



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:50 PM GMT

PDB ID : 4Q47
Title : Structure of the DrRecQ Catalytic Core in complex with ADP
Authors : Chen, S.C.; Yang, C.S.; Chen, Y.
Deposited on : 2014-04-14
Resolution : 2.90 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

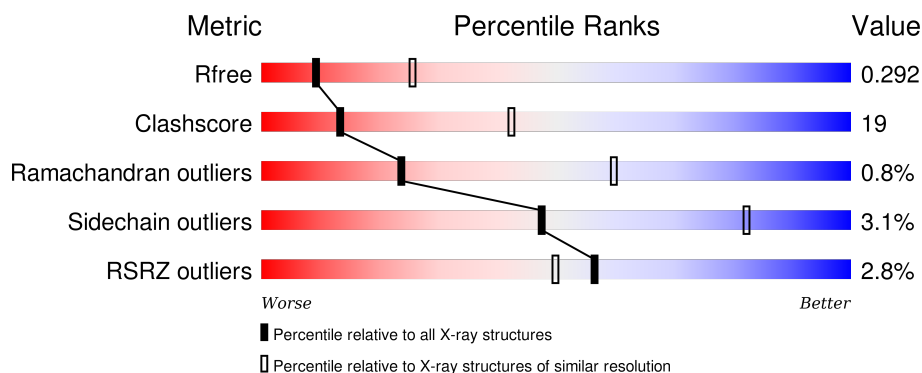
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 $\leq 5\%$. 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	525	<div> <div></div> <div>66%</div> <div>30%</div> <div>..</div> </div>
1	B	525	<div> <div>4%</div> <div>57%</div> <div>33%</div> <div>...</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7999 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 DNA helicase RecQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	0	0	0
			4012	2522	728	746	16			
1	B	502	Total	C	N	O	S	0	0	0
			3931	2469	713	733	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	518	LEU	-	EXPRESSION TAG	UNP Q9RUU2
A	519	GLU	-	EXPRESSION TAG	UNP Q9RUU2
A	520	HIS	-	EXPRESSION TAG	UNP Q9RUU2
A	521	HIS	-	EXPRESSION TAG	UNP Q9RUU2
A	522	HIS	-	EXPRESSION TAG	UNP Q9RUU2
A	523	HIS	-	EXPRESSION TAG	UNP Q9RUU2
A	524	HIS	-	EXPRESSION TAG	UNP Q9RUU2
A	525	HIS	-	EXPRESSION TAG	UNP Q9RUU2
B	518	LEU	-	EXPRESSION TAG	UNP Q9RUU2
B	519	GLU	-	EXPRESSION TAG	UNP Q9RUU2
B	520	HIS	-	EXPRESSION TAG	UNP Q9RUU2
B	521	HIS	-	EXPRESSION TAG	UNP Q9RUU2
B	522	HIS	-	EXPRESSION TAG	UNP Q9RUU2
B	523	HIS	-	EXPRESSION TAG	UNP Q9RUU2
B	524	HIS	-	EXPRESSION TAG	UNP Q9RUU2
B	525	HIS	-	EXPRESSION TAG	UNP Q9RUU2

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



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

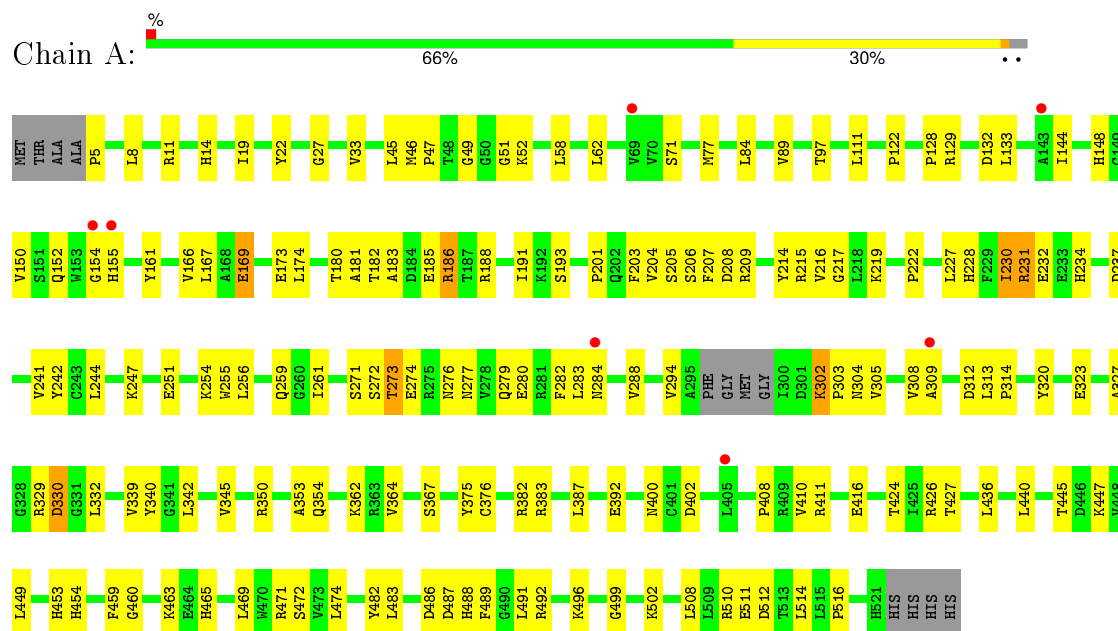
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

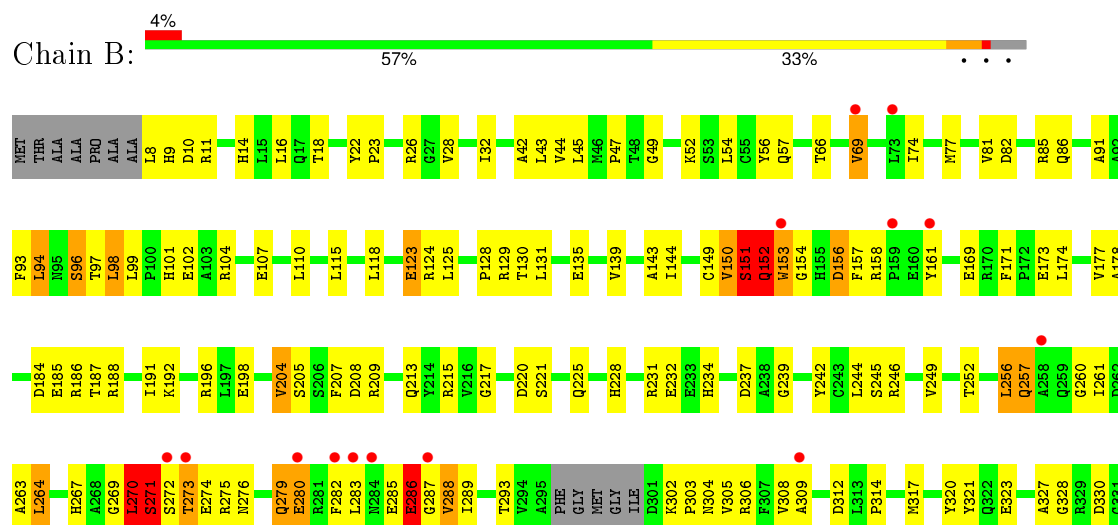
3 Residue-property plots

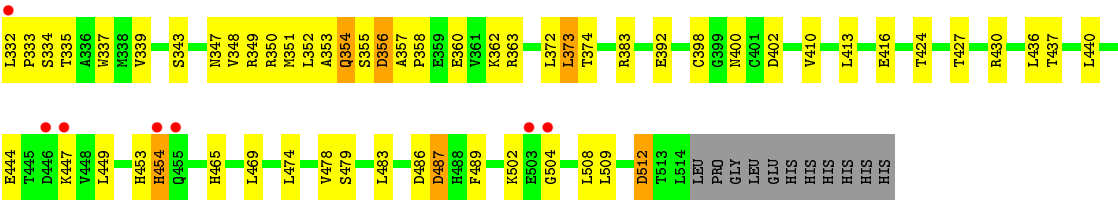
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: DNA helicase RecQ



• Molecule 1: DNA helicase RecQ





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.76Å 95.61Å 183.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.56 – 2.90 27.56 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (27.56-2.90) 96.7 (27.56-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.222 , 0.295 0.223 , 0.292	Depositor DCC
R_{free} test set	1940 reflections (5.93%)	DCC
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 33755 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7999	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, 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	0.53	0/4090	0.78	0/5546
1	B	0.58	1/4005 (0.0%)	0.93	15/5429 (0.3%)
All	All	0.55	1/8095 (0.0%)	0.85	15/10975 (0.1%)

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	4
1	B	0	11
All	All	0	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	152	GLN	CG-CD	-7.10	1.34	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	GLN	N-CA-CB	-10.85	91.08	110.60
1	B	152	GLN	N-CA-C	8.49	133.93	111.00
1	B	94	LEU	CA-CB-CG	7.56	132.68	115.30
1	B	354	GLN	N-CA-C	7.38	130.93	111.00
1	B	288	VAL	CG1-CB-CG2	-6.20	100.98	110.90
1	B	270	LEU	N-CA-CB	-5.90	98.60	110.40
1	B	151	SER	N-CA-CB	-5.69	101.97	110.50
1	B	270	LEU	CA-CB-CG	5.60	128.19	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	354	GLN	CB-CA-C	-5.48	99.44	110.40
1	B	272	SER	C-N-CA	-5.42	108.15	121.70
1	B	280	GLU	CA-CB-CG	-5.36	101.61	113.40
1	B	154	GLY	N-CA-C	5.33	126.42	113.10
1	B	98	LEU	N-CA-C	-5.30	96.70	111.00
1	B	264	LEU	CA-CB-CG	5.17	127.19	115.30
1	B	373	LEU	CB-CG-CD1	-5.17	102.21	111.00

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	ARG	Peptide
1	A	230	ILE	Peptide
1	A	272	SER	Peptide
1	A	329	ARG	Peptide
1	B	150	VAL	Peptide
1	B	151	SER	Peptide
1	B	257	GLN	Peptide
1	B	270	LEU	Peptide
1	B	271	SER	Peptide
1	B	273	THR	Peptide
1	B	286	GLU	Peptide
1	B	302	LYS	Peptide
1	B	454	HIS	Peptide
1	B	486	ASP	Peptide
1	B	487	ASP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4012	0	4014	122	0
1	B	3931	0	3933	179	0
2	A	27	0	12	6	0
2	B	27	0	12	4	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
All	All	7999	0	7971	300	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 19.

All (300) 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:22:TYR:OH	2:A:601:ADP:H2'	1.20	1.29
1:A:22:TYR:OH	2:A:601:ADP:C2'	2.03	1.04
1:A:22:TYR:CZ	2:A:601:ADP:H2'	2.01	0.94
1:B:184:ASP:HB3	1:B:187:THR:HG23	1.52	0.91
1:A:499:GLY:HA2	1:A:502:LYS:HE2	1.58	0.85
1:B:308:VAL:HG23	1:B:327:ALA:HB2	1.58	0.84
1:A:314:PRO:HG2	1:A:320:TYR:HB2	1.59	0.84
1:A:271:SER:HG	1:A:273:THR:HG1	1.26	0.83
1:B:305:VAL:HB	1:B:327:ALA:HA	1.61	0.82
1:B:270:LEU:HD11	1:B:275:ARG:HG2	1.61	0.82
1:A:383:ARG:HH21	1:A:400:ASN:HB3	1.44	0.82
1:A:486:ASP:OD1	1:A:487:ASP:N	2.11	0.81
1:B:276:ASN:HA	1:B:279:GLN:HG3	1.62	0.79
1:B:152:GLN:NE2	1:B:187:THR:HG22	1.97	0.78
1:B:213:GLN:HB3	1:B:335:THR:HG22	1.67	0.76
1:B:256:LEU:HG	1:B:261:ILE:HD11	1.66	0.76
1:B:169:GLU:HG3	1:B:196:ARG:HH12	1.50	0.76
1:A:410:VAL:HG21	1:A:508:LEU:HD13	1.65	0.76
1:B:271:SER:OG	1:B:274:GLU:OE1	2.05	0.75
1:B:502:LYS:HG2	1:B:504:GLY:H	1.49	0.75
1:B:152:GLN:NE2	1:B:153:TRP:O	2.20	0.74
1:A:353:ALA:O	1:A:362:LYS:NZ	2.20	0.74
1:B:152:GLN:CD	1:B:153:TRP:H	1.92	0.73
1:B:152:GLN:OE1	1:B:153:TRP:CE3	2.42	0.72
1:A:247:LYS:NZ	1:A:251:GLU:OE2	2.18	0.72
1:B:512:ASP:N	1:B:512:ASP:OD1	2.23	0.71
1:A:241:VAL:HG22	1:A:309:ALA:HB3	1.73	0.70
1:B:279:GLN:O	1:B:282:PHE:HB3	1.92	0.69
1:A:510:ARG:NH1	1:A:512:ASP:OD2	2.25	0.69
1:A:129:ARG:O	1:A:133:LEU:HB2	1.92	0.69
1:A:375:TYR:O	1:A:382:ARG:NH1	2.26	0.68
1:B:413:LEU:HD13	1:B:509:LEU:HD22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:GLN:CD	1:B:153:TRP:N	2.48	0.67
1:B:257:GLN:NE2	1:B:261:ILE:O	2.27	0.67
1:B:123:GLU:HG2	1:B:124:ARG:N	2.09	0.67
1:B:45:LEU:HD11	1:B:188:ARG:HD3	1.77	0.66
1:B:124:ARG:HG3	1:B:124:ARG:HH11	1.61	0.65
1:B:184:ASP:HB3	1:B:187:THR:CG2	2.25	0.65
1:B:192:LYS:HD2	1:B:198:GLU:HG2	1.77	0.65
1:B:306:ARG:NH2	1:B:330:ASP:OD1	2.31	0.64
1:B:244:LEU:HD13	1:B:312:ASP:HB3	1.78	0.64
1:A:350:ARG:O	1:A:354:GLN:HG3	1.97	0.64
1:B:220:ASP:OD1	1:B:221:SER:N	2.29	0.63
1:A:209:ARG:NH2	1:A:327:ALA:O	2.32	0.63
1:A:427:THR:OG1	1:A:453:HIS:NE2	2.32	0.63
1:B:271:SER:O	1:B:271:SER:OG	2.11	0.62
1:B:208:ASP:OD1	1:B:209:ARG:N	2.32	0.62
1:B:283:LEU:HA	1:B:285:GLU:OE2	1.99	0.62
1:B:152:GLN:OE1	1:B:153:TRP:CD2	2.53	0.62
1:A:487:ASP:OD1	1:A:488:HIS:HA	2.00	0.62
1:A:185:GLU:HA	1:A:188:ARG:NH2	2.15	0.62
1:B:82:ASP:O	1:B:86:GLN:HG3	2.00	0.61
1:A:302:LYS:HE3	1:A:304:ASN:OD1	2.00	0.61
1:A:208:ASP:OD1	1:A:209:ARG:N	2.33	0.61
1:B:263:ALA:HB1	1:B:289:ILE:O	2.01	0.61
1:B:8:LEU:O	1:B:11:ARG:N	2.31	0.61
1:B:267:HIS:O	1:B:270:LEU:HD22	2.01	0.60
1:B:208:ASP:N	1:B:392:GLU:OE2	2.35	0.60
1:B:85:ARG:NE	1:B:91:ALA:O	2.34	0.60
1:B:332:LEU:HB3	1:B:333:PRO:HD2	1.84	0.60
1:A:387:LEU:HB3	1:A:392:GLU:HB3	1.84	0.59
1:B:246:ARG:HG3	1:B:267:HIS:CD2	2.36	0.59
1:A:228:HIS:HA	1:A:231:ARG:HD3	1.84	0.59
1:A:46:MET:O	1:A:181:ALA:HA	2.03	0.59
1:A:47:PRO:HD2	1:A:206:SER:HB2	1.85	0.59
2:B:601:ADP:H3'	2:B:601:ADP:O1A	2.02	0.59
1:A:308:VAL:HG23	1:A:327:ALA:HB2	1.84	0.59
1:B:125:LEU:HA	1:B:130:THR:HG21	1.85	0.59
1:B:317:MET:HG3	1:B:372:LEU:HD13	1.84	0.58
1:B:124:ARG:HG3	1:B:124:ARG:NH1	2.17	0.58
1:A:152:GLN:H	1:A:152:GLN:CD	2.07	0.58
1:A:201:PRO:HB2	1:A:203:PHE:HE1	1.69	0.58
1:B:273:THR:HG23	1:B:276:ASN:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ARG:NH2	1:A:62:LEU:O	2.37	0.57
1:B:54:LEU:HA	1:B:57:GLN:HB2	1.85	0.57
1:A:302:LYS:HG2	1:A:305:VAL:HG23	1.85	0.57
1:A:234:HIS:HB3	1:A:237:ASP:HB2	1.86	0.57
1:B:192:LYS:HB3	1:B:198:GLU:HG3	1.87	0.57
1:A:128:PRO:O	1:A:129:ARG:HB3	2.05	0.57
1:B:104:ARG:HA	1:B:107:GLU:HB2	1.87	0.56
1:B:26:ARG:NH1	1:B:49:GLY:O	2.38	0.56
1:A:313:LEU:HD21	1:A:345:VAL:HG22	1.86	0.56
1:A:155:HIS:HD2	1:A:155:HIS:O	1.87	0.56
1:B:207:PHE:O	1:B:321:TYR:OH	2.13	0.56
1:B:355:SER:N	1:B:356:ASP:HA	2.19	0.56
1:B:410:VAL:HG21	1:B:508:LEU:HD13	1.87	0.56
1:B:288:VAL:O	1:B:289:ILE:HD13	2.06	0.56
1:A:155:HIS:ND1	1:A:182:THR:OG1	2.29	0.55
1:A:486:ASP:HB3	1:A:492:ARG:CZ	2.37	0.55
1:A:242:TYR:CE2	1:A:323:GLU:HB3	2.42	0.55
1:B:96:SER:HB3	1:B:124:ARG:HH12	1.71	0.55
1:A:183:ALA:HB1	1:A:188:ARG:HG3	1.89	0.54
1:A:364:VAL:O	1:A:367:SER:HB3	2.07	0.54
1:A:201:PRO:HB2	1:A:203:PHE:CE1	2.43	0.54
1:B:449:LEU:HD23	1:B:454:HIS:CG	2.43	0.54
1:B:304:ASN:HB2	1:B:330:ASP:OD2	2.07	0.54
1:A:111:LEU:HD21	1:A:133:LEU:HD23	1.88	0.53
1:B:221:SER:O	1:B:225:GLN:HG3	2.08	0.53
1:B:157:PHE:CG	1:B:158:ARG:N	2.76	0.53
1:B:14:HIS:O	1:B:18:THR:OG1	2.17	0.53
1:B:465:HIS:CG	1:B:469:LEU:HD23	2.43	0.53
1:A:340:TYR:HE2	1:A:342:LEU:HD23	1.74	0.53
1:A:148:HIS:ND1	1:A:180:THR:OG1	2.36	0.53
1:B:184:ASP:OD1	1:B:185:GLU:N	2.42	0.53
1:B:314:PRO:HG3	1:B:320:TYR:HB2	1.90	0.53
1:B:427:THR:HG23	1:B:453:HIS:NE2	2.24	0.52
1:B:263:ALA:CB	1:B:289:ILE:HB	2.39	0.52
1:A:52:LYS:HZ2	1:A:180:THR:C	2.13	0.52
1:B:234:HIS:HB3	1:B:237:ASP:HB2	1.91	0.52
1:B:152:GLN:CD	1:B:187:THR:HG22	2.29	0.52
1:A:22:TYR:OH	2:A:601:ADP:C3'	2.57	0.52
1:B:153:TRP:CZ3	1:B:186:ARG:HG3	2.44	0.52
1:B:171:PHE:HD2	1:B:174:LEU:HD12	1.75	0.52
1:B:273:THR:HG23	1:B:276:ASN:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LYS:HB3	1:B:198:GLU:CG	2.40	0.51
1:B:156:ASP:OD1	1:B:157:PHE:N	2.43	0.51
1:A:122:PRO:HG3	1:A:161:TYR:HE1	1.76	0.51
1:B:156:ASP:O	1:B:157:PHE:HB3	2.10	0.51
1:A:383:ARG:NH2	1:A:400:ASN:HB3	2.21	0.51
1:B:151:SER:CA	1:B:152:GLN:HB3	2.39	0.51
1:A:256:LEU:HD22	1:A:261:ILE:HG12	1.93	0.51
1:B:424:THR:HG21	1:B:483:LEU:HD21	1.92	0.51
1:A:5:PRO:HD2	1:A:8:LEU:HB2	1.92	0.51
1:B:239:GLY:HA2	1:B:305:VAL:HG13	1.94	0.50
1:A:330:ASP:OD1	1:A:330:ASP:N	2.44	0.50
1:A:217:GLY:O	1:A:339:VAL:HA	2.11	0.50
1:A:45:LEU:O	1:A:204:VAL:HA	2.12	0.50
1:B:169:GLU:HG3	1:B:196:ARG:NH1	2.24	0.50
1:A:411:ARG:NH2	1:A:511:GLU:OE2	2.39	0.50
1:A:445:THR:HG22	1:A:447:LYS:H	1.77	0.50
1:B:215:ARG:HG2	1:B:402:ASP:HB3	1.93	0.50
1:B:151:SER:OG	1:B:152:GLN:HB3	2.11	0.49
1:B:96:SER:CB	1:B:124:ARG:HH12	2.25	0.49
1:A:227:LEU:O	1:A:231:ARG:HB2	2.11	0.49
1:B:153:TRP:CH2	1:B:186:ARG:NE	2.79	0.49
1:A:204:VAL:HG21	1:A:392:GLU:HA	1.95	0.49
1:B:276:ASN:CA	1:B:279:GLN:HG3	2.39	0.49
1:B:449:LEU:HG	1:B:454:HIS:HB3	1.95	0.49
1:B:360:GLU:HA	1:B:363:ARG:CZ	2.43	0.49
1:A:186:ARG:NH2	1:A:486:ASP:O	2.46	0.49
1:B:52:LYS:HE3	2:B:601:ADP:PB	2.52	0.49
1:B:374:THR:HG21	1:B:479:SER:HB2	1.94	0.49
1:B:52:LYS:HB2	2:B:601:ADP:O2B	2.13	0.49
1:B:173:GLU:HG2	1:B:174:LEU:HG	1.93	0.49
1:A:330:ASP:C	1:A:332:LEU:H	2.16	0.48
1:A:460:GLY:O	1:A:463:LYS:HE3	2.13	0.48
1:A:49:GLY:O	2:A:601:ADP:H5'2	2.13	0.48
1:B:188:ARG:HB3	1:B:192:LYS:NZ	2.29	0.48
1:B:257:GLN:HA	1:B:260:GLY:H	1.79	0.48
1:B:99:LEU:HD12	1:B:102:GLU:H	1.78	0.48
1:A:150:VAL:HG21	1:A:191:ILE:HA	1.96	0.48
1:A:155:HIS:CD2	1:A:155:HIS:O	2.66	0.48
1:B:149:CYS:C	1:B:151:SER:H	2.16	0.48
1:A:215:ARG:HG2	1:A:402:ASP:HB3	1.96	0.48
1:B:151:SER:CB	1:B:152:GLN:HB3	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:GLU:OE2	1:A:465:HIS:NE2	2.46	0.47
1:A:129:ARG:HA	1:A:132:ASP:HB2	1.95	0.47
1:B:280:GLU:HA	1:B:283:LEU:H	1.79	0.47
1:B:22:TYR:OH	2:B:601:ADP:H2'	2.14	0.47
1:B:99:LEU:HD12	1:B:102:GLU:HG2	1.96	0.47
1:A:154:GLY:O	1:A:155:HIS:HB3	2.15	0.47
1:B:416:GLU:OE2	1:B:465:HIS:NE2	2.46	0.47
1:B:508:LEU:O	1:B:509:LEU:HD12	2.14	0.47
1:B:66:THR:OG1	1:B:115:LEU:O	2.13	0.47
1:A:340:TYR:CE1	1:A:376:CYS:HB3	2.49	0.47
1:A:274:GLU:O	1:A:277:ASN:HB3	2.15	0.46
1:A:436:LEU:O	1:A:440:LEU:HD12	2.15	0.46
1:B:263:ALA:O	1:B:264:LEU:HD12	2.14	0.46
1:B:252:THR:O	1:B:256:LEU:HD13	2.15	0.46
1:B:306:ARG:O	1:B:334:SER:OG	2.24	0.46
1:A:483:LEU:HD22	1:A:491:LEU:HB3	1.96	0.46
1:A:302:LYS:HG2	1:A:305:VAL:CG2	2.45	0.46
1:B:99:LEU:CD1	1:B:102:GLU:HG2	2.45	0.46
1:B:81:VAL:HG21	1:B:93:PHE:HB3	1.98	0.46
1:A:282:PHE:HA	1:A:288:VAL:HG11	1.97	0.46
1:A:487:ASP:HB3	1:A:488:HIS:ND1	2.30	0.46
1:B:217:GLY:O	1:B:339:VAL:HA	2.15	0.46
1:A:216:VAL:HB	1:A:382:ARG:NH2	2.31	0.46
1:A:186:ARG:CZ	1:A:486:ASP:O	2.63	0.46
1:B:188:ARG:HB3	1:B:192:LYS:HZ3	1.81	0.46
1:A:313:LEU:HA	1:A:314:PRO:HD3	1.81	0.46
1:B:427:THR:HG23	1:B:453:HIS:HE2	1.80	0.46
1:A:465:HIS:HB3	1:A:469:LEU:HD23	1.97	0.46
1:A:33:VAL:HG21	1:A:58:LEU:HD23	1.98	0.46
1:B:347:ASN:HA	1:B:350:ARG:NH2	2.31	0.46
1:A:273:THR:OG1	1:A:274:GLU:N	2.42	0.46
1:A:45:LEU:HD11	1:A:188:ARG:HD3	1.97	0.46
1:A:271:SER:OG	1:A:273:THR:OG1	2.07	0.45
1:B:270:LEU:HD23	1:B:270:LEU:O	2.16	0.45
1:B:280:GLU:HG2	1:B:283:LEU:HD13	1.97	0.45
1:B:487:ASP:OD1	1:B:487:ASP:N	2.47	0.45
1:B:9:HIS:CD2	1:B:10:ASP:H	2.34	0.45
1:B:449:LEU:HD23	1:B:454:HIS:ND1	2.31	0.45
1:A:256:LEU:O	1:A:261:ILE:HG13	2.17	0.45
1:B:447:LYS:HA	1:B:447:LYS:HD3	1.60	0.45
1:B:128:PRO:O	1:B:129:ARG:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLU:HG3	1:B:196:ARG:HH22	1.81	0.45
1:A:166:VAL:HG13	1:A:167:LEU:HD23	1.98	0.45
1:A:279:GLN:O	1:A:283:LEU:HD13	2.16	0.45
1:A:173:GLU:HG2	1:A:174:LEU:N	2.30	0.45
1:B:487:ASP:HA	1:B:489:PHE:H	1.82	0.45
1:A:445:THR:O	1:A:449:LEU:HG	2.17	0.45
1:B:74:ILE:O	1:B:77:MET:HG2	2.16	0.45
1:B:349:ARG:NH2	1:B:373:LEU:HD22	2.31	0.45
1:A:27:GLY:HA3	1:A:205:SER:OG	2.16	0.45
1:B:353:ALA:C	1:B:354:GLN:HG3	2.37	0.45
1:B:8:LEU:HA	1:B:8:LEU:HD12	1.80	0.44
1:B:28:VAL:HG12	1:B:32:ILE:HG13	1.98	0.44
1:B:150:VAL:CG2	1:B:151:SER:HB2	2.48	0.44
1:B:305:VAL:H	1:B:328:GLY:H	1.64	0.44
1:A:228:HIS:NE2	1:A:232:GLU:OE2	2.49	0.44
1:B:356:ASP:HB2	1:B:362:LYS:CE	2.47	0.44
1:B:43:LEU:HD12	1:B:44:VAL:H	1.82	0.44
1:A:454:HIS:HA	1:A:459:PHE:CD1	2.52	0.44
1:A:276:ASN:O	1:A:280:GLU:HG2	2.18	0.44
1:A:186:ARG:NH1	1:A:487:ASP:OD2	2.51	0.44
1:A:330:ASP:C	1:A:332:LEU:N	2.71	0.44
1:B:42:ALA:O	1:B:177:VAL:HA	2.18	0.44
1:A:14:HIS:O	1:A:14:HIS:ND1	2.51	0.44
1:A:19:ILE:HD11	1:B:246:ARG:NH2	2.33	0.44
1:A:207:PHE:HB2	1:A:392:GLU:OE1	2.18	0.44
1:B:263:ALA:HB2	1:B:289:ILE:HB	1.99	0.44
1:B:97:THR:O	1:B:97:THR:OG1	2.34	0.44
1:B:231:ARG:HD3	1:B:232:GLU:HG3	2.00	0.44
1:A:244:LEU:HD12	1:A:312:ASP:HB3	1.99	0.44
1:B:131:LEU:O	1:B:135:GLU:HG2	2.18	0.44
1:B:357:ALA:HB1	1:B:358:PRO:HD2	1.99	0.44
1:A:465:HIS:CG	1:A:469:LEU:HD23	2.53	0.43
1:B:352:LEU:HA	1:B:354:GLN:HG2	1.99	0.43
1:B:249:VAL:HG21	1:B:293:THR:HG22	2.00	0.43
1:B:129:ARG:O	1:B:129:ARG:HD2	2.19	0.43
1:B:437:THR:HA	1:B:440:LEU:HD12	2.01	0.43
1:B:228:HIS:NE2	1:B:232:GLU:OE1	2.50	0.43
1:A:254:LYS:HB3	1:A:254:LYS:HE3	1.54	0.43
1:A:256:LEU:HB3	1:A:261:ILE:HD11	2.00	0.43
1:B:444:GLU:HB3	1:B:449:LEU:HD11	2.01	0.43
1:B:99:LEU:HD13	1:B:101:HIS:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ALA:HA	1:B:337:TRP:O	2.19	0.43
1:B:273:THR:CG2	1:B:276:ASN:HB2	2.48	0.43
1:B:47:PRO:HG3	1:B:207:PHE:HA	2.00	0.43
1:B:144:ILE:HD12	1:B:144:ILE:N	2.33	0.43
1:A:129:ARG:HG2	1:A:129:ARG:O	2.19	0.43
1:B:56:TYR:CE1	1:B:57:GLN:HG3	2.54	0.43
1:B:43:LEU:HD13	1:B:178:ALA:HB3	2.00	0.43
1:B:436:LEU:O	1:B:440:LEU:HD12	2.19	0.43
1:A:51:GLY:HA2	2:A:601:ADP:H5'1	2.00	0.42
1:B:69:VAL:HA	1:B:143:ALA:O	2.20	0.42
1:B:152:GLN:HE22	1:B:153:TRP:HB2	1.83	0.42
1:A:71:SER:H	1:A:77:MET:HE1	1.84	0.42
1:B:213:GLN:HG3	1:B:400:ASN:O	2.19	0.42
1:A:424:THR:HA	1:A:427:THR:HG22	2.01	0.42
1:B:246:ARG:CZ	1:B:269:GLY:HA3	2.48	0.42
1:B:286:GLU:HG2	1:B:287:GLY:C	2.39	0.42
1:A:8:LEU:HD12	1:A:8:LEU:HA	1.87	0.42
1:A:19:ILE:HD11	1:B:246:ARG:CZ	2.49	0.42
1:B:355:SER:HB2	1:B:356:ASP:HA	2.02	0.42
1:B:383:ARG:HD2	1:B:398:CYS:CB	2.50	0.42
1:A:471:ARG:HA	1:A:471:ARG:HD2	1.73	0.42
1:B:282:PHE:HA	1:B:288:VAL:HG21	2.02	0.42
1:A:144:ILE:HD12	1:A:144:ILE:N	2.35	0.42
1:A:474:LEU:HA	1:A:474:LEU:HD23	1.78	0.42
1:B:98:LEU:HG	1:B:102:GLU:HG3	2.01	0.42
1:B:74:ILE:HG12	1:B:77:MET:HE1	2.01	0.42
1:B:110:LEU:HD22	1:B:118:LEU:HD22	2.01	0.42
1:A:84:LEU:HD22	1:A:89:VAL:HG11	2.01	0.42
1:B:267:HIS:O	1:B:270:LEU:HB3	2.20	0.41
1:B:306:ARG:HA	1:B:334:SER:HB2	2.01	0.41
1:A:411:ARG:HD2	1:A:514:LEU:HD13	2.02	0.41
1:B:245:SER:O	1:B:249:VAL:HG23	2.20	0.41
1:A:424:THR:O	1:A:427:THR:HG22	2.19	0.41
1:B:171:PHE:CD2	1:B:174:LEU:HD12	2.56	0.41
1:B:173:GLU:HG2	1:B:174:LEU:N	2.34	0.41
1:A:280:GLU:HB2	1:A:284:ASN:OD1	2.20	0.41
1:B:474:LEU:O	1:B:478:VAL:HG23	2.20	0.41
1:A:219:LYS:HB3	1:A:222:PRO:HG3	2.02	0.41
1:A:487:ASP:HA	1:A:489:PHE:N	2.35	0.41
1:B:502:LYS:HG2	1:B:504:GLY:N	2.26	0.41
1:B:205:SER:HA	1:B:392:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:TYR:HA	1:B:23:PRO:HD3	1.84	0.41
1:B:487:ASP:C	1:B:489:PHE:H	2.24	0.41
1:A:427:THR:HG1	1:A:453:HIS:CD2	2.38	0.41
1:B:282:PHE:O	1:B:288:VAL:HG21	2.21	0.41
1:B:123:GLU:CG	1:B:124:ARG:N	2.81	0.41
1:B:242:TYR:CE2	1:B:323:GLU:HB3	2.55	0.41
1:A:204:VAL:HG21	1:A:392:GLU:CA	2.51	0.41
1:B:16:LEU:HG	1:B:22:TYR:HB2	2.02	0.41
1:B:321:TYR:CD1	1:B:321:TYR:C	2.94	0.41
1:B:270:LEU:HD21	1:B:275:ARG:HD3	2.01	0.41
1:B:149:CYS:HB2	1:B:161:TYR:CE2	2.56	0.40
1:A:214:TYR:HE1	1:A:383:ARG:NH1	2.19	0.40
1:B:45:LEU:HD12	1:B:204:VAL:CG1	2.50	0.40
1:B:98:LEU:HA	1:B:98:LEU:HD12	1.91	0.40
1:A:255:TRP:O	1:A:259:GLN:HG2	2.21	0.40
1:B:139:VAL:HG11	1:B:174:LEU:HD13	2.04	0.40
1:B:43:LEU:HD12	1:B:44:VAL:N	2.36	0.40
1:A:169:GLU:H	1:A:169:GLU:HG2	1.75	0.40
1:A:408:PRO:HB3	1:A:510:ARG:NH2	2.36	0.40
1:B:150:VAL:HG21	1:B:191:ILE:HA	2.04	0.40
1:B:348:VAL:O	1:B:352:LEU:HB2	2.22	0.40
1:A:482:TYR:CZ	1:A:496:LYS:HE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	509/525 (97%)	486 (96%)	18 (4%)	5 (1%)	19	54
1	B	498/525 (95%)	468 (94%)	27 (5%)	3 (1%)	30	67
All	All	1007/1050 (96%)	954 (95%)	45 (4%)	8 (1%)	24	60

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	156	ASP
1	B	271	SER
1	A	230	ILE
1	A	231	ARG
1	A	273	THR
1	A	302	LYS
1	B	303	PRO
1	A	303	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	428/436 (98%)	420 (98%)	8 (2%)	65	89
1	B	420/436 (96%)	402 (96%)	18 (4%)	35	71
All	All	848/872 (97%)	822 (97%)	26 (3%)	47	82

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	THR
1	A	169	GLU
1	A	193	SER
1	A	294	VAL
1	A	330	ASP
1	A	426	ARG
1	A	472	SER
1	A	516	PRO
1	B	69	VAL
1	B	94	LEU
1	B	96	SER
1	B	123	GLU
1	B	151	SER
1	B	152	GLN
1	B	153	TRP

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Mol	Chain	Res	Type
1	B	204	VAL
1	B	256	LEU
1	B	270	LEU
1	B	271	SER
1	B	279	GLN
1	B	286	GLU
1	B	343	SER
1	B	351	MET
1	B	356	ASP
1	B	430	ARG
1	B	512	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	435	HIS
1	B	267	HIS
1	B	276	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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
2	ADP	A	601	-	22,29,29	2.09	7 (31%)	27,45,45	2.01	8 (29%)
2	ADP	B	601	-	22,29,29	2.13	7 (31%)	27,45,45	2.26	11 (40%)

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	601	-	-	0/12/32/32	0/3/3/3
2	ADP	B	601	-	-	0/12/32/32	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	O4'-C4'	-4.10	1.35	1.45
2	A	601	ADP	O4'-C1'	-2.65	1.37	1.41
2	A	601	ADP	O5'-C5'	-2.46	1.34	1.44
2	B	601	ADP	O3'-C3'	-2.45	1.37	1.43
2	B	601	ADP	O5'-C5'	-2.42	1.34	1.44
2	A	601	ADP	O3'-C3'	-2.16	1.37	1.43
2	B	601	ADP	O4'-C1'	-2.13	1.38	1.41
2	A	601	ADP	C4-N3	2.24	1.38	1.35
2	B	601	ADP	C2-N3	2.49	1.36	1.32
2	B	601	ADP	C2-N1	2.53	1.38	1.33
2	A	601	ADP	C2-N1	3.04	1.39	1.33
2	A	601	ADP	O4'-C4'	3.39	1.52	1.45
2	A	601	ADP	PA-O5'	6.07	1.86	1.59
2	B	601	ADP	PA-O5'	6.26	1.87	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	PA-O3A-PB	-4.13	118.82	132.67
2	A	601	ADP	C4'-O4'-C1'	-3.71	105.64	109.72
2	A	601	ADP	O5'-PA-O1A	-3.58	95.72	109.62
2	A	601	ADP	PA-O3A-PB	-3.54	120.80	132.67
2	B	601	ADP	O5'-PA-O1A	-3.36	96.56	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	C5'-C4'-C3'	-2.59	104.91	115.21
2	B	601	ADP	C4'-O4'-C1'	-2.52	106.95	109.72
2	B	601	ADP	O2A-PA-O5'	-2.13	97.73	108.46
2	A	601	ADP	O2A-PA-O5'	-2.07	98.00	108.46
2	B	601	ADP	O3B-PB-O2B	2.00	115.01	107.38
2	B	601	ADP	O4'-C4'-C3'	2.04	109.26	105.15
2	A	601	ADP	O3B-PB-O2B	2.08	115.31	107.38
2	A	601	ADP	O2A-PA-O3A	2.64	117.05	105.09
2	B	601	ADP	O2A-PA-O3A	2.73	117.47	105.09
2	B	601	ADP	O3'-C3'-C4'	2.83	119.53	111.05
2	A	601	ADP	O3'-C3'-C4'	3.32	121.00	111.05
2	B	601	ADP	C2'-C1'-N9	3.96	120.34	114.29
2	A	601	ADP	O4'-C1'-N9	4.85	118.26	108.10
2	B	601	ADP	O4'-C1'-N9	6.00	120.65	108.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ADP	6	0
2	B	601	ADP	4	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(Å ²)	Q<0.9
1	A	513/525 (97%)	-0.06	7 (1%) 78 76	40, 63, 87, 99	0
1	B	502/525 (95%)	0.16	21 (4%) 40 33	42, 74, 116, 149	0
All	All	1015/1050 (96%)	0.05	28 (2%) 56 50	40, 67, 105, 149	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	454	HIS	3.6
1	B	153	TRP	3.3
1	A	155	HIS	3.3
1	B	161	TYR	3.1
1	B	283	LEU	2.8
1	B	503	GLU	2.8
1	B	282	PHE	2.7
1	B	287	GLY	2.7
1	A	69	VAL	2.7
1	B	159	PRO	2.6
1	B	332	LEU	2.5
1	B	272	SER	2.4
1	B	280	GLU	2.4
1	A	143	ALA	2.4
1	B	504	GLY	2.3
1	B	455	GLN	2.3
1	B	258	ALA	2.3
1	B	447	LYS	2.2
1	A	284	ASN	2.2
1	B	284	ASN	2.2
1	A	309	ALA	2.2
1	A	154	GLY	2.2
1	B	273	THR	2.2
1	B	446	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	73	LEU	2.1
1	B	69	VAL	2.0
1	A	405	LEU	2.0
1	B	309	ALA	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 carbohydrates 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. 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(\AA^2)	Q<0.9
3	ZN	A	602	1/1	0.99	0.14	-0.47	63,63,63,63	0
2	ADP	A	601	27/27	0.93	0.17	-0.53	63,75,90,95	0
2	ADP	B	601	27/27	0.96	0.14	-0.97	52,67,75,82	0
3	ZN	B	602	1/1	0.99	0.11	-1.17	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.