



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:55 PM GMT

PDB ID : 1VRT  
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 : 2.20 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

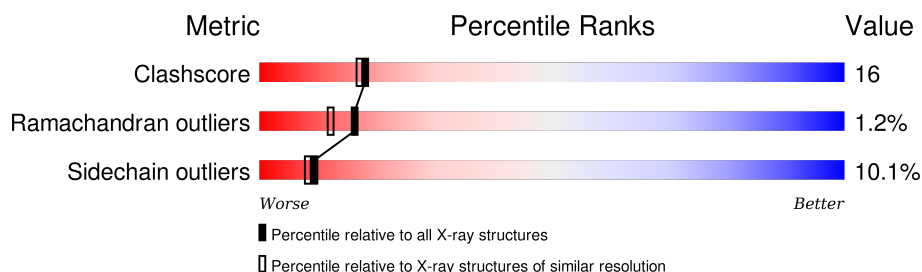
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	
2	B	440	

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7953 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
1	A	525	Total	C	N	O	S	0	0	0
			4310	2792	714	796	8			

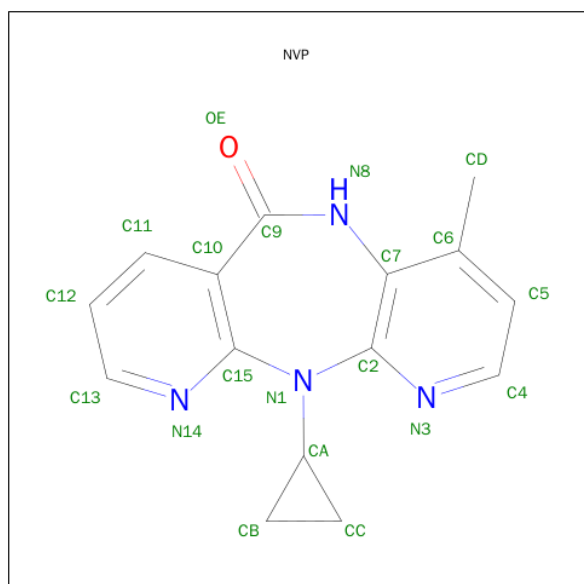
- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	401	Total	C	N	O	S	0	0	0
			3317	2161	548	602	6			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 11-CYCLOPROPYL-5,11-DIHYDRO-4-METHYL-6H-DIPYRIDO[3,2-B:2',3'-E][1,4]DIAZEPIN-6-ONE (three-letter code: NVP) (formula: C<sub>15</sub>H<sub>14</sub>N<sub>4</sub>O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			20	15	4	1		

- Molecule 5 is water.

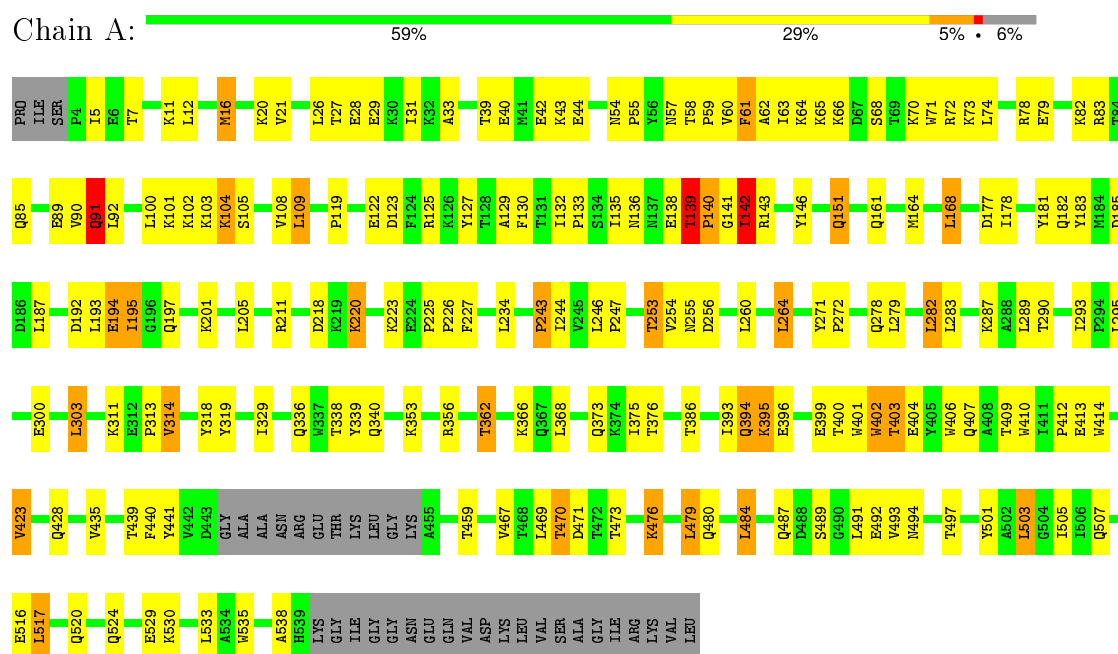
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	161	Total	O	0	0
			161	161		
5	B	144	Total	O	0	0
			144	144		

### 3 Residue-property plots

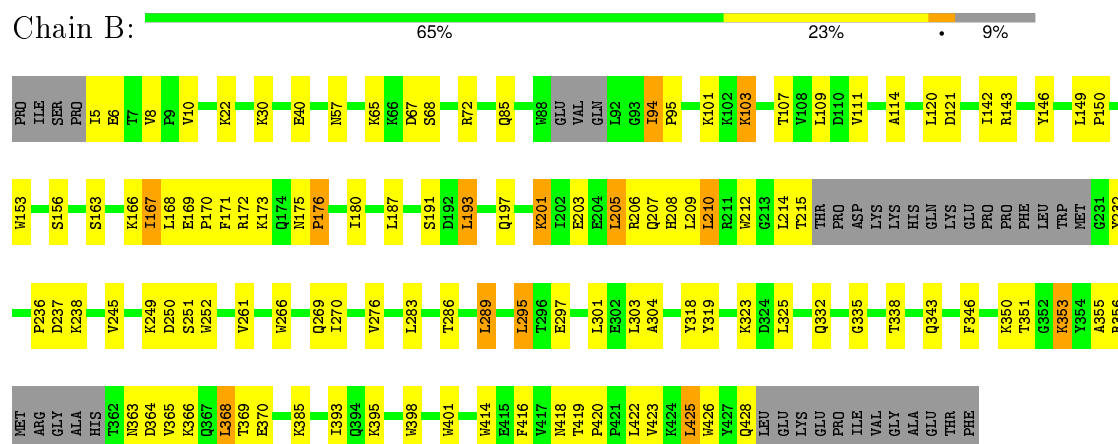
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

#### • Molecule 1: HIV-1 REVERSE TRANSCRIPTASE



#### • Molecule 2: HIV-1 REVERSE TRANSCRIPTASE



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	141.80 Å   116.70 Å   66.40 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	25.00 – 2.20	Depositor
% Data completeness (in resolution range)	87.1 (25.00-2.20)	Depositor
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.186 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7953	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	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: CSD, MG, NVP

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	0.71	0/4417	0.86	0/6005
2	B	0.70	0/3409	0.85	2/4630 (0.0%)
All	All	0.71	0/7826	0.86	2/10635 (0.0%)

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	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	425	LEU	CA-CB-CG	6.46	130.15	115.30
2	B	356	ARG	N-CA-C	5.97	127.13	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	339	TYR	Sidechain

### 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	4310	0	4342	156	0
2	B	3317	0	3349	90	0
3	A	1	0	0	0	0
4	A	20	0	14	1	0
5	A	161	0	0	5	0
5	B	144	0	0	5	0
All	All	7953	0	7705	241	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 16.

All (241) 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:469:LEU:HD21	1:A:480:GLN:HG3	1.38	1.01
1:A:467:VAL:HG21	1:A:484:LEU:HD11	1.53	0.91
2:B:30:LYS:HE3	5:B:1297:HOH:O	1.74	0.86
1:A:142:ILE:H	1:A:142:ILE:HD13	1.42	0.85
2:B:353:LYS:NZ	2:B:428:GLN:HG3	1.95	0.80
1:A:246:LEU:HD22	1:A:260:LEU:HD11	1.63	0.78
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.19	0.78
2:B:173:LYS:HA	2:B:176:PRO:HG3	1.70	0.74
1:A:138:GLU:HG3	1:A:138:GLU:O	1.88	0.74
2:B:261:VAL:HG13	2:B:276:VAL:HG11	1.70	0.72
2:B:353:LYS:HZ3	2:B:428:GLN:HG3	1.54	0.71
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.71	0.71
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.57	0.70
2:B:295:LEU:HD12	2:B:295:LEU:H	1.57	0.69
2:B:193:LEU:HD23	2:B:197:GLN:HB3	1.74	0.69
1:A:101:LYS:N	1:A:101:LYS:HD2	2.08	0.68
1:A:406:TRP:CZ3	1:A:407:GLN:HG3	2.29	0.68
2:B:169:GLU:N	2:B:170:PRO:HD2	2.09	0.67
1:A:72:ARG:HG2	1:A:72:ARG:HH11	1.58	0.67
2:B:209:LEU:HD22	2:B:214:LEU:HD23	1.76	0.67
2:B:366:LYS:O	2:B:370:GLU:HG3	1.95	0.66
2:B:295:LEU:HD12	2:B:295:LEU:N	2.09	0.66
2:B:94:ILE:H	2:B:95:PRO:CD	2.08	0.66
1:A:311:LYS:O	1:A:313:PRO:HD3	1.96	0.65
1:A:395:LYS:HD2	1:A:395:LYS:H	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:GLU:HB2	5:B:1186:HOH:O	1.97	0.64
1:A:136:ASN:HB3	1:A:139:THR:OG1	1.98	0.64
2:B:207:GLN:HA	2:B:210:LEU:HB2	1.80	0.64
1:A:132:ILE:HB	1:A:142:ILE:HG12	1.80	0.63
2:B:5:ILE:HG22	2:B:6:GLU:H	1.62	0.63
1:A:63:ILE:HD13	1:A:74:LEU:HD13	1.80	0.63
1:A:393:ILE:HG13	1:A:423:VAL:HG22	1.80	0.63
2:B:395:LYS:HD2	2:B:416:PHE:CE2	2.34	0.62
2:B:175:ASN:N	2:B:176:PRO:HD3	2.14	0.62
1:A:139:THR:HG22	1:A:140:PRO:CD	2.29	0.62
2:B:167:ILE:HD11	2:B:209:LEU:HD23	1.81	0.61
2:B:425:LEU:HD22	2:B:426:TRP:CD1	2.35	0.61
1:A:139:THR:HG22	1:A:140:PRO:HD3	1.82	0.60
1:A:487:GLN:HA	1:A:524:GLN:NE2	2.16	0.60
1:A:435:VAL:HG23	5:A:1136:HOH:O	2.00	0.60
2:B:94:ILE:H	2:B:95:PRO:HD3	1.66	0.60
1:A:395:LYS:CD	1:A:395:LYS:H	2.13	0.60
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.36	0.60
2:B:103:LYS:HG2	2:B:191:SER:N	2.16	0.60
1:A:476:LYS:HD3	1:A:517:LEU:HD12	1.84	0.59
1:A:60:VAL:CG2	1:A:130:PHE:HB2	2.31	0.59
2:B:295:LEU:H	2:B:295:LEU:CD1	2.16	0.59
1:A:79:GLU:HG3	1:A:83:ARG:NH1	2.18	0.59
1:A:220:LYS:HB3	1:A:220:LYS:NZ	2.17	0.58
1:A:72:ARG:HG2	1:A:72:ARG:NH1	2.19	0.58
1:A:125:ARG:HG2	1:A:146:TYR:O	2.04	0.58
1:A:5:ILE:HG23	1:A:119:PRO:HD2	1.83	0.58
1:A:63:ILE:HG22	1:A:64:LYS:N	2.19	0.58
1:A:406:TRP:HH2	2:B:418:ASN:HA	1.68	0.58
1:A:66:LYS:HB3	1:A:66:LYS:NZ	2.20	0.57
1:A:395:LYS:HD2	1:A:395:LYS:N	2.19	0.57
2:B:420:PRO:O	2:B:423:VAL:HG12	2.05	0.57
1:A:362:THR:HG22	1:A:366:LYS:HD3	1.87	0.57
1:A:469:LEU:HD21	1:A:480:GLN:CG	2.25	0.57
2:B:65:LYS:HB2	2:B:68:SER:HB3	1.85	0.57
1:A:399:GLU:O	1:A:403:THR:HB	2.06	0.56
1:A:282:LEU:HD21	1:A:295:LEU:CD2	2.36	0.56
2:B:332:GLN:HB3	2:B:428:GLN:HE22	1.70	0.56
1:A:101:LYS:HE3	1:A:319:TYR:HD2	1.70	0.56
2:B:205:LEU:HD22	2:B:209:LEU:HG	1.87	0.56
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:LEU:CD2	1:A:480:GLN:HG3	2.25	0.56
1:A:253:THR:HG22	1:A:255:ASN:N	2.21	0.55
2:B:353:LYS:HZ2	2:B:428:GLN:HG3	1.69	0.55
1:A:40:GLU:O	1:A:44:GLU:HG3	2.05	0.55
2:B:249:LYS:HD3	2:B:251:SER:O	2.07	0.55
1:A:467:VAL:CG2	1:A:484:LEU:HD11	2.32	0.55
2:B:210:LEU:HD13	2:B:214:LEU:O	2.07	0.55
2:B:323:LYS:O	2:B:385:LYS:NZ	2.39	0.54
2:B:203:GLU:O	2:B:206:ARG:HB2	2.08	0.54
1:A:27:THR:HG22	1:A:29:GLU:H	1.72	0.54
1:A:63:ILE:HG22	1:A:64:LYS:H	1.72	0.54
2:B:172:ARG:O	2:B:176:PRO:HG3	2.08	0.53
1:A:220:LYS:HZ2	1:A:220:LYS:HB3	1.71	0.53
1:A:491:LEU:O	1:A:529:GLU:HB2	2.09	0.53
1:A:376:THR:HG23	1:A:386:THR:HG22	1.90	0.53
1:A:195:ILE:HD13	1:A:195:ILE:N	2.24	0.53
2:B:261:VAL:HG22	2:B:276:VAL:HG13	1.92	0.52
1:A:193:LEU:HB3	1:A:197:GLN:HB3	1.91	0.52
1:A:497:THR:O	1:A:535:TRP:HA	2.09	0.52
1:A:194:GLU:HG3	1:A:197:GLN:HB2	1.91	0.51
1:A:400:THR:O	1:A:404:GLU:HG2	2.10	0.51
2:B:5:ILE:HG22	2:B:6:GLU:N	2.26	0.51
2:B:266:TRP:O	2:B:269:GLN:HG2	2.11	0.51
1:A:73:LYS:NZ	1:A:146:TYR:OH	2.43	0.51
2:B:107:THR:HG22	2:B:109:LEU:HD12	1.93	0.51
2:B:103:LYS:O	2:B:236:PRO:HG2	2.11	0.50
1:A:410:TRP:CE3	2:B:363:ASN:HB2	2.47	0.50
1:A:476:LYS:HD2	1:A:476:LYS:O	2.11	0.50
2:B:94:ILE:N	2:B:95:PRO:CD	2.74	0.50
1:A:63:ILE:HD12	1:A:63:ILE:N	2.27	0.50
1:A:362:THR:CG2	1:A:366:LYS:HD3	2.41	0.50
2:B:167:ILE:HD12	2:B:212:TRP:HB2	1.93	0.50
2:B:142:ILE:HD12	2:B:142:ILE:N	2.26	0.50
2:B:167:ILE:O	2:B:167:ILE:HG13	2.10	0.49
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.94	0.49
1:A:39:THR:O	1:A:43:LYS:HG2	2.12	0.49
1:A:195:ILE:H	1:A:195:ILE:HD13	1.77	0.49
2:B:252:TRP:CD1	2:B:295:LEU:HD11	2.47	0.49
1:A:100:LEU:O	1:A:318:TYR:HB3	2.12	0.49
1:A:211:ARG:HD2	5:A:1061:HOH:O	2.12	0.49
2:B:270:ILE:HG12	2:B:346:PHE:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:HB	1:A:140:PRO:HD2	1.95	0.49
1:A:83:ARG:HH11	1:A:83:ARG:HG3	1.77	0.49
2:B:332:GLN:HB3	2:B:428:GLN:NE2	2.27	0.49
2:B:338:THR:HG22	2:B:353:LYS:HD3	1.94	0.49
1:A:151:GLN:HE21	1:A:151:GLN:N	2.10	0.48
2:B:163:SER:O	2:B:167:ILE:HG23	2.13	0.48
1:A:278:GLN:HA	1:A:278:GLN:HE21	1.78	0.48
1:A:61:PHE:N	1:A:61:PHE:CD1	2.82	0.47
2:B:175:ASN:ND2	2:B:201:LYS:HD3	2.29	0.47
1:A:65:LYS:CB	1:A:68:SER:HB3	2.44	0.47
1:A:42:GLU:HG2	1:A:42:GLU:O	2.13	0.47
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.49	0.47
1:A:530:LYS:HA	5:A:1135:HOH:O	2.13	0.47
2:B:295:LEU:CD1	2:B:295:LEU:N	2.76	0.47
1:A:62:ALA:C	1:A:63:ILE:HD12	2.34	0.47
2:B:419:THR:HA	2:B:420:PRO:HD3	1.81	0.47
1:A:503:LEU:HD13	1:A:507:GLN:NE2	2.30	0.47
1:A:439:THR:HG22	1:A:441:TYR:CE1	2.50	0.47
2:B:85:GLN:O	2:B:85:GLN:HG3	2.12	0.47
1:A:401:TRP:CD1	5:A:1123:HOH:O	2.68	0.47
1:A:393:ILE:O	1:A:414:TRP:HZ3	1.98	0.46
2:B:335:GLY:O	2:B:355:ALA:HA	2.15	0.46
1:A:373:GLN:HG2	5:B:1292:HOH:O	2.15	0.46
1:A:89:GLU:OE2	1:A:92:LEU:HB2	2.15	0.46
1:A:178:ILE:HD13	1:A:178:ILE:N	2.29	0.46
1:A:393:ILE:O	1:A:414:TRP:CZ3	2.69	0.46
1:A:151:GLN:CA	1:A:151:GLN:HE21	2.28	0.46
1:A:253:THR:CG2	1:A:255:ASN:H	2.29	0.46
1:A:338:THR:HG22	1:A:353:LYS:HG2	1.98	0.46
1:A:517:LEU:HA	1:A:520:GLN:HE21	1.81	0.46
1:A:401:TRP:CE3	1:A:402:TRP:N	2.84	0.46
1:A:72:ARG:NH1	1:A:74:LEU:HD12	2.31	0.46
1:A:253:THR:HB	1:A:256:ASP:OD2	2.16	0.46
1:A:399:GLU:HA	1:A:402:TRP:HE3	1.81	0.45
1:A:439:THR:O	1:A:459:THR:HA	2.17	0.45
1:A:399:GLU:HA	1:A:402:TRP:CE3	2.51	0.45
1:A:440:PHE:CZ	1:A:489:SER:HB3	2.52	0.45
1:A:91:GLN:HG2	1:A:91:GLN:O	2.16	0.45
1:A:65:LYS:HZ1	1:A:72:ARG:HG3	1.82	0.45
2:B:142:ILE:HD12	2:B:142:ILE:H	1.81	0.45
2:B:169:GLU:N	2:B:170:PRO:CD	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:THR:HG22	1:A:255:ASN:H	1.80	0.45
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.99	0.45
1:A:409:THR:O	2:B:364:ASP:HB2	2.17	0.45
2:B:368:LEU:HD23	2:B:368:LEU:HA	1.78	0.45
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.98	0.44
2:B:318:TYR:HE1	5:B:1278:HOH:O	1.99	0.44
1:A:271:TYR:OH	1:A:313:PRO:HA	2.17	0.44
1:A:253:THR:HG22	1:A:256:ASP:H	1.83	0.44
1:A:393:ILE:CG1	1:A:423:VAL:HG22	2.48	0.44
1:A:218:ASP:OD2	1:A:220:LYS:HB2	2.17	0.44
1:A:253:THR:HG23	1:A:289:LEU:O	2.17	0.44
2:B:237:ASP:OD2	2:B:238:LYS:HG3	2.18	0.44
2:B:214:LEU:HD12	2:B:215:THR:H	1.83	0.44
1:A:108:VAL:HG11	1:A:223:LYS:HE2	1.99	0.44
2:B:208:HIS:ND1	2:B:208:HIS:O	2.51	0.44
2:B:319:TYR:CD1	2:B:343:GLN:NE2	2.86	0.44
1:A:469:LEU:HD11	1:A:480:GLN:HE21	1.83	0.44
1:A:516:GLU:O	1:A:520:GLN:HG3	2.17	0.44
1:A:467:VAL:HG11	1:A:484:LEU:HD21	1.99	0.43
1:A:246:LEU:HA	1:A:247:PRO:HD3	1.80	0.43
2:B:172:ARG:NH2	2:B:180:ILE:O	2.51	0.43
1:A:142:ILE:H	1:A:142:ILE:CD1	2.13	0.43
1:A:136:ASN:CB	1:A:139:THR:OG1	2.63	0.43
2:B:385:LYS:HD3	5:B:1286:HOH:O	2.18	0.43
1:A:58:THR:HA	1:A:59:PRO:HD3	1.87	0.43
1:A:480:GLN:HG2	1:A:517:LEU:HD11	2.00	0.43
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.53	0.43
1:A:494:ASN:HB3	2:B:289:LEU:HD22	2.00	0.43
2:B:209:LEU:HB3	2:B:214:LEU:HB3	2.00	0.43
1:A:104:LYS:NZ	1:A:104:LYS:HB3	2.33	0.43
1:A:109:LEU:HA	1:A:109:LEU:HD12	1.73	0.43
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.72	0.43
2:B:146:TYR:CD2	2:B:150:PRO:HB3	2.54	0.43
1:A:90:VAL:O	1:A:92:LEU:HD23	2.19	0.43
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.83	0.43
2:B:10:VAL:HG11	2:B:153:TRP:CH2	2.54	0.43
1:A:72:ARG:HH11	1:A:74:LEU:HD12	1.84	0.43
1:A:83:ARG:HH11	1:A:83:ARG:CG	2.32	0.43
1:A:27:THR:HG22	1:A:29:GLU:HB3	2.01	0.43
1:A:503:LEU:O	1:A:507:GLN:HB2	2.18	0.43
1:A:11:LYS:O	1:A:85:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:PRO:HG2	2:B:208:HIS:CE1	2.54	0.43
1:A:470:THR:O	1:A:471:ASP:HB2	2.19	0.43
1:A:394:GLN:H	1:A:394:GLN:HG2	1.66	0.43
1:A:61:PHE:N	1:A:61:PHE:HD1	2.17	0.42
2:B:422:LEU:O	2:B:425:LEU:HB3	2.19	0.42
1:A:78:ARG:O	1:A:82:LYS:HG3	2.19	0.42
1:A:271:TYR:CE1	1:A:314:VAL:HG13	2.54	0.42
1:A:225:PRO:HA	1:A:226:PRO:C	2.40	0.42
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.73	0.42
2:B:369:THR:HG22	2:B:398:TRP:CH2	2.54	0.42
1:A:64:LYS:HA	1:A:70:LYS:O	2.18	0.42
1:A:79:GLU:OE2	1:A:83:ARG:NH1	2.52	0.42
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.55	0.42
2:B:365:VAL:HG11	2:B:401:TRP:HB2	2.01	0.42
1:A:65:LYS:HB3	1:A:68:SER:HB3	2.01	0.42
1:A:16:MET:HE2	1:A:83:ARG:HA	2.02	0.42
2:B:350:LYS:HG3	2:B:351:THR:N	2.35	0.42
1:A:122:GLU:HA	1:A:125:ARG:HD2	2.01	0.42
1:A:90:VAL:O	1:A:92:LEU:N	2.53	0.42
1:A:31:ILE:CD1	1:A:133:PRO:HG2	2.50	0.42
2:B:94:ILE:HG13	2:B:94:ILE:O	2.19	0.41
2:B:323:LYS:HD2	2:B:323:LYS:HA	1.81	0.41
2:B:393:ILE:HD13	2:B:398:TRP:HE3	1.84	0.41
1:A:264:LEU:HA	1:A:264:LEU:HD12	1.86	0.41
2:B:149:LEU:HD13	2:B:156:SER:HA	2.02	0.41
1:A:57:ASN:OD1	1:A:143:ARG:NH1	2.53	0.41
1:A:31:ILE:HG12	1:A:133:PRO:HG2	2.03	0.41
1:A:164:MET:SD	1:A:168:LEU:HD22	2.61	0.41
1:A:501:TYR:CZ	1:A:505:ILE:HD11	2.56	0.41
1:A:70:LYS:HD2	1:A:70:LYS:HA	1.80	0.41
1:A:181:TYR:CD2	4:A:999:NVP:C5	3.04	0.41
2:B:289:LEU:HD12	2:B:289:LEU:HA	1.75	0.41
1:A:492:GLU:HA	1:A:530:LYS:O	2.21	0.41
1:A:28:GLU:HG3	1:A:135:ILE:HD13	2.03	0.41
2:B:173:LYS:O	2:B:176:PRO:HD3	2.21	0.41
2:B:167:ILE:HD11	2:B:209:LEU:CD2	2.49	0.41
2:B:210:LEU:HD13	2:B:210:LEU:HA	1.80	0.41
1:A:254:VAL:HG23	1:A:293:ILE:CD1	2.51	0.41
2:B:366:LYS:HE3	2:B:370:GLU:OE2	2.22	0.40
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.70	0.40
2:B:57:ASN:HD22	2:B:143:ARG:HH12	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:TRP:CD1	1:A:402:TRP:C	2.94	0.40
2:B:350:LYS:CG	2:B:351:THR:N	2.83	0.40
2:B:301:LEU:O	2:B:304:ALA:HB3	2.21	0.40
1:A:246:LEU:HD13	1:A:303:LEU:CD2	2.50	0.40
2:B:208:HIS:CG	2:B:208:HIS:O	2.74	0.40
1:A:108:VAL:HG12	1:A:227:PHE:CE1	2.56	0.40
1:A:394:GLN:HG2	5:A:1106:HOH:O	2.21	0.40
2:B:120:LEU:O	2:B:121:ASP:C	2.60	0.40
1:A:33:ALA:HB2	1:A:71:TRP:CD1	2.56	0.40
1:A:54:ASN:ND2	1:A:129:ALA:HB2	2.36	0.40
1:A:54:ASN:HA	1:A:55:PRO:HD2	1.90	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	520/560 (93%)	486 (94%)	26 (5%)	8 (2%)	13	9
2	B	393/440 (89%)	371 (94%)	19 (5%)	3 (1%)	24	22
All	All	913/1000 (91%)	857 (94%)	45 (5%)	11 (1%)	16	12

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	THR
1	A	538	ALA
1	A	142	ILE
2	B	193	LEU
1	A	91	GLN
1	A	141	GLY
2	B	94	ILE

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Mol	Chain	Res	Type
1	A	140	PRO
1	A	412	PRO
2	B	176	PRO
1	A	243	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	473/499 (95%)	414 (88%)	59 (12%)	6	4
2	B	365/400 (91%)	339 (93%)	26 (7%)	18	19
All	All	838/899 (93%)	753 (90%)	85 (10%)	9	8

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	16	MET
1	A	20	LYS
1	A	21	VAL
1	A	61	PHE
1	A	91	GLN
1	A	102	LYS
1	A	104	LYS
1	A	105	SER
1	A	109	LEU
1	A	123	ASP
1	A	139	THR
1	A	142	ILE
1	A	151	GLN
1	A	161	GLN
1	A	168	LEU
1	A	177	ASP
1	A	182	GLN
1	A	185	ASP

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Mol	Chain	Res	Type
1	A	187	LEU
1	A	194	GLU
1	A	195	ILE
1	A	205	LEU
1	A	220	LYS
1	A	234	LEU
1	A	243	PRO
1	A	244	ILE
1	A	253	THR
1	A	264	LEU
1	A	279	LEU
1	A	282	LEU
1	A	283	LEU
1	A	287	LYS
1	A	290	THR
1	A	300	GLU
1	A	303	LEU
1	A	314	VAL
1	A	336	GLN
1	A	340	GLN
1	A	356	ARG
1	A	362	THR
1	A	368	LEU
1	A	394	GLN
1	A	395	LYS
1	A	396	GLU
1	A	402	TRP
1	A	403	THR
1	A	413	GLU
1	A	423	VAL
1	A	428	GLN
1	A	470	THR
1	A	473	THR
1	A	476	LYS
1	A	479	LEU
1	A	484	LEU
1	A	493	VAL
1	A	503	LEU
1	A	517	LEU
1	A	533	LEU
2	B	8	VAL
2	B	22	LYS

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Mol	Chain	Res	Type
2	B	67	ASP
2	B	72	ARG
2	B	101	LYS
2	B	103	LYS
2	B	166	LYS
2	B	167	ILE
2	B	168	LEU
2	B	171	PHE
2	B	201	LYS
2	B	205	LEU
2	B	210	LEU
2	B	232	TYR
2	B	245	VAL
2	B	250	ASP
2	B	283	LEU
2	B	286	THR
2	B	289	LEU
2	B	295	LEU
2	B	297	GLU
2	B	303	LEU
2	B	325	LEU
2	B	353	LYS
2	B	368	LEU
2	B	414	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
1	A	222	GLN
1	A	278	GLN
1	A	336	GLN
1	A	480	GLN
1	A	507	GLN
1	A	520	GLN
2	B	57	ASN
2	B	147	ASN
2	B	269	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	0.91	0	3,8,10	8.32	1 (33%)

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	-	1/2/6/8	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	14.29	129.22	105.40

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	NVP	A	999	-	18,23,23	0.83	0	18,34,34	1.13	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
4	NVP	A	999	-	-	0/0/6/6	0/2/4/4

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	999	NVP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.