WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:16 pm GMT

PDB ID	:	2G2I
Title	:	A Src-like Inactive Conformation in the Abl Tyrosine Kinase Domain
Authors	:	Levinson, N.M.; Kuchment, O.
Deposited on	:	2006-02-16
Resolution	:	3.12 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 3.12 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	Percentile Ranks	Value
Rfree		0.293
Clashscore		29
Ramachandran outliers		5.2%
Sidechain outliers		6.5%
RSRZ outliers		2.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
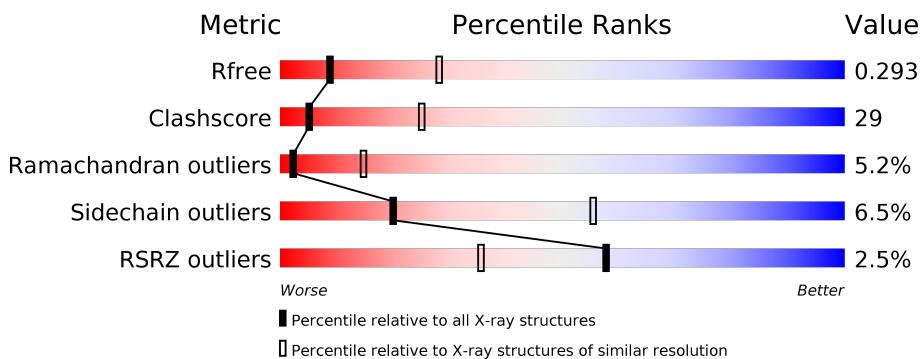
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1000 (3.14-3.10)
Clashscore	112137	1099 (3.14-3.10)
Ramachandran outliers	110173	1060 (3.14-3.10)
Sidechain outliers	110143	1060 (3.14-3.10)
RSRZ outliers	101464	1005 (3.14-3.10)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	287	2% 51% 37% 5% · 6%
1	B	287	3% 41% 45% 5% · 8%
2	C	13	54% 8% 38%
2	D	13	46% 8% 46%
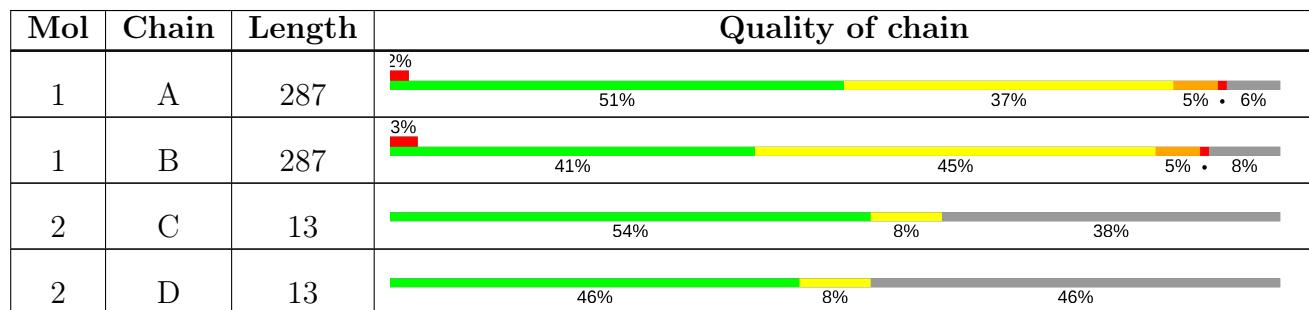
2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 4518 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 Abl Tyrosine Kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	271	Total	C	N	O	S	0	0	0
			2203	1419	357	410	17			
1	B	265	Total	C	N	O	S	0	0	0
			2164	1396	350	401	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	226	GLY	-	CLONING ARTIFACT	UNP P00519
A	227	HIS	-	CLONING ARTIFACT	UNP P00519
A	228	MET	-	CLONING ARTIFACT	UNP P00519
A	396	PRO	HIS	ENGINEERED	UNP P00519
B	226	GLY	-	CLONING ARTIFACT	UNP P00519
B	227	HIS	-	CLONING ARTIFACT	UNP P00519
B	228	MET	-	CLONING ARTIFACT	UNP P00519
B	396	PRO	HIS	ENGINEERED	UNP P00519

- Molecule 2 is a protein called ATP-Peptide Conjugate.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	0	0	0
			48	32	8	8			
2	D	7	Total	C	N	O	0	0	0
			49	35	7	7			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

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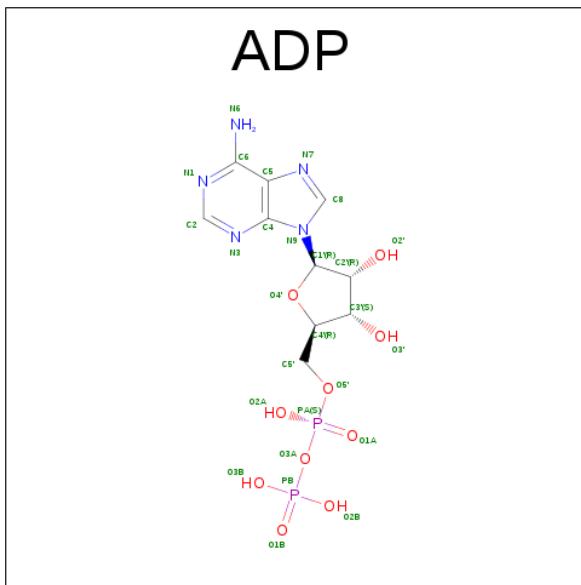
| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: Abl Tyrosine Kinase
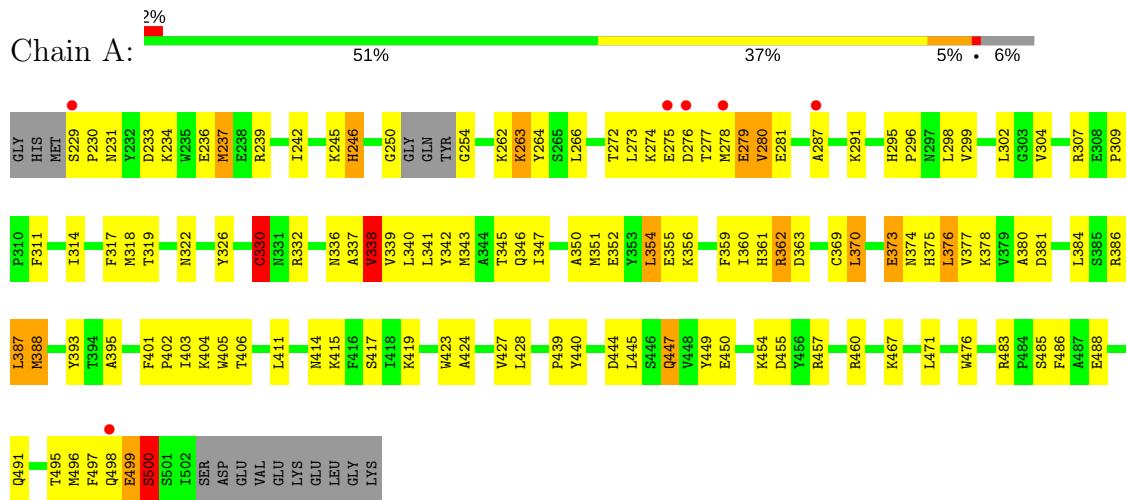
- Molecule 1: Abl Tyrosine Kinase
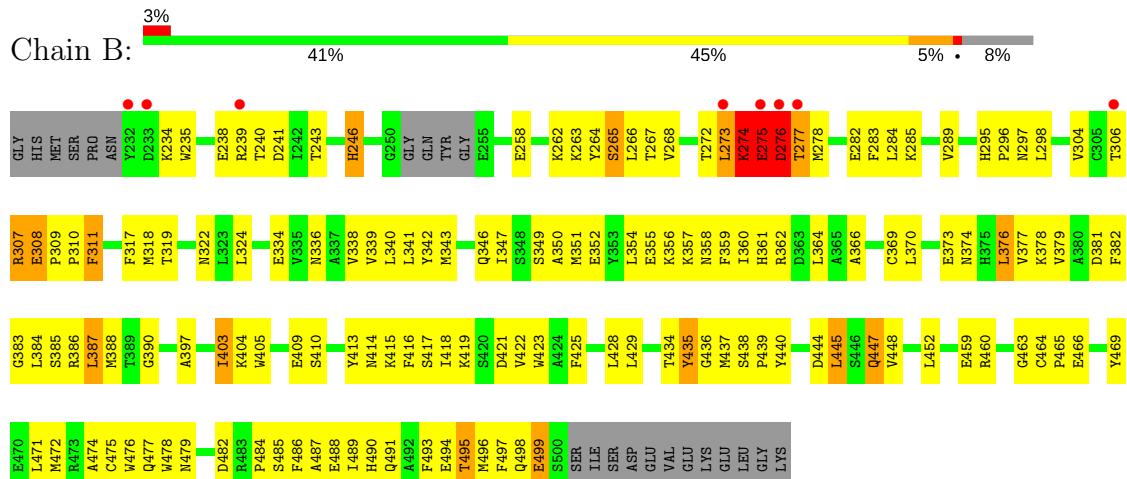
- Molecule 2: ATP-Peptide Conjugate

• Molecule 2: ATP-Peptide Conjugate

Chain D:

46%   8%   46%
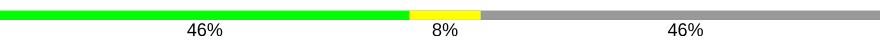
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.46Å 88.46Å 235.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.12 49.03 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.12) 93.4 (49.03-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.81 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.308 0.239 , 0.293	Depositor DCC
R_{free} test set	867 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	77.5	Xtriage
Anisotropy	0.457	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 89.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4518	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \|L\| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.44	0/2259	0.78	3/3058 (0.1%)
1	B	0.41	0/2219	0.75	2/3003 (0.1%)
2	C	0.54	0/48	0.59	0/64
2	D	0.55	0/50	0.59	0/66
All	All	0.43	0/4576	0.76	5/6191 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	500	SER	N-CA-C	9.54	136.76	111.00
1	A	499	GLU	C-N-CA	9.20	144.70	121.70
1	A	500	SER	CB-CA-C	-6.54	97.67	110.10
1	B	276	ASP	C-N-CA	5.06	134.35	121.70
1	B	390	GLY	N-CA-C	-5.04	100.50	113.10

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	2203	0	2160	122	1
1	B	2164	0	2123	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	48	0	32	1	0
2	D	49	0	37	1	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
All	All	4518	0	4376	262	1

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 29.

All (262) 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:250:GLY:C	1:A:254:GLY:O	1.90	1.10
1:A:336:ASN:OD1	1:A:338:VAL:HG13	1.52	1.09
1:B:274:LYS:O	1:B:275:GLU:HB3	1.61	0.97
1:A:336:ASN:OD1	1:A:339:VAL:HG23	1.71	0.90
1:A:345:THR:HG21	1:B:336:ASN:ND2	1.89	0.88
1:A:299:VAL:HG21	1:A:380:ALA:HB2	1.54	0.88
1:B:275:GLU:O	1:B:276:ASP:C	2.06	0.87
1:B:387:LEU:HD22	1:B:387:LEU:H	1.38	0.85
1:A:277:THR:O	1:A:279:GLU:HG2	1.78	0.83
1:A:495:THR:CG2	1:A:498:GLN:HB3	2.09	0.83
1:B:274:LYS:O	1:B:275:GLU:CB	2.25	0.83
1:A:229:SER:N	1:A:230:PRO:HD3	1.94	0.83
1:A:336:ASN:CG	1:A:338:VAL:CG1	2.49	0.81
1:A:336:ASN:OD1	1:A:338:VAL:CG1	2.27	0.80
1:A:491:GLN:HG2	1:A:499:GLU:HG2	1.64	0.78
1:A:345:THR:HG21	1:B:336:ASN:HD21	1.48	0.76
1:B:275:GLU:O	1:B:277:THR:N	2.19	0.75
1:A:499:GLU:OE2	1:A:500:SER:HB3	1.86	0.75
1:B:266:LEU:HD23	1:B:267:THR:N	2.01	0.75
1:B:336:ASN:OD1	1:B:339:VAL:HG23	1.89	0.73
1:B:308:GLU:CD	1:B:308:GLU:H	1.92	0.73
1:A:239:ARG:HB2	1:A:239:ARG:NH1	2.05	0.72
1:A:299:VAL:CG2	1:A:380:ALA:HB2	2.19	0.72
1:B:410:SER:HB3	1:B:416:PHE:HE1	1.54	0.72
1:B:349:SER:HA	1:B:490:HIS:CD2	2.25	0.72
1:A:387:LEU:O	1:A:388:MET:HB2	1.88	0.71
1:A:336:ASN:ND2	1:B:494:GLU:OE2	2.24	0.71
1:A:336:ASN:ND2	1:A:338:VAL:CG1	2.55	0.70
1:A:362:ARG:HD3	1:A:384:LEU:O	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:HD11	1:A:279:GLU:HG3	1.73	0.69
1:B:273:LEU:HD23	1:B:311:PHE:HB2	1.74	0.69
1:A:230:PRO:HD2	1:A:234:LYS:O	1.93	0.69
1:A:491:GLN:CG	1:A:499:GLU:HG2	2.23	0.69
1:B:275:GLU:O	1:B:275:GLU:HG3	1.92	0.69
1:B:362:ARG:HD3	1:B:384:LEU:O	1.92	0.69
1:A:295:HIS:CG	1:A:296:PRO:HD2	2.29	0.68
1:A:317:PHE:HE2	1:A:319:THR:HA	1.58	0.68
1:A:495:THR:HG21	1:A:498:GLN:HB3	1.75	0.68
1:A:298:LEU:HD11	1:A:354:LEU:HD13	1.74	0.67
1:B:410:SER:HB3	1:B:416:PHE:CE1	2.30	0.67
1:B:352:GLU:HG3	1:B:487:ALA:HA	1.76	0.67
1:B:318:MET:HG3	1:B:370:LEU:HB3	1.75	0.67
1:B:447:GLN:N	1:B:447:GLN:HE21	1.92	0.66
1:A:245:LYS:O	1:A:246:HIS:HB3	1.95	0.65
1:A:277:THR:O	1:A:279:GLU:N	2.28	0.65
1:A:460:ARG:HH11	1:A:460:ARG:HB3	1.61	0.65
1:B:434:THR:OG1	1:B:437:MET:HB2	1.97	0.65
1:A:298:LEU:HD21	1:A:350:ALA:HB1	1.80	0.64
1:A:495:THR:HG22	1:A:495:THR:O	1.96	0.64
1:B:273:LEU:HD22	1:B:283:PHE:CD2	2.33	0.64
1:A:336:ASN:CG	1:A:338:VAL:HG13	2.11	0.64
1:B:349:SER:HA	1:B:490:HIS:HD2	1.60	0.63
1:B:495:THR:O	1:B:498:GLN:HB3	1.97	0.63
1:B:318:MET:HG3	1:B:370:LEU:CB	2.28	0.63
1:A:457:ARG:HG2	1:A:457:ARG:HH11	1.64	0.63
1:B:404:LYS:HG3	1:B:440:TYR:HD1	1.64	0.63
1:B:336:ASN:OD1	1:B:339:VAL:N	2.25	0.62
1:B:304:VAL:HB	1:B:306:THR:HG23	1.81	0.62
1:A:317:PHE:CE2	1:A:319:THR:HA	2.35	0.62
1:A:495:THR:HG22	1:A:498:GLN:HB3	1.81	0.62
1:A:419:LYS:NZ	1:A:483:ARG:O	2.33	0.61
1:A:491:GLN:NE2	1:A:499:GLU:HG2	2.15	0.61
1:B:340:LEU:HD23	1:B:343:MET:CE	2.30	0.61
1:A:314:ILE:N	1:A:314:ILE:HD12	2.16	0.61
1:A:336:ASN:ND2	1:A:338:VAL:HG11	2.15	0.61
1:A:450:GLU:O	1:A:454:LYS:HG2	2.01	0.61
1:A:239:ARG:HB2	1:A:239:ARG:HH11	1.65	0.60
1:B:410:SER:HG	1:B:416:PHE:HD1	1.47	0.60
1:A:352:GLU:HG2	1:A:356:LYS:HE2	1.83	0.60
1:A:309:PRO:HG3	1:A:311:PHE:CZ	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:VAL:O	1:B:475:CYS:HB3	2.02	0.59
1:B:340:LEU:HD23	1:B:343:MET:HE3	1.85	0.59
1:B:460:ARG:HD2	1:B:469:TYR:CD2	2.37	0.58
1:B:355:GLU:OE2	1:B:485:SER:HB2	2.02	0.58
1:B:418:ILE:O	1:B:422:VAL:HG23	2.04	0.58
1:B:311:PHE:N	1:B:311:PHE:CD1	2.73	0.57
1:A:376:LEU:HD23	1:A:377:VAL:N	2.19	0.57
1:A:359:PHE:CZ	1:A:387:LEU:HG	2.40	0.57
1:A:387:LEU:O	1:A:388:MET:CB	2.53	0.57
1:A:387:LEU:HD22	1:A:388:MET:H	1.68	0.57
1:A:467:LYS:HG3	1:A:497:PHE:CD2	2.40	0.57
1:B:381:ASP:C	1:B:383:GLY:H	2.06	0.57
1:B:239:ARG:NH2	1:B:310:PRO:O	2.36	0.57
1:B:404:LYS:HG3	1:B:440:TYR:CD1	2.39	0.57
1:B:495:THR:HB	1:B:498:GLN:O	2.04	0.57
1:B:413:TYR:O	1:B:415:LYS:HG3	2.05	0.57
1:B:296:PRO:O	1:B:378:LYS:HE2	2.05	0.56
1:B:362:ARG:HE	1:B:416:PHE:HE2	1.50	0.56
1:A:298:LEU:CD2	1:A:350:ALA:HB1	2.35	0.55
1:B:386:ARG:HG2	1:B:387:LEU:HD22	1.86	0.55
1:B:362:ARG:NE	1:B:416:PHE:CE2	2.74	0.55
1:B:285:LYS:O	1:B:289:VAL:HG23	2.06	0.55
1:A:276:ASP:O	1:A:277:THR:HG23	2.07	0.55
1:A:262:LYS:O	1:A:264:TYR:N	2.40	0.55
1:B:239:ARG:O	1:B:239:ARG:HG2	2.07	0.55
1:B:469:TYR:O	1:B:472:MET:HB2	2.06	0.54
1:A:393:TYR:HE2	1:A:395:ALA:HA	1.72	0.54
1:B:264:TYR:O	1:B:265:SER:C	2.46	0.54
1:A:424:ALA:O	1:A:427:VAL:N	2.38	0.54
1:A:491:GLN:CD	1:A:499:GLU:HG2	2.27	0.54
1:B:498:GLN:HG2	1:B:499:GLU:HG2	1.89	0.54
1:B:362:ARG:HG2	1:B:416:PHE:CD2	2.42	0.53
1:B:298:LEU:HD23	1:B:379:VAL:HB	1.90	0.53
1:A:229:SER:N	1:A:230:PRO:CD	2.69	0.53
1:B:423:TRP:CE3	1:B:476:TRP:HA	2.43	0.53
1:B:474:ALA:O	1:B:477:GLN:HG2	2.09	0.53
1:A:355:GLU:OE2	1:A:485:SER:HB2	2.09	0.53
1:A:387:LEU:CD2	1:A:388:MET:H	2.22	0.53
1:A:485:SER:OG	1:A:488:GLU:HG3	2.08	0.53
1:A:491:GLN:HG2	1:A:499:GLU:CG	2.34	0.53
1:B:416:PHE:O	1:B:417:SER:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ASN:HD21	1:B:338:VAL:HB	1.74	0.52
1:B:369:CYS:C	1:B:370:LEU:HD12	2.30	0.52
1:A:386:ARG:C	1:A:387:LEU:O	2.46	0.52
1:B:405:TRP:HZ3	2:D:106:ILE:HG23	1.75	0.52
1:B:429:LEU:HD12	1:B:472:MET:HG3	1.91	0.52
1:B:447:GLN:HE21	1:B:447:GLN:CA	2.22	0.51
1:A:457:ARG:HG2	1:A:457:ARG:NH1	2.25	0.51
1:B:421:ASP:HB3	1:B:486:PHE:HZ	1.75	0.51
1:A:491:GLN:HG2	1:A:499:GLU:CB	2.41	0.51
1:B:387:LEU:HD22	1:B:387:LEU:N	2.17	0.51
1:B:295:HIS:HB3	1:B:298:LEU:HD12	1.93	0.51
1:B:282:GLU:O	1:B:285:LYS:HB2	2.10	0.50
1:B:346:GLN:O	1:B:349:SER:HB3	2.12	0.50
1:A:359:PHE:CE1	1:A:387:LEU:HG	2.47	0.50
1:A:495:THR:HG22	1:A:498:GLN:CB	2.41	0.50
1:B:369:CYS:O	1:B:370:LEU:HD12	2.12	0.50
1:B:387:LEU:HD13	1:B:387:LEU:N	2.27	0.50
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.75	0.50
1:B:479:ASN:O	1:B:482:ASP:HB2	2.12	0.50
1:B:359:PHE:CE2	1:B:387:LEU:HD12	2.47	0.50
1:B:403:ILE:HB	1:B:445:LEU:HD22	1.93	0.50
1:A:361:HIS:O	1:A:363:ASP:N	2.45	0.49
1:B:356:LYS:C	1:B:358:ASN:H	2.15	0.49
1:B:488:GLU:O	1:B:491:GLN:HB3	2.12	0.49
1:B:243:THR:OG1	1:B:262:LYS:HE3	2.13	0.49
1:B:349:SER:CA	1:B:490:HIS:HD2	2.23	0.49
1:A:277:THR:HB	1:A:279:GLU:CD	2.33	0.49
1:B:356:LYS:C	1:B:358:ASN:N	2.66	0.49
1:B:434:THR:O	1:B:435:TYR:C	2.51	0.49
1:B:263:LYS:HE2	1:B:264:TYR:CE1	2.48	0.49
1:A:279:GLU:O	1:A:281:GLU:N	2.46	0.48
1:A:393:TYR:CE2	1:A:395:ALA:HA	2.48	0.48
1:A:454:LYS:O	1:A:455:ASP:HB2	2.12	0.48
1:A:417:SER:C	1:A:419:LYS:H	2.17	0.48
1:B:318:MET:SD	1:B:378:LYS:HD2	2.53	0.48
1:B:422:VAL:HG11	1:B:484:PRO:O	2.13	0.48
1:B:362:ARG:HB2	1:B:384:LEU:HB3	1.94	0.48
1:B:297:ASN:HB2	1:B:350:ALA:HB2	1.94	0.48
1:B:434:THR:O	1:B:436:GLY:N	2.47	0.48
1:A:360:ILE:HD11	1:A:386:ARG:HB2	1.96	0.48
1:B:317:PHE:CE2	1:B:319:THR:HA	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ASN:OD1	1:B:324:LEU:HB3	2.14	0.48
1:B:361:HIS:HA	1:B:385:SER:OG	2.14	0.47
1:A:496:MET:O	1:A:497:PHE:HB2	2.14	0.47
1:A:274:LYS:O	1:A:276:ASP:N	2.48	0.47
1:B:382:PHE:O	1:B:385:SER:HB2	2.14	0.47
1:A:362:ARG:HB2	1:A:384:LEU:CB	2.45	0.47
1:A:405:TRP:CZ2	1:A:439:PRO:HG2	2.49	0.47
1:B:351:MET:CE	1:B:364:LEU:HD22	2.44	0.47
1:A:362:ARG:HB2	1:A:384:LEU:HB2	1.97	0.47
1:A:351:MET:HB3	1:A:486:PHE:CG	2.50	0.47
1:B:295:HIS:ND1	1:B:296:PRO:HD2	2.30	0.47
1:B:336:ASN:ND2	1:B:338:VAL:HB	2.29	0.47
1:A:339:VAL:O	1:A:343:MET:HG3	2.16	0.46
1:B:283:PHE:HD2	1:B:284:LEU:HD12	1.80	0.46
1:B:298:LEU:HD11	1:B:354:LEU:HD13	1.95	0.46
1:A:340:LEU:HD23	1:A:343:MET:CE	2.45	0.46
1:B:307:ARG:HH11	1:B:307:ARG:HG2	1.81	0.46
1:A:326:TYR:O	1:A:330:CYS:HB3	2.16	0.46
1:A:337:ALA:O	1:B:496:MET:HG2	2.16	0.46
1:B:318:MET:CG	1:B:370:LEU:HB3	2.43	0.46
1:B:295:HIS:ND1	1:B:296:PRO:CD	2.78	0.46
1:A:245:LYS:O	1:A:246:HIS:CB	2.62	0.46
1:A:386:ARG:NE	1:A:393:TYR:CE1	2.84	0.46
1:B:347:ILE:HG22	1:B:425:PHE:HE1	1.80	0.46
1:A:237:MET:HE3	1:A:314:ILE:HG12	1.99	0.45
1:B:452:LEU:HB3	1:B:478:TRP:HZ3	1.82	0.45
1:A:471:LEU:HD23	1:A:471:LEU:O	2.17	0.45
1:A:336:ASN:HD21	1:A:338:VAL:HG11	1.82	0.45
1:B:238:GLU:HG3	1:B:240:THR:H	1.80	0.45
1:A:403:ILE:HB	1:A:445:LEU:HD22	1.99	0.45
1:B:463:GLY:O	1:B:464:CYS:C	2.55	0.45
1:A:279:GLU:O	1:A:280:VAL:C	2.55	0.45
1:B:239:ARG:HB2	1:B:239:ARG:NH1	2.31	0.45
1:B:359:PHE:O	1:B:418:ILE:HD11	2.15	0.45
1:B:347:ILE:HD11	1:B:377:VAL:HG11	1.98	0.45
1:B:386:ARG:CG	1:B:387:LEU:HD22	2.47	0.45
1:B:266:LEU:C	1:B:266:LEU:HD23	2.37	0.45
1:B:356:LYS:HB2	1:B:356:LYS:HE3	1.79	0.45
1:A:287:ALA:O	1:A:291:LYS:HG3	2.18	0.44
1:B:357:LYS:HB3	1:B:359:PHE:CD1	2.52	0.44
1:A:428:LEU:O	1:A:428:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:318:MET:CB	1:B:370:LEU:HB3	2.48	0.44
1:B:382:PHE:HB3	1:B:385:SER:HB2	1.98	0.44
1:B:410:SER:OG	1:B:416:PHE:HD1	1.98	0.44
1:B:464:CYS:HA	1:B:465:PRO:HD2	1.86	0.44
1:B:274:LYS:HB2	1:B:278:MET:HG3	1.99	0.44
1:A:287:ALA:HB1	1:A:304:VAL:HG11	1.99	0.43
1:B:295:HIS:CG	1:B:296:PRO:HD2	2.53	0.43
1:B:404:LYS:CG	1:B:440:TYR:HD1	2.31	0.43
2:C:107:PHE:CD1	2:C:107:PHE:N	2.86	0.43
1:B:419:LYS:HD3	1:B:419:LYS:HA	1.75	0.43
1:A:447:GLN:NE2	1:A:447:GLN:CA	2.82	0.43
1:B:362:ARG:NE	1:B:416:PHE:HE2	2.10	0.43
1:B:274:LYS:HB3	1:B:274:LYS:HE2	1.44	0.43
1:B:381:ASP:C	1:B:383:GLY:N	2.72	0.43
1:B:273:LEU:HD23	1:B:311:PHE:CB	2.43	0.43
1:B:284:LEU:HD21	1:B:306:THR:HB	1.99	0.43
1:B:349:SER:CA	1:B:490:HIS:CD2	2.98	0.43
1:A:354:LEU:HD12	1:A:354:LEU:HA	1.91	0.43
1:B:241:ASP:OD2	1:B:263:LYS:HG3	2.19	0.43
1:A:230:PRO:HG3	1:A:302:LEU:O	2.19	0.43
1:B:479:ASN:HB3	1:B:482:ASP:OD2	2.19	0.43
1:A:318:MET:HE3	1:A:378:LYS:HD2	2.01	0.42
1:A:393:TYR:O	1:A:415:LYS:HA	2.19	0.42
1:B:387:LEU:CD2	1:B:387:LEU:H	2.11	0.42
1:B:409:GLU:HG2	1:B:410:SER:N	2.35	0.42
1:A:233:ASP:HB3	1:A:236:GLU:HB2	2.00	0.42
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.34	0.42
1:A:345:THR:HG21	1:B:336:ASN:HD22	1.80	0.42
1:B:308:GLU:CD	1:B:308:GLU:N	2.68	0.42
1:A:496:MET:CE	1:B:341:LEU:HD22	2.49	0.42
1:A:336:ASN:CG	1:A:338:VAL:HG12	2.36	0.42
1:B:471:LEU:HD21	1:B:489:ILE:HG12	2.01	0.42
1:B:366:ALA:N	1:B:428:LEU:HD13	2.34	0.42
1:B:439:PRO:O	1:B:440:TYR:C	2.58	0.42
1:A:262:LYS:O	1:A:263:LYS:C	2.58	0.42
1:A:449:TYR:CD2	1:A:449:TYR:C	2.92	0.42
1:A:341:LEU:HD22	1:B:496:MET:CE	2.49	0.42
1:A:237:MET:CE	1:A:242:ILE:HD11	2.49	0.42
1:A:343:MET:O	1:A:347:ILE:HG13	2.20	0.42
1:B:351:MET:HE2	1:B:364:LEU:HD22	2.02	0.42
1:B:376:LEU:HD11	1:B:378:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:ILE:HG12	1:B:388:MET:HG3	2.01	0.42
1:A:417:SER:C	1:A:419:LYS:N	2.72	0.42
1:A:460:ARG:NH1	1:A:460:ARG:HB3	2.32	0.42
1:A:233:ASP:OD1	1:A:234:LYS:N	2.50	0.42
1:A:439:PRO:O	1:A:440:TYR:C	2.57	0.42
1:B:397:ALA:HA	1:B:414:ASN:HD21	1.84	0.42
1:A:406:THR:HG22	1:A:411:LEU:HG	2.02	0.41
1:A:404:LYS:HE2	1:A:445:LEU:HD23	2.00	0.41
1:B:307:ARG:HG2	1:B:307:ARG:NH1	2.35	0.41
1:B:352:GLU:HA	1:B:486:PHE:HB2	2.02	0.41
1:B:234:LYS:CG	1:B:235:TRP:N	2.84	0.41
1:A:375:HIS:HD2	1:B:342:TYR:OH	2.03	0.41
1:B:266:LEU:HD22	1:B:268:VAL:HG13	2.01	0.41
1:B:246:HIS:HE1	1:B:258:GLU:OE2	2.04	0.41
1:B:460:ARG:HE	1:B:466:GLU:HA	1.86	0.41
1:A:322:ASN:HA	1:A:369:CYS:O	2.20	0.41
1:B:370:LEU:HD21	3:B:821:ADP:C5	2.55	0.41
1:A:423:TRP:CE3	1:A:476:TRP:HA	2.56	0.41
1:B:384:LEU:HA	1:B:384:LEU:HD23	1.81	0.41
1:A:471:LEU:HD23	1:A:471:LEU:C	2.40	0.40
1:A:373:GLU:CB	1:B:374:ASN:ND2	2.84	0.40
1:B:397:ALA:HA	1:B:414:ASN:ND2	2.36	0.40
1:A:250:GLY:O	1:A:254:GLY:O	2.33	0.40
1:A:342:TYR:O	1:A:346:GLN:HG3	2.21	0.40
1:B:493:PHE:CE1	1:B:497:PHE:HZ	2.38	0.40
1:A:369:CYS:O	1:A:370:LEU:HD12	2.22	0.40
1:A:395:ALA:N	1:A:414:ASN:O	2.52	0.40
1:B:266:LEU:HD23	1:B:267:THR:C	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:SER:OG	1:A:229:SER:OG[7_555]	2.18	0.02

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	267/287 (93%)	225 (84%)	27 (10%)	15 (6%)	2	13
1	B	261/287 (91%)	213 (82%)	35 (13%)	13 (5%)	2	16
2	C	6/13 (46%)	5 (83%)	1 (17%)	0	100	100
2	D	5/13 (38%)	5 (100%)	0	0	100	100
All	All	539/600 (90%)	448 (83%)	63 (12%)	28 (5%)	2	15

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	275	GLU
1	A	278	MET
1	A	330	CYS
1	A	338	VAL
1	A	362	ARG
1	A	500	SER
1	B	277	THR
1	B	307	ARG
1	B	435	TYR
1	B	448	VAL
1	A	263	LYS
1	A	280	VAL
1	A	332	ARG
1	B	274	LYS
1	B	276	ASP
1	B	309	PRO
1	B	445	LEU
1	A	246	HIS
1	A	387	LEU
1	B	275	GLU
1	A	388	MET

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Mol	Chain	Res	Type
1	B	308	GLU
1	B	499	GLU
1	A	381	ASP
1	B	403	ILE
1	A	402	PRO
1	B	265	SER

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	238/251 (95%)	223 (94%)	15 (6%)	21	56
1	B	233/251 (93%)	217 (93%)	16 (7%)	18	53
2	C	2/10 (20%)	2 (100%)	0	100	100
2	D	3/10 (30%)	3 (100%)	0	100	100
All	All	476/522 (91%)	445 (94%)	31 (6%)	20	55

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	MET
1	A	266	LEU
1	A	272	THR
1	A	279	GLU
1	A	330	CYS
1	A	338	VAL
1	A	354	LEU
1	A	370	LEU
1	A	373	GLU
1	A	374	ASN
1	A	376	LEU
1	A	401	PHE
1	A	444	ASP
1	A	447	GLN
1	A	500	SER

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Mol	Chain	Res	Type
1	B	246	HIS
1	B	272	THR
1	B	273	LEU
1	B	274	LYS
1	B	275	GLU
1	B	276	ASP
1	B	311	PHE
1	B	334	GLU
1	B	373	GLU
1	B	376	LEU
1	B	387	LEU
1	B	438	SER
1	B	444	ASP
1	B	447	GLN
1	B	459	GLU
1	B	495	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	A	331	ASN
1	A	374	ASN
1	A	375	HIS
1	A	447	GLN
1	A	491	GLN
1	B	246	HIS
1	B	297	ASN
1	B	358	ASN
1	B	361	HIS
1	B	374	ASN
1	B	447	GLN
1	B	477	GLN
1	B	490	HIS

5.3.3 RNA (i)

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 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	ADP	A	820	-	25,29,29	1.22	3 (12%)	24,45,45	1.96	2 (8%)
3	ADP	B	821	-	25,29,29	1.23	2 (8%)	24,45,45	2.02	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	A	820	-	-	0/12/32/32	0/3/3/3
3	ADP	B	821	-	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	820	ADP	C8-N7	-2.32	1.30	1.34
3	B	821	ADP	C8-N7	-2.23	1.30	1.34
3	A	820	ADP	O4'-C1'	2.53	1.44	1.41
3	A	820	ADP	PB-O3A	2.89	1.64	1.60
3	B	821	ADP	O4'-C1'	3.61	1.46	1.41

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All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	820	ADP	N3-C2-N1	-8.73	121.25	128.86
3	B	821	ADP	N3-C2-N1	-8.69	121.29	128.86
3	B	821	ADP	C4-C5-N7	-2.36	107.13	109.41
3	A	820	ADP	C4-C5-N7	-2.12	107.36	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	821	ADP	1	0

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(Å²)	Q<0.9
1	A	271/287 (94%)	-0.00	6 (2%)	62	41	39, 68, 133, 181	0
1	B	265/287 (92%)	0.09	8 (3%)	51	27	44, 78, 137, 200	0
2	C	8/13 (61%)	-0.02	0	100	100	75, 94, 124, 133	0
2	D	7/13 (53%)	-0.11	0	100	100	86, 96, 107, 128	0
All	All	551/600 (91%)	0.04	14 (2%)	58	35	39, 75, 137, 200	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	TYR	6.1
1	A	275	GLU	4.4
1	A	278	MET	4.0
1	A	276	ASP	3.9
1	B	277	THR	3.8
1	B	275	GLU	3.8
1	A	229	SER	3.4
1	B	276	ASP	3.3
1	B	273	LEU	2.6
1	B	306	THR	2.6
1	A	287	ALA	2.5
1	B	233	ASP	2.3
1	A	498	GLN	2.0
1	B	239	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	ADP	B	821	27/27	0.90	0.18	-0.73	77,80,96,100	0
3	ADP	A	820	27/27	0.94	0.16	-1.05	74,76,92,95	0

6.5 Other polymers ⓘ

There are no such residues in this entry.