Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:52 PM 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 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

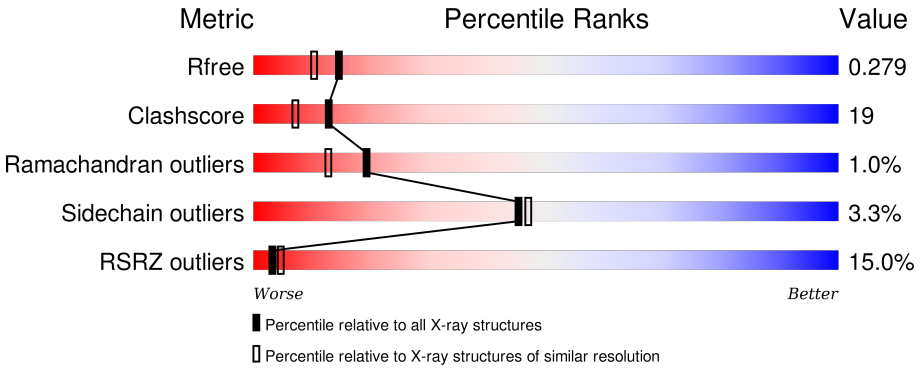
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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. 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	525	14% 68% 30%
1	B	525	16% 62% 35%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8607 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.

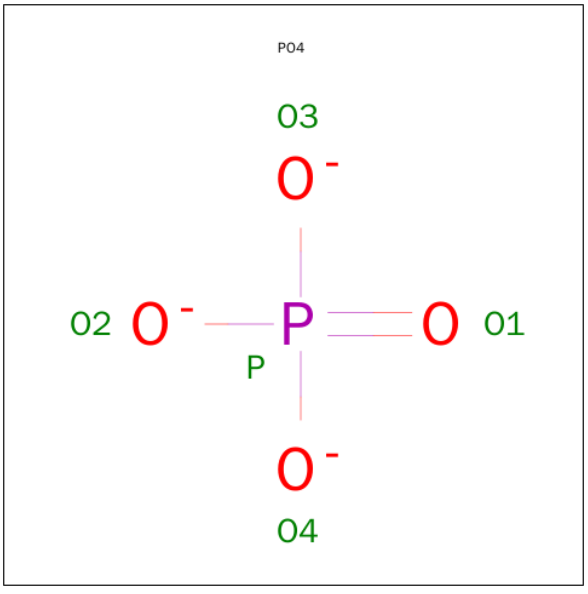
- Molecule 1 is a protein called 5'-NUCLEOTIDASE.

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).

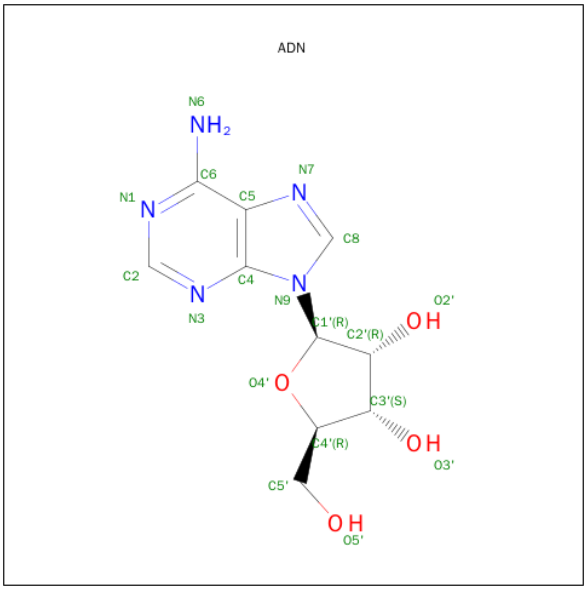
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is ADENOSINE (three-letter code: ADN) (formula: $C_{10}H_{13}N_5O_4$).



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

- Molecule 5 is water.

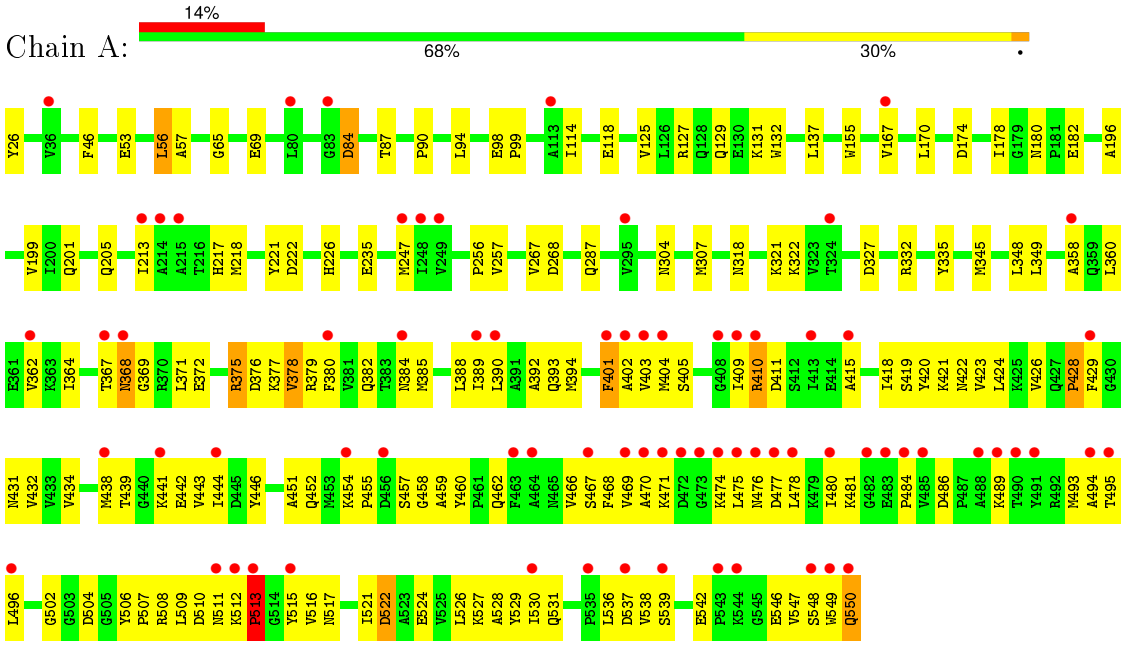
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	238	Total O 238 238	0	0
5	B	117	Total O 117 117	0	0

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 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.

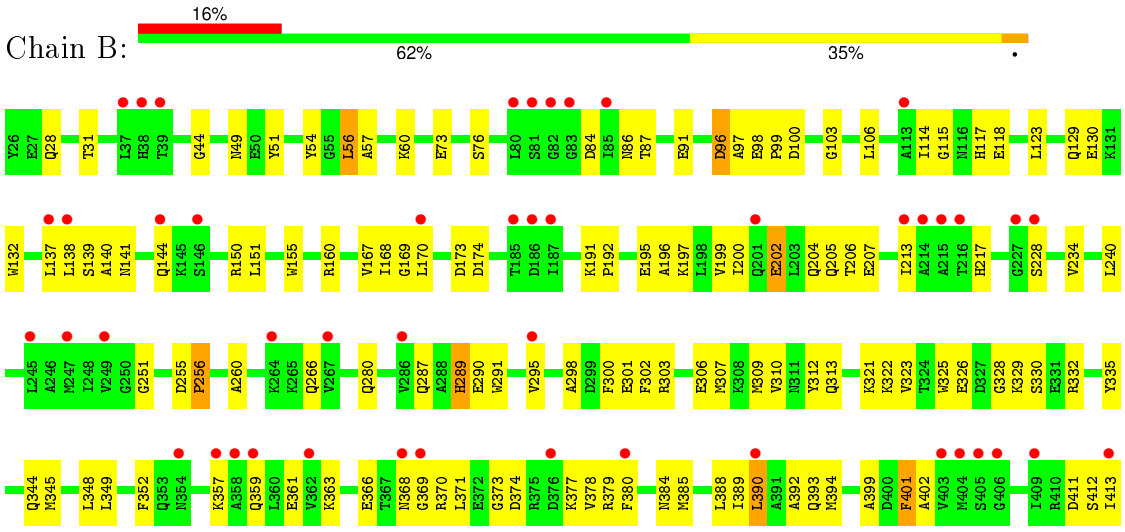
- Molecule 1: 5'-NUCLEOTIDASE

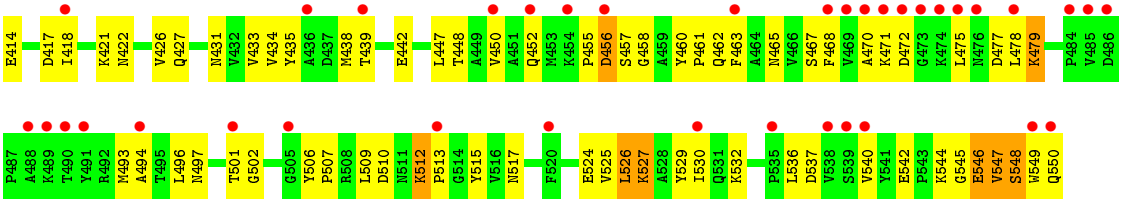
Chain A:



- Molecule 1: 5'-NUCLEOTIDASE

Chain B:




E414 D417 T418 K421 N422 V426 Q427 N431 V432 Y433 V434 Y435 A436 D437 M438 T439 E442 L447 T448 A449 V450 A451 Q452 N453 K454 P455 D456 S457 G458 A459 Y460 P461 Q462 P463 A464 N465 V466 S467 F468 V469 A470 K471 D472 G473 K474 L475 N476 D477 L478 K479 P484 V485 D486
P487 A488 K489 T490 Y491 R492 M493 A494 T495 L496 N497 T501 G502 G505 Y506 P507 R508 L509 D510 N511 K512 P513 G514 Y515 V516 N517 P520 E524 V525 L526 K527 A528 Y529 I530 Q531 K532 P535 L536 D537 V538 S539 V540 Y541 E542 P543 K544 G545 E546 V547 S548 W549 Q550

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.32 , 50.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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 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	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
3	A	5	0	0	0	0
3	B	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 (313) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:MET:HE3	1:B:348:LEU:HD23	1.82	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	24	17
1	B	523/525 (100%)	481 (92%)	36 (7%)	6 (1%)	17	11
All	All	1046/1050 (100%)	971 (93%)	65 (6%)	10 (1%)	19	13

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%)	46	48
1	B	433/433 (100%)	418 (96%)	15 (4%)	43	44
All	All	866/866 (100%)	837 (97%)	29 (3%)	45	47

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
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

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Mol	Chain	Res	Type
1	B	129	GLN
1	B	144	GLN
1	B	266	GLN
1	B	279	GLN
1	B	359	GLN
1	B	393	GLN
1	B	427	GLN
1	B	452	GLN
1	B	476	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 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	0.94	0	6,6,6	0.28	0
4	ADN	A	1604	-	16,21,21	0.59	0	16,31,31	0.62	0
3	PO4	B	2603	2	4,4,4	1.01	0	6,6,6	0.27	0
4	ADN	B	2604	-	16,21,21	0.61	0	16,31,31	0.49	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	-	-	0/2/22/22	0/3/3/3
3	PO4	B	2603	2	-	0/0/0/0	0/0/0/0
4	ADN	B	2604	-	-	0/2/22/22	0/3/3/3

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1604	ADN	1	0
3	B	2603	PO4	1	0
4	B	2604	ADN	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, 95^{th} 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%)	0.73	74 (14%) 4 5	16, 34, 76, 91	0
1	B	525/525 (100%)	0.90	84 (16%) 3 4	24, 48, 74, 86	0
All	All	1050/1050 (100%)	0.81	158 (15%) 3 5	16, 44, 75, 91	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	469	VAL	7.8
1	B	358	ALA	7.5
1	A	473	GLY	7.5
1	A	549	TRP	7.3
1	B	485	VAL	5.9
1	B	185	THR	5.8
1	A	530	ILE	5.6
1	A	488	ALA	5.5
1	A	472	ASP	5.0
1	A	464	ALA	4.6
1	A	380	PHE	4.6
1	B	478	LEU	4.6
1	B	488	ALA	4.4
1	A	441	LYS	4.4
1	B	471	LYS	4.3
1	A	475	LEU	4.2
1	B	454	LYS	4.1
1	A	408	GLY	4.1
1	A	484	PRO	4.0
1	B	490	THR	4.0
1	A	403	VAL	3.9
1	B	390	LEU	3.9
1	A	470	ALA	3.9
1	A	513	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	489	LYS	3.9
1	B	113	ALA	3.8
1	B	249	VAL	3.7
1	A	358	ALA	3.7
1	A	463	PHE	3.7
1	B	473	GLY	3.7
1	B	215	ALA	3.7
1	B	146	SER	3.6
1	B	418	ILE	3.6
1	A	444	ILE	3.6
1	A	544	LYS	3.5
1	B	267	VAL	3.4
1	A	474	LYS	3.4
1	B	530	ILE	3.4
1	A	548	SER	3.3
1	B	80	LEU	3.3
1	B	469	VAL	3.3
1	A	489	LYS	3.2
1	A	535	PRO	3.3
1	B	452	GLN	3.2
1	B	539	SER	3.2
1	A	550	GLN	3.2
1	A	368	ASN	3.2
1	A	482	GLY	3.1
1	B	85	ILE	3.1
1	B	369	GLY	3.1
1	B	187	ILE	3.1
1	B	144	GLN	3.1
1	B	484	PRO	3.0
1	B	550	GLN	3.0
1	A	390	LEU	3.0
1	B	368	ASN	3.0
1	B	413	ILE	2.9
1	A	496	LEU	2.9
1	B	403	VAL	2.9
1	A	515	TYR	2.9
1	B	228	SER	2.9
1	B	264	LYS	2.9
1	B	81	SER	2.9
1	A	413	ILE	2.9
1	B	247	MET	2.8
1	A	409	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	491	TYR	2.8
1	A	389	ILE	2.8
1	A	537	ASP	2.8
1	B	491	TYR	2.8
1	B	463	PHE	2.7
1	B	82	GLY	2.7
1	A	80	LEU	2.7
1	B	472	ASP	2.7
1	A	249	VAL	2.7
1	A	404	MET	2.7
1	A	480	ILE	2.6
1	A	324	THR	2.6
1	B	501	THR	2.6
1	A	362	VAL	2.6
1	A	478	LEU	2.6
1	B	138	LEU	2.6
1	B	186	ASP	2.6
1	A	476	ASN	2.6
1	B	474	LYS	2.6
1	A	213	ILE	2.6
1	B	476	ASN	2.6
1	B	376	ASP	2.6
1	A	494	ALA	2.6
1	B	540	VAL	2.6
1	B	535	PRO	2.5
1	A	214	ALA	2.5
1	B	362	VAL	2.5
1	A	512	LYS	2.5
1	B	201	GLN	2.5
1	A	36	VAL	2.5
1	B	286	VAL	2.5
1	B	513	PRO	2.5
1	A	438	MET	2.5
1	B	494	ALA	2.5
1	A	471	LYS	2.5
1	A	539	SER	2.5
1	A	415	ALA	2.4
1	B	456	ASP	2.4
1	A	485	VAL	2.4
1	B	470	ALA	2.4
1	B	380	PHE	2.4
1	A	367	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	215	ALA	2.4
1	B	83	GLY	2.4
1	B	38	HIS	2.4
1	B	538	VAL	2.4
1	B	354	ASN	2.4
1	B	505	GLY	2.4
1	A	456	ASP	2.3
1	A	511	ASN	2.3
1	A	429	PHE	2.3
1	A	467	SER	2.3
1	B	486	ASP	2.3
1	B	409	ILE	2.3
1	B	170	LEU	2.3
1	B	450	VAL	2.2
1	A	490	THR	2.2
1	A	83	GLY	2.2
1	B	214	ALA	2.2
1	B	475	LEU	2.2
1	A	543	PRO	2.2
1	B	227	GLY	2.2
1	B	357	LYS	2.2
1	B	37	LEU	2.2
1	B	39	THR	2.2
1	B	520	PHE	2.2
1	A	167	VAL	2.2
1	A	248	ILE	2.2
1	B	137	LEU	2.2
1	A	401	PHE	2.1
1	A	410	ARG	2.1
1	A	113	ALA	2.1
1	A	495	THR	2.1
1	B	439	THR	2.1
1	B	245	LEU	2.1
1	B	436	ALA	2.1
1	B	406	GLY	2.1
1	A	483	GLU	2.1
1	B	213	ILE	2.1
1	B	404	MET	2.1
1	B	549	TRP	2.1
1	B	216	THR	2.1
1	B	359	GLN	2.1
1	B	405	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	468	PHE	2.1
1	B	295	VAL	2.1
1	A	454	LYS	2.0
1	A	402	ALA	2.0
1	A	247	MET	2.0
1	A	295	VAL	2.0
1	A	384	ASN	2.0
1	A	477	ASP	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, 95^{th} 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
4	ADN	B	2604	19/19	0.85	0.19	0.70	59,62,62,63	0
4	ADN	A	1604	19/19	0.89	0.22	0.43	46,52,56,57	0
2	MN	A	1601	1/1	1.00	0.17	-0.47	25,25,25,25	0
3	PO4	B	2603	5/5	0.95	0.13	-0.75	60,61,62,62	0
2	MN	B	2601	1/1	0.99	0.10	-1.55	38,38,38,38	0
3	PO4	A	1603	5/5	0.97	0.12	-1.55	23,31,37,39	0
2	MN	A	1602	1/1	0.99	0.13	-2.13	23,23,23,23	0
2	MN	B	2602	1/1	0.98	0.10	-2.97	41,41,41,41	0

6.5 Other polymers (i)

There are no such residues in this entry.