Full wwPDB X-ray Structure Validation Report (i)

May 29, 2024 – 01:38 PM EDT

PDB ID	:	1VRU
Title	:	HIGH RESOLUTION STRUCTURES OF HIV-1 RT FROM FOUR RT-INHIBITOR COMPLEXES
Authors	:	Ren, J.; Esnouf, R.; Garman, E.; Somers, D.; Ross, C.; Kirby, I.; Keeling, J.; Darby, G.; Jones, Y.; Stuart, D.; Stammers, D.
Deposited on	:	1995-04-19
Resolution	:	2.40 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 (i) 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 (1)) were used in the production of this report:

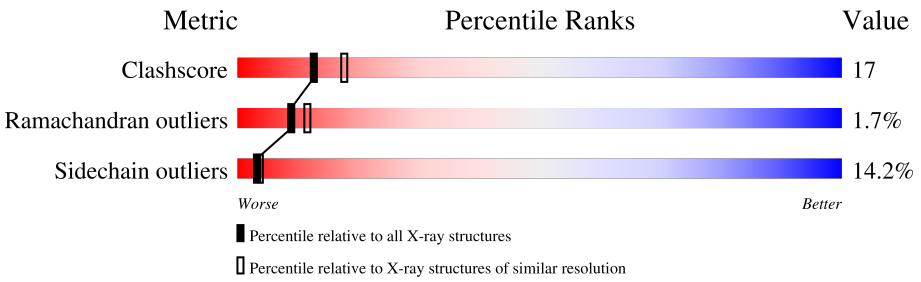
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.40 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	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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	560	54% 33% 7% • 6%
2	B	440	59% 30% • 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7852 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.

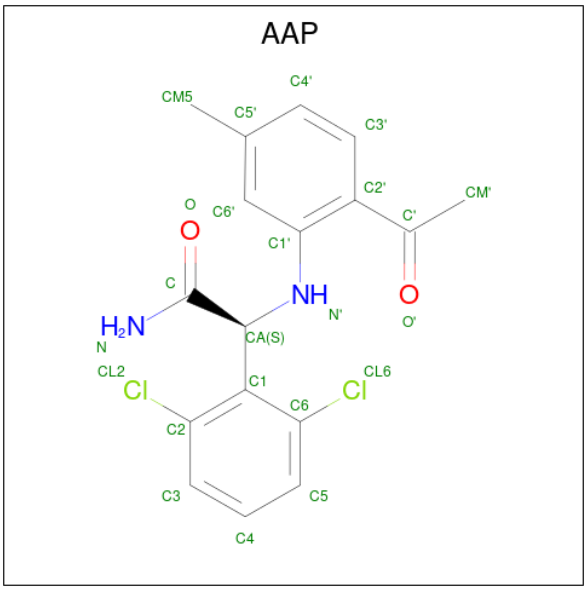
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	526	4316	2795	715	798	8	0	0	0

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	410	3382	2201	560	615	6	0	0	0

- Molecule 3 is ALPHA-(2,6-DICHLOROPHENYL)-ALPHA-(2-ACETYL-5-METHYLANILINO)ACETAMIDE (three-letter code: AAP) (formula: $C_{17}H_{16}Cl_2N_2O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	23	17	2	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	72	72	72	0	0
			Total	O		
4	B	59	59	59	0	0

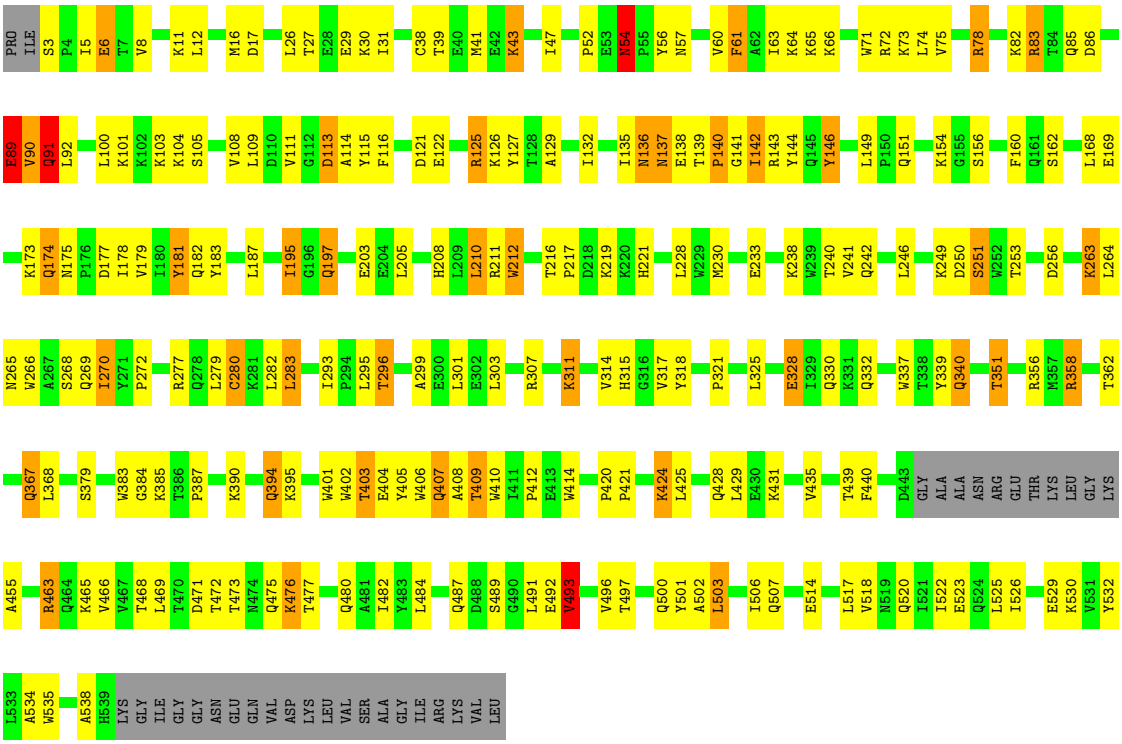
3 Residue-property plots (i)

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.

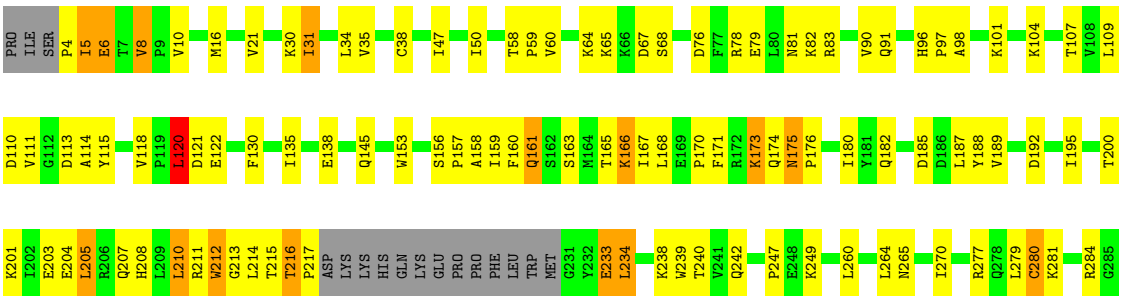
• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE

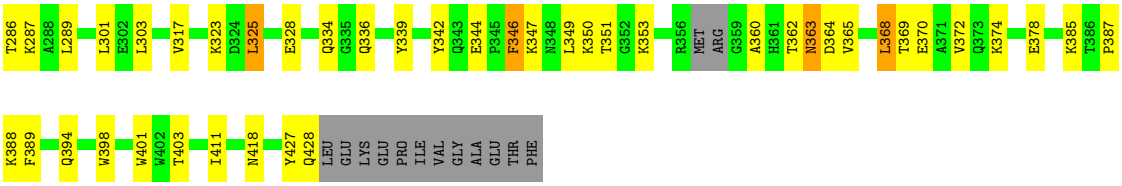
Chain A: 54% 33% 7% • 6%



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE

Chain B: 59% 30% • 7%




T286
K287
A288
L289
L301
E302
L303
V317
K323
D324
L325
E328
Q334
G335
Q336
Y339
Y342
Q343
E344
P345
F346
K347
N348
L349
K350
T351
G352
K353
R356
MET
ARG
G359
A360
H361
T362
N363
D364
V365
L368
T369
E370
A371
V372
Q373
K374
E378
K385
T386
P387
K388
F389
Q394
W398
W401
W402
T403
I411
N418
Y427
Q428
LEU
GLU
LYS
GLU
PRO
ILE
VAL
GLY
ALA
GLU
THR
PHE

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	143.20Å 116.80Å 66.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40	Depositor
% Data completeness (in resolution range)	86.5 (25.00-2.40)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7852	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

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: AAP, CSD

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	0.76	0/4423	0.92	6/6014 (0.1%)
2	B	0.77	0/3478	0.90	4/4727 (0.1%)
All	All	0.77	0/7901	0.91	10/10741 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	54	ASN	N-CA-C	-9.38	85.69	111.00
1	A	538	ALA	N-CA-C	6.87	129.55	111.00
1	A	210	LEU	CA-CB-CG	-5.80	101.95	115.30
2	B	279	LEU	CA-CB-CG	-5.66	102.28	115.30
1	A	141	GLY	N-CA-C	-5.40	99.59	113.10
1	A	493	VAL	CB-CA-C	-5.30	101.33	111.40
2	B	185	ASP	CB-CG-OD1	5.23	123.00	118.30
2	B	120	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	358	ARG	N-CA-C	-5.13	97.14	111.00
2	B	34	LEU	CB-CG-CD1	-5.12	102.30	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	TYR	Sidechain
1	A	181	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4316	0	4347	162	0
2	B	3382	0	3410	102	0
3	A	23	0	16	2	0
4	A	72	0	0	4	0
4	B	59	0	0	2	0
All	All	7852	0	7773	258	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 17.

All (258) 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:406:TRP:CZ3	1:A:407:GLN:HG3	1.99	0.97
2:B:280:CYS:HB3	2:B:284:ARG:HH21	1.32	0.93
1:A:472:THR:HG22	1:A:476:LYS:HD2	1.48	0.92
1:A:315:HIS:HB3	4:A:1036:HOH:O	1.71	0.90
1:A:330:GLN:HE22	1:A:340:GLN:HE21	1.20	0.87
2:B:65:LYS:HB2	2:B:68:SER:HB2	1.56	0.86
1:A:503:LEU:O	1:A:507:GLN:HB2	1.76	0.85
1:A:503:LEU:HD13	1:A:535:TRP:HB2	1.59	0.83
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.15	0.81
1:A:296:THR:HG22	1:A:299:ALA:H	1.46	0.80
2:B:64:LYS:HD3	2:B:65:LYS:H	1.47	0.79
2:B:210:LEU:HA	2:B:214:LEU:O	1.85	0.77
1:A:197:GLN:HE21	1:A:197:GLN:HA	1.49	0.76
1:A:63:ILE:HG22	1:A:74:LEU:HD11	1.68	0.76
1:A:139:THR:CG2	1:A:140:PRO:HD2	2.16	0.76
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.25	0.75
1:A:78:ARG:HG2	1:A:78:ARG:HH11	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:LYS:HG2	2:B:192:ASP:OD1	1.86	0.75
1:A:241:VAL:HG13	1:A:266:TRP:HE1	1.51	0.74
1:A:113:ASP:HB2	1:A:116:PHE:HD2	1.53	0.74
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.70	0.74
1:A:111:VAL:HG12	1:A:114:ALA:HB2	1.70	0.73
1:A:139:THR:HG22	1:A:140:PRO:HD2	1.70	0.73
2:B:163:SER:O	2:B:167:ILE:HG13	1.89	0.73
2:B:362:THR:O	2:B:363:ASN:HB3	1.90	0.71
2:B:203:GLU:HG2	2:B:207:GLN:HE22	1.54	0.71
2:B:280:CYS:HB3	2:B:284:ARG:NH2	2.05	0.71
1:A:39:THR:O	1:A:43:LYS:HE2	1.90	0.71
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.25	0.71
1:A:330:GLN:HE22	1:A:340:GLN:NE2	1.88	0.70
2:B:161:GLN:HE21	2:B:161:GLN:HA	1.56	0.70
1:A:115:TYR:HB2	1:A:151:GLN:HE22	1.56	0.68
1:A:125:ARG:HB3	1:A:146:TYR:O	1.91	0.68
2:B:334:GLN:HA	2:B:360:ALA:HB2	1.74	0.68
1:A:64:LYS:HB3	1:A:71:TRP:HA	1.74	0.68
1:A:91:GLN:O	1:A:91:GLN:HG2	1.94	0.67
1:A:142:ILE:HD13	1:A:142:ILE:H	1.60	0.66
1:A:332:GLN:O	1:A:332:GLN:HG2	1.95	0.66
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.31	0.65
1:A:16:MET:HG3	1:A:83:ARG:HG3	1.79	0.65
1:A:491:LEU:O	1:A:529:GLU:HB2	1.95	0.65
1:A:27:THR:HG23	1:A:30:LYS:HB2	1.78	0.65
2:B:173:LYS:HA	2:B:176:PRO:HG3	1.79	0.65
2:B:5:ILE:HG13	2:B:6:GLU:H	1.62	0.65
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.32	0.64
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.77	0.64
1:A:241:VAL:HG13	1:A:266:TRP:NE1	2.13	0.64
1:A:268:SER:O	1:A:351:THR:HG22	1.97	0.64
1:A:402:TRP:CZ3	1:A:409:THR:HB	2.33	0.64
2:B:175:ASN:HD22	2:B:201:LYS:NZ	1.97	0.63
1:A:101:LYS:HE3	1:A:321:PRO:HG3	1.80	0.63
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.80	0.62
1:A:136:ASN:HB3	1:A:139:THR:OG1	1.99	0.62
1:A:197:GLN:HA	1:A:197:GLN:NE2	2.14	0.62
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.80	0.62
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.80	0.62
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.82	0.61
2:B:167:ILE:HG23	2:B:212:TRP:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:CG2	1:A:30:LYS:HB2	2.30	0.61
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.36	0.60
2:B:350:LYS:HG3	2:B:351:THR:N	2.16	0.60
2:B:334:GLN:C	2:B:360:ALA:HB2	2.22	0.60
1:A:132:ILE:HB	1:A:142:ILE:HG12	1.83	0.60
2:B:277:ARG:O	2:B:281:LYS:HG3	2.02	0.60
1:A:469:LEU:HD23	4:A:1066:HOH:O	2.00	0.60
1:A:139:THR:HG22	1:A:140:PRO:CD	2.31	0.59
1:A:113:ASP:HB2	1:A:116:PHE:CD2	2.34	0.59
1:A:465:LYS:HZ3	1:A:484:LEU:HD22	1.66	0.59
2:B:212:TRP:HA	2:B:212:TRP:CE3	2.36	0.59
1:A:114:ALA:HB1	1:A:160:PHE:HE1	1.67	0.59
1:A:518:VAL:O	1:A:522:ILE:HG13	2.02	0.59
1:A:73:LYS:HE2	1:A:75:VAL:HG22	1.84	0.59
2:B:64:LYS:HD3	2:B:65:LYS:N	2.16	0.59
1:A:379:SER:CB	1:A:387:PRO:HD3	2.33	0.58
1:A:47:ILE:HD12	1:A:144:TYR:CD2	2.38	0.58
1:A:517:LEU:HA	1:A:520:GLN:NE2	2.19	0.58
2:B:161:GLN:HE21	2:B:161:GLN:CA	2.14	0.58
2:B:260:LEU:O	2:B:264:LEU:HB2	2.03	0.58
1:A:3:SER:OG	1:A:212:TRP:HB3	2.04	0.57
1:A:401:TRP:HZ3	1:A:402:TRP:CZ2	2.22	0.57
2:B:175:ASN:HD22	2:B:201:LYS:HZ1	1.52	0.57
2:B:334:GLN:CA	2:B:360:ALA:HB2	2.34	0.57
2:B:38:CYS:O	2:B:47:ILE:HD11	2.04	0.57
2:B:110:ASP:O	2:B:216:THR:HG22	2.02	0.57
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.69	0.57
1:A:492:GLU:HA	1:A:530:LYS:O	2.05	0.57
1:A:497:THR:O	1:A:535:TRP:HA	2.04	0.57
2:B:167:ILE:HG23	2:B:212:TRP:CB	2.34	0.57
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.39	0.57
1:A:12:LEU:HD11	1:A:127:TYR:CE2	2.39	0.57
1:A:174:GLN:HE21	1:A:174:GLN:HA	1.69	0.57
1:A:465:LYS:NZ	1:A:484:LEU:HD22	2.20	0.57
1:A:129:ALA:HA	1:A:144:TYR:O	2.04	0.57
1:A:27:THR:HG23	1:A:30:LYS:H	1.70	0.56
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.40	0.56
2:B:344:GLU:HB2	2:B:347:LYS:HB2	1.86	0.56
1:A:522:ILE:O	1:A:526:ILE:HG13	2.06	0.56
2:B:65:LYS:CB	2:B:68:SER:HB2	2.32	0.56
2:B:428:GLN:NE2	2:B:428:GLN:HA	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:PHE:HD1	1:A:61:PHE:N	2.05	0.55
1:A:263:LYS:N	1:A:263:LYS:HE3	2.22	0.55
1:A:65:LYS:HG3	1:A:66:LYS:N	2.22	0.55
2:B:212:TRP:HA	2:B:212:TRP:HE3	1.71	0.55
2:B:59:PRO:HG2	2:B:76:ASP:HB3	1.88	0.55
2:B:233:GLU:HB2	4:B:1103:HOH:O	2.06	0.54
1:A:17:ASP:O	1:A:83:ARG:HG2	2.07	0.54
1:A:406:TRP:CH2	1:A:407:GLN:HG3	2.42	0.54
2:B:200:THR:O	2:B:204:GLU:HG2	2.07	0.54
2:B:158:ALA:O	2:B:161:GLN:HB3	2.08	0.54
2:B:203:GLU:HG2	2:B:207:GLN:NE2	2.22	0.54
2:B:211:ARG:O	2:B:212:TRP:HE3	1.91	0.54
2:B:328:GLU:O	2:B:339:TYR:HA	2.08	0.54
1:A:61:PHE:N	1:A:61:PHE:CD1	2.76	0.54
1:A:270:ILE:HD12	1:A:270:ILE:H	1.73	0.53
2:B:79:GLU:O	2:B:83:ARG:HG3	2.07	0.53
1:A:115:TYR:CB	1:A:151:GLN:HE22	2.22	0.53
2:B:98:ALA:O	2:B:101:LYS:HG2	2.08	0.53
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.90	0.53
1:A:89:GLU:CB	1:A:92:LEU:HD12	2.39	0.53
1:A:89:GLU:CD	1:A:92:LEU:HB2	2.29	0.52
1:A:5:ILE:HG13	1:A:6:GLU:N	2.24	0.52
3:A:999:AAP:HM'1	2:B:138:GLU:HG2	1.91	0.52
1:A:424:LYS:HG2	1:A:425:LEU:N	2.24	0.52
1:A:270:ILE:O	1:A:272:PRO:HD3	2.10	0.51
2:B:175:ASN:ND2	2:B:201:LYS:NZ	2.57	0.51
2:B:284:ARG:O	2:B:287:LYS:NZ	2.44	0.51
1:A:401:TRP:HZ3	1:A:402:TRP:CE2	2.29	0.51
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.45	0.51
1:A:463:ARG:NH1	1:A:463:ARG:HG2	2.26	0.51
1:A:465:LYS:HG2	1:A:466:VAL:N	2.26	0.51
1:A:115:TYR:CD2	1:A:156:SER:HB3	2.46	0.51
1:A:64:LYS:HA	1:A:72:ARG:HD3	1.93	0.51
1:A:406:TRP:HH2	1:A:407:GLN:HE21	1.59	0.50
2:B:64:LYS:HE2	2:B:68:SER:O	2.11	0.50
1:A:78:ARG:O	1:A:82:LYS:HG3	2.11	0.50
1:A:78:ARG:HG2	1:A:78:ARG:NH1	2.23	0.49
1:A:270:ILE:HD12	1:A:270:ILE:N	2.27	0.49
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.42	0.49
1:A:86:ASP:HA	1:A:154:LYS:HE2	1.95	0.49
1:A:395:LYS:HA	1:A:414:TRP:CH2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:LYS:HE2	2:B:166:LYS:O	2.12	0.49
1:A:39:THR:HG23	1:A:43:LYS:CE	2.42	0.49
2:B:180:ILE:CD1	2:B:205:LEU:HD11	2.43	0.49
1:A:208:HIS:O	1:A:212:TRP:CD1	2.65	0.49
2:B:207:GLN:O	2:B:210:LEU:HG	2.13	0.49
1:A:63:ILE:O	1:A:72:ARG:HB2	2.13	0.49
1:A:142:ILE:HD13	1:A:142:ILE:N	2.27	0.48
1:A:384:GLY:HA3	2:B:135:ILE:HD13	1.95	0.48
1:A:337:TRP:HE1	1:A:367:GLN:NE2	2.11	0.48
2:B:114:ALA:HB1	2:B:160:PHE:CE2	2.49	0.48
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.96	0.48
2:B:170:PRO:O	2:B:174:GLN:HB2	2.13	0.48
1:A:11:LYS:O	1:A:85:GLN:HG2	2.14	0.48
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.96	0.48
2:B:78:ARG:O	2:B:82:LYS:HG3	2.13	0.48
1:A:29:GLU:HG3	1:A:30:LYS:N	2.28	0.47
1:A:108:VAL:HA	1:A:187:LEU:O	2.12	0.47
2:B:115:TYR:OH	2:B:157:PRO:HB3	2.13	0.47
2:B:120:LEU:O	2:B:121:ASP:C	2.51	0.47
2:B:216:THR:HA	2:B:217:PRO:HD3	1.76	0.47
1:A:8:VAL:O	1:A:121:ASP:HB2	2.13	0.47
1:A:103:LYS:HE3	1:A:179:VAL:HG21	1.97	0.47
1:A:111:VAL:CG1	1:A:114:ALA:HB2	2.43	0.47
1:A:402:TRP:CD2	1:A:409:THR:HG21	2.50	0.47
2:B:58:THR:HG23	2:B:76:ASP:O	2.14	0.47
1:A:500:GLN:HB2	4:A:1071:HOH:O	2.15	0.47
1:A:463:ARG:HG2	1:A:463:ARG:HH11	1.80	0.46
2:B:180:ILE:HD11	2:B:205:LEU:HD11	1.96	0.46
1:A:73:LYS:HE2	1:A:75:VAL:CG2	2.44	0.46
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.50	0.46
1:A:38:CYS:SG	1:A:132:ILE:CD1	3.01	0.46
2:B:187:LEU:HD12	2:B:187:LEU:HA	1.72	0.46
1:A:330:GLN:NE2	1:A:340:GLN:NE2	2.62	0.46
2:B:370:GLU:O	2:B:374:LYS:HD3	2.15	0.46
1:A:11:LYS:HD2	4:A:1024:HOH:O	2.15	0.46
1:A:328:GLU:O	1:A:339:TYR:HA	2.15	0.46
2:B:76:ASP:HA	2:B:411:ILE:HD12	1.97	0.46
1:A:401:TRP:CZ3	1:A:402:TRP:CE2	3.04	0.45
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.47	0.45
2:B:389:PHE:CD1	2:B:389:PHE:N	2.84	0.45
1:A:465:LYS:HZ3	1:A:484:LEU:CD2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:180:ILE:HG12	2:B:189:VAL:HG13	1.97	0.45
1:A:57:ASN:ND2	1:A:143:ARG:NH1	2.64	0.45
2:B:31:ILE:O	2:B:35:VAL:HG23	2.17	0.45
1:A:403:THR:HG22	1:A:404:GLU:N	2.32	0.45
2:B:180:ILE:HA	2:B:188:TYR:O	2.17	0.45
1:A:26:LEU:HB3	1:A:31:ILE:HG13	1.99	0.45
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.99	0.45
2:B:16:MET:HE2	2:B:83:ARG:HG2	1.98	0.45
1:A:100:LEU:O	1:A:318:TYR:HB3	2.17	0.44
1:A:169:GLU:O	1:A:173:LYS:HD3	2.16	0.44
1:A:379:SER:OG	1:A:387:PRO:HD3	2.17	0.44
2:B:8:VAL:HG21	2:B:159:ILE:HG12	1.99	0.44
1:A:266:TRP:O	1:A:269:GLN:HG2	2.18	0.44
2:B:96:HIS:HA	2:B:97:PRO:HD3	1.69	0.44
1:A:358:ARG:NH2	2:B:394:GLN:HG2	2.32	0.44
2:B:214:LEU:HD12	2:B:215:THR:H	1.82	0.44
1:A:56:TYR:O	1:A:143:ARG:NH2	2.44	0.44
1:A:89:GLU:HB3	1:A:92:LEU:HD12	1.99	0.44
1:A:424:LYS:HE2	1:A:424:LYS:HB3	1.71	0.44
2:B:81:ASN:OD1	2:B:153:TRP:HD1	2.01	0.44
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.52	0.44
3:A:999:AAP:CL6	3:A:999:AAP:H6'	2.55	0.44
1:A:54:ASN:C	1:A:54:ASN:HD22	2.20	0.44
2:B:428:GLN:HA	2:B:428:GLN:HE21	1.81	0.44
1:A:115:TYR:O	1:A:149:LEU:HB2	2.18	0.44
1:A:135:ILE:HG13	1:A:135:ILE:O	2.17	0.44
1:A:263:LYS:HE3	1:A:263:LYS:CA	2.47	0.44
1:A:293:ILE:N	1:A:293:ILE:HD12	2.33	0.44
1:A:402:TRP:CE3	1:A:409:THR:CG2	3.00	0.44
2:B:323:LYS:O	2:B:385:LYS:NZ	2.47	0.44
2:B:353:LYS:NZ	2:B:428:GLN:HG2	2.33	0.44
1:A:455:ALA:HB2	1:A:477:THR:HG23	2.00	0.43
1:A:139:THR:HG22	1:A:140:PRO:HG2	2.00	0.43
2:B:158:ALA:O	2:B:161:GLN:CB	2.66	0.43
1:A:394:GLN:HE21	1:A:394:GLN:HB2	1.71	0.43
1:A:12:LEU:HD22	1:A:83:ARG:HB3	2.00	0.43
1:A:54:ASN:HD22	1:A:56:TYR:H	1.66	0.43
2:B:60:VAL:HG21	2:B:130:PHE:CD2	2.54	0.43
2:B:211:ARG:O	2:B:212:TRP:CE3	2.71	0.43
2:B:342:TYR:HA	2:B:349:LEU:HD13	2.01	0.43
1:A:137:ASN:ND2	1:A:138:GLU:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:427:TYR:O	2:B:428:GLN:HB2	2.19	0.42
1:A:39:THR:HG23	1:A:43:LYS:HE3	2.02	0.42
1:A:328:GLU:HG3	1:A:390:LYS:HD3	2.00	0.42
2:B:166:LYS:HE2	2:B:166:LYS:C	2.39	0.42
1:A:482:ILE:HD12	1:A:502:ALA:HB1	2.01	0.42
2:B:168:LEU:HD21	2:B:180:ILE:HG21	2.00	0.42
1:A:104:LYS:HE3	1:A:104:LYS:HB2	1.89	0.42
1:A:420:PRO:HA	1:A:421:PRO:C	2.39	0.42
1:A:89:GLU:HB2	1:A:92:LEU:HD12	2.02	0.42
1:A:402:TRP:CZ3	1:A:405:TYR:HD2	2.37	0.42
1:A:520:GLN:O	1:A:523:GLU:HB2	2.20	0.42
1:A:103:LYS:HD3	1:A:103:LYS:HA	1.43	0.42
1:A:253:THR:O	1:A:256:ASP:HB2	2.20	0.41
1:A:296:THR:HG22	1:A:299:ALA:N	2.26	0.41
2:B:270:ILE:HG12	2:B:346:PHE:HB3	2.02	0.41
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.85	0.41
2:B:208:HIS:O	2:B:208:HIS:CG	2.74	0.41
2:B:325:LEU:HB3	2:B:387:PRO:HB3	2.02	0.41
2:B:284:ARG:HG3	2:B:284:ARG:NH1	2.33	0.41
2:B:368:LEU:O	2:B:372:VAL:HG23	2.21	0.41
1:A:217:PRO:HB2	1:A:221:HIS:HB2	2.02	0.41
1:A:249:LYS:HG3	1:A:251:SER:O	2.21	0.41
1:A:280:CSD:O	1:A:283:LEU:HB2	2.21	0.41
2:B:114:ALA:CA	2:B:214:LEU:HD13	2.50	0.41
1:A:139:THR:HG22	1:A:140:PRO:CG	2.51	0.41
1:A:246:LEU:HB3	1:A:307:ARG:NH1	2.36	0.41
1:A:233:GLU:N	1:A:240:THR:O	2.48	0.40
1:A:489:SER:HB2	1:A:493:VAL:HG13	2.01	0.40
2:B:118:VAL:HG21	2:B:160:PHE:HD1	1.86	0.40
1:A:41:MET:HB3	1:A:47:ILE:HG12	2.02	0.40
2:B:215:THR:O	2:B:216:THR:HG23	2.21	0.40
1:A:114:ALA:CB	1:A:160:PHE:CE1	3.04	0.40
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.56	0.40
2:B:247:PRO:HG3	4:B:1107:HOH:O	2.21	0.40
1:A:311:LYS:HA	1:A:311:LYS:HD3	1.89	0.40
1:A:476:LYS:HD3	1:A:480:GLN: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	521/560 (93%)	491 (94%)	21 (4%)	9 (2%)	9 11
2	B	404/440 (92%)	367 (91%)	30 (7%)	7 (2%)	9 11
All	All	925/1000 (92%)	858 (93%)	51 (6%)	16 (2%)	9 11

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	113	ASP
1	A	140	PRO
1	A	219	LYS
2	B	363	ASN
1	A	412	PRO
2	B	195	ILE
1	A	91	GLN
2	B	234	LEU
1	A	89	GLU
1	A	195	ILE
2	B	346	PHE
1	A	90	VAL
1	A	137	ASN
2	B	90	VAL
2	B	213	GLY
2	B	175	ASN

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	474/499 (95%)	396 (84%)	78 (16%)	2 2
2	B	372/400 (93%)	330 (89%)	42 (11%)	6 8
All	All	846/899 (94%)	726 (86%)	120 (14%)	3 4

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	43	LYS
1	A	52	PRO
1	A	54	ASN
1	A	61	PHE
1	A	78	ARG
1	A	83	ARG
1	A	89	GLU
1	A	90	VAL
1	A	91	GLN
1	A	105	SER
1	A	109	LEU
1	A	122	GLU
1	A	125	ARG
1	A	126	LYS
1	A	136	ASN
1	A	142	ILE
1	A	162	SER
1	A	168	LEU
1	A	174	GLN
1	A	177	ASP
1	A	182	GLN
1	A	195	ILE
1	A	197	GLN
1	A	203	GLU
1	A	205	LEU
1	A	210	LEU
1	A	211	ARG
1	A	212	TRP
1	A	216	THR
1	A	228	LEU
1	A	230	MET
1	A	238	LYS
1	A	242	GLN
1	A	250	ASP

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Mol	Chain	Res	Type
1	A	251	SER
1	A	263	LYS
1	A	264	LEU
1	A	265	ASN
1	A	270	ILE
1	A	277	ARG
1	A	279	LEU
1	A	282	LEU
1	A	283	LEU
1	A	295	LEU
1	A	296	THR
1	A	301	LEU
1	A	303	LEU
1	A	311	LYS
1	A	314	VAL
1	A	317	VAL
1	A	328	GLU
1	A	340	GLN
1	A	351	THR
1	A	356	ARG
1	A	362	THR
1	A	367	GLN
1	A	368	LEU
1	A	385	LYS
1	A	394	GLN
1	A	403	THR
1	A	407	GLN
1	A	409	THR
1	A	424	LYS
1	A	428	GLN
1	A	431	LYS
1	A	435	VAL
1	A	463	ARG
1	A	468	THR
1	A	471	ASP
1	A	473	THR
1	A	476	LYS
1	A	487	GLN
1	A	493	VAL
1	A	496	VAL
1	A	503	LEU
1	A	514	GLU

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Mol	Chain	Res	Type
1	A	525	LEU
2	B	4	PRO
2	B	5	ILE
2	B	6	GLU
2	B	8	VAL
2	B	10	VAL
2	B	30	LYS
2	B	31	ILE
2	B	67	ASP
2	B	91	GLN
2	B	107	THR
2	B	109	LEU
2	B	113	ASP
2	B	120	LEU
2	B	122	GLU
2	B	156	SER
2	B	161	GLN
2	B	165	THR
2	B	166	LYS
2	B	171	PHE
2	B	173	LYS
2	B	182	GLN
2	B	205	LEU
2	B	210	LEU
2	B	212	TRP
2	B	216	THR
2	B	233	GLU
2	B	234	LEU
2	B	238	LYS
2	B	240	THR
2	B	242	GLN
2	B	249	LYS
2	B	265	ASN
2	B	280	CYS
2	B	286	THR
2	B	301	LEU
2	B	303	LEU
2	B	317	VAL
2	B	325	LEU
2	B	336	GLN
2	B	368	LEU
2	B	388	LYS

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Mol	Chain	Res	Type
2	B	403	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	137	ASN
1	A	151	GLN
1	A	174	GLN
1	A	197	GLN
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	340	GLN
1	A	367	GLN
1	A	373	GLN
1	A	394	GLN
1	A	520	GLN
1	A	524	GLN
2	B	57	ASN
2	B	91	GLN
2	B	96	HIS
2	B	145	GLN
2	B	147	ASN
2	B	151	GLN
2	B	161	GLN
2	B	175	ASN
2	B	207	GLN
2	B	242	GLN
2	B	278	GLN
2	B	336	GLN
2	B	418	ASN
2	B	428	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSD	A	280	1	3,7,8	1.08	0	1,8,10	10.43	1 (100%)

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
1	CSD	A	280	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	CSD	OD1-SG-CB	10.43	125.38	105.54

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	AAP	A	999	-	24,24,24	1.05	1 (4%)	27,34,34	1.25	3 (11%)

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	AAP	A	999	-	-	4/16/16/16	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	AAP	C2'-C'	3.22	1.55	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999	AAP	C6-C1-C2	3.83	119.33	114.91
3	A	999	AAP	C3-C2-C1	-2.53	119.23	122.39
3	A	999	AAP	C1-C2-CL2	2.48	122.89	120.49

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	AAP	O-C-CA-C1
3	A	999	AAP	N-C-CA-C1
3	A	999	AAP	O-C-CA-N'
3	A	999	AAP	N-C-CA-N'

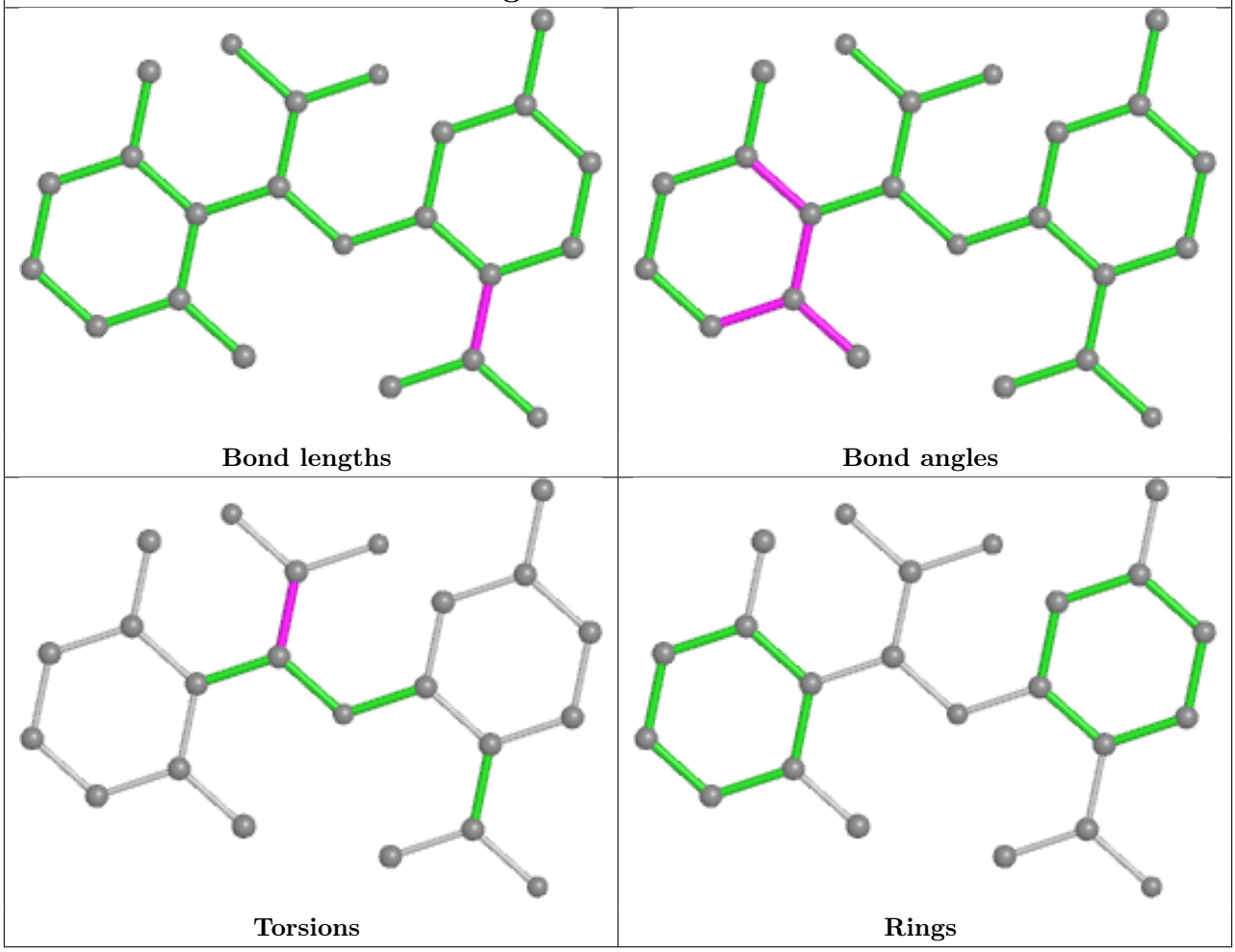
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	AAP	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 AAP A 999



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.