



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:55 PM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

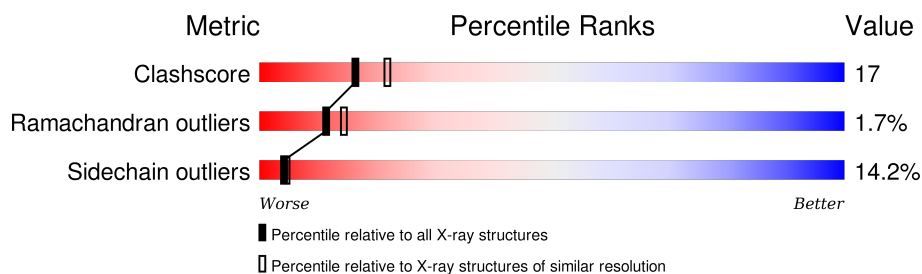
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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 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 $\leq 5\%$. 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 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.

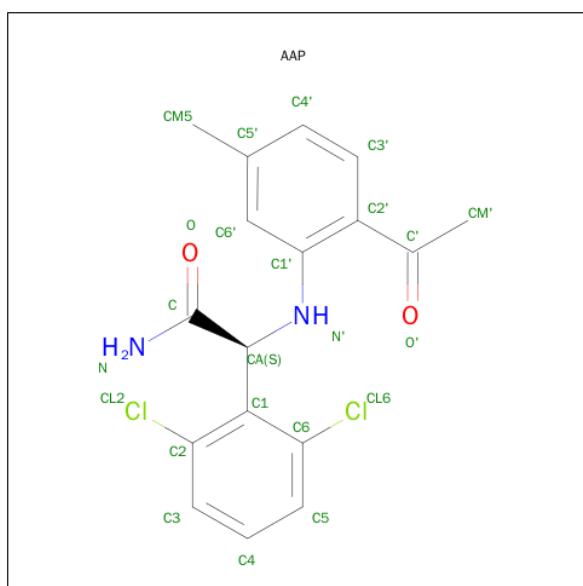
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

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

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

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

- Molecule 3 is ALPHA-(2,6-DICHLOROPHENYL)-ALPHA-(2-ACETYL-5-METHYLANILINO)ACETAMIDE (three-letter code: AAP) (formula: C₁₇H₁₆Cl₂N₂O₂).



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

- Molecule 4 is water.

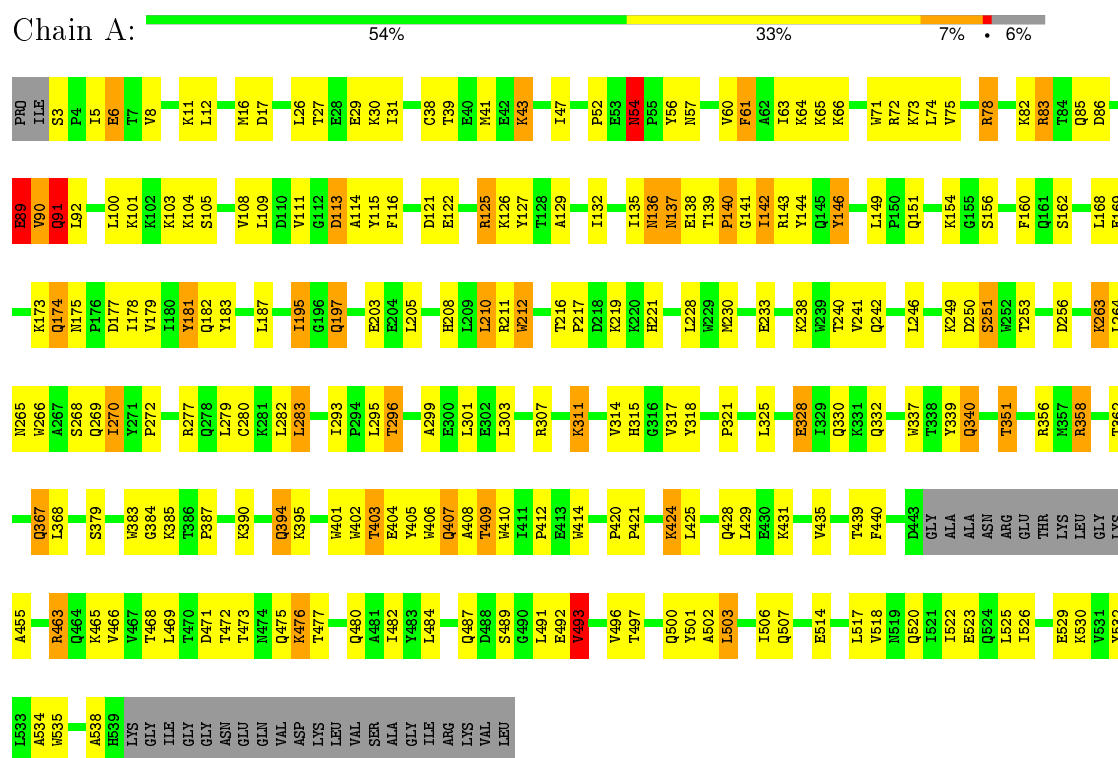
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total 72	O 72	0	0
4	B	59	Total 59	O 59	0	0

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



K368	F389	Q394	W398	W401	W402	T403	I411	M418	Y427	Q428	LEU	GLU	LVS	GLU	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE																									
T286	A287	L289	L301	E302	L303	V317	K323	D324	L325	E328	Q334	G335	Q336	Y339	Y342	Q343	G344	P345	F346	K347	P348	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

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, α , β , γ	143.20 Å 116.80 Å 66.40 Å 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, AAP

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($^{\circ}$)	Ideal($^{\circ}$)
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 ⓘ

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

Continued on next page...

Continued from previous page...

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:HA	2:B:161:GLN:HE21	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:HG2	1:A:91:GLN:O	1.94	0.67
1:A:142:ILE:H	1:A:142:ILE:HD13	1.60	0.66
1:A:332:GLN:HG2	1:A:332:GLN:O	1.95	0.66
1:A:475:GLN:HB3	1:A:501:TYR:CE2	2.31	0.65
1:A:491:LEU:O	1:A:529:GLU:HB2	1.95	0.65
1:A:16:MET:HG3	1:A:83:ARG:HG3	1.79	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
2:B:114:ALA:HB2	2:B:214:LEU:HD13	1.77	0.64
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.32	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:NE2	1:A:197:GLN:HA	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
2:B:167:ILE:HG23	2:B:212:TRP:HB3	1.82	0.61
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.82	0.61

Continued on next page...

Continued from previous page...

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
2:B:64:LYS:HD3	2:B:65:LYS:N	2.16	0.59
1:A:73:LYS:HE2	1:A:75:VAL:HG22	1.84	0.59
1:A:379:SER:CB	1:A:387:PRO:HD3	2.33	0.58
2:B:161:GLN:CA	2:B:161:GLN:HE21	2.14	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:260:LEU:O	2:B:264:LEU:HB2	2.03	0.58
2:B:334:GLN:CA	2:B:360:ALA:HB2	2.34	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
1:A:3:SER:OG	1:A:212:TRP:HB3	2.04	0.57
2:B:284:ARG:HH11	2:B:284:ARG:HG3	1.69	0.57
2:B:110:ASP:O	2:B:216:THR:HG22	2.02	0.57
2:B:38:CYS:O	2:B:47:ILE:HD11	2.04	0.57
1:A:497:THR:O	1:A:535:TRP:HA	2.04	0.57
1:A:492:GLU:HA	1:A:530:LYS:O	2.05	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:465:LYS:NZ	1:A:484:LEU:HD22	2.20	0.57
1:A:174:GLN:HE21	1:A:174:GLN:HA	1.69	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
2:B:65:LYS:CB	2:B:68:SER:HB2	2.32	0.56
1:A:522:ILE:O	1:A:526:ILE:HG13	2.06	0.56
2:B:428:GLN:HA	2:B:428:GLN:NE2	2.22	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:LYS:N	1:A:263:LYS:HE3	2.22	0.55
1:A:61:PHE:N	1:A:61:PHE:HD1	2.05	0.55
1:A:65:LYS:HG3	1:A:66:LYS:N	2.22	0.55
2:B:212:TRP:HE3	2:B:212:TRP:HA	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
2:B:79:GLU:O	2:B:83:ARG:HG3	2.07	0.53
1:A:270:ILE:H	1:A:270:ILE:HD12	1.73	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
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.45	0.51
1:A:401:TRP:HZ3	1:A:402:TRP:CE2	2.29	0.51
1:A:465:LYS:HG2	1:A:466:VAL:N	2.26	0.51
1:A:463:ARG:NH1	1:A:463:ARG:HG2	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:NH1	1:A:78:ARG:HG2	2.23	0.49
1:A:270:ILE:N	1:A:270:ILE:HD12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:LYS:O	2:B:166:LYS:HE2	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
2:B:207:GLN:O	2:B:210:LEU:HG	2.13	0.49
1:A:208:HIS:O	1:A:212:TRP:CD1	2.65	0.49
1:A:63:ILE:O	1:A:72:ARG:HB2	2.13	0.49
1:A:142:ILE:N	1:A:142:ILE:HD13	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
2:B:78:ARG:O	2:B:82:LYS:HG3	2.13	0.48
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.96	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:216:THR:HA	2:B:217:PRO:HD3	1.76	0.47
2:B:120:LEU:O	2:B:121:ASP:C	2.51	0.47
1:A:8:VAL:O	1:A:121:ASP:HB2	2.13	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:103:LYS:HE3	1:A:179:VAL:HG21	1.97	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:HA	2:B:187:LEU:HD12	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
2:B:76:ASP:HA	2:B:411:ILE:HD12	1.97	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
1:A:401:TRP:CZ3	1:A:402:TRP:CE2	3.04	0.45
2:B:389:PHE:CD1	2:B:389:PHE:N	2.84	0.45
2:B:50:ILE:CG2	2:B:145:GLN:HG2	2.47	0.45
1:A:465:LYS:HZ3	1:A:484:LEU:CD2	2.29	0.45

Continued on next page...

Continued from previous page...

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
2:B:16:MET:HE2	2:B:83:ARG:HG2	1.98	0.45
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.99	0.45
1:A:26:LEU:HB3	1:A:31:ILE:HG13	1.99	0.45
1:A:379:SER:OG	1:A:387:PRO:HD3	2.17	0.44
1:A:100:LEU:O	1:A:318:TYR:HB3	2.17	0.44
2:B:8:VAL:HG21	2:B:159:ILE:HG12	1.99	0.44
1:A:169:GLU:O	1:A:173:LYS:HD3	2.16	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
2:B:214:LEU:HD12	2:B:215:THR:H	1.82	0.44
1:A:358:ARG:NH2	2:B:394:GLN:HG2	2.32	0.44
1:A:89:GLU:HB3	1:A:92:LEU:HD12	1.99	0.44
1:A:424:LYS:HB3	1:A:424:LYS:HE2	1.71	0.44
1:A:56:TYR:O	1:A:143:ARG:NH2	2.44	0.44
2:B:239:TRP:CH2	2:B:378:GLU:HG2	2.52	0.44
2:B:81:ASN:OD1	2:B:153:TRP:HD1	2.01	0.44
3:A:999:AAP:CL6	3:A:999:AAP:H6'	2.55	0.44
2:B:428:GLN:HA	2:B:428:GLN:HE21	1.81	0.44
1:A:54:ASN:HD22	1:A:54:ASN:C	2.20	0.44
1:A:115:TYR:O	1:A:149:LEU:HB2	2.18	0.44
1:A:135:ILE:O	1:A:135:ILE:HG13	2.17	0.44
1:A:402:TRP:CE3	1:A:409:THR:CG2	3.00	0.44
2:B:353:LYS:NZ	2:B:428:GLN:HG2	2.33	0.44
1:A:263:LYS:CA	1:A:263:LYS:HE3	2.47	0.44
1:A:293:ILE:N	1:A:293:ILE:HD12	2.33	0.44
2:B:323:LYS:O	2:B:385:LYS:NZ	2.47	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:211:ARG:O	2:B:212:TRP:CE3	2.71	0.43
2:B:60:VAL:HG21	2:B:130:PHE:CD2	2.54	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

Continued on next page...

Continued from previous page...

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
2:B:166:LYS:C	2:B:166:LYS:HE2	2.39	0.42
1:A:328:GLU:HG3	1:A:390:LYS:HD3	2.00	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: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:89:GLU:HB2	1:A:92:LEU:HD12	2.02	0.42
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.43	0.42
1:A:296:THR:HG22	1:A:299:ALA:N	2.26	0.41
1:A:253:THR:O	1:A:256:ASP:HB2	2.20	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:CG	2:B:208:HIS:O	2.74	0.41
2:B:325:LEU:HB3	2:B:387:PRO:HB3	2.02	0.41
2:B:284:ARG:NH1	2:B:284:ARG:HG3	2.33	0.41
2:B:368:LEU:O	2:B:372:VAL:HG23	2.21	0.41
2:B:114:ALA:CA	2:B:214:LEU:HD13	2.50	0.41
1:A:280:CSD:O	1:A:283:LEU:HB2	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: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
2:B:118:VAL:HG21	2:B:160:PHE:HD1	1.86	0.40
1:A:489:SER:HB2	1:A:493:VAL:HG13	2.01	0.40
1:A:233:GLU:N	1:A:240:THR:O	2.48	0.40
2:B:215:THR:O	2:B:216:THR:HG23	2.21	0.40
1:A:41:MET:HB3	1:A:47:ILE:HG12	2.02	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:476:LYS:HD3	1:A:480:GLN:HG2	2.03	0.40
1:A:311:LYS:HA	1:A:311:LYS:HD3	1.89	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	521/560 (93%)	491 (94%)	21 (4%)	9 (2%)	11	14
2	B	404/440 (92%)	367 (91%)	30 (7%)	7 (2%)	11	14
All	All	925/1000 (92%)	858 (93%)	51 (6%)	16 (2%)	11	14

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

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%)	3	3
2	B	372/400 (93%)	330 (89%)	42 (11%)	7	10
All	All	846/899 (94%)	726 (86%)	120 (14%)	4	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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	403	THR

Some 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 ⓘ

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	1.02	0	3,8,10	6.97	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	11.99	125.38	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.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	-	23,24,24	1.00	1 (4%)	29,34,34	1.28	5 (17%)

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	-	-	0/16/16/16	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'	3.14	1.55	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	AAP	C3-C2-C1	-2.55	119.23	122.45
3	A	999	AAP	C6'-C1'-N'	-2.06	118.90	121.89
3	A	999	AAP	C1'-N'-CA	2.25	127.16	121.69
3	A	999	AAP	C1-C2-CL2	2.36	122.89	120.45
3	A	999	AAP	C6-C1-C2	3.25	119.33	114.92

There are no chirality outliers.

There are no torsion outliers.

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

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 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.