



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 03:45 AM GMT

PDB ID : 1HO5
Title : 5'-NUCLEOTIDASE (E. COLI) IN COMPLEX WITH ADENOSINE AND PHOSPHATE
Authors : Knoefel, T.; Straeter, N.
Deposited on : 2000-12-08
Resolution : 2.10 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

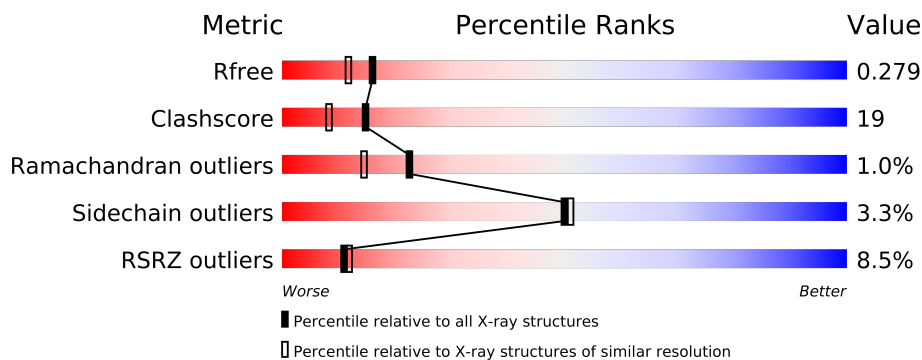
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.10 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}	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	525	
1	B	525	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8607 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

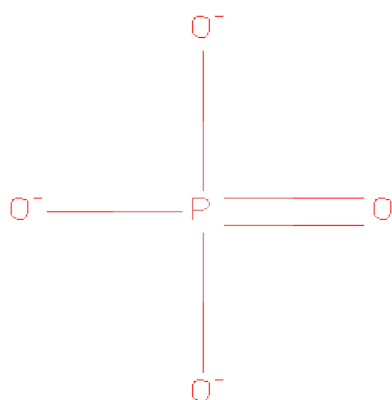
- Molecule 1 is a protein called 5'-NUCLEOTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	525	Total	C	N	O	S	0	0	0
			4100	2590	703	790	17			
1	B	525	Total	C	N	O	S	0	0	0
			4100	2590	703	790	17			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

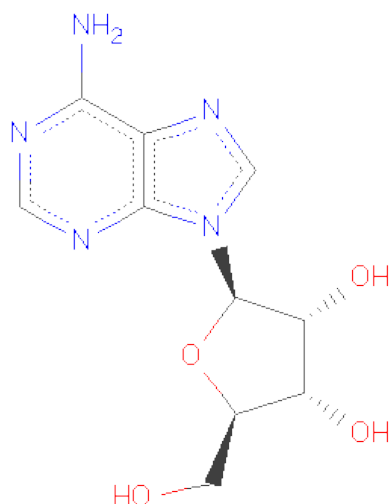
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is ADENOSINE (three-letter code: ADN) (formula: C₁₀H₁₃N₅O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			19	10	5	4		
4	B	1	Total	C	N	O	0	0
			19	10	5	4		

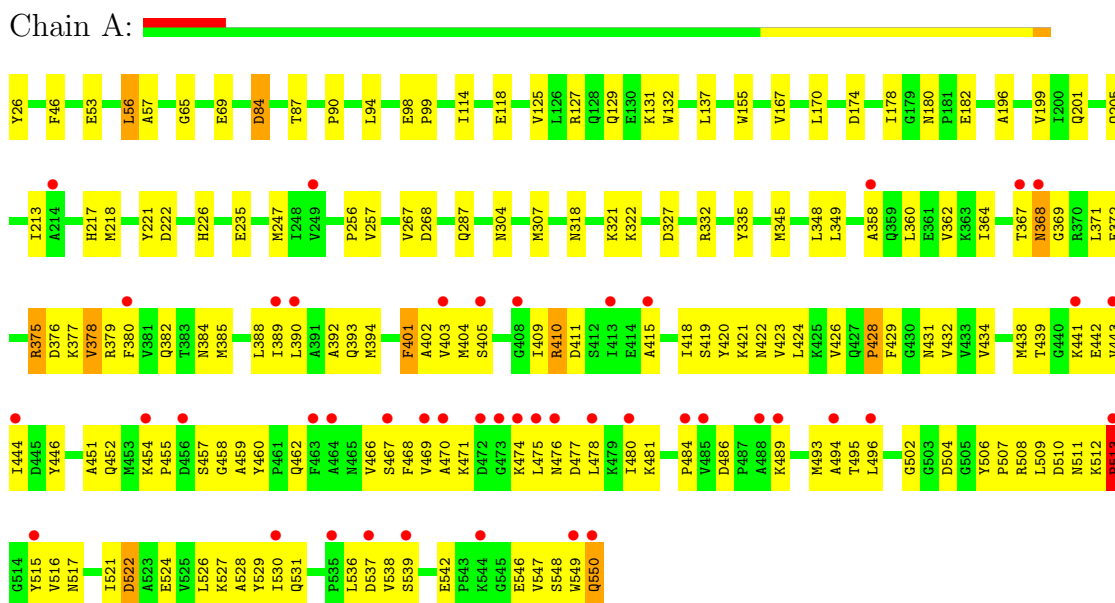
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	238	Total	O	0	0
			238	238		
5	B	117	Total	O	0	0
			117	117		

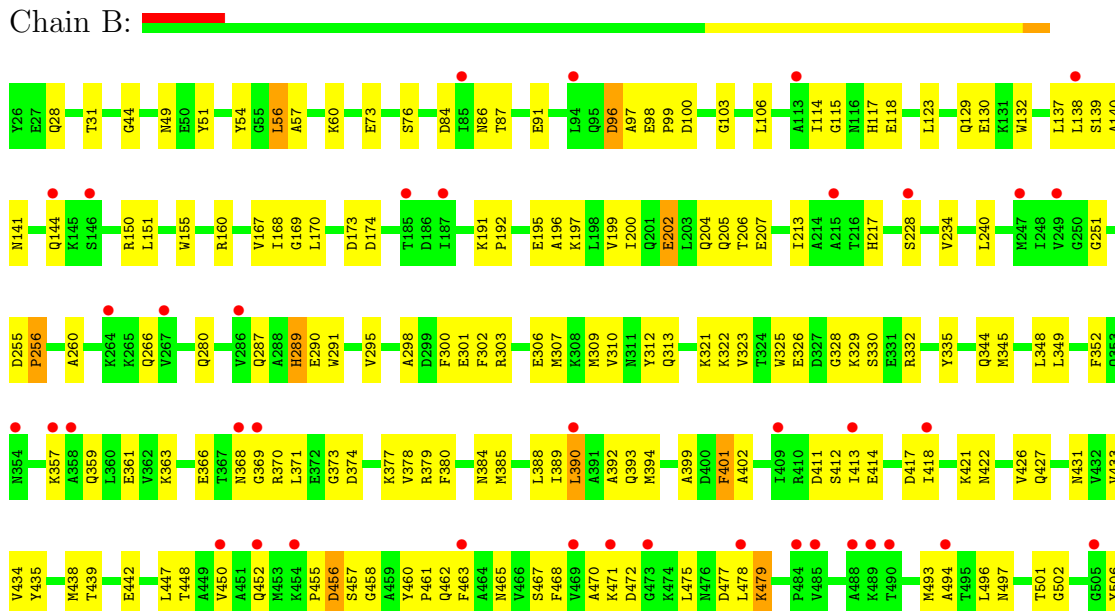
3 Residue-property plots

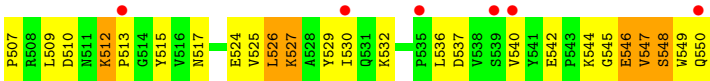
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: 5'-NUCLEOTIDASE



• Molecule 1: 5'-NUCLEOTIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.90Å 75.70Å 221.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.56 – 2.10 29.56 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.5 (29.56-2.10) 98.9 (29.56-1.99)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.238 , 0.279 0.238 , 0.279	Depositor DCC
R_{free} test set	2116 reflections (3.06%)	DCC
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 81150 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8607	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ADN, PO4, MN

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	0.69	0/4188	0.79	1/5666 (0.0%)
1	B	0.53	0/4188	0.73	2/5666 (0.0%)
All	All	0.62	0/8376	0.76	3/11332 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	PRO	N-CA-C	-6.45	95.33	112.10
1	A	256	PRO	N-CA-C	-6.33	95.65	112.10
1	B	295	VAL	N-CA-C	-5.60	95.88	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4100	0	4019	150	0
1	B	4100	0	4019	163	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	5	0	0	0	0
3	B	5	0	0	1	0
4	A	19	0	13	1	0
4	B	19	0	13	1	0
5	A	238	0	0	2	0
5	B	117	0	0	1	0
All	All	8607	0	8064	313	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (313) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:218:MET:CE	1:A:218:MET:SD	2.02	1.47
1:A:444:ILE:HG12	1:A:478:LEU:HD23	1.46	0.97
1:A:345:MET:HE1	1:A:348:LEU:HD23	1.48	0.96
1:A:368:ASN:HD22	1:A:537:ASP:HA	1.36	0.89
1:A:521:ILE:HB	1:A:524:GLU:HG3	1.58	0.85
1:B:206:THR:HG23	1:B:207:GLU:HG2	1.59	0.83
1:B:114:ILE:HG12	1:B:138:LEU:O	1.80	0.82
1:B:345:MET:CE	1:B:348:LEU:HD23	2.09	0.82
1:B:345:MET:HE2	1:B:349:LEU:HG	1.59	0.82
1:B:477:ASP:O	1:B:479:LYS:HD2	1.79	0.82
1:B:234:VAL:HG13	1:B:280:GLN:HG3	1.61	0.81
1:A:512:LYS:HB3	1:A:513:PRO:HD2	1.62	0.80
1:B:345:MET:HE1	1:B:348:LEU:HD23	1.63	0.80
1:A:345:MET:HE2	1:A:349:LEU:HD21	1.63	0.80
1:B:363:LYS:NZ	1:B:366:GLU:HB3	1.95	0.80
1:B:363:LYS:HZ1	1:B:366:GLU:HB3	1.48	0.79
1:A:379:ARG:HD2	1:A:458:GLY:HA2	1.64	0.79
1:A:423:VAL:HG13	1:A:526:LEU:HD23	1.64	0.79
1:B:197:LYS:HG2	1:B:240:LEU:HD23	1.65	0.79
1:B:374:ASP:HB2	1:B:377:LYS:HD3	1.65	0.78
1:B:202:GLU:O	1:B:206:THR:HG22	1.85	0.76
1:B:357:LYS:HE3	1:B:361:GLU:OE2	1.86	0.76
1:B:144:GLN:HB2	1:B:151:LEU:HD21	1.67	0.75
1:A:434:VAL:HG12	1:A:517:ASN:HA	1.70	0.73
1:A:451:ALA:HB1	1:A:549:TRP:HE1	1.53	0.73
1:A:114:ILE:HD11	1:A:137:LEU:HB3	1.70	0.72
1:A:322:LYS:HE2	1:A:332:ARG:NH1	2.05	0.71
1:B:455:PRO:O	1:B:456:ASP:HB3	1.89	0.71
1:A:401:PHE:CZ	1:A:493:MET:HB2	2.26	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:363:LYS:HZ3	1:B:417:ASP:CG	1.95	0.70
1:B:303:ARG:O	1:B:306:GLU:HG2	1.92	0.70
1:A:345:MET:HE3	1:A:349:LEU:HG	1.74	0.69
1:B:530:ILE:HD12	1:B:536:LEU:HD11	1.73	0.69
1:A:46:PHE:HA	1:A:56:LEU:HD22	1.76	0.68
1:B:31:THR:OG1	1:B:303:ARG:HD2	1.93	0.68
1:A:467:SER:HB3	1:A:546:GLU:HB2	1.76	0.67
1:B:141:ASN:ND2	1:B:192:PRO:HG3	2.10	0.67
1:A:345:MET:CE	1:A:349:LEU:HG	2.25	0.67
1:A:410:ARG:HG3	1:A:428:PRO:CD	2.25	0.66
1:A:411:ASP:O	1:A:426:VAL:HG22	1.95	0.66
1:A:345:MET:HE2	1:A:349:LEU:CD2	2.25	0.66
1:B:392:ALA:HA	1:B:529:TYR:CD1	2.30	0.66
1:A:444:ILE:HG12	1:A:478:LEU:CD2	2.22	0.66
1:B:130:GLU:HG2	1:B:137:LEU:HD22	1.77	0.65
1:A:180:ASN:HD21	1:A:182:GLU:CG	2.09	0.65
1:A:507:PRO:O	1:A:509:LEU:HD13	1.97	0.65
1:A:404:MET:SD	1:A:409:ILE:HD11	2.37	0.65
1:B:547:VAL:O	1:B:548:SER:HB3	1.97	0.64
1:B:114:ILE:CD1	1:B:137:LEU:HB3	2.28	0.64
1:B:57:ALA:HA	1:B:345:MET:HG2	1.80	0.64
1:A:180:ASN:ND2	1:A:182:GLU:HG2	2.12	0.64
1:B:98:GLU:N	1:B:99:PRO:HD2	2.13	0.64
1:A:127:ARG:O	1:A:131:LYS:HG3	1.98	0.63
1:A:367:THR:HA	1:A:536:LEU:HB2	1.80	0.63
1:A:438:MET:HB2	1:A:442:GLU:HB2	1.81	0.63
1:A:364:ILE:HG12	1:A:418:ILE:O	1.99	0.62
1:A:403:VAL:HG23	1:A:462:GLN:O	1.98	0.62
1:A:379:ARG:HD2	1:A:458:GLY:CA	2.30	0.62
1:A:452:GLN:OE1	1:A:452:GLN:HA	2.00	0.62
1:A:431:ASN:HB2	1:A:522:ASP:OD2	2.00	0.62
1:A:368:ASN:ND2	1:A:537:ASP:HA	2.13	0.61
1:B:370:ARG:HG3	1:B:414:GLU:HA	1.81	0.61
1:A:480:ILE:O	1:A:481:LYS:HB2	2.00	0.61
1:A:431:ASN:OD1	4:A:1604:ADN:H2	2.00	0.61
1:A:468:PHE:CZ	1:A:547:VAL:HG13	2.36	0.60
1:A:527:LYS:O	1:A:530:ILE:HG12	2.02	0.60
1:B:300:PHE:HB3	1:B:307:MET:HE2	1.82	0.60
1:A:345:MET:HE2	1:A:349:LEU:CG	2.32	0.60
1:B:389:ILE:HG12	1:B:526:LEU:HD21	1.83	0.60
1:A:510:ASP:HA	1:A:515:TYR:CD2	2.35	0.60
1:B:345:MET:HE3	1:B:348:LEU:HD23	1.82	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:403:VAL:HA	1:A:462:GLN:O	2.02	0.59
1:A:380:PHE:HA	1:A:455:PRO:HB3	1.84	0.59
1:A:257:VAL:HG23	1:A:287:GLN:HB3	1.85	0.59
1:B:114:ILE:HD11	1:B:137:LEU:HB3	1.85	0.59
1:B:402:ALA:HB2	1:B:494:ALA:HB3	1.85	0.58
1:A:364:ILE:CD1	1:A:530:ILE:HD11	2.33	0.58
1:B:114:ILE:CG1	1:B:139:SER:HB2	2.34	0.58
1:B:467:SER:OG	1:B:479:LYS:HG2	2.04	0.58
1:B:379:ARG:HD2	1:B:458:GLY:HA2	1.85	0.58
1:B:545:GLY:O	1:B:547:VAL:O	2.21	0.57
1:B:388:LEU:HD21	1:B:530:ILE:HD11	1.86	0.57
1:B:388:LEU:O	1:B:388:LEU:HD23	2.04	0.57
1:B:60:LYS:HE2	1:B:106:LEU:HG	1.87	0.57
1:B:371:LEU:HA	1:B:384:ASN:HD21	1.69	0.57
1:B:200:ILE:HD12	1:B:240:LEU:HD22	1.87	0.56
1:B:526:LEU:O	1:B:530:ILE:HG12	2.04	0.56
1:B:450:VAL:O	1:B:461:PRO:HG2	2.04	0.56
1:B:28:GLN:HG3	5:B:2712:HOH:O	2.04	0.56
1:B:363:LYS:NZ	1:B:417:ASP:HA	2.20	0.56
1:B:300:PHE:HB3	1:B:307:MET:CE	2.34	0.56
1:B:371:LEU:HA	1:B:384:ASN:ND2	2.21	0.56
1:B:439:THR:OG1	1:B:442:GLU:HG3	2.05	0.56
1:B:173:ASP:OD2	1:B:191:LYS:HD3	2.05	0.56
1:B:385:MET:O	1:B:389:ILE:HG13	2.05	0.56
1:A:382:GLN:HA	1:A:462:GLN:HE22	1.70	0.56
1:B:433:VAL:HG21	1:B:525:VAL:HG21	1.86	0.56
1:A:495:THR:HG23	1:A:496:LEU:N	2.21	0.56
1:B:496:LEU:HD22	1:B:496:LEU:N	2.21	0.56
1:A:376:ASP:OD1	1:A:377:LYS:HG2	2.06	0.55
1:A:379:ARG:CD	1:A:458:GLY:HA2	2.35	0.55
1:A:98:GLU:HG3	1:A:132:TRP:CE2	2.42	0.55
1:A:454:LYS:HB3	1:A:455:PRO:CD	2.37	0.55
1:A:471:LYS:HE2	1:A:550:GLN:HE21	1.70	0.54
1:B:401:PHE:CE2	1:B:493:MET:HE3	2.41	0.54
1:B:373:GLY:HA3	1:B:411:ASP:O	2.08	0.54
1:B:345:MET:CE	1:B:349:LEU:HG	2.35	0.54
1:B:363:LYS:HZ2	1:B:417:ASP:HA	1.72	0.54
1:A:180:ASN:ND2	1:A:182:GLU:CG	2.70	0.54
1:B:447:LEU:HD21	1:B:493:MET:HE3	1.90	0.53
1:A:201:GLN:HG2	1:A:205:GLN:NE2	2.23	0.53
1:B:388:LEU:HD22	1:B:526:LEU:HD11	1.90	0.53
1:B:427:GLN:NE2	1:B:526:LEU:HD23	2.24	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:410:ARG:HD2	1:A:429:PHE:CE2	2.44	0.53
1:A:364:ILE:HD12	1:A:530:ILE:HD11	1.91	0.53
1:B:390:LEU:O	1:B:394:MET:HB2	2.07	0.53
1:A:459:ALA:CB	1:A:504:ASP:HB3	2.38	0.53
1:A:548:SER:O	1:A:549:TRP:HB2	2.09	0.53
1:B:51:TYR:HB3	1:B:332:ARG:HD2	1.90	0.53
1:B:115:GLY:O	1:B:118:GLU:HB2	2.09	0.52
1:B:502:GLY:HA2	1:B:506:TYR:O	2.08	0.52
1:B:98:GLU:HG3	1:B:132:TRP:CE2	2.45	0.52
1:B:298:ALA:HA	1:B:309:MET:HE1	1.91	0.52
1:A:410:ARG:HA	1:A:410:ARG:HE	1.74	0.52
1:B:329:LYS:HG2	1:B:330:SER:N	2.25	0.52
1:B:76:SER:HB3	1:B:160:ARG:HD2	1.92	0.52
1:A:470:ALA:HB3	1:A:549:TRP:HA	1.92	0.52
1:A:98:GLU:N	1:A:99:PRO:HD2	2.25	0.52
1:A:345:MET:CE	1:A:349:LEU:CG	2.88	0.51
1:A:486:ASP:OD2	1:A:489:LYS:HG2	2.10	0.51
1:B:371:LEU:HD12	1:B:413:ILE:HB	1.92	0.51
1:B:461:PRO:HB2	1:B:463:PHE:CE1	2.45	0.51
1:B:290:GLU:HG3	1:B:291:TRP:CG	2.44	0.51
1:A:549:TRP:O	1:A:550:GLN:HB3	2.09	0.51
1:A:368:ASN:HB2	1:A:538:VAL:H	1.75	0.51
1:B:393:GLN:HE22	1:B:496:LEU:HD21	1.76	0.51
1:B:325:TRP:O	1:B:328:GLY:N	2.41	0.51
1:A:401:PHE:CE1	1:A:493:MET:HB2	2.46	0.51
1:A:439:THR:OG1	1:A:442:GLU:HG3	2.11	0.51
1:B:379:ARG:CD	1:B:458:GLY:HA2	2.40	0.51
1:B:413:ILE:HG21	1:B:418:ILE:HG12	1.93	0.51
1:A:174:ASP:O	1:A:178:ILE:HG12	2.11	0.51
1:B:542:GLU:O	1:B:544:LYS:HG3	2.11	0.51
1:A:438:MET:HG3	1:A:443:VAL:CG2	2.42	0.50
1:A:546:GLU:CD	1:A:546:GLU:H	2.14	0.50
1:B:332:ARG:HH11	1:B:332:ARG:HG2	1.76	0.50
1:B:298:ALA:CA	1:B:309:MET:HE1	2.41	0.50
1:A:394:MET:HG3	1:A:402:ALA:HB2	1.93	0.50
1:B:115:GLY:N	1:B:118:GLU:OE1	2.45	0.50
1:B:529:TYR:HA	1:B:532:LYS:HE2	1.92	0.50
1:B:390:LEU:HD21	1:B:462:GLN:O	2.12	0.50
1:B:256:PRO:HD3	1:B:289:HIS:CG	2.45	0.50
1:A:392:ALA:HA	1:A:529:TYR:CD1	2.47	0.50
1:A:477:ASP:O	1:A:477:ASP:CG	2.50	0.49
1:A:432:VAL:HG11	1:A:517:ASN:OD1	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:140:ALA:C	1:B:195:GLU:HG2	2.32	0.49
1:A:372:GLU:CD	1:A:377:LYS:HG3	2.33	0.49
1:B:323:VAL:O	1:B:330:SER:HA	2.12	0.49
1:A:371:LEU:HD13	1:A:388:LEU:CD2	2.43	0.49
1:B:388:LEU:HD23	1:B:388:LEU:C	2.33	0.49
1:A:65:GLY:O	1:A:69:GLU:HG3	2.12	0.49
1:A:539:SER:HA	1:A:542:GLU:OE2	2.12	0.49
1:A:502:GLY:HA2	1:A:506:TYR:O	2.12	0.49
1:A:379:ARG:HD2	1:A:457:SER:C	2.32	0.48
1:A:434:VAL:HB	1:A:516:VAL:O	2.13	0.48
1:A:495:THR:HG23	1:A:496:LEU:O	2.14	0.48
1:A:439:THR:OG1	1:A:441:LYS:HB3	2.13	0.48
1:B:468:PHE:C	1:B:468:PHE:CD1	2.86	0.48
1:A:419:SER:O	1:A:422:ASN:HB2	2.14	0.48
1:A:57:ALA:HA	1:A:345:MET:HG2	1.94	0.48
1:A:389:ILE:CD1	1:A:409:ILE:HD12	2.42	0.48
1:A:470:ALA:O	1:A:549:TRP:O	2.32	0.48
1:B:452:GLN:O	1:B:452:GLN:HG2	2.14	0.48
1:A:466:VAL:HG12	1:A:467:SER:N	2.29	0.48
1:A:321:LYS:HB3	1:A:335:TYR:CZ	2.49	0.48
1:A:378:VAL:HG11	1:A:409:ILE:HG21	1.96	0.47
1:A:114:ILE:CD1	1:A:137:LEU:HB3	2.42	0.47
1:A:358:ALA:O	1:A:362:VAL:HG23	2.14	0.47
1:A:218:MET:CG	1:A:218:MET:CE	2.91	0.47
1:B:312:TYR:CD1	1:B:313:GLN:N	2.83	0.47
1:B:168:ILE:HG22	1:B:169:GLY:N	2.29	0.47
1:A:371:LEU:HD23	1:A:384:ASN:ND2	2.29	0.47
1:B:141:ASN:N	1:B:195:GLU:HG2	2.29	0.47
1:B:170:LEU:HB3	1:B:192:PRO:HB3	1.97	0.47
1:B:394:MET:HE1	1:B:402:ALA:N	2.30	0.47
1:B:510:ASP:HA	1:B:515:TYR:CD2	2.49	0.47
1:A:521:ILE:HD13	1:A:521:ILE:N	2.30	0.47
1:B:322:LYS:HG2	1:B:332:ARG:NH1	2.30	0.47
1:B:84:ASP:CG	1:B:217:HIS:CE1	2.87	0.47
1:A:471:LYS:HE2	1:A:550:GLN:NE2	2.29	0.47
1:B:117:HIS:NE2	3:B:2603:PO4:O1	2.48	0.47
1:A:53:GLU:HG2	1:A:318:ASN:O	2.15	0.47
1:A:375:ARG:NE	1:A:379:ARG:NH2	2.63	0.46
1:B:470:ALA:HB3	1:B:549:TRP:CD1	2.50	0.46
1:A:459:ALA:HB2	1:A:504:ASP:HB3	1.97	0.46
1:B:363:LYS:HZ2	1:B:366:GLU:HB3	1.79	0.46
1:A:420:TYR:CD1	1:A:527:LYS:HD3	2.49	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:446:TYR:CE1	1:A:509:LEU:HD11	2.51	0.46
1:B:394:MET:SD	1:B:465:ASN:ND2	2.88	0.46
1:B:448:THR:HA	1:B:475:LEU:HD11	1.96	0.46
1:B:524:GLU:O	1:B:527:LYS:HG3	2.15	0.46
1:B:345:MET:HE3	1:B:348:LEU:HB3	1.97	0.46
1:B:545:GLY:O	1:B:547:VAL:N	2.49	0.46
1:B:368:ASN:ND2	1:B:537:ASP:HA	2.30	0.46
1:B:204:GLN:OE1	1:B:204:GLN:HA	2.15	0.46
1:B:170:LEU:HD11	1:B:196:ALA:HB2	1.98	0.46
1:B:56:LEU:HD23	1:B:103:GLY:HA3	1.97	0.46
1:A:385:MET:HE1	1:A:426:VAL:HG11	1.98	0.46
1:A:467:SER:CB	1:A:546:GLU:HB2	2.45	0.46
1:B:141:ASN:CG	1:B:192:PRO:HG3	2.37	0.46
1:B:298:ALA:HB1	1:B:309:MET:CE	2.46	0.46
1:B:114:ILE:HG12	1:B:139:SER:HB2	1.97	0.45
1:B:368:ASN:OD1	1:B:369:GLY:N	2.49	0.45
1:B:130:GLU:CG	1:B:137:LEU:HD22	2.42	0.45
1:B:251:GLY:HA2	1:B:287:GLN:CD	2.37	0.45
1:A:125:VAL:O	1:A:129:GLN:HG3	2.16	0.45
1:A:475:LEU:HD13	1:A:478:LEU:HD13	1.97	0.45
1:B:380:PHE:CE2	1:B:456:ASP:HA	2.51	0.45
1:A:385:MET:HE2	1:A:389:ILE:HD11	1.97	0.45
1:A:401:PHE:HB2	1:A:466:VAL:CG2	2.46	0.45
1:A:364:ILE:HD11	1:A:530:ILE:HD11	1.97	0.45
1:B:302:PHE:HB2	1:B:307:MET:CE	2.46	0.45
1:B:456:ASP:OD1	1:B:456:ASP:C	2.54	0.45
1:B:150:ARG:NH2	1:B:195:GLU:OE2	2.47	0.45
1:A:508:ARG:HD2	1:A:510:ASP:OD1	2.17	0.45
1:A:367:THR:HG23	1:A:415:ALA:HA	1.99	0.45
1:A:438:MET:HG3	1:A:443:VAL:HG22	1.98	0.45
1:B:167:VAL:HA	1:B:213:ILE:O	2.16	0.45
1:A:486:ASP:HB3	1:A:489:LYS:HB2	1.98	0.44
1:A:90:PRO:O	1:A:94:LEU:HG	2.17	0.44
1:A:375:ARG:HA	1:A:378:VAL:HG22	1.99	0.44
1:B:377:LYS:HD2	1:B:377:LYS:N	2.32	0.44
1:A:390:LEU:HD11	1:A:404:MET:HG2	2.00	0.44
1:A:469:VAL:HG23	1:A:477:ASP:HB3	1.99	0.44
1:A:155:TRP:CE3	1:A:199:VAL:HG13	2.52	0.44
1:B:99:PRO:HB3	1:B:352:PHE:CD2	2.53	0.44
1:B:394:MET:HA	1:B:399:ALA:HB3	2.00	0.44
1:A:394:MET:CG	1:A:402:ALA:HB2	2.48	0.44
1:A:26:TYR:N	5:A:1809:HOH:O	2.49	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:221:TYR:O	1:A:222:ASP:C	2.56	0.44
1:B:49:ASN:HB3	1:B:54:TYR:CE1	2.53	0.43
1:A:213:ILE:HG12	1:A:247:MET:HG2	1.99	0.43
1:A:528:ALA:HA	1:A:531:GLN:OE1	2.17	0.43
1:A:476:ASN:O	1:A:477:ASP:HB3	2.18	0.43
1:A:375:ARG:O	1:A:379:ARG:HB2	2.19	0.43
1:B:98:GLU:N	1:B:99:PRO:CD	2.79	0.43
1:B:302:PHE:HB2	1:B:307:MET:HE3	2.01	0.43
1:B:512:LYS:HG3	1:B:513:PRO:HD2	2.00	0.43
1:B:380:PHE:CZ	1:B:456:ASP:HA	2.53	0.43
1:A:439:THR:O	1:A:443:VAL:HG23	2.18	0.43
1:B:321:LYS:HB3	1:B:335:TYR:CZ	2.53	0.43
1:A:378:VAL:O	1:A:460:TYR:HD2	2.02	0.43
1:A:369:GLY:HA2	1:A:415:ALA:HB2	2.01	0.43
1:B:438:MET:HB2	1:B:442:GLU:HB2	2.01	0.43
1:A:170:LEU:HD11	1:A:196:ALA:HB2	2.00	0.43
1:A:379:ARG:HD2	1:A:458:GLY:N	2.34	0.43
1:A:511:ASN:OD1	1:A:512:LYS:HG3	2.19	0.43
1:B:301:GLU:HG3	1:B:310:VAL:HG11	2.01	0.43
1:A:454:LYS:HB3	1:A:455:PRO:HD2	2.00	0.42
1:A:267:VAL:O	1:A:268:ASP:HB2	2.20	0.42
1:A:405:SER:HB3	1:A:458:GLY:O	2.19	0.42
1:B:348:LEU:O	1:B:348:LEU:HG	2.20	0.42
1:B:545:GLY:O	1:B:546:GLU:C	2.57	0.42
1:A:493:MET:HG2	1:A:494:ALA:N	2.35	0.42
1:B:115:GLY:CA	1:B:118:GLU:OE1	2.68	0.42
1:B:255:ASP:O	1:B:287:GLN:HG2	2.19	0.42
1:B:357:LYS:C	1:B:359:GLN:H	2.22	0.42
1:B:106:LEU:HD21	1:B:344:GLN:HG2	2.02	0.42
1:B:345:MET:CE	1:B:348:LEU:HB3	2.50	0.42
1:B:359:GLN:NE2	1:B:359:GLN:HA	2.35	0.42
1:A:401:PHE:HB2	1:A:466:VAL:HG23	2.02	0.42
1:B:434:VAL:HG12	1:B:517:ASN:HA	2.01	0.42
1:B:312:TYR:CD1	1:B:312:TYR:C	2.93	0.42
1:A:384:ASN:HD22	1:A:538:VAL:HG13	1.83	0.41
1:B:431:ASN:OD1	4:B:2604:ADN:H2	2.19	0.41
1:B:260:ALA:HB2	1:B:266:GLN:HA	2.02	0.41
1:B:379:ARG:HD2	1:B:458:GLY:CA	2.49	0.41
1:B:460:TYR:HA	1:B:461:PRO:HD3	1.69	0.41
1:B:86:ASN:HD21	1:B:129:GLN:HE22	1.69	0.41
1:B:96:ASP:O	1:B:97:ALA:HB3	2.20	0.41
1:B:507:PRO:O	1:B:509:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:86:ASN:ND2	1:B:129:GLN:HE22	2.18	0.41
1:A:474:LYS:HE3	1:A:474:LYS:HB2	1.91	0.41
1:B:155:TRP:CE3	1:B:199:VAL:HG13	2.56	0.41
1:A:389:ILE:O	1:A:393:GLN:HG3	2.21	0.41
1:A:521:ILE:HB	1:A:524:GLU:CG	2.41	0.41
1:A:401:PHE:N	1:A:401:PHE:CD1	2.89	0.41
1:A:360:LEU:HD12	1:A:421:LYS:HB2	2.01	0.41
1:A:389:ILE:HD12	1:A:409:ILE:HD12	2.03	0.41
1:B:379:ARG:HD2	1:B:457:SER:C	2.41	0.41
1:A:360:LEU:HD11	1:A:424:LEU:HD12	2.03	0.41
1:A:401:PHE:CG	1:A:480:ILE:HD12	2.55	0.41
1:B:371:LEU:O	1:B:412:SER:HB3	2.21	0.41
1:B:435:TYR:HA	1:B:493:MET:O	2.20	0.41
1:A:84:ASP:CG	1:A:217:HIS:CE1	2.94	0.41
1:A:57:ALA:CA	1:A:345:MET:HG2	2.51	0.41
1:A:167:VAL:HA	1:A:213:ILE:O	2.21	0.41
1:A:226:HIS:NE2	5:A:1684:HOH:O	2.37	0.41
1:B:91:GLU:OE2	1:B:421:LYS:HD2	2.20	0.41
1:B:151:LEU:HA	1:B:151:LEU:HD23	1.90	0.41
1:B:326:GLU:C	1:B:328:GLY:H	2.22	0.41
1:B:123:LEU:HA	1:B:123:LEU:HD12	1.89	0.41
1:B:497:ASN:O	1:B:501:THR:HG23	2.21	0.41
1:B:422:ASN:O	1:B:426:VAL:HG23	2.21	0.41
1:B:475:LEU:HD13	1:B:478:LEU:HD13	2.04	0.40
1:B:86:ASN:HD21	1:B:129:GLN:NE2	2.19	0.40
1:B:471:LYS:HE2	1:B:550:GLN:HG3	2.03	0.40
1:A:468:PHE:CE1	1:A:547:VAL:HG13	2.55	0.40
1:B:540:VAL:HG12	1:B:540:VAL:O	2.21	0.40
1:B:141:ASN:CA	1:B:195:GLU:HG2	2.52	0.40
1:B:173:ASP:N	1:B:173:ASP:OD1	2.53	0.40
1:A:26:TYR:CE1	1:A:304:ASN:HA	2.57	0.40
1:B:44:GLY:HA2	1:B:100:ASP:OD2	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	523/525 (100%)	490 (94%)	29 (6%)	4 (1%)	27	20
1	B	523/525 (100%)	481 (92%)	36 (7%)	6 (1%)	21	13
All	All	1046/1050 (100%)	971 (93%)	65 (6%)	10 (1%)	22	14

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	513	PRO
1	B	546	GLU
1	A	87	THR
1	B	548	SER
1	B	289	HIS
1	B	87	THR
1	B	378	VAL
1	B	472	ASP
1	A	378	VAL
1	A	484	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	433/433 (100%)	419 (97%)	14 (3%)	51	52
1	B	433/433 (100%)	418 (96%)	15 (4%)	48	48
All	All	866/866 (100%)	837 (97%)	29 (3%)	50	51

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	LEU
1	A	84	ASP
1	A	118	GLU
1	A	235	GLU
1	A	307	MET

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Mol	Chain	Res	Type
1	A	327	ASP
1	A	368	ASN
1	A	375	ARG
1	A	401	PHE
1	A	410	ARG
1	A	428	PRO
1	A	513	PRO
1	A	522	ASP
1	A	550	GLN
1	B	56	LEU
1	B	73	GLU
1	B	96	ASP
1	B	174	ASP
1	B	202	GLU
1	B	205	GLN
1	B	228	SER
1	B	390	LEU
1	B	401	PHE
1	B	456	ASP
1	B	479	LYS
1	B	512	LYS
1	B	526	LEU
1	B	527	LYS
1	B	547	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	180	ASN
1	A	204	GLN
1	A	368	ASN
1	A	462	GLN
1	A	476	ASN
1	A	550	GLN
1	B	86	ASN
1	B	129	GLN
1	B	144	GLN
1	B	266	GLN
1	B	279	GLN
1	B	359	GLN
1	B	393	GLN

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Mol	Chain	Res	Type
1	B	427	GLN
1	B	452	GLN
1	B	476	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	PO4	A	1603	2	4,4,4	0.72	0	6,6,6	0.32	0
4	ADN	A	1604	-	21,21,21	0.56	0	31,31,31	0.70	0
3	PO4	B	2603	2	4,4,4	0.78	0	6,6,6	0.31	0
4	ADN	B	2604	-	21,21,21	0.55	0	31,31,31	0.67	0

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	PO4	A	1603	2	-	0/0/0/0	0/0/0/0
4	ADN	A	1604	-	-	0/6/22/22	0/1/3/3
3	PO4	B	2603	2	-	0/0/0/0	0/0/0/0
4	ADN	B	2604	-	-	0/6/22/22	0/1/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	525/525 (100%)	0.52	45 (8%)	11 11	16, 34, 76, 91	0
1	B	525/525 (100%)	0.69	45 (8%)	11 11	24, 48, 74, 86	0
All	All	1050/1050 (100%)	0.60	90 (8%)	11 11	16, 44, 75, 91	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	VAL	6.8
1	B	358	ALA	5.9
1	A	549	TRP	5.4
1	A	473	GLY	5.3
1	B	485	VAL	4.9
1	B	185	THR	4.8
1	A	530	ILE	4.6
1	A	475	LEU	4.5
1	B	454	LYS	4.4
1	A	488	ALA	4.4
1	A	441	LYS	4.3
1	A	464	ALA	4.1
1	A	444	ILE	4.1
1	B	488	ALA	3.9
1	B	490	THR	3.8
1	A	472	ASP	3.6
1	B	478	LEU	3.6
1	B	471	LYS	3.6
1	B	473	GLY	3.5
1	B	489	LYS	3.5
1	A	380	PHE	3.5
1	B	418	ILE	3.4
1	B	390	LEU	3.4
1	A	408	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	544	LYS	3.3
1	A	403	VAL	3.3
1	A	474	LYS	3.3
1	B	530	ILE	3.3
1	B	113	ALA	3.3
1	B	505	GLY	3.0
1	B	267	VAL	3.0
1	A	367	THR	3.0
1	A	368	ASN	3.0
1	B	452	GLN	2.9
1	B	539	SER	2.9
1	A	463	PHE	2.9
1	A	513	PRO	2.8
1	A	485	VAL	2.8
1	A	550	GLN	2.8
1	A	470	ALA	2.7
1	A	476	ASN	2.6
1	B	484	PRO	2.6
1	A	535	PRO	2.6
1	B	540	VAL	2.6
1	B	369	GLY	2.6
1	A	478	LEU	2.6
1	B	249	VAL	2.6
1	A	537	ASP	2.6
1	B	215	ALA	2.6
1	B	264	LYS	2.5
1	B	187	ILE	2.5
1	A	484	PRO	2.5
1	B	413	ILE	2.5
1	A	489	LYS	2.4
1	B	368	ASN	2.4
1	A	390	LEU	2.4
1	A	496	LEU	2.4
1	A	413	ILE	2.4
1	A	494	ALA	2.4
1	B	463	PHE	2.4
1	B	513	PRO	2.4
1	B	469	VAL	2.3
1	A	480	ILE	2.3
1	B	550	GLN	2.3
1	A	358	ALA	2.3
1	B	144	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	456	ASP	2.3
1	B	535	PRO	2.2
1	A	515	TYR	2.2
1	B	85	ILE	2.2
1	B	146	SER	2.2
1	B	247	MET	2.2
1	A	539	SER	2.2
1	B	494	ALA	2.2
1	A	405	SER	2.2
1	A	214	ALA	2.1
1	B	94	LEU	2.1
1	A	467	SER	2.1
1	B	228	SER	2.1
1	B	354	ASN	2.1
1	A	454	LYS	2.1
1	A	389	ILE	2.1
1	B	286	VAL	2.1
1	A	249	VAL	2.0
1	A	443	VAL	2.0
1	B	450	VAL	2.0
1	B	357	LYS	2.0
1	B	409	ILE	2.0
1	A	415	ALA	2.0
1	B	138	LEU	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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ADN	B	2604	19/19	0.17	0.39	59,62,62,63	0
4	ADN	A	1604	19/19	0.19	0.26	46,52,56,57	0
3	PO4	B	2603	5/5	0.14	-0.52	60,61,62,62	0
2	MN	A	1601	1/1	0.17	-0.69	25,25,25,25	0
3	PO4	A	1603	5/5	0.14	-1.37	23,31,37,39	0
2	MN	B	2601	1/1	0.10	-1.60	38,38,38,38	0
2	MN	B	2602	1/1	0.10	-2.51	41,41,41,41	0
2	MN	A	1602	1/1	0.13	-2.62	23,23,23,23	0

6.5 Other polymers

There are no such residues in this entry.