602	ATP	C5-N7	-2.17	1.35	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	602	ATP	C5-C4-N3	-6.16	118.23	126.72
4	A	602	ATP	C5-C4-N3	-5.73	118.83	126.72
4	B	602	ATP	N3-C4-N9	5.08	135.81	127.17
4	A	602	ATP	N3-C4-N9	4.71	135.18	127.17
4	B	602	ATP	C2-N3-C4	3.88	121.31	111.83
4	A	602	ATP	C2-N3-C4	3.60	120.63	111.83
4	B	602	ATP	N3-C2-N1	-3.54	123.22	128.58
4	A	602	ATP	C4-C5-N7	-3.27	106.84	110.58
4	B	602	ATP	C4-C5-N7	-3.14	106.99	110.58
4	A	602	ATP	N3-C2-N1	-3.14	123.84	128.58
4	A	602	ATP	C4-N9-C8	2.82	108.70	105.74
4	B	602	ATP	C2'-C1'-N9	-2.52	107.04	113.30
4	A	602	ATP	C2'-C1'-N9	-2.47	107.17	113.30
4	B	602	ATP	C4-N9-C8	2.46	108.32	105.74
4	A	602	ATP	C5-N7-C8	2.45	107.30	103.45
4	B	602	ATP	C5-N7-C8	2.39	107.21	103.45
4	B	602	ATP	C2-N1-C6	2.09	122.17	118.73
4	B	602	ATP	O4'-C1'-N9	2.01	111.95	108.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

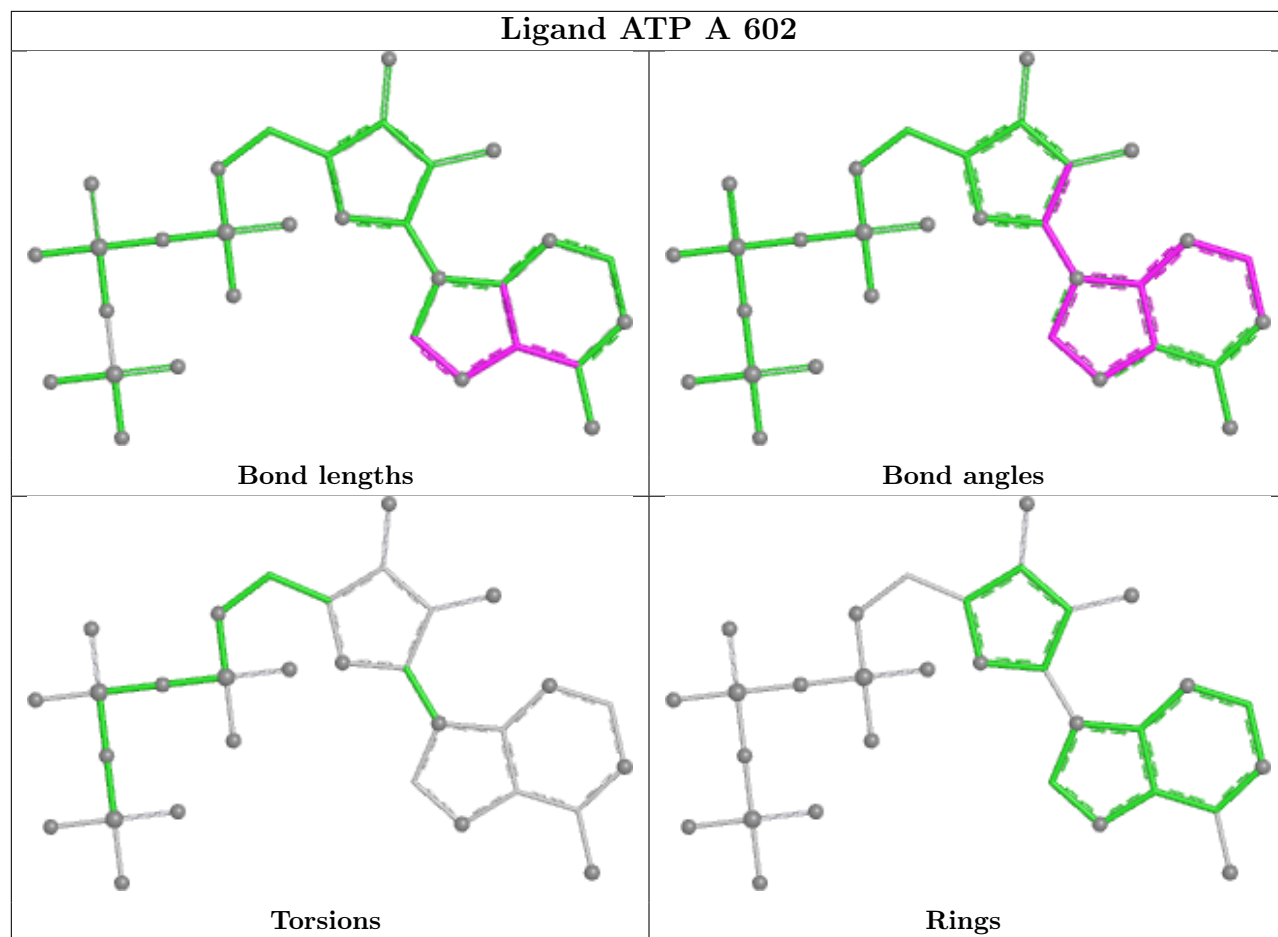
Mol	Chain	Res	Type	Atoms
4	B	602	ATP	O4'-C1'-N9-C8
4	B	602	ATP	O4'-C1'-N9-C4
4	B	602	ATP	PG-O3B-PB-O2B

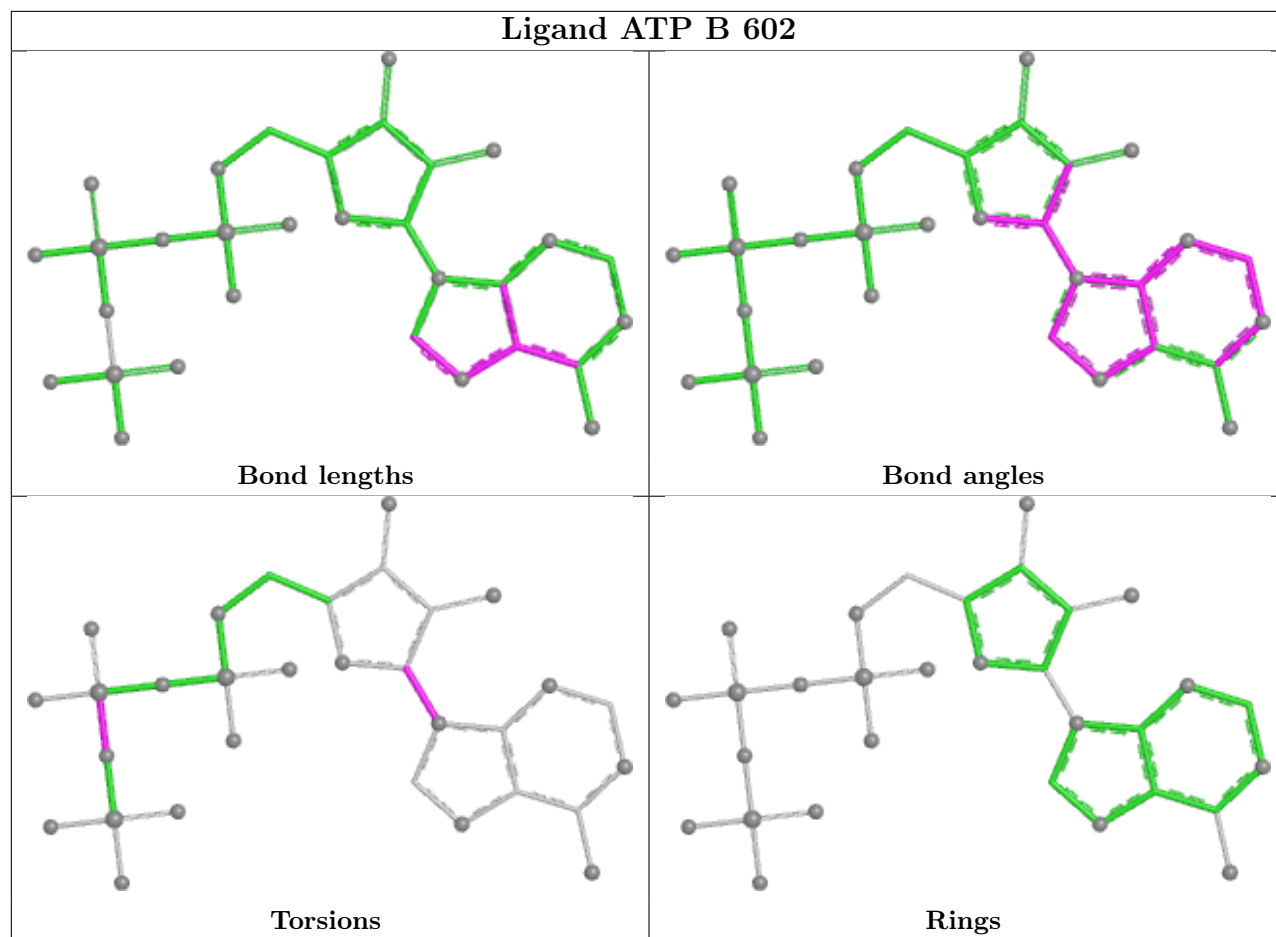
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	ATP	1	0
4	B	602	ATP	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	510/549 (92%)	0.37	16 (3%) 51 35	177, 244, 305, 345	0
1	B	511/549 (93%)	0.47	21 (4%) 41 27	178, 242, 352, 466	0
2	C	7/8 (87%)	1.21	2 (28%) 1 1	231, 274, 337, 344	0
2	D	5/8 (62%)	0.75	0 100 100	228, 249, 302, 304	0
All	All	1033/1114 (92%)	0.42	39 (3%) 44 30	177, 244, 334, 466	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	PHE	4.9
1	A	298	CYS	4.7
1	B	51	LEU	4.7
1	A	409	LEU	4.6
1	B	68	LEU	3.9
1	B	115	LEU	3.5
1	A	293	LEU	3.5
1	A	32	GLY	3.4
1	A	77	TYR	3.3
1	A	530	PRO	3.0
1	A	472	THR	3.0
1	A	51	LEU	2.9
1	B	10	LEU	2.9
1	A	275	VAL	2.8
1	A	158	HIS	2.8
1	B	18	ILE	2.6
1	A	29	TYR	2.6
2	C	754	CYS	2.5
1	B	121	LEU	2.5
1	A	191	LYS	2.5
1	B	274	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	427	ASP	2.4
1	B	460	ILE	2.4
1	A	302	LEU	2.3
1	B	36	PHE	2.2
1	B	253	VAL	2.2
1	B	70	PRO	2.2
1	B	351	LEU	2.1
1	A	394	ALA	2.1
1	B	108	PRO	2.1
1	B	52	GLU	2.1
1	B	57	PHE	2.1
1	B	23	PRO	2.1
1	B	282	SER	2.1
2	C	753	LEU	2.1
1	A	487	ILE	2.0
1	A	470	ALA	2.0
1	B	393	LEU	2.0
1	B	72	ILE	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](#)

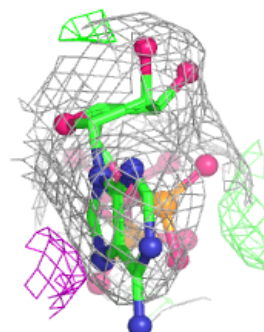
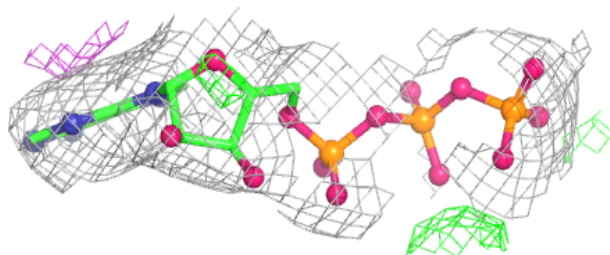
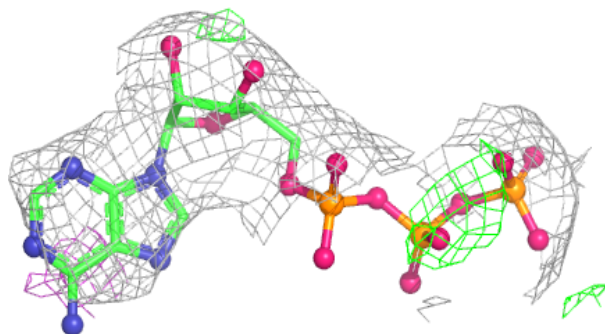
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

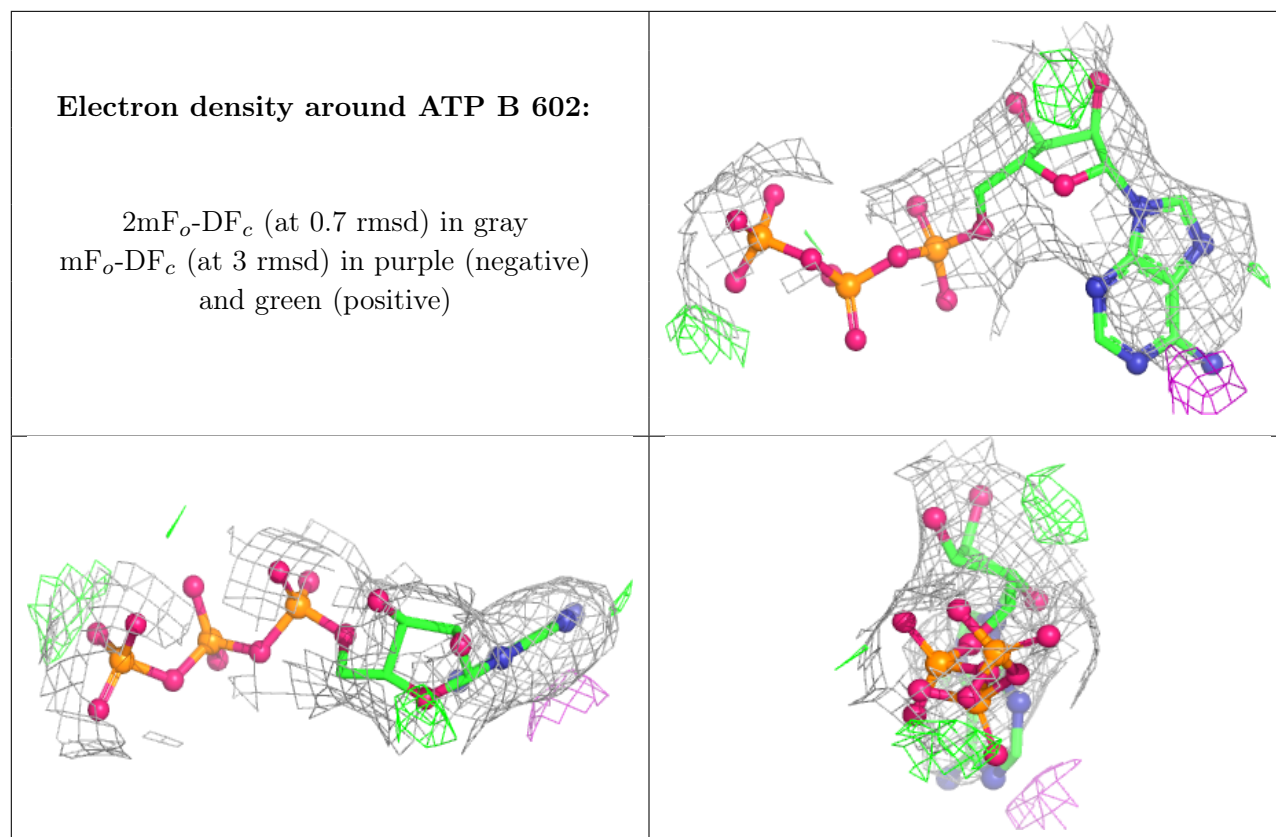
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	601	1/1	0.81	0.21	176,176,176,176	0
3	MG	B	601	1/1	0.87	0.18	168,168,168,168	0
4	ATP	A	602	31/31	0.94	0.10	157,214,239,249	0
4	ATP	B	602	31/31	0.94	0.11	184,209,243,250	0

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 ATP A 602:

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.