



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:41 AM JST

PDB ID : 5FHH / pdb_00005fhh
Title : Structure of human Pif1 helicase domain residues 200-641
Authors : Zhou, X.; Ren, W.; Bharath, S.R.; Song, H.
Deposited on : 2015-12-22
Resolution : 3.60 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

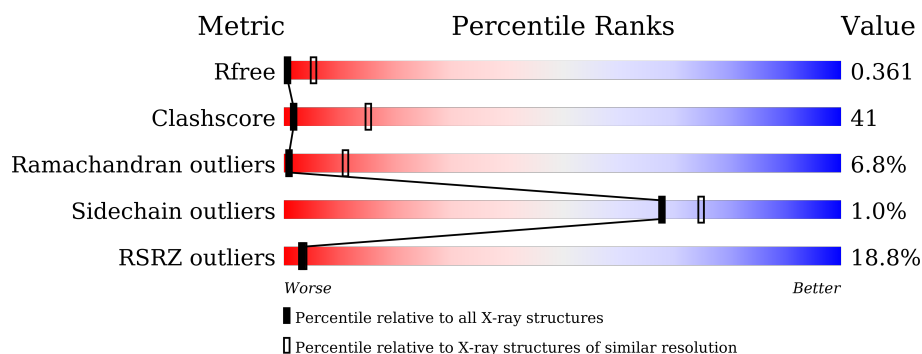
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	442	
1	B	442	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ALF	A	702	-	-	X	-
3	ALF	B	702	-	-	X	-

2 Entry composition [i](#)

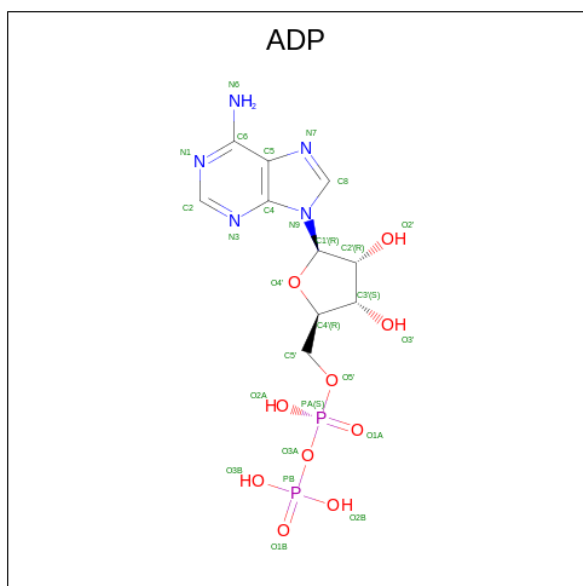
There are 3 unique types of molecules in this entry. The entry contains 5128 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ATP-dependent DNA helicase PIF1.

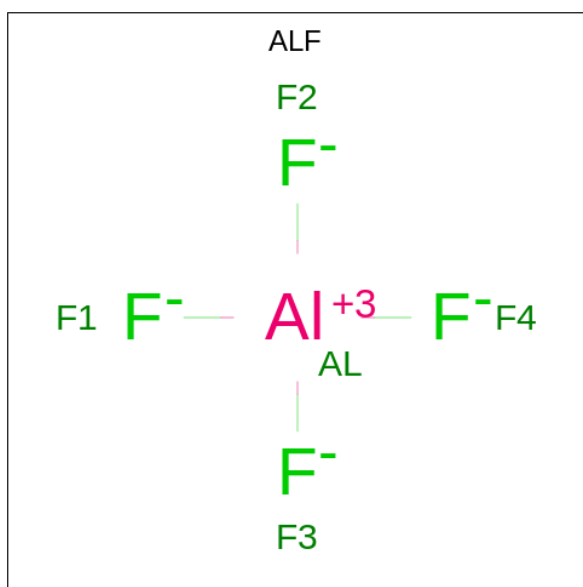
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			2622	1656	470	482	14			
1	B	393	Total	C	N	O	S	0	0	0
			2442	1536	430	465	11			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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		

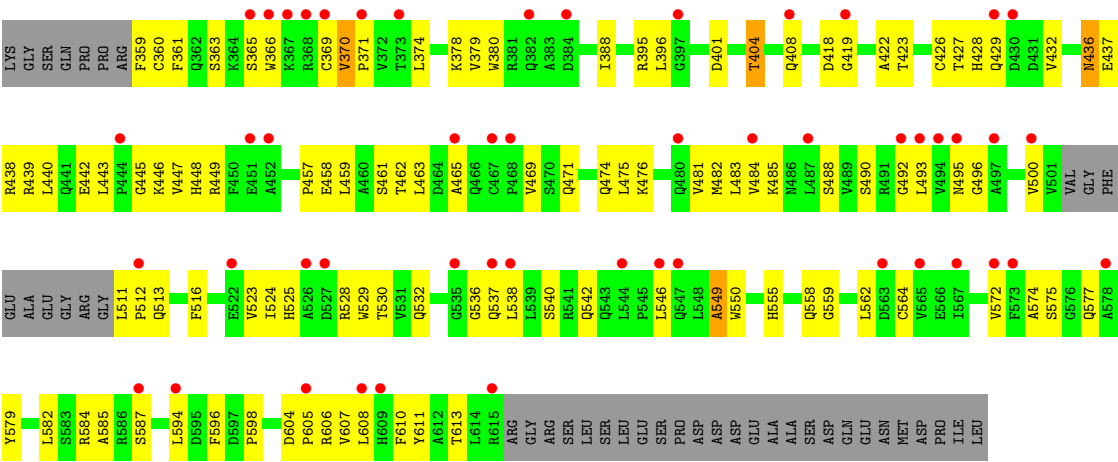
- Molecule 3 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Al	F	0	0
			5	1	4		
3	B	1	Total	Al	F	0	0
			5	1	4		

- Molecule 1: ATP-dependent DNA helicase PIF1





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	204.75Å 204.75Å 77.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.06 – 3.60 47.06 – 3.60	Depositor EDS
% Data completeness (in resolution range)	94.2 (47.06-3.60) 94.2 (47.06-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.57Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.310 , 0.355 0.323 , 0.361	Depositor DCC
R_{free} test set	1043 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	76.6	Xtriage
Anisotropy	1.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 148.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for -h,-k,l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	5128	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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, ALF

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	0.34	0/2669	0.77	5/3661 (0.1%)
1	B	0.30	0/2485	0.81	10/3434 (0.3%)
All	All	0.32	0/5154	0.79	15/7095 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	SER	N-CA-C	9.03	124.07	112.34
1	A	246	PRO	N-CA-C	7.83	120.26	110.70
1	A	291	PRO	N-CA-C	7.32	127.55	112.47
1	B	303	LEU	CA-C-N	-7.15	113.56	122.93
1	B	303	LEU	C-N-CA	-7.15	113.56	122.93
1	B	549	ALA	N-CA-C	6.99	122.67	113.30
1	B	235	SER	N-CA-C	-6.32	105.05	112.89
1	A	516	PHE	N-CA-C	-6.17	100.21	109.96
1	A	528	ARG	N-CA-C	6.00	118.72	109.07
1	B	305	ILE	N-CA-C	-5.88	100.94	109.29
1	B	291	PRO	CA-C-N	-5.21	117.24	123.44
1	B	291	PRO	C-N-CA	-5.21	117.24	123.44
1	B	341	CYS	CA-CB-SG	5.15	126.24	114.40
1	B	231	GLY	CA-C-N	5.02	131.13	121.54
1	B	231	GLY	C-N-CA	5.02	131.13	121.54

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	2622	0	2314	216	0
1	B	2442	0	1983	171	0
2	A	27	0	12	6	0
2	B	27	0	12	8	0
3	A	5	0	0	3	0
3	B	5	0	0	7	0
All	All	5128	0	4321	385	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 41.

All (385) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:TRP:CZ2	1:A:323:ALA:HA	1.54	1.41
1:B:378:LYS:O	1:B:380:TRP:CD1	1.76	1.38
1:A:297:TRP:HZ2	1:A:323:ALA:CA	1.37	1.36
1:A:290:ARG:CG	1:A:291:PRO:HD2	1.59	1.29
1:A:290:ARG:HG2	1:A:291:PRO:CD	1.67	1.25
1:A:297:TRP:HZ2	1:A:323:ALA:CB	1.49	1.24
1:B:423:THR:HG23	1:B:549:ALA:O	1.05	1.20
1:B:423:THR:CG2	1:B:549:ALA:O	1.95	1.12
1:B:333:PHE:HE2	1:B:336:ILE:HG21	1.13	1.10
1:A:297:TRP:CZ2	1:A:323:ALA:CB	2.34	1.09
1:A:297:TRP:CZ2	1:A:323:ALA:CA	2.21	1.06
1:A:407:LEU:HD23	1:A:407:LEU:H	1.20	1.05
1:A:297:TRP:CE2	1:A:323:ALA:HA	1.92	1.04
1:B:333:PHE:CE2	1:B:336:ILE:CG2	2.40	1.03
1:B:333:PHE:HE2	1:B:336:ILE:CG2	1.72	1.02
1:B:333:PHE:CD2	1:B:336:ILE:HG22	1.93	1.02
1:B:333:PHE:CE2	1:B:336:ILE:HG21	1.95	1.01
1:B:378:LYS:O	1:B:380:TRP:NE1	2.03	0.90
1:A:297:TRP:CZ2	1:A:323:ALA:HB2	2.07	0.87
1:B:378:LYS:O	1:B:380:TRP:HD1	1.50	0.87
1:A:517:LEU:C	1:A:519:GLY:H	1.84	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLY:O	1:B:235:SER:N	2.08	0.86
1:A:246:PRO:O	1:A:247:PRO:O	1.95	0.85
1:A:407:LEU:O	1:A:410:THR:N	2.10	0.85
1:A:346:GLN:NE2	3:A:702:ALF:F1	2.00	0.84
1:B:333:PHE:HD2	1:B:336:ILE:HG22	1.41	0.83
1:B:333:PHE:CE2	1:B:336:ILE:HG22	2.13	0.80
1:A:229:SER:HA	1:A:395:ARG:NH1	1.98	0.79
1:B:235:SER:OG	2:B:701:ADP:H5'2	1.84	0.78
2:B:701:ADP:O1A	3:B:702:ALF:F3	1.90	0.78
1:A:297:TRP:HD1	1:A:326:VAL:CG1	1.97	0.77
2:B:701:ADP:O3B	3:B:702:ALF:F1	1.94	0.76
1:A:412:SER:O	1:A:413:HIS:O	2.04	0.76
1:B:436:ASN:O	1:B:438:ARG:N	2.20	0.75
1:A:569:LEU:O	1:A:595:ASP:HB3	1.86	0.75
1:A:228:GLY:N	1:A:234:LYS:HD3	2.02	0.75
1:A:528:ARG:HD2	1:B:292:GLY:HA2	1.69	0.75
1:A:574:ALA:O	1:A:576:GLY:N	2.20	0.74
1:B:238:LEU:O	1:B:242:LEU:N	2.17	0.74
1:A:297:TRP:CD1	1:A:326:VAL:HB	2.22	0.74
1:B:320:GLU:HG2	1:B:333:PHE:HA	1.67	0.74
1:A:453:MET:O	1:A:455:SER:N	2.21	0.74
1:B:294:ARG:O	1:B:298:LEU:N	2.20	0.74
1:B:369:CYS:C	1:B:371:PRO:HD2	2.14	0.73
1:B:426:CYS:HB2	1:B:432:VAL:HG12	1.68	0.73
1:B:305:ILE:O	1:B:340:ILE:HA	1.89	0.73
1:B:231:GLY:O	1:B:233:GLY:N	2.22	0.72
1:B:482:MET:HA	1:B:495:ASN:HA	1.71	0.72
1:A:401:ASP:O	1:A:405:ARG:N	2.15	0.72
1:A:407:LEU:H	1:A:407:LEU:CD2	2.01	0.72
1:A:420:ILE:HD12	1:A:496:GLY:HA2	1.72	0.71
1:A:392:GLN:HA	1:A:395:ARG:HB3	1.72	0.71
1:A:410:THR:O	1:A:412:SER:N	2.23	0.71
1:A:597:ASP:O	1:A:599:MET:N	2.23	0.71
1:A:320:GLU:HA	1:A:333:PHE:HE1	1.56	0.71
1:A:407:LEU:HD23	1:A:407:LEU:N	2.03	0.70
1:A:277:GLY:O	1:A:318:LYS:NZ	2.23	0.70
1:A:407:LEU:O	1:A:408:GLN:C	2.28	0.70
1:A:331:LYS:HB3	1:A:332:PRO:HD2	1.74	0.70
1:B:378:LYS:CB	1:B:380:TRP:NE1	2.55	0.69
1:A:297:TRP:HD1	1:A:326:VAL:HG11	1.57	0.69
1:A:253:THR:HG22	1:A:254:ALA:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:GLY:O	1:B:447:VAL:N	2.21	0.69
1:B:306:ASP:O	1:B:341:CYS:O	2.11	0.69
1:B:333:PHE:CD2	1:B:333:PHE:O	2.46	0.69
1:B:308:ILE:O	1:B:310:MET:N	2.27	0.68
1:A:290:ARG:CG	1:A:291:PRO:CD	2.44	0.68
1:A:306:ASP:OD1	1:A:307:GLU:N	2.27	0.68
1:A:425:LEU:HB2	1:A:567:ILE:HG22	1.76	0.67
1:B:233:GLY:O	3:B:702:ALF:F2	2.03	0.67
1:A:412:SER:O	1:A:413:HIS:C	2.37	0.67
1:B:260:ALA:O	1:B:264:GLY:N	2.29	0.66
1:B:559:GLY:HA2	2:B:701:ADP:O3A	1.95	0.66
1:B:233:GLY:O	3:B:702:ALF:F3	2.04	0.66
1:A:267:THR:O	1:A:269:HIS:N	2.29	0.66
1:B:429:GLN:O	1:B:432:VAL:HG22	1.95	0.66
1:A:297:TRP:CH2	1:A:323:ALA:HB2	2.31	0.66
1:B:208:SER:HB3	1:B:211:GLN:HG3	1.78	0.65
1:A:229:SER:HA	1:A:395:ARG:HH12	1.58	0.65
1:A:281:LEU:O	1:A:285:VAL:N	2.16	0.65
1:B:379:VAL:HG21	1:B:388:ILE:HG13	1.77	0.65
1:A:598:PRO:O	1:A:599:MET:O	2.14	0.65
1:A:407:LEU:HG	1:A:408:GLN:H	1.61	0.65
1:A:402:GLU:O	1:A:406:GLN:NE2	2.28	0.65
1:A:407:LEU:HB2	1:A:593:VAL:HG11	1.77	0.65
1:A:599:MET:O	1:A:601:VAL:N	2.27	0.64
1:B:317:ASP:OD1	1:B:363:SER:HB2	1.98	0.64
1:B:320:GLU:HG2	1:B:333:PHE:CA	2.27	0.64
1:B:318:LYS:O	1:B:322:VAL:HG23	1.98	0.63
1:B:238:LEU:HD12	1:B:306:ASP:OD1	1.98	0.63
1:A:214:VAL:HB	1:A:237:LEU:HD21	1.81	0.63
1:A:392:GLN:N	1:A:392:GLN:OE1	2.31	0.63
1:B:339:ILE:O	1:B:340:ILE:CB	2.46	0.63
1:B:449:ARG:HA	1:B:474:GLN:HA	1.80	0.62
1:A:542:GLN:HB3	1:B:291:PRO:HB2	1.81	0.62
2:B:701:ADP:O4'	3:B:702:ALF:F4	2.07	0.62
1:A:246:PRO:O	1:A:247:PRO:C	2.43	0.62
1:A:297:TRP:NE1	1:A:323:ALA:HA	2.13	0.62
1:B:379:VAL:HG11	1:B:388:ILE:HG21	1.80	0.62
1:B:231:GLY:O	3:B:702:ALF:F4	2.08	0.62
1:B:295:GLN:O	1:B:299:ASN:N	2.29	0.62
1:A:391:LEU:O	1:A:395:ARG:N	2.23	0.62
1:A:403:VAL:HA	1:A:406:GLN:HE22	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ASN:O	1:A:516:PHE:HB3	2.00	0.61
1:A:343:ASP:OD2	1:A:395:ARG:NH1	2.34	0.61
1:A:517:LEU:O	1:A:519:GLY:N	2.33	0.61
1:A:598:PRO:O	1:A:599:MET:C	2.44	0.60
1:B:605:PRO:HG2	1:B:607:VAL:HB	1.83	0.60
1:B:395:ARG:HB2	1:B:579:TYR:HE1	1.67	0.60
1:A:426:CYS:HB2	1:A:432:VAL:HG13	1.82	0.60
2:A:701:ADP:O2B	3:A:702:ALF:F4	2.09	0.60
1:B:238:LEU:CD1	1:B:306:ASP:OD1	2.50	0.60
1:A:246:PRO:C	1:A:247:PRO:O	2.45	0.59
1:A:347:LEU:HG	1:A:580:VAL:HG21	1.85	0.59
1:B:308:ILE:HD12	1:B:344:PHE:CE1	2.37	0.59
1:A:252:ALA:HA	1:A:304:VAL:HG22	1.85	0.59
1:B:579:TYR:O	1:B:582:LEU:N	2.35	0.59
1:B:315:LEU:O	1:B:319:LEU:N	2.32	0.58
1:B:440:LEU:HA	1:B:443:LEU:HD12	1.85	0.58
1:A:274:ILE:HG21	1:A:284:CYS:SG	2.43	0.58
1:B:308:ILE:C	1:B:310:MET:H	2.11	0.58
1:B:463:LEU:HD21	1:B:471:GLN:H	1.68	0.58
1:B:559:GLY:HA2	2:B:701:ADP:PA	2.43	0.58
1:A:228:GLY:C	1:A:234:LYS:HZ1	2.12	0.58
1:B:215:LEU:O	1:B:219:LEU:HD12	2.03	0.58
1:A:470:SER:H	1:A:543:GLN:HE22	1.52	0.58
1:B:395:ARG:HH12	1:B:611:TYR:HE2	1.50	0.58
1:A:297:TRP:CD1	1:A:326:VAL:CB	2.87	0.57
1:A:215:LEU:O	1:A:219:LEU:HD13	2.05	0.57
1:B:513:GLN:HA	1:B:523:VAL:HA	1.86	0.57
1:A:291:PRO:HG3	1:B:542:GLN:HB3	1.85	0.57
1:A:360:CYS:SG	1:A:366:TRP:NE1	2.77	0.57
1:A:549:ALA:O	1:A:551:ALA:N	2.30	0.57
1:B:481:VAL:O	1:B:496:GLY:N	2.36	0.57
1:A:400:SER:OG	1:A:403:VAL:HG23	2.04	0.57
1:B:238:LEU:HD13	1:B:304:VAL:CG2	2.35	0.57
1:A:516:PHE:N	1:A:516:PHE:CD2	2.73	0.57
1:B:308:ILE:HG13	1:B:309:SER:H	1.69	0.56
1:A:233:GLY:HA2	2:A:701:ADP:C8	2.41	0.56
1:B:524:ILE:HG12	1:B:546:LEU:HD21	1.86	0.56
1:A:304:VAL:HG12	1:A:339:ILE:HD12	1.88	0.56
1:A:370:VAL:N	1:A:371:PRO:HD3	2.21	0.56
1:B:361:PHE:C	1:B:363:SER:H	2.14	0.56
1:A:235:SER:HB2	2:A:701:ADP:O1A	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ARG:HD2	1:B:292:GLY:CA	2.36	0.56
1:B:447:VAL:HA	1:B:476:LYS:HA	1.88	0.56
1:A:482:MET:HA	1:A:495:ASN:HA	1.88	0.55
1:B:378:LYS:CB	1:B:380:TRP:CE2	2.89	0.55
1:A:384:ASP:OD1	1:A:386:THR:OG1	2.23	0.55
1:B:235:SER:N	3:B:702:ALF:F3	2.28	0.55
1:A:288:ALA:HA	1:A:293:VAL:HG11	1.89	0.55
1:B:300:CYS:SG	1:B:336:ILE:HD11	2.46	0.55
1:A:247:PRO:O	1:A:248:THR:OG1	2.24	0.55
1:A:297:TRP:CD1	1:A:326:VAL:HG11	2.40	0.55
1:B:226:PHE:O	1:B:341:CYS:HB2	2.06	0.55
1:B:448:HIS:N	1:B:475:LEU:O	2.39	0.55
1:B:347:LEU:HB2	1:B:558:GLN:OE1	2.06	0.55
1:B:418:ASP:OD2	1:B:419:GLY:N	2.31	0.54
1:A:246:PRO:HG2	1:A:302:ARG:NH2	2.23	0.54
1:A:294:ARG:HH12	1:B:525:HIS:CE1	2.25	0.54
1:A:432:VAL:O	1:A:436:ASN:HB2	2.06	0.54
1:A:392:GLN:O	1:A:396:LEU:HD12	2.08	0.54
1:B:462:THR:HG23	1:B:463:LEU:N	2.23	0.54
1:B:322:VAL:O	1:B:326:VAL:HG23	2.07	0.54
1:B:484:VAL:HA	1:B:493:LEU:HA	1.90	0.54
1:A:448:HIS:HB3	1:A:475:LEU:O	2.07	0.53
1:A:598:PRO:C	1:A:599:MET:O	2.49	0.53
1:A:246:PRO:HG2	1:A:302:ARG:HH22	1.74	0.53
1:A:332:PRO:HB2	1:A:369:CYS:HA	1.91	0.53
1:B:226:PHE:HA	1:B:374:LEU:O	2.08	0.53
1:A:300:CYS:O	1:A:327:ARG:NH1	2.33	0.53
1:B:401:ASP:O	1:B:404:THR:OG1	2.21	0.53
1:A:387:PHE:CE1	1:A:391:LEU:HD21	2.44	0.52
1:A:297:TRP:HD1	1:A:326:VAL:CB	2.22	0.52
1:A:406:GLN:OE1	1:A:407:LEU:CD2	2.58	0.52
1:A:517:LEU:HD12	1:A:517:LEU:H	1.75	0.52
1:B:308:ILE:O	1:B:311:VAL:HG22	2.09	0.52
1:A:517:LEU:C	1:A:519:GLY:N	2.48	0.52
1:B:378:LYS:CB	1:B:380:TRP:HE1	2.22	0.52
1:A:304:VAL:HA	1:A:339:ILE:HB	1.92	0.52
1:B:218:VAL:HG11	1:B:241:ILE:HD13	1.92	0.52
1:B:320:GLU:HA	1:B:333:PHE:HD1	1.75	0.52
1:A:415:VAL:HG12	1:A:564:CYS:HB2	1.92	0.51
1:A:452:ALA:C	1:A:454:ASP:H	2.17	0.51
1:A:233:GLY:HA2	2:A:701:ADP:H8	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:PHE:O	1:B:613:THR:OG1	2.28	0.51
1:B:261:CYS:SG	1:B:485:LYS:HA	2.50	0.51
1:B:349:PRO:HD3	1:B:359:PHE:CE1	2.46	0.51
1:A:316:PHE:O	1:A:320:GLU:N	2.44	0.51
1:A:343:ASP:OD1	1:A:345:LEU:N	2.41	0.51
1:B:238:LEU:HA	1:B:241:ILE:HB	1.92	0.51
1:A:290:ARG:HG2	1:A:291:PRO:HD2	0.72	0.51
1:B:427:THR:HG23	1:B:428:HIS:ND1	2.25	0.51
1:B:596:PHE:O	1:B:598:PRO:HD3	2.10	0.51
1:A:302:ARG:HA	1:A:337:GLN:O	2.11	0.51
1:A:400:SER:N	1:A:403:VAL:HB	2.26	0.51
1:A:225:PHE:CD2	1:A:366:TRP:HH2	2.29	0.51
1:A:443:LEU:HD12	1:A:444:PRO:HD2	1.93	0.51
1:B:309:SER:OG	1:B:344:PHE:HA	2.12	0.50
1:A:224:ILE:HD11	1:A:374:LEU:HD22	1.94	0.50
1:A:605:PRO:HG2	1:A:607:VAL:HG12	1.92	0.50
1:A:258:VAL:HA	1:A:261:CYS:SG	2.51	0.50
1:A:407:LEU:HG	1:A:408:GLN:N	2.26	0.50
1:A:320:GLU:HA	1:A:333:PHE:CE1	2.41	0.50
1:B:463:LEU:HD12	1:B:463:LEU:H	1.76	0.50
1:B:562:LEU:O	1:B:585:ALA:HA	2.12	0.50
1:A:382:GLN:NE2	1:A:391:LEU:HD11	2.28	0.49
1:A:406:GLN:HG2	1:A:407:LEU:N	2.27	0.49
1:A:576:GLY:O	1:A:580:VAL:HG23	2.12	0.49
1:B:252:ALA:HA	1:B:304:VAL:HG13	1.94	0.49
1:B:333:PHE:CD2	1:B:336:ILE:CG2	2.69	0.49
1:A:315:LEU:O	1:A:319:LEU:HB2	2.11	0.49
1:B:226:PHE:CE2	1:B:237:LEU:HD23	2.48	0.49
1:B:422:ALA:HA	1:B:564:CYS:SG	2.53	0.49
1:A:429:GLN:OE1	1:A:432:VAL:HG23	2.12	0.49
1:B:293:VAL:CG1	1:B:297:TRP:HD1	2.26	0.49
1:A:427:THR:HG23	1:A:572:VAL:HG23	1.94	0.49
1:B:366:TRP:HA	1:B:369:CYS:O	2.13	0.48
1:A:402:GLU:C	1:A:406:GLN:HE22	2.20	0.48
1:B:427:THR:HB	1:B:572:VAL:HG12	1.95	0.48
1:B:333:PHE:O	1:B:333:PHE:CG	2.65	0.48
1:B:427:THR:C	1:B:428:HIS:HD1	2.21	0.48
1:A:424:ARG:O	1:A:551:ALA:HA	2.14	0.48
1:A:450:PHE:HD1	1:A:451:GLU:O	1.97	0.48
1:B:223:SER:OG	1:B:338:LEU:N	2.40	0.48
1:B:292:GLY:HA3	1:B:536:GLY:HA2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ILE:C	1:B:310:MET:N	2.70	0.48
1:A:401:ASP:C	1:A:403:VAL:N	2.70	0.48
1:A:450:PHE:CD1	1:A:451:GLU:O	2.67	0.48
1:B:378:LYS:C	1:B:380:TRP:CD1	2.80	0.48
1:B:344:PHE:CE2	1:B:361:PHE:CD2	3.02	0.47
1:A:228:GLY:CA	1:A:234:LYS:HD3	2.43	0.47
1:A:253:THR:HG21	1:A:268:LEU:HD23	1.97	0.47
1:A:582:LEU:HD12	1:A:582:LEU:H	1.78	0.47
1:A:228:GLY:C	1:A:234:LYS:NZ	2.72	0.47
1:A:395:ARG:HD2	1:A:579:TYR:CE2	2.50	0.47
1:A:609:HIS:O	1:A:613:THR:HG23	2.14	0.47
1:B:579:TYR:C	1:B:579:TYR:CD2	2.91	0.47
1:A:251:VAL:HG11	1:A:271:PHE:CE1	2.49	0.47
1:B:359:PHE:HD1	1:B:360:CYS:N	2.12	0.47
1:B:436:ASN:HA	1:B:550:TRP:CE3	2.50	0.47
1:A:211:GLN:OE1	2:A:701:ADP:N6	2.45	0.47
1:B:236:TYR:HB2	2:B:701:ADP:N7	2.30	0.47
1:A:251:VAL:HG22	1:A:303:LEU:HA	1.96	0.46
1:A:403:VAL:HA	1:A:406:GLN:NE2	2.29	0.46
1:A:407:LEU:O	1:A:409:ALA:N	2.48	0.46
1:B:496:GLY:HA3	1:B:516:PHE:HA	1.98	0.46
1:B:253:THR:HG22	1:B:266:THR:H	1.80	0.46
1:B:604:ASP:C	1:B:606:ARG:H	2.21	0.46
1:A:424:ARG:HA	1:A:566:GLU:O	2.15	0.46
1:A:569:LEU:HA	1:A:572:VAL:HG12	1.97	0.46
1:B:365:SER:O	1:B:369:CYS:N	2.48	0.46
1:B:492:GLY:C	1:B:493:LEU:HD12	2.40	0.46
1:A:297:TRP:CD1	1:A:326:VAL:CG1	2.88	0.46
1:B:575:SER:C	1:B:577:GLN:H	2.23	0.46
1:B:359:PHE:HD1	1:B:360:CYS:H	1.63	0.46
1:A:443:LEU:HD21	1:A:478:GLY:H	1.81	0.46
1:A:448:HIS:NE2	1:A:500:VAL:HG11	2.31	0.46
1:A:572:VAL:O	1:A:572:VAL:HG13	2.15	0.46
1:A:311:VAL:HG13	1:A:315:LEU:HD23	1.98	0.46
1:A:401:ASP:C	1:A:403:VAL:H	2.24	0.46
1:A:290:ARG:HD2	1:A:535:GLY:C	2.42	0.45
1:A:406:GLN:HG2	1:A:407:LEU:CD2	2.46	0.45
1:A:401:ASP:O	1:A:404:THR:N	2.49	0.45
1:A:253:THR:HG22	1:A:254:ALA:N	2.29	0.45
1:A:432:VAL:HG21	1:A:553:SER:HB3	1.99	0.45
1:A:347:LEU:HD12	1:A:558:GLN:HG3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:LEU:HA	1:A:467:CYS:SG	2.57	0.45
1:B:238:LEU:HD13	1:B:304:VAL:HG21	1.98	0.45
1:B:293:VAL:O	1:B:295:GLN:N	2.49	0.45
1:B:308:ILE:HD12	1:B:344:PHE:HE1	1.80	0.45
1:A:246:PRO:HG2	1:A:302:ARG:NH1	2.31	0.45
1:A:308:ILE:HG22	1:A:342:GLY:HA3	1.99	0.45
1:A:424:ARG:HG3	1:A:425:LEU:N	2.32	0.45
1:B:347:LEU:HD21	1:B:555:HIS:HA	1.98	0.45
1:B:462:THR:O	1:B:465:ALA:N	2.50	0.45
1:A:252:ALA:HA	1:A:304:VAL:CG2	2.46	0.45
1:A:305:ILE:HB	1:A:340:ILE:HD13	1.98	0.45
1:A:523:VAL:HG13	1:A:525:HIS:HE1	1.81	0.45
1:B:230:ALA:HA	2:B:701:ADP:O3B	2.17	0.45
1:A:406:GLN:CD	1:A:406:GLN:H	2.25	0.45
1:A:470:SER:H	1:A:543:GLN:NE2	2.12	0.45
1:A:390:LEU:O	1:A:394:VAL:HG23	2.16	0.44
1:B:226:PHE:O	1:B:341:CYS:CB	2.65	0.44
1:B:229:SER:O	1:B:232:THR:OG1	2.34	0.44
1:B:528:ARG:NH1	1:B:530:THR:CG2	2.80	0.44
1:A:226:PHE:CE2	1:A:237:LEU:HD23	2.52	0.44
1:A:385:GLN:HA	1:A:388:ILE:HB	1.99	0.44
1:A:290:ARG:HD2	1:A:535:GLY:O	2.17	0.44
1:A:242:LEU:HD21	1:A:304:VAL:HG11	1.98	0.44
1:A:360:CYS:O	1:A:363:SER:OG	2.22	0.44
1:A:556:LYS:O	1:A:560:MET:HE3	2.16	0.44
1:A:273:GLY:O	1:A:287:LEU:HD22	2.17	0.44
1:B:237:LEU:O	1:B:240:ARG:N	2.50	0.44
1:B:251:VAL:HG22	1:B:302:ARG:O	2.17	0.44
1:B:347:LEU:CD2	1:B:555:HIS:HA	2.48	0.44
1:B:267:THR:O	1:B:268:LEU:HB3	2.18	0.44
1:B:379:VAL:HG21	1:B:388:ILE:CG1	2.47	0.44
1:B:458:GLU:O	1:B:459:LEU:HD22	2.18	0.44
1:A:228:GLY:O	1:A:234:LYS:NZ	2.43	0.44
1:A:304:VAL:HG12	1:A:339:ILE:CD1	2.48	0.44
1:A:309:SER:OG	1:A:343:ASP:O	2.29	0.44
1:A:369:CYS:C	1:A:371:PRO:HD3	2.43	0.44
1:A:227:THR:C	1:A:234:LYS:HD3	2.42	0.43
1:A:452:ALA:O	1:A:454:ASP:N	2.44	0.43
1:B:395:ARG:NH1	1:B:611:TYR:HE2	2.14	0.43
1:A:274:ILE:HG22	1:A:275:GLY:N	2.33	0.43
1:A:348:PRO:HB2	1:A:349:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:SER:H	1:A:403:VAL:HB	1.83	0.43
1:A:415:VAL:CG1	1:A:564:CYS:HB2	2.48	0.43
1:B:260:ALA:HB1	1:B:265:GLY:O	2.18	0.43
1:B:528:ARG:HH12	1:B:530:THR:HG21	1.82	0.43
1:B:226:PHE:CZ	1:B:238:LEU:HD21	2.53	0.43
1:B:315:LEU:O	1:B:319:LEU:HB2	2.18	0.43
1:B:511:LEU:N	1:B:512:PRO:HD3	2.34	0.43
1:A:263:ILE:HD11	1:A:306:ASP:OD2	2.17	0.43
1:A:557:SER:HA	1:A:560:MET:SD	2.59	0.43
1:A:368:ARG:C	1:A:370:VAL:H	2.26	0.43
1:A:528:ARG:CD	1:B:292:GLY:HA2	2.45	0.43
1:B:436:ASN:HA	1:B:550:TRP:HE3	1.83	0.43
1:A:246:PRO:HG2	1:A:302:ARG:CZ	2.48	0.43
1:A:333:PHE:CD2	1:A:338:LEU:HD22	2.52	0.43
1:A:451:GLU:CB	1:A:472:LEU:HA	2.47	0.43
1:B:396:LEU:O	1:B:608:LEU:HD11	2.19	0.43
1:A:294:ARG:NH1	1:B:525:HIS:CE1	2.87	0.43
1:A:361:PHE:CD1	1:A:361:PHE:C	2.97	0.43
1:B:281:LEU:O	1:B:285:VAL:HG23	2.19	0.43
1:B:459:LEU:HB3	1:B:461:SER:OG	2.18	0.43
1:A:218:VAL:O	1:A:337:GLN:NE2	2.46	0.43
1:A:301:GLN:O	1:A:337:GLN:N	2.51	0.43
1:A:210:GLU:OE2	1:A:377:THR:OG1	2.32	0.43
1:A:366:TRP:C	1:A:368:ARG:H	2.26	0.43
1:B:308:ILE:HG12	1:B:341:CYS:O	2.19	0.43
1:A:229:SER:O	1:A:234:LYS:NZ	2.51	0.42
1:A:406:GLN:HG2	1:A:407:LEU:HD23	2.01	0.42
1:A:410:THR:O	1:A:413:HIS:N	2.47	0.42
1:B:252:ALA:O	1:B:265:GLY:HA3	2.19	0.42
1:B:379:VAL:O	1:B:380:TRP:CG	2.72	0.42
1:B:395:ARG:HB2	1:B:579:TYR:CE1	2.52	0.42
1:A:224:ILE:HG13	1:A:374:LEU:HD13	2.00	0.42
1:A:408:GLN:OE1	1:A:596:PHE:CB	2.68	0.42
1:A:492:GLY:C	1:A:493:LEU:HD12	2.44	0.42
1:B:532:GLN:HA	1:B:537:GLN:CB	2.49	0.42
1:B:359:PHE:CD1	1:B:360:CYS:N	2.88	0.42
1:B:378:LYS:CB	1:B:380:TRP:CZ2	3.02	0.42
1:A:246:PRO:HG2	1:A:302:ARG:HH12	1.85	0.42
1:A:291:PRO:HG2	1:A:292:GLY:H	1.85	0.42
1:A:438:ARG:O	1:A:442:GLU:HG3	2.19	0.42
1:A:511:LEU:N	1:A:512:PRO:HD3	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:VAL:HG12	1:B:297:TRP:HD1	1.85	0.42
1:B:226:PHE:HZ	1:B:238:LEU:HD21	1.83	0.42
1:B:439:ARG:O	1:B:442:GLU:HG3	2.19	0.42
1:B:483:LEU:CB	1:B:546:LEU:HD23	2.50	0.42
1:B:404:THR:O	1:B:408:GLN:N	2.29	0.42
1:A:267:THR:HG21	1:A:466:GLN:HA	2.02	0.41
1:A:218:VAL:HG11	1:A:241:ILE:HD13	2.02	0.41
1:A:289:GLN:HG2	1:A:326:VAL:HG22	2.02	0.41
1:A:562:LEU:O	1:A:585:ALA:HA	2.20	0.41
1:A:210:GLU:HB3	1:A:376:LEU:HD23	2.02	0.41
1:A:473:LEU:HD23	1:A:473:LEU:HA	1.83	0.41
1:B:215:LEU:HD13	1:B:241:ILE:HG12	2.02	0.41
1:B:423:THR:HG23	1:B:549:ALA:C	2.14	0.41
1:A:289:GLN:HA	1:A:294:ARG:CG	2.50	0.41
1:A:463:LEU:HD12	1:A:463:LEU:H	1.86	0.41
1:A:401:ASP:C	1:A:404:THR:H	2.28	0.41
1:A:347:LEU:HB2	1:A:558:GLN:OE1	2.21	0.41
1:B:529:TRP:O	1:B:540:SER:HA	2.21	0.41
1:A:281:LEU:O	1:A:285:VAL:HG12	2.20	0.41
1:B:379:VAL:C	1:B:380:TRP:CG	2.98	0.41
1:A:359:PHE:O	1:A:362:GLN:HG3	2.21	0.41
1:A:418:ASP:HB3	1:A:419:GLY:H	1.56	0.41
2:A:701:ADP:O2B	3:A:702:ALF:F2	2.29	0.41
1:B:214:VAL:HB	1:B:237:LEU:HD21	2.02	0.41
1:B:232:THR:HG22	1:B:232:THR:O	2.21	0.41
1:B:361:PHE:C	1:B:363:SER:N	2.78	0.41
1:B:379:VAL:HG11	1:B:388:ILE:HG12	2.02	0.41
1:B:462:THR:HG23	1:B:463:LEU:H	1.86	0.41
1:A:289:GLN:HA	1:A:294:ARG:HG3	2.03	0.41
1:B:443:LEU:HD13	1:B:476:LYS:CB	2.51	0.41
1:B:274:ILE:HD12	1:B:284:CYS:HB3	2.03	0.40
1:B:370:VAL:N	1:B:371:PRO:HD2	2.35	0.40
1:B:313:ALA:HB2	1:B:359:PHE:O	2.21	0.40
1:A:294:ARG:O	1:A:297:TRP:N	2.54	0.40
1:A:385:GLN:HA	1:A:388:ILE:HD12	2.04	0.40
1:B:225:PHE:HB2	1:B:340:ILE:O	2.21	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	389/442 (88%)	301 (77%)	59 (15%)	29 (8%)	1	9
1	B	387/442 (88%)	297 (77%)	66 (17%)	24 (6%)	1	12
All	All	776/884 (88%)	598 (77%)	125 (16%)	53 (7%)	1	11

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	PRO
1	A	411	ALA
1	A	413	HIS
1	A	417	ARG
1	A	430	ASP
1	A	452	ALA
1	A	454	ASP
1	A	484	VAL
1	A	575	SER
1	A	597	ASP
1	A	599	MET
1	B	232	THR
1	B	309	SER
1	B	340	ILE
1	B	437	GLU
1	B	446	LYS
1	B	469	VAL
1	B	500	VAL
1	B	538	LEU
1	B	574	ALA
1	A	266	THR
1	A	268	LEU
1	A	453	MET
1	A	464	ASP
1	A	549	ALA

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Mol	Chain	Res	Type
1	B	252	ALA
1	B	436	ASN
1	B	488	SER
1	B	490	SER
1	A	346	GLN
1	A	517	LEU
1	A	574	ALA
1	A	578	ALA
1	B	234	LYS
1	B	594	LEU
1	A	337	GLN
1	A	466	GLN
1	A	598	PRO
1	B	268	LEU
1	B	294	ARG
1	B	404	THR
1	A	282	ALA
1	A	291	PRO
1	B	370	VAL
1	B	457	PRO
1	B	584	ARG
1	B	587	SER
1	A	264	GLY
1	A	369	CYS
1	A	468	PRO
1	B	274	ILE
1	B	290	ARG
1	A	457	PRO

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	216/363 (60%)	213 (99%)	3 (1%)	59	71
1	B	175/363 (48%)	174 (99%)	1 (1%)	78	79
All	All	391/726 (54%)	387 (99%)	4 (1%)	68	75

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	407	LEU
1	A	516	PHE
1	A	517	LEU
1	B	306	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

4 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	A	701	3	27,29,29	1.45	4 (14%)	42,45,45	1.94	10 (23%)
3	ALF	B	702	2,1	0,4,4	-	-	-		
2	ADP	B	701	3	27,29,29	1.36	4 (14%)	42,45,45	2.32	13 (30%)
3	ALF	A	702	2	0,4,4	-	-	-		

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	701	3	-	3/16/32/32	0/3/3/3
2	ADP	B	701	3	-	4/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ADP	C5-C4	4.87	1.48	1.39
2	B	701	ADP	C5-C4	4.43	1.47	1.39
2	A	701	ADP	C5-C6	3.10	1.49	1.41
2	A	701	ADP	C8-N7	2.86	1.37	1.31
2	B	701	ADP	C5-C6	2.64	1.48	1.41
2	B	701	ADP	C8-N7	2.27	1.35	1.31
2	B	701	ADP	C5-N7	-2.26	1.34	1.39
2	A	701	ADP	C5-N7	-2.08	1.35	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	ADP	C5-C4-N3	-6.66	118.06	126.75
2	A	701	ADP	C5-C4-N3	-6.10	118.80	126.75
2	B	701	ADP	N3-C4-N9	4.95	135.25	127.08
2	B	701	ADP	C2'-C1'-N9	-4.61	101.63	113.30
2	A	701	ADP	N3-C4-N9	4.53	134.55	127.08
2	A	701	ADP	C2-N3-C4	4.03	121.28	111.75
2	B	701	ADP	PA-O3A-PB	-3.91	119.41	132.83
2	B	701	ADP	C2-N3-C4	3.81	120.75	111.75
2	B	701	ADP	C4-C5-N7	-3.63	106.20	110.62
2	B	701	ADP	O4'-C1'-N9	3.62	115.19	108.06
2	B	701	ADP	C3'-C2'-C1'	3.38	107.85	101.43
2	A	701	ADP	PA-O3A-PB	-3.29	121.52	132.83
2	A	701	ADP	C4-C5-N7	-3.18	106.74	110.62
2	B	701	ADP	C5-N7-C8	3.12	107.94	103.51
2	B	701	ADP	O5'-C5'-C4'	2.82	118.69	108.99
2	B	701	ADP	N3-C2-N1	-2.81	124.21	128.60
2	A	701	ADP	N3-C2-N1	-2.74	124.31	128.60
2	A	701	ADP	C3'-C2'-C1'	2.67	106.51	101.43
2	A	701	ADP	C6-C5-N7	2.61	136.88	132.02
2	A	701	ADP	C5-N7-C8	2.38	106.89	103.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	ADP	C4-N9-C8	2.21	108.12	105.73
2	B	701	ADP	N9-C8-N7	-2.11	111.03	113.91
2	A	701	ADP	C4-N9-C8	2.09	108.00	105.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

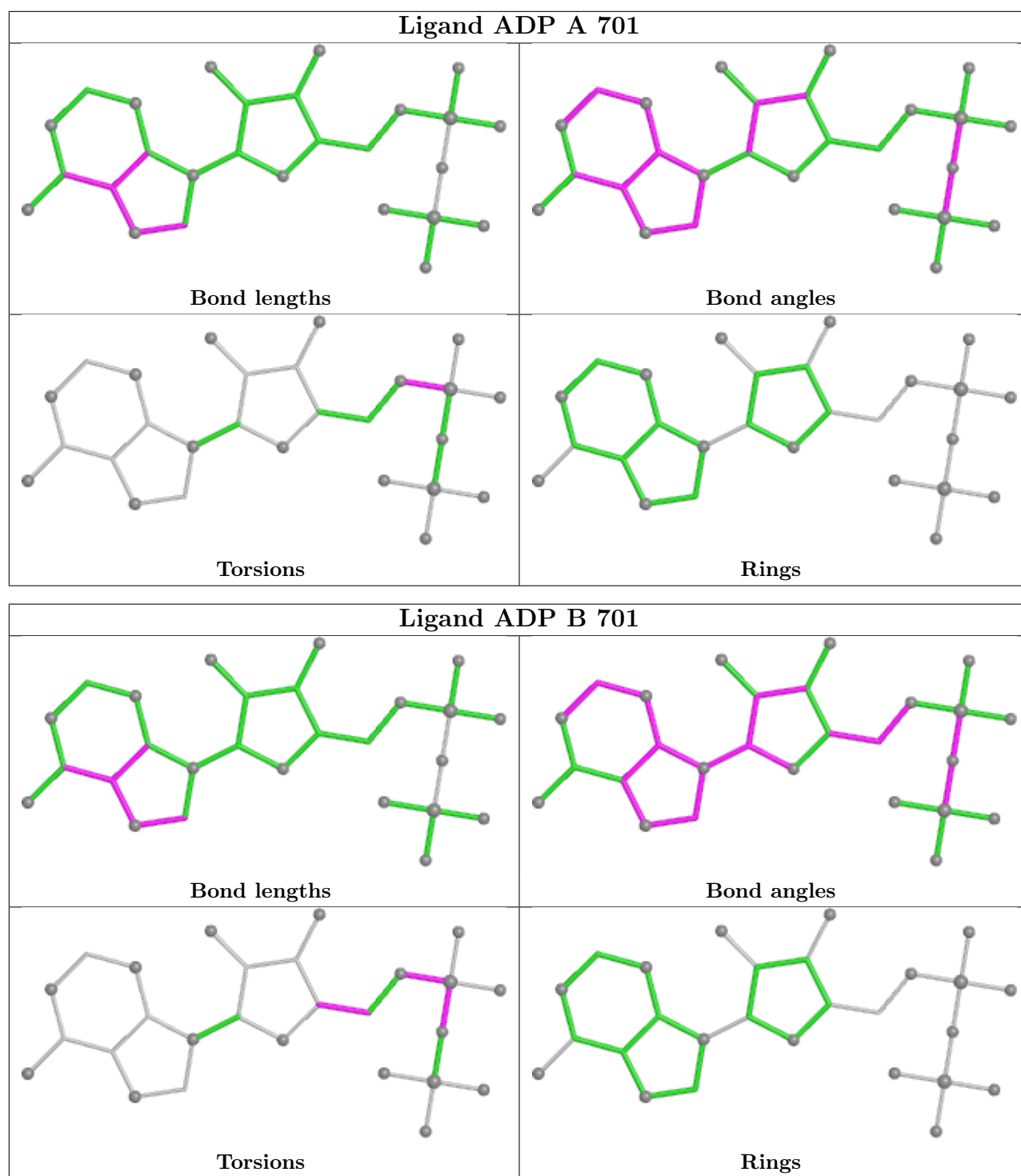
Mol	Chain	Res	Type	Atoms
2	A	701	ADP	C5'-O5'-PA-O1A
2	A	701	ADP	C5'-O5'-PA-O2A
2	B	701	ADP	PB-O3A-PA-O5'
2	B	701	ADP	C5'-O5'-PA-O1A
2	B	701	ADP	C3'-C4'-C5'-O5'
2	A	701	ADP	C5'-O5'-PA-O3A
2	B	701	ADP	C5'-O5'-PA-O3A

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	ADP	6	0
3	B	702	ALF	7	0
2	B	701	ADP	8	0
3	A	702	ALF	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 ⓘ

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	395/442 (89%)	1.11	71 (17%) 3 4	31, 81, 121, 147	0
1	B	393/442 (88%)	1.32	77 (19%) 3 3	57, 118, 171, 217	0
All	All	788/884 (89%)	1.21	148 (18%) 3 3	31, 100, 160, 217	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	518	CYS	6.6
1	B	341	CYS	6.3
1	A	297	TRP	6.2
1	B	292	GLY	5.7
1	B	343	ASP	5.4
1	A	597	ASP	5.3
1	A	413	HIS	4.9
1	B	578	ALA	4.8
1	B	335	GLY	4.7
1	B	269	HIS	4.4
1	B	493	LEU	4.3
1	B	369	CYS	4.2
1	B	465	ALA	4.1
1	B	467	CYS	4.0
1	B	282	ALA	3.9
1	A	409	ALA	3.8
1	B	367	LYS	3.7
1	A	493	LEU	3.6
1	B	368	ARG	3.6
1	A	463	LEU	3.6
1	A	399	CYS	3.5
1	A	527	ASP	3.4
1	B	371	PRO	3.4
1	B	547	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	484	VAL	3.4
1	A	528	ARG	3.3
1	A	450	PHE	3.3
1	A	519	GLY	3.2
1	B	340	ILE	3.2
1	B	605	PRO	3.2
1	B	480	GLN	3.2
1	A	370	VAL	3.2
1	B	330	ASN	3.2
1	B	452	ALA	3.2
1	A	410	THR	3.1
1	A	501	VAL	3.1
1	A	533	ALA	3.0
1	A	541	ARG	3.0
1	A	447	VAL	3.0
1	A	322	VAL	3.0
1	A	451	GLU	2.9
1	B	594	LEU	2.9
1	B	608	LEU	2.9
1	A	442	GLU	2.9
1	A	317	ASP	2.8
1	B	500	VAL	2.8
1	A	595	ASP	2.8
1	B	587	SER	2.7
1	A	357	PRO	2.7
1	A	248	THR	2.7
1	B	267	THR	2.7
1	A	520	VAL	2.7
1	B	565	VAL	2.7
1	B	572	VAL	2.7
1	A	250	THR	2.7
1	A	261	CYS	2.7
1	B	495	ASN	2.7
1	B	333	PHE	2.7
1	B	365	SER	2.6
1	B	293	VAL	2.6
1	B	609	HIS	2.6
1	A	570	GLY	2.6
1	B	563	ASP	2.6
1	B	346	GLN	2.6
1	B	535	GLY	2.6
1	B	339	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	486	ASN	2.6
1	A	441	GLN	2.6
1	A	489	VAL	2.5
1	A	596	PHE	2.5
1	A	470	SER	2.5
1	A	494	VAL	2.5
1	A	571	ARG	2.5
1	A	495	ASN	2.5
1	B	526	ALA	2.4
1	A	483	LEU	2.4
1	B	342	GLY	2.4
1	B	397	GLY	2.4
1	A	537	GLN	2.4
1	B	497	ALA	2.4
1	B	573	PHE	2.4
1	B	210	GLU	2.4
1	A	411	ALA	2.4
1	B	382	GLN	2.4
1	B	373	THR	2.4
1	B	544	LEU	2.4
1	B	527	ASP	2.4
1	B	615	ARG	2.4
1	A	366	TRP	2.3
1	B	419	GLY	2.3
1	A	511	LEU	2.3
1	A	550	TRP	2.3
1	A	598	PRO	2.3
1	B	250	THR	2.3
1	A	472	LEU	2.3
1	A	365	SER	2.3
1	A	349	PRO	2.3
1	A	262	HIS	2.2
1	B	235	SER	2.2
1	A	342	GLY	2.2
1	A	435	THR	2.2
1	B	291	PRO	2.2
1	B	487	LEU	2.2
1	B	253	THR	2.2
1	A	563	ASP	2.2
1	B	325	ALA	2.2
1	A	371	PRO	2.2
1	B	444	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	448	HIS	2.2
1	A	548	LEU	2.2
1	A	500	VAL	2.2
1	B	494	VAL	2.1
1	A	427	THR	2.1
1	A	498	ARG	2.1
1	B	309	SER	2.1
1	B	408	GLN	2.1
1	B	429	GLN	2.1
1	B	537	GLN	2.1
1	B	321	ALA	2.1
1	A	572	VAL	2.1
1	A	431	ASP	2.1
1	B	546	LEU	2.1
1	A	574	ALA	2.1
1	B	384	ASP	2.1
1	A	605	PRO	2.1
1	A	360	CYS	2.1
1	A	587	SER	2.1
1	A	456	ASN	2.1
1	A	480	GLN	2.1
1	A	589	GLN	2.1
1	B	283	GLN	2.1
1	B	512	PRO	2.1
1	A	284	CYS	2.1
1	A	517	LEU	2.1
1	B	236	TYR	2.0
1	B	366	TRP	2.0
1	B	468	PRO	2.0
1	A	449	ARG	2.0
1	B	323	ALA	2.0
1	B	538	LEU	2.0
1	B	492	GLY	2.0
1	B	451	GLU	2.0
1	B	522	GLU	2.0
1	A	283	GLN	2.0
1	B	299	ASN	2.0
1	B	567	ILE	2.0
1	B	430	ASP	2.0
1	B	484	VAL	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](#)

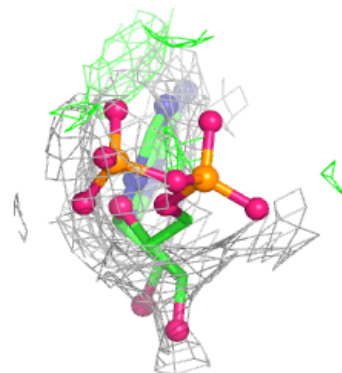
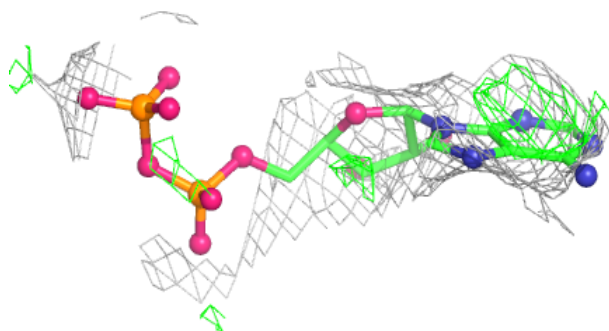
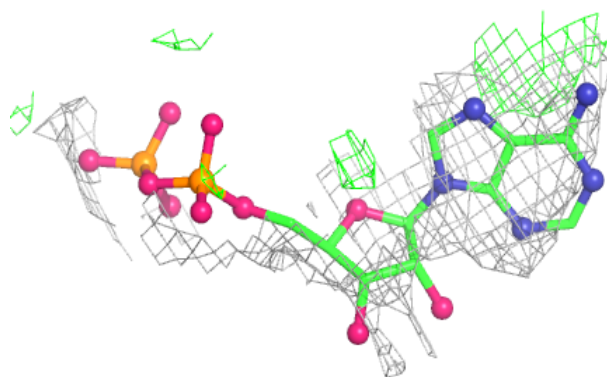
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B	701	27/27	0.76	0.20	129,150,155,157	0
3	ALF	B	702	5/5	0.78	0.12	131,133,139,146	0
3	ALF	A	702	5/5	0.81	0.27	91,108,116,118	0
2	ADP	A	701	27/27	0.90	0.20	37,75,114,125	0

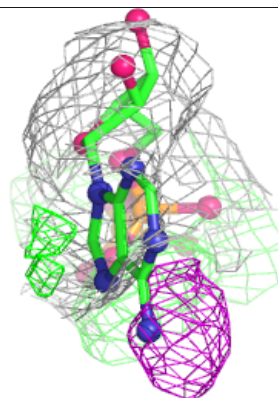
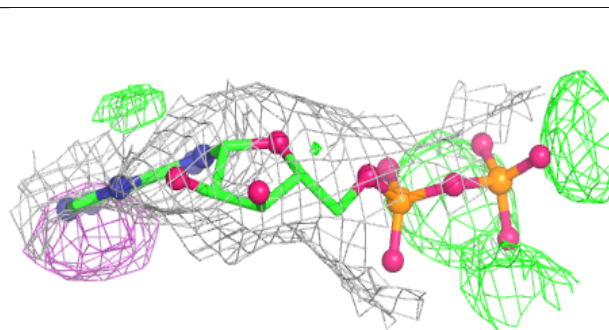
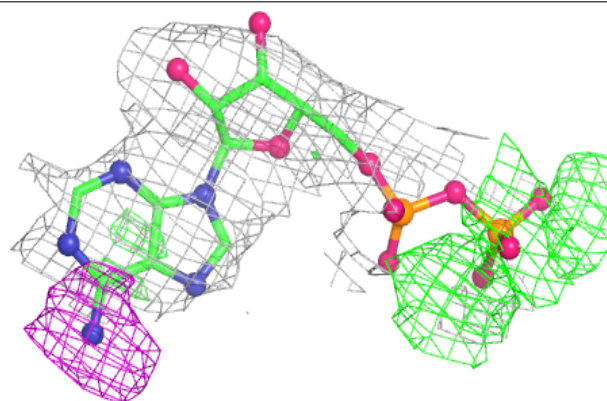
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP B 701:

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

**Electron density around ADP A 701:**

$2mF_o-DF_c$ (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.