Full wwPDB X-ray Structure Validation Report ⓘ

Jan 29, 2024 – 09:50 PM EST

PDB ID	:	1FA0
Title	:	STRUCTURE OF YEAST POLY(A) POLYMERASE BOUND TO MANGANATE AND 3'-DATP
Authors	:	Bard, J.; Zhelkovsky, A.M.; Helmling, S.; Moore, C.L.; Bohm, A.
Deposited on	:	2000-07-11
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

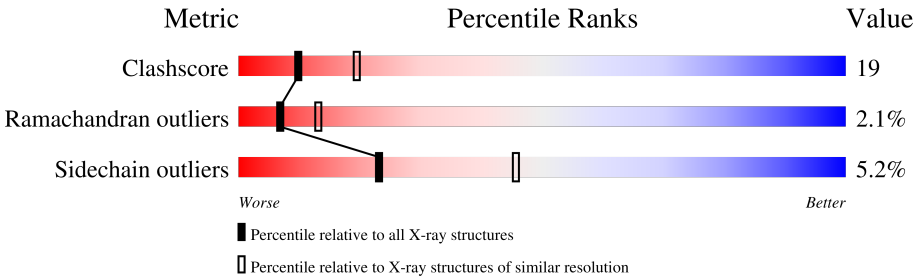
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	537	60% 32% · 5%
1	B	537	61% 32% · 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8250 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.

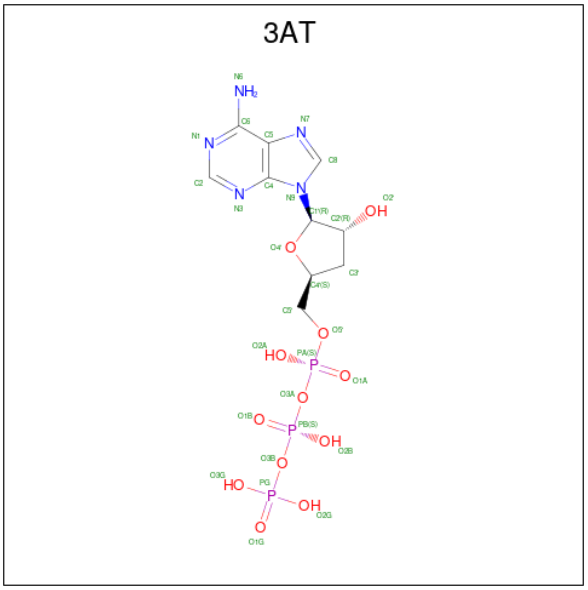
- Molecule 1 is a protein called POLY(A)-POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	14	0	0
			4025	2593	679	737	16			
1	B	511	Total	C	N	O	S	0	0	0
			4034	2598	680	740	16			

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

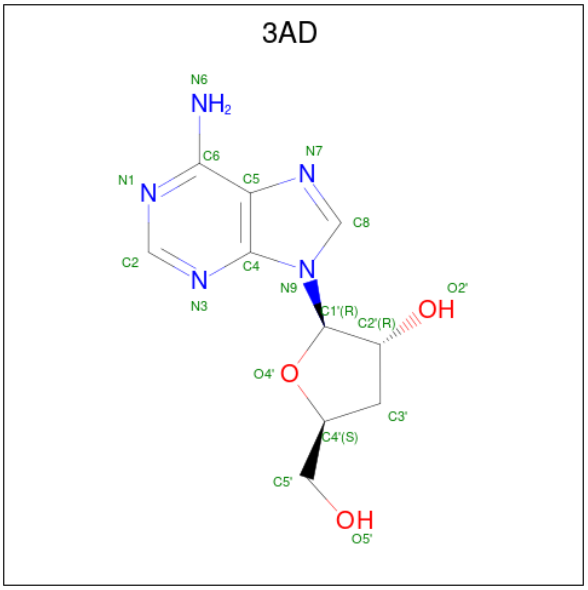
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

- Molecule 3 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: 3AT) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



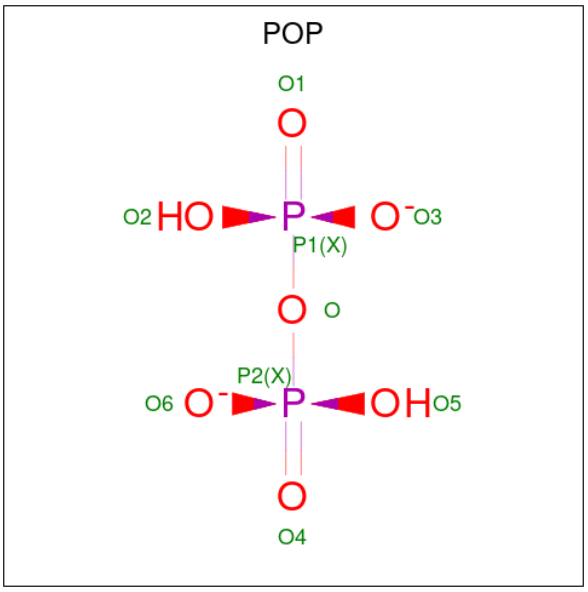
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 4 is 3'-DEOXYADENOSINE (three-letter code: 3AD) (formula: $C_{10}H_{13}N_5O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			18	10	5	3		
4	B	1	Total	C	N	O	0	0
			18	10	5	3		

- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 9 7 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	54	Total O 54 54	0	0
6	B	28	Total O 28 28	0	0

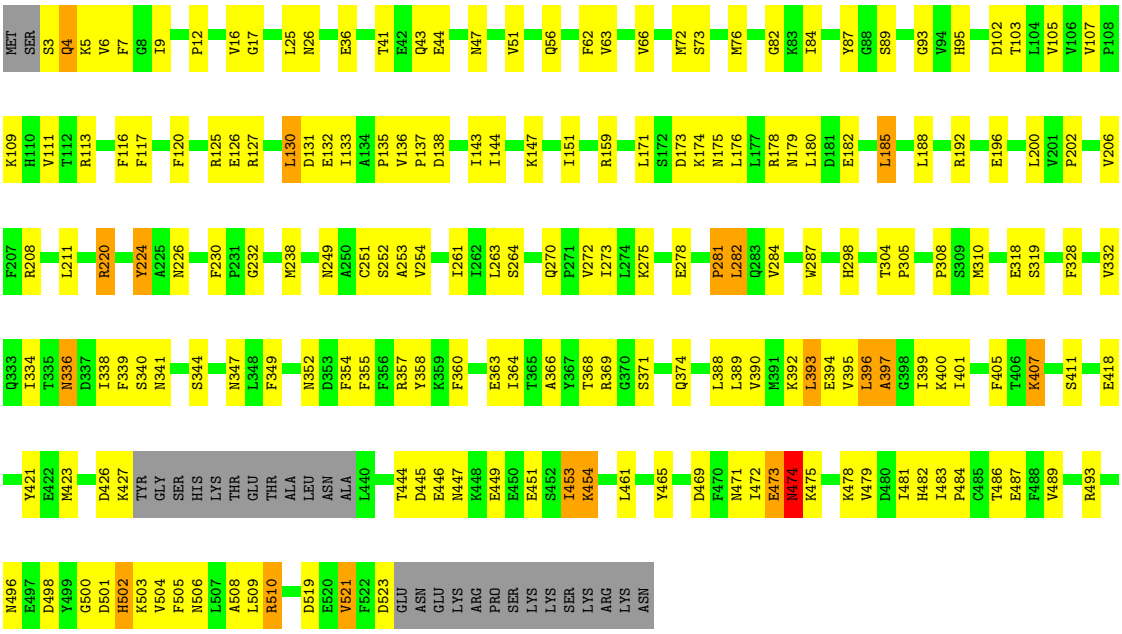
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

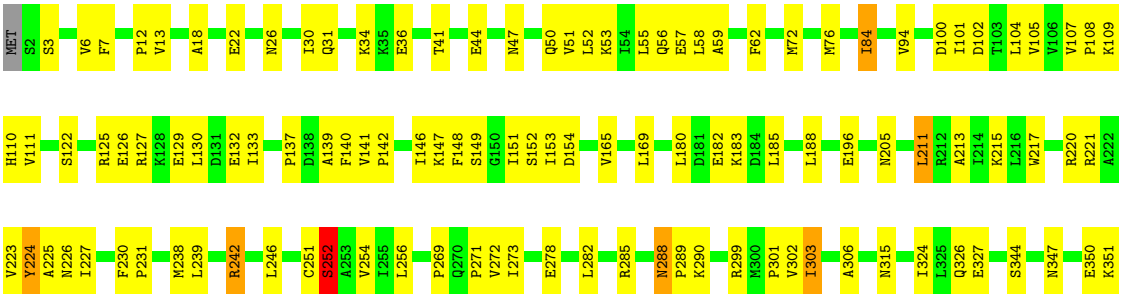
• Molecule 1: POLY(A)-POLYMERASE

Chain A:



• Molecule 1: POLY(A)-POLYMERASE

Chain B:




N352 D353 F354 F355 F356 R357 I364 R369 G370 S371 Q374 H375 L376 K377 W378 L381 V382 E383 S384 K385 V386 R387 L388 L389 V390 M391 K392 L393 E394 V395 L396 A397 G398 I399 K400 P404 F405 Y413 C414 C415 P416 M423 D426 K427 Y428 G429 S430 T433 E434 T435 A436
L437 N438 A439 L440 K441 L442 V443 T444 ASP GLU ASN LYS GLU GLU GLU SER ILE LYS ASP ALA P457 Y460 L461 S462 T463 D469 I472 GLU ASN LYS LYS GLU LYS V479 C485 F488 V489 R493 S494 F495 D498 Y499 G500 D501 H502 K503 V504 L507 A508 L509 R510 F511
V512 D516 V521 E526 K527 S530 LYS LYS SER LYS ARG LYS ASN

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.80Å 109.10Å 238.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	84.0 (20.00-2.60)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8250	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 3AT, 3AD, MN, POP

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	0.40	0/4116	0.63	0/5586
1	B	0.40	0/4127	0.63	0/5604
All	All	0.40	0/8243	0.63	0/11190

There are no bond length outliers.

There are no bond angle outliers.

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	4025	0	3979	147	0
1	B	4034	0	3979	160	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	30	0	12	1	0
3	B	30	0	12	1	0
4	A	18	0	13	1	0
4	B	18	0	13	2	0
5	A	9	0	0	0	0
6	A	54	0	0	5	0
6	B	28	0	0	1	0
All	All	8250	0	8008	309	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 (309) 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:133:ILE:HG12	1:A:135:PRO:HD3	1.44	0.98
1:B:251:CYS:O	1:B:252:SER:HB2	1.67	0.92
1:A:496:ASN:HD22	1:A:498:ASP:H	1.18	0.91
1:A:496:ASN:ND2	1:A:498:ASP:H	1.69	0.90
1:A:444:THR:HB	1:A:446:GLU:HG2	1.53	0.89
1:B:41:THR:OG1	1:B:44:GLU:HG3	1.81	0.79
1:A:396:LEU:HD21	1:A:481:ILE:HG22	1.65	0.78
1:B:7:PHE:HB3	1:B:12:PRO:HD3	1.66	0.77
1:A:501:ASP:O	1:A:502:HIS:HB2	1.86	0.76
1:A:496:ASN:HD22	1:A:498:ASP:N	1.85	0.75
1:B:125:ARG:HH11	1:B:125:ARG:HG3	1.52	0.75
1:A:352:ASN:HD22	1:A:354:PHE:H	1.33	0.74
1:A:84:ILE:CD1	1:A:105:VAL:HG22	2.18	0.73
1:A:483:ILE:HB	1:A:484:PRO:HD3	1.70	0.73
1:B:125:ARG:HE	1:B:133:ILE:HG21	1.54	0.73
1:A:56:GLN:HE22	1:A:84:ILE:H	1.37	0.72
1:A:473:GLU:HG3	1:A:474:ASN:H	1.56	0.70
1:A:308:PRO:HG2	1:A:310:MET:HE2	1.71	0.70
1:A:282:LEU:HB2	1:A:284:VAL:HG22	1.76	0.68
1:A:89:SER:OG	1:A:95:HIS:HA	1.94	0.68
1:A:461:LEU:O	1:A:461:LEU:HD12	1.93	0.68
1:B:122:SER:O	1:B:126:GLU:HG3	1.94	0.68
1:B:273:ILE:HG13	1:B:303:ILE:CD1	2.25	0.67
1:A:3:SER:O	1:A:4:GLN:HB2	1.94	0.67
1:B:510:ARG:HG2	1:B:510:ARG:HH11	1.59	0.67
1:A:7:PHE:HB3	1:A:12:PRO:HD3	1.76	0.67
1:A:87:TYR:O	1:A:102:ASP:HB2	1.95	0.66
1:B:282:LEU:HB3	1:B:285:ARG:HD2	1.78	0.66
1:A:224:TYR:HD2	1:A:224:TYR:O	1.77	0.66
1:A:363:GLU:HG3	1:A:465:TYR:CE2	2.31	0.65
1:B:84:ILE:HD11	1:B:105:VAL:HG22	1.78	0.65
1:B:59:ALA:O	1:B:62:PHE:HB3	1.96	0.65
1:B:375:HIS:CD2	1:B:460:TYR:HB2	2.32	0.64
1:A:89:SER:HB3	6:A:871:HOH:O	1.98	0.64
1:B:217:TRP:O	1:B:221:ARG:HG2	1.98	0.64
1:A:125:ARG:HA	1:A:130:LEU:HD12	1.80	0.63
1:A:287:TRP:HE1	1:A:298:HIS:HD2	1.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:LYS:HE2	1:A:471:ASN:HA	1.81	0.63
1:B:288:ASN:C	1:B:288:ASN:HD22	2.03	0.62
1:B:485:CYS:HB3	1:B:509:LEU:HD22	1.81	0.62
1:A:9:ILE:HD13	1:A:273:ILE:HD11	1.80	0.62
1:A:41:THR:OG1	1:A:44:GLU:HG3	1.99	0.62
1:A:396:LEU:C	1:A:396:LEU:HD12	2.19	0.62
1:B:381:LEU:O	1:B:381:LEU:HD23	1.99	0.62
1:B:501:ASP:HB3	1:B:504:VAL:HG12	1.82	0.61
1:B:51:VAL:HG21	1:B:151:ILE:HD13	1.83	0.61
1:B:414:CYS:O	1:B:416:PRO:HD3	2.01	0.61
1:A:287:TRP:HE1	1:A:298:HIS:CD2	2.19	0.61
1:B:58:LEU:HD11	1:B:127:ARG:HD2	1.83	0.60
1:A:369:ARG:O	1:A:504:VAL:HG13	2.00	0.60
1:A:109:LYS:O	1:A:159:ARG:NH2	2.34	0.60
1:A:366:ALA:O	1:A:461:LEU:HA	2.02	0.60
1:B:142:PRO:HD3	1:B:183:LYS:HD3	1.84	0.60
1:A:444:THR:CB	1:A:446:GLU:HG2	2.29	0.60
1:A:132:GLU:HG2	1:A:147:LYS:HB3	1.84	0.60
1:A:16:VAL:HG12	1:A:17:GLY:O	2.02	0.59
1:B:389:LEU:HG	1:B:393:LEU:HD22	1.85	0.59
1:A:56:GLN:NE2	6:A:844:HOH:O	2.36	0.59
1:A:232:GLY:N	6:A:846:HOH:O	2.34	0.58
1:B:507:LEU:HD12	1:B:509:LEU:HD11	1.85	0.58
1:A:173:ASP:OD2	1:A:175:ASN:HB2	2.02	0.58
1:B:413:TYR:CD2	1:B:442:LEU:HA	2.38	0.58
1:A:352:ASN:ND2	1:A:354:PHE:H	2.01	0.58
1:B:400:LYS:HD3	1:B:469:ASP:OD2	2.03	0.58
1:A:397:ALA:HB3	1:A:479:VAL:HG21	1.85	0.58
1:A:135:PRO:C	1:A:137:PRO:HD3	2.25	0.57
1:B:47:ASN:O	1:B:51:VAL:HG23	2.05	0.57
1:B:396:LEU:C	1:B:396:LEU:HD12	2.26	0.56
1:B:107:VAL:CG2	1:B:111:VAL:HB	2.36	0.56
1:B:125:ARG:HG3	1:B:125:ARG:NH1	2.21	0.56
1:A:238:MET:SD	1:A:304:THR:HA	2.45	0.56
1:A:447:ASN:O	1:A:453:ILE:HG21	2.05	0.56
1:B:53:LYS:O	1:B:57:GLU:HG3	2.06	0.56
1:B:273:ILE:HG13	1:B:303:ILE:HD11	1.88	0.56
1:A:113:ARG:O	1:A:116:PHE:HB3	2.06	0.55
1:A:444:THR:HG22	1:A:445:ASP:N	2.22	0.55
1:B:390:VAL:HG21	1:B:404:PRO:HG3	1.88	0.55
1:B:132:GLU:HG3	1:B:147:LYS:CB	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ASP:O	1:A:502:HIS:CB	2.55	0.54
1:B:428:TYR:HB2	1:B:437:LEU:HD21	1.88	0.54
1:A:174:LYS:NZ	1:A:278:GLU:OE2	2.41	0.54
1:A:224:TYR:O	1:A:224:TYR:CD2	2.58	0.54
1:B:231:PRO:HD3	1:B:324:ILE:HD11	1.89	0.54
1:B:133:ILE:HG13	1:B:146:ILE:HG22	1.90	0.54
1:B:396:LEU:HD12	1:B:399:ILE:HD13	1.89	0.54
1:A:447:ASN:HB2	1:A:453:ILE:HG13	1.89	0.54
1:B:273:ILE:HG13	1:B:303:ILE:HD12	1.90	0.54
1:B:101:ILE:HB	1:B:153:ILE:CD1	2.38	0.54
1:A:25:LEU:HD12	1:A:339:PHE:CD1	2.42	0.53
1:A:226:ASN:HA	1:A:230:PHE:O	2.08	0.53
1:B:271:PRO:HG2	1:B:273:ILE:HD11	1.90	0.53
1:B:51:VAL:HG13	1:B:148:PHE:CD2	2.44	0.53
1:A:411:SER:OG	1:A:461:LEU:HD11	2.08	0.53
1:B:390:VAL:HG21	1:B:404:PRO:CG	2.38	0.52
1:B:427:LYS:CD	1:B:433:THR:HB	2.39	0.52
1:A:93:GLY:O	1:A:208:ARG:HD3	2.09	0.52
1:B:30:ILE:O	1:B:34:LYS:HG2	2.09	0.52
1:B:72:MET:HE2	1:B:76:MET:HB3	1.91	0.52
1:B:108:PRO:O	1:B:111:VAL:HG23	2.09	0.52
1:B:385:LYS:O	1:B:388:LEU:HB2	2.09	0.52
1:A:473:GLU:CG	1:A:474:ASN:H	2.21	0.52
1:A:508:ALA:C	1:A:509:LEU:HD12	2.30	0.52
1:B:299:ARG:HH11	1:B:299:ARG:HG3	1.73	0.52
1:A:421:TYR:C	1:A:423:MET:H	2.11	0.52
1:B:213:ALA:HB3	1:B:256:LEU:HD21	1.91	0.52
1:B:273:ILE:CG1	1:B:303:ILE:HD11	2.40	0.52
1:A:136:VAL:HG13	1:A:143:ILE:HG23	1.92	0.52
1:A:446:GLU:CG	1:A:447:ASN:H	2.23	0.52
1:A:178:ARG:HG3	1:A:179:ASN:HD22	1.75	0.52
1:A:371:SER:OG	1:A:374:GLN:HG3	2.10	0.52
1:B:7:PHE:HB2	6:B:625:HOH:O	2.10	0.52
1:A:73:SER:HB3	1:A:76:MET:HB2	1.92	0.52
1:A:493:ARG:HD3	1:A:500:GLY:HA2	1.92	0.52
1:B:26:ASN:ND2	1:B:252:SER:HB2	2.25	0.52
1:B:427:LYS:HD2	1:B:433:THR:HB	1.91	0.52
1:B:430:SER:O	1:B:434:GLU:HB2	2.10	0.52
1:B:501:ASP:C	1:B:503:LYS:H	2.13	0.51
1:A:390:VAL:O	1:A:394:GLU:HG2	2.10	0.51
1:B:180:LEU:HB2	1:B:185:LEU:HD21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:351:LYS:HG2	1:B:352:ASN:N	2.25	0.51
1:A:192:ARG:HG2	1:A:192:ARG:HH11	1.75	0.51
1:B:390:VAL:CG2	1:B:404:PRO:HG3	2.38	0.51
1:A:6:VAL:HG13	1:A:6:VAL:O	2.10	0.51
1:B:498:ASP:C	1:B:500:GLY:H	2.14	0.51
1:A:26:ASN:HD22	1:A:253:ALA:H	1.58	0.51
1:A:275:LYS:HE2	1:A:305:PRO:O	2.11	0.51
1:B:101:ILE:HB	1:B:153:ILE:HD13	1.92	0.51
1:B:129:GLU:HB3	1:B:149:SER:OG	2.11	0.51
1:A:364:ILE:HG13	1:A:509:LEU:HG	1.93	0.50
1:A:446:GLU:HG3	1:A:447:ASN:N	2.26	0.50
1:B:132:GLU:HG3	1:B:147:LYS:HB3	1.93	0.50
1:A:421:TYR:O	1:A:423:MET:N	2.39	0.50
1:A:116:PHE:O	1:A:120:PHE:HB3	2.12	0.50
1:A:449:GLU:HA	1:A:454:LYS:HD2	1.94	0.50
1:B:142:PRO:CD	1:B:183:LYS:HD3	2.41	0.50
1:B:507:LEU:HD12	1:B:509:LEU:CD1	2.41	0.50
1:A:136:VAL:HG22	1:A:136:VAL:O	2.11	0.50
1:B:165:VAL:HG13	1:B:169:LEU:HD23	1.92	0.50
1:B:381:LEU:HD23	1:B:381:LEU:C	2.32	0.50
1:A:84:ILE:HD11	1:A:105:VAL:HG22	1.92	0.50
1:A:318:GLU:HB3	1:A:394:GLU:OE1	2.10	0.50
1:A:482:HIS:O	1:A:486:THR:HG22	2.11	0.49
1:B:508:ALA:C	1:B:509:LEU:HD12	2.32	0.49
1:A:47:ASN:O	1:A:51:VAL:HG23	2.13	0.49
1:B:413:TYR:HD2	1:B:442:LEU:HA	1.76	0.49
1:A:185:LEU:HD11	1:A:282:LEU:HD13	1.95	0.49
1:B:102:ASP:HA	1:B:154:ASP:HB2	1.94	0.49
1:A:282:LEU:CB	1:A:284:VAL:HG22	2.43	0.49
1:A:389:LEU:O	1:A:393:LEU:HB2	2.13	0.49
1:B:226:ASN:HA	1:B:230:PHE:O	2.13	0.49
1:A:397:ALA:CB	1:A:479:VAL:HG11	2.43	0.48
1:B:141:VAL:O	1:B:141:VAL:HG13	2.13	0.48
1:B:369:ARG:O	1:B:504:VAL:HG23	2.13	0.48
1:A:446:GLU:CG	1:A:447:ASN:N	2.76	0.48
1:B:251:CYS:SG	1:B:254:VAL:HG23	2.53	0.48
1:B:354:PHE:O	1:B:357:ARG:HG2	2.13	0.48
1:A:3:SER:O	1:A:4:GLN:CB	2.60	0.48
1:A:319:SER:N	1:A:394:GLU:OE1	2.46	0.48
1:A:344:SER:O	1:A:347:ASN:HB2	2.11	0.48
1:A:407:LYS:HD2	1:A:407:LYS:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:THR:O	1:A:489:VAL:HB	2.13	0.48
1:B:100:ASP:HB2	1:B:152:SER:O	2.13	0.48
1:B:315:ASN:HB3	1:B:387:ARG:HD3	1.95	0.48
1:B:107:VAL:HB	1:B:111:VAL:HG21	1.96	0.48
1:A:281:PRO:O	1:A:282:LEU:O	2.31	0.48
1:B:288:ASN:HD22	1:B:290:LYS:H	1.62	0.48
1:A:62:PHE:O	1:A:66:VAL:HG23	2.14	0.48
1:A:6:VAL:O	1:A:6:VAL:CG1	2.62	0.48
1:A:51:VAL:HG21	1:A:151:ILE:HD12	1.96	0.48
1:B:364:ILE:O	1:B:463:THR:HA	2.13	0.48
1:A:63:VAL:HG21	1:A:82:GLY:HA3	1.96	0.47
1:A:84:ILE:HD12	1:A:105:VAL:HG22	1.93	0.47
1:A:143:ILE:HG12	1:A:144:ILE:N	2.29	0.47
1:A:364:ILE:HD12	1:A:364:ILE:N	2.29	0.47
1:B:139:ALA:O	1:B:140:PHE:C	2.52	0.47
1:A:36:GLU:OE2	1:A:220:ARG:NH2	2.48	0.47
1:A:501:ASP:OD2	1:A:503:LYS:N	2.47	0.47
1:A:446:GLU:HG3	1:A:447:ASN:H	1.80	0.47
1:B:509:LEU:HD12	1:B:509:LEU:N	2.29	0.47
1:A:72:MET:HG2	1:A:76:MET:HB3	1.96	0.47
1:B:36:GLU:CD	1:B:220:ARG:HH22	2.17	0.47
1:B:104:LEU:HD21	1:B:188:LEU:HD12	1.96	0.47
3:B:605:3AT:H5'2	4:B:607:3AD:H5'1	1.96	0.47
1:A:397:ALA:HB1	1:A:479:VAL:HG11	1.95	0.47
1:B:18:ALA:HB2	1:B:251:CYS:HB3	1.97	0.47
1:B:26:ASN:O	1:B:30:ILE:HG12	2.15	0.47
1:B:182:GLU:OE1	1:B:285:ARG:NH2	2.39	0.47
1:B:423:MET:HA	1:B:426:ASP:OD1	2.14	0.47
1:A:206:VAL:HG21	6:A:859:HOH:O	2.14	0.46
1:B:3:SER:O	1:B:6:VAL:HG22	2.15	0.46
1:A:401:ILE:HG22	1:A:469:ASP:CB	2.45	0.46
1:A:396:LEU:HD12	1:A:397:ALA:N	2.30	0.46
1:A:107:VAL:CG2	1:A:111:VAL:HB	2.45	0.46
1:B:129:GLU:HB2	1:B:148:PHE:CZ	2.51	0.46
1:B:223:VAL:HG11	1:B:327:GLU:HG3	1.97	0.46
1:A:336:ASN:HD22	1:A:336:ASN:HA	1.53	0.46
1:B:288:ASN:HD21	1:B:290:LYS:HB2	1.81	0.46
1:A:125:ARG:HA	1:A:130:LEU:CD1	2.43	0.46
1:B:94:VAL:HG21	1:B:211:LEU:HD13	1.98	0.46
1:B:355:PHE:CD1	1:B:521:VAL:HG13	2.50	0.46
1:B:384:SER:OG	1:B:385:LYS:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:ARG:NH2	1:A:506:ASN:HA	2.30	0.45
1:A:132:GLU:HG2	1:A:147:LYS:CB	2.46	0.45
1:B:18:ALA:CB	1:B:251:CYS:HB3	2.46	0.45
1:B:132:GLU:HG3	1:B:147:LYS:HB2	1.99	0.45
1:B:299:ARG:HG3	1:B:299:ARG:NH1	2.32	0.45
1:B:347:ASN:HA	1:B:350:GLU:OE2	2.16	0.45
1:A:363:GLU:HG3	1:A:465:TYR:CZ	2.52	0.45
1:B:101:ILE:HD12	1:B:153:ILE:HD11	1.98	0.45
1:B:107:VAL:HG21	1:B:111:VAL:HB	1.98	0.45
1:B:52:LEU:HD23	1:B:55:LEU:HD12	1.98	0.45
1:B:353:ASP:OD1	1:B:353:ASP:O	2.33	0.45
1:B:435:THR:HA	1:B:438:ASN:HD22	1.82	0.45
1:A:196:GLU:O	1:A:200:LEU:HG	2.17	0.45
1:A:474:ASN:HD22	1:A:474:ASN:HA	1.54	0.45
1:B:180:LEU:HB2	1:B:185:LEU:CD2	2.46	0.45
1:B:396:LEU:CD1	1:B:399:ILE:HD13	2.47	0.45
1:A:334:ILE:O	1:A:338:ILE:HG13	2.17	0.45
1:B:125:ARG:HE	1:B:133:ILE:CG2	2.26	0.45
1:A:220:ARG:HD2	1:A:349:PHE:O	2.17	0.45
1:B:110:HIS:CD2	1:B:110:HIS:H	2.35	0.45
1:B:251:CYS:O	1:B:252:SER:CB	2.50	0.45
1:B:485:CYS:O	1:B:489:VAL:HG23	2.17	0.45
1:B:211:LEU:O	1:B:215:LYS:HB2	2.17	0.45
1:A:421:TYR:C	1:A:423:MET:N	2.70	0.44
1:B:141:VAL:HG11	4:B:607:3AD:C5	2.48	0.44
1:B:224:TYR:C	1:B:224:TYR:CD2	2.91	0.44
1:B:510:ARG:NH1	1:B:512:VAL:HG12	2.32	0.44
1:B:51:VAL:HG13	1:B:148:PHE:HD2	1.83	0.44
1:B:460:TYR:CD1	1:B:460:TYR:N	2.85	0.44
1:B:288:ASN:ND2	1:B:290:LYS:H	2.14	0.44
1:B:381:LEU:HD11	1:B:495:PHE:CG	2.53	0.44
1:A:6:VAL:HG13	1:A:202:PRO:HG3	1.99	0.44
1:A:125:ARG:C	1:A:127:ARG:H	2.21	0.44
1:B:354:PHE:CE2	1:B:405:PHE:HB2	2.53	0.44
1:A:251:CYS:SG	1:A:254:VAL:HG23	2.58	0.44
1:B:227:ILE:HD11	1:B:384:SER:HA	1.99	0.43
1:B:344:SER:O	1:B:347:ASN:HB2	2.18	0.43
1:B:399:ILE:N	1:B:399:ILE:HD12	2.33	0.43
1:B:493:ARG:HG2	1:B:493:ARG:HH11	1.83	0.43
1:A:395:VAL:O	1:A:395:VAL:HG12	2.18	0.43
1:A:486:THR:HG23	1:A:487:GLU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:PRO:O	1:A:137:PRO:HD3	2.18	0.43
1:B:125:ARG:NE	1:B:133:ILE:HG21	2.27	0.43
1:B:133:ILE:HA	1:B:146:ILE:HG22	2.01	0.43
1:B:427:LYS:HB3	1:B:436:ALA:HB3	2.01	0.43
1:B:238:MET:HE1	1:B:302:VAL:HG12	2.00	0.43
1:B:31:GLN:O	1:B:34:LYS:HB2	2.19	0.43
1:A:264:SER:HB3	1:A:328:PHE:HB3	2.01	0.43
1:A:368:THR:HG23	1:A:505:PHE:CE1	2.53	0.43
1:B:165:VAL:HG13	1:B:169:LEU:CD2	2.49	0.43
1:B:220:ARG:HG3	1:B:220:ARG:HH11	1.84	0.43
1:A:131:ASP:O	1:A:132:GLU:HB3	2.19	0.42
1:A:84:ILE:HG23	1:A:103:THR:CG2	2.50	0.42
1:A:281:PRO:O	1:A:282:LEU:C	2.57	0.42
1:A:473:GLU:HG3	1:A:475:LYS:HG2	2.00	0.42
1:B:100:ASP:HB3	1:B:152:SER:HB2	2.01	0.42
1:B:461:LEU:HD12	1:B:461:LEU:N	2.34	0.42
1:A:171:LEU:HA	1:A:176:LEU:CD1	2.49	0.42
1:B:371:SER:H	1:B:374:GLN:HE21	1.66	0.42
1:A:360:PHE:CZ	1:A:478:LYS:HE2	2.54	0.42
1:A:355:PHE:CG	1:A:521:VAL:HG13	2.55	0.42
1:B:180:LEU:HD12	1:B:185:LEU:HD23	2.01	0.42
1:B:269:PRO:O	1:B:301:PRO:HG2	2.20	0.42
1:A:444:THR:CG2	1:A:446:GLU:HG2	2.49	0.42
1:A:396:LEU:HG	1:A:399:ILE:HG13	2.01	0.42
1:A:444:THR:HG22	1:A:446:GLU:H	1.84	0.42
1:B:196:GLU:OE2	1:B:306:ALA:HA	2.19	0.42
1:B:510:ARG:HG2	1:B:510:ARG:NH1	2.32	0.42
1:B:510:ARG:HH11	1:B:512:VAL:HG12	1.85	0.42
1:B:460:TYR:C	1:B:461:LEU:HD12	2.40	0.42
1:B:108:PRO:HG2	1:B:111:VAL:CG2	2.49	0.41
1:B:485:CYS:O	1:B:488:PHE:HB3	2.20	0.41
1:B:59:ALA:HB2	1:B:84:ILE:HD13	2.02	0.41
1:B:108:PRO:HG2	1:B:111:VAL:HG23	2.02	0.41
1:A:180:LEU:CD1	1:A:188:LEU:HD12	2.50	0.41
1:B:371:SER:OG	1:B:374:GLN:HB2	2.20	0.41
1:B:381:LEU:HD13	1:B:499:TYR:CE1	2.54	0.41
1:B:510:ARG:HH11	1:B:510:ARG:CG	2.28	0.41
1:A:282:LEU:HD22	6:A:851:HOH:O	2.20	0.41
1:A:340:SER:O	1:A:341:ASN:HB2	2.21	0.41
1:A:493:ARG:HG3	1:A:493:ARG:HH11	1.85	0.41
1:A:426:ASP:O	1:A:427:LYS:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:PRO:HG2	1:B:273:ILE:CD1	2.50	0.41
1:B:526:GLU:HB2	1:B:527:LYS:H	1.75	0.41
1:A:261:ILE:HG12	1:A:332:VAL:HG13	2.01	0.41
1:B:56:GLN:HE22	1:B:84:ILE:H	1.68	0.41
1:B:242:ARG:HG2	1:B:272:VAL:HG13	2.03	0.41
1:B:288:ASN:C	1:B:288:ASN:ND2	2.73	0.41
1:A:89:SER:OG	1:A:95:HIS:CA	2.67	0.41
3:A:604:3AT:O4'	4:A:606:3AD:H2'	2.21	0.41
1:B:13:VAL:HG23	1:B:246:LEU:HB3	2.01	0.41
1:B:430:SER:HB2	1:B:516:ASP:OD2	2.21	0.41
1:B:493:ARG:CZ	1:B:502:HIS:NE2	2.84	0.41
1:B:501:ASP:HB3	1:B:504:VAL:CG1	2.50	0.41
1:B:501:ASP:O	1:B:502:HIS:HB2	2.21	0.41
1:A:401:ILE:HG22	1:A:469:ASP:HB3	2.02	0.41
1:A:501:ASP:OD2	1:A:504:VAL:N	2.48	0.41
1:B:288:ASN:HA	1:B:289:PRO:HD2	1.91	0.41
1:B:326:GLN:HE22	1:B:357:ARG:HH22	1.69	0.41
1:B:378:TRP:O	1:B:382:VAL:HG23	2.21	0.41
1:A:136:VAL:N	1:A:137:PRO:HD3	2.36	0.40
1:A:363:GLU:HB3	1:A:510:ARG:HG3	2.03	0.40
1:B:18:ALA:HA	1:B:22:GLU:OE2	2.20	0.40
1:A:354:PHE:CE2	1:A:405:PHE:HB2	2.56	0.40
1:A:26:ASN:HD21	1:A:252:SER:HB2	1.87	0.40
1:A:117:PHE:CD2	1:A:137:PRO:HG3	2.57	0.40
1:A:357:ARG:HG3	1:A:358:TYR:CE1	2.57	0.40
1:B:391:MET:HA	1:B:394:GLU:HG2	2.03	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	505/537 (94%)	456 (90%)	38 (8%)	11 (2%)	6 12
1	B	505/537 (94%)	450 (89%)	45 (9%)	10 (2%)	7 14
All	All	1010/1074 (94%)	906 (90%)	83 (8%)	21 (2%)	7 13

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	LEU
1	A	397	ALA
1	A	474	ASN
1	B	494	SER
1	B	527	LYS
1	A	4	GLN
1	A	281	PRO
1	A	502	HIS
1	B	225	ALA
1	B	252	SER
1	B	397	ALA
1	B	499	TYR
1	B	526	GLU
1	A	126	GLU
1	A	454	LYS
1	A	451	GLU
1	A	473	GLU
1	B	416	PRO
1	B	443	VAL
1	A	472	ILE
1	B	137	PRO

5.3.2 Protein sidechains (i)

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	432/479 (90%)	406 (94%)	26 (6%)	19 39
1	B	434/479 (91%)	415 (96%)	19 (4%)	28 53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	866/958 (90%)	821 (95%)	45 (5%)	23 46

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	43	GLN
1	A	130	LEU
1	A	138	ASP
1	A	182	GLU
1	A	185	LEU
1	A	211	LEU
1	A	220	ARG
1	A	224	TYR
1	A	249	ASN
1	A	263	LEU
1	A	270	GLN
1	A	272	VAL
1	A	336	ASN
1	A	388	LEU
1	A	392	LYS
1	A	393	LEU
1	A	396	LEU
1	A	407	LYS
1	A	418	GLU
1	A	453	ILE
1	A	474	ASN
1	A	510	ARG
1	A	519	ASP
1	A	521	VAL
1	A	523	ASP
1	B	50	GLN
1	B	84	ILE
1	B	109	LYS
1	B	130	LEU
1	B	205	ASN
1	B	211	LEU
1	B	224	TYR
1	B	239	LEU
1	B	242	ARG
1	B	252	SER
1	B	278	GLU

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Mol	Chain	Res	Type
1	B	288	ASN
1	B	303	ILE
1	B	376	LEU
1	B	393	LEU
1	B	435	THR
1	B	440	LEU
1	B	507	LEU
1	B	521	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	26	ASN
1	A	47	ASN
1	A	56	GLN
1	A	60	GLN
1	A	162	GLN
1	A	179	ASN
1	A	245	GLN
1	A	298	HIS
1	A	333	GLN
1	A	336	ASN
1	A	352	ASN
1	A	425	GLN
1	A	447	ASN
1	A	474	ASN
1	A	490	ASN
1	A	496	ASN
1	B	4	GLN
1	B	26	ASN
1	B	110	HIS
1	B	162	GLN
1	B	164	GLN
1	B	189	ASN
1	B	205	ASN
1	B	267	ASN
1	B	270	GLN
1	B	288	ASN
1	B	326	GLN
1	B	336	ASN
1	B	374	GLN

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Mol	Chain	Res	Type
1	B	375	HIS
1	B	438	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	$\#\|Z\| > 2$
4	3AD	A	606	-	17,20,20	0.69	0	16,29,29	0.79	1 (6%)
3	3AT	B	605	2	25,32,32	1.20	3 (12%)	28,50,50	1.14	3 (10%)
3	3AT	A	604	2	25,32,32	1.27	4 (16%)	28,50,50	1.49	4 (14%)
5	POP	A	817	-	6,8,8	1.19	0	13,13,13	0.75	0
4	3AD	B	607	-	17,20,20	0.68	0	16,29,29	0.81	1 (6%)

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
4	3AD	A	606	-	-	0/2/18/18	0/3/3/3
3	3AT	B	605	2	-	2/18/34/34	0/3/3/3
3	3AT	A	604	2	-	6/18/34/34	0/3/3/3
5	POP	A	817	-	-	1/6/6/6	-
4	3AD	B	607	-	-	1/2/18/18	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	604	3AT	C4-N3	3.21	1.40	1.35
3	B	605	3AT	C4-N3	3.13	1.40	1.35
3	A	604	3AT	C2-N3	2.43	1.36	1.32
3	A	604	3AT	C2'-C1'	2.17	1.56	1.54
3	A	604	3AT	PG-O3G	-2.14	1.46	1.54
3	B	605	3AT	C8-N7	-2.14	1.30	1.34
3	B	605	3AT	C2-N3	2.05	1.35	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	604	3AT	O3G-PG-O2G	3.54	121.17	107.64
3	A	604	3AT	O2G-PG-O3B	-3.53	92.81	104.64
3	A	604	3AT	O3B-PG-O1G	-2.58	96.89	111.19
4	B	607	3AD	C5-C6-N6	2.20	123.70	120.35
4	A	606	3AD	C5-C6-N6	2.18	123.67	120.35
3	B	605	3AT	C4-C5-N7	2.18	111.67	109.40
3	B	605	3AT	O3G-PG-O2G	2.05	115.48	107.64
3	B	605	3AT	O4'-C4'-C5'	-2.02	106.20	109.52
3	A	604	3AT	O4'-C1'-C2'	-2.00	104.00	106.93

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	604	3AT	PB-O3B-PG-O3G
3	A	604	3AT	PB-O3A-PA-O5'
3	A	604	3AT	C5'-O5'-PA-O1A
3	B	605	3AT	O4'-C4'-C5'-O5'
3	B	605	3AT	C3'-C4'-C5'-O5'
3	A	604	3AT	C5'-O5'-PA-O3A
3	A	604	3AT	C5'-O5'-PA-O2A
3	A	604	3AT	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
5	A	817	POP	P1-O-P2-O4
4	B	607	3AD	O4'-C4'-C5'-O5'

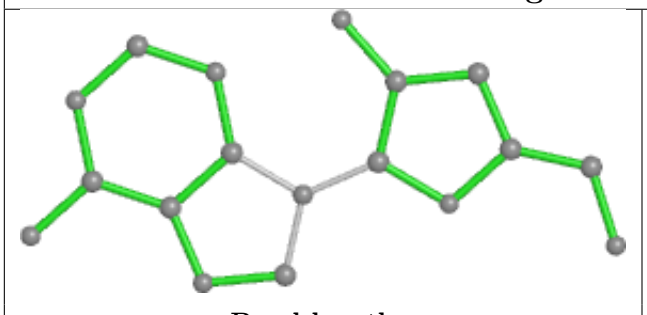
There are no ring outliers.

4 monomers are involved in 3 short contacts:

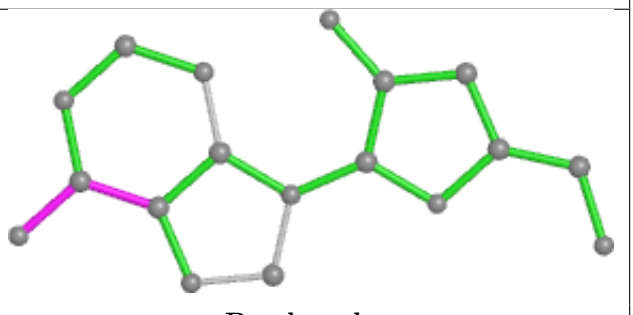
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	606	3AD	1	0
3	B	605	3AT	1	0
3	A	604	3AT	1	0
4	B	607	3AD	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

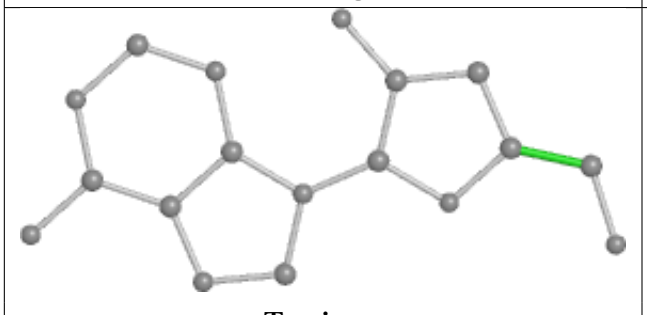
Ligand 3AD A 606



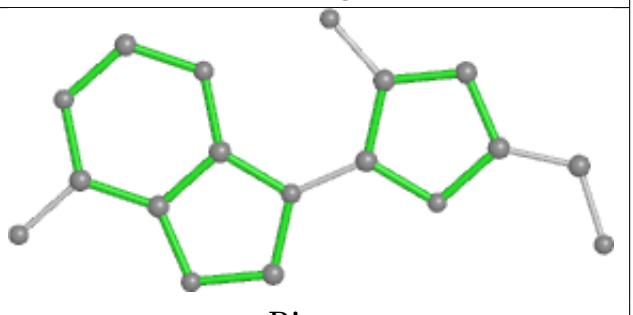
Bond lengths



Bond angles

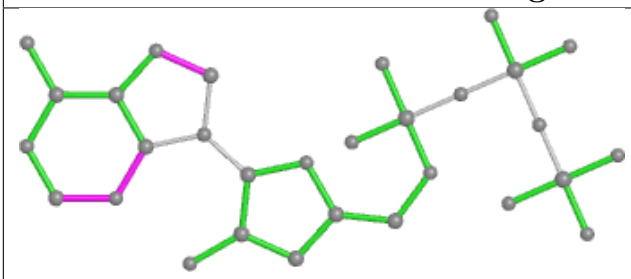


Torsions

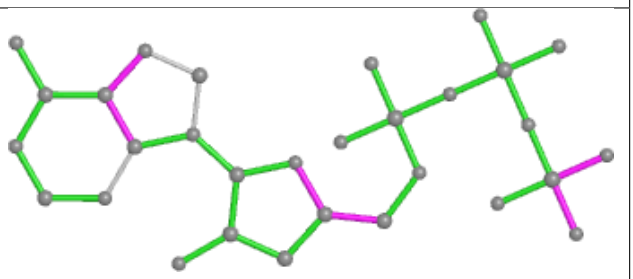


Rings

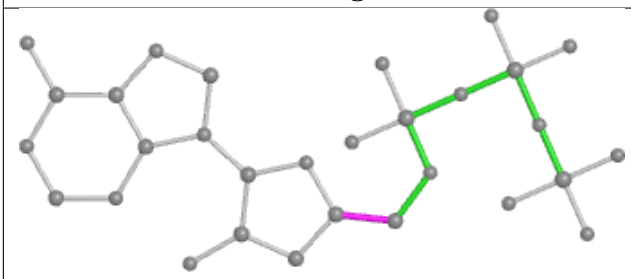
Ligand 3AT B 605



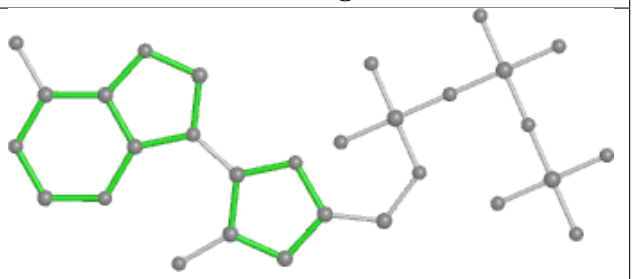
Bond lengths



Bond angles

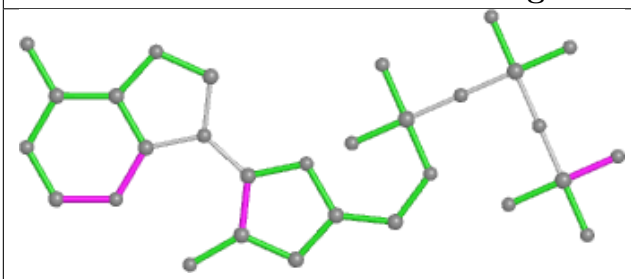


Torsions

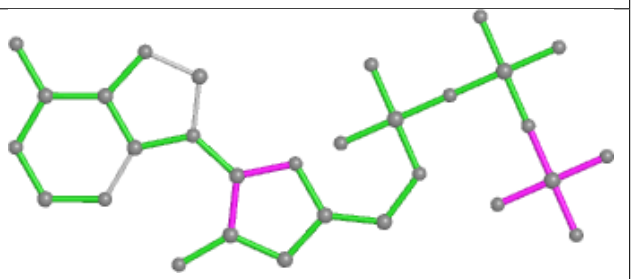


Rings

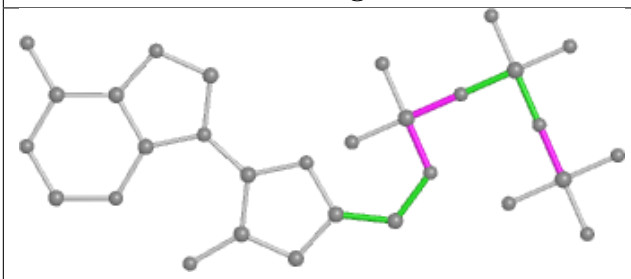
Ligand 3AT A 604



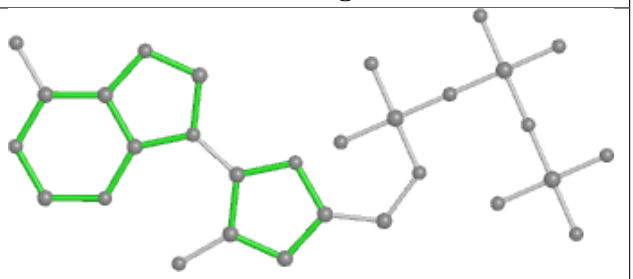
Bond lengths



Bond angles

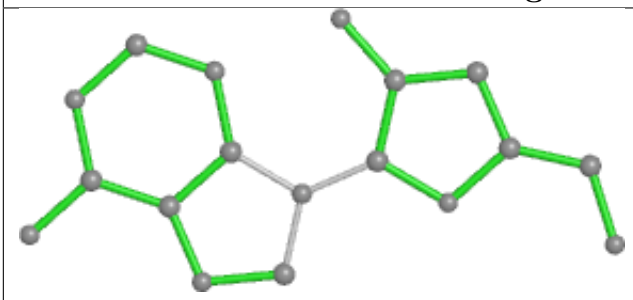


Torsions

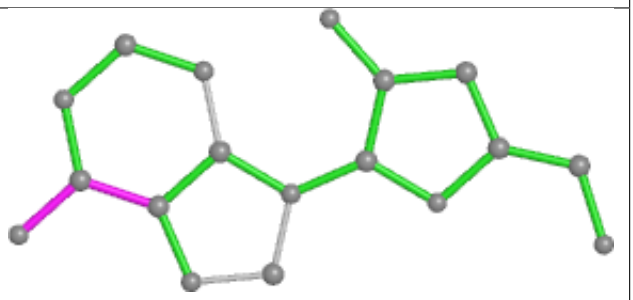


Rings

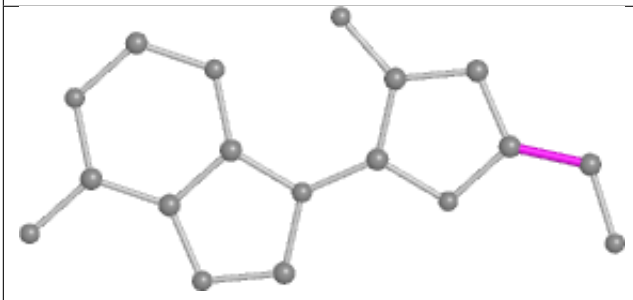
Ligand 3AD B 607



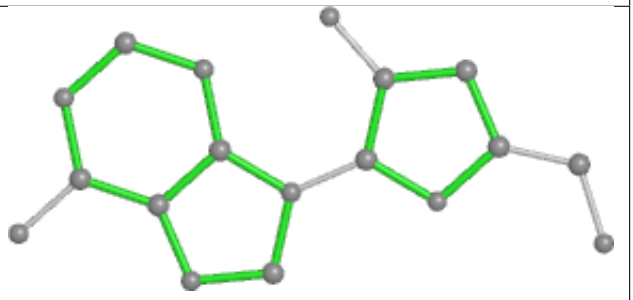
Bond lengths



Bond angles



Torsions



Rings

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.