



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:11 AM UTC

PDB ID : 1VRU / pdb_00001vru
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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

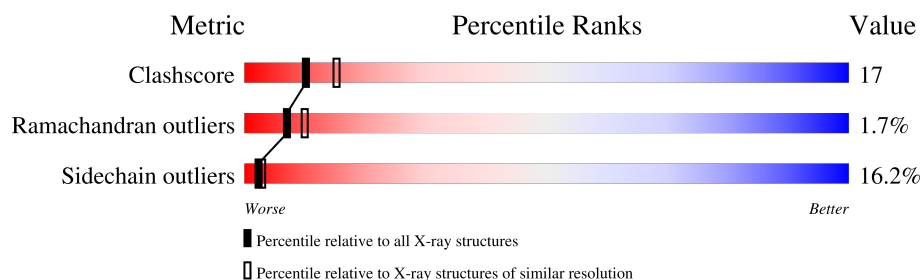
1 Overall quality at a glance

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	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (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 $\leq 5\%$

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.

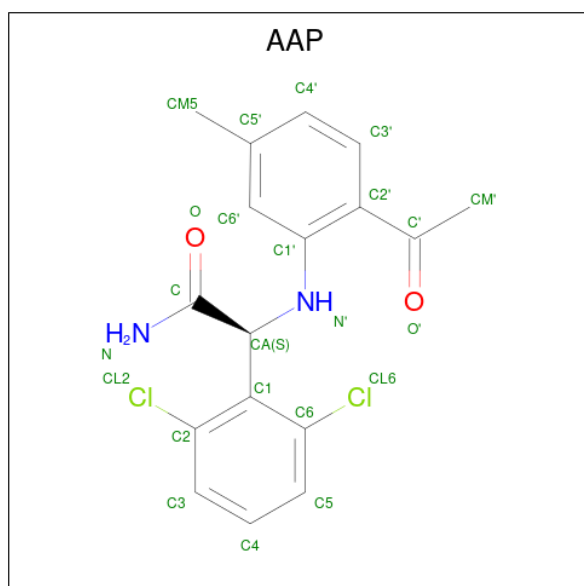
- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

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 (CCD ID: AAP) (formula: $C_{17}H_{16}Cl_2N_2O_2$).



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.

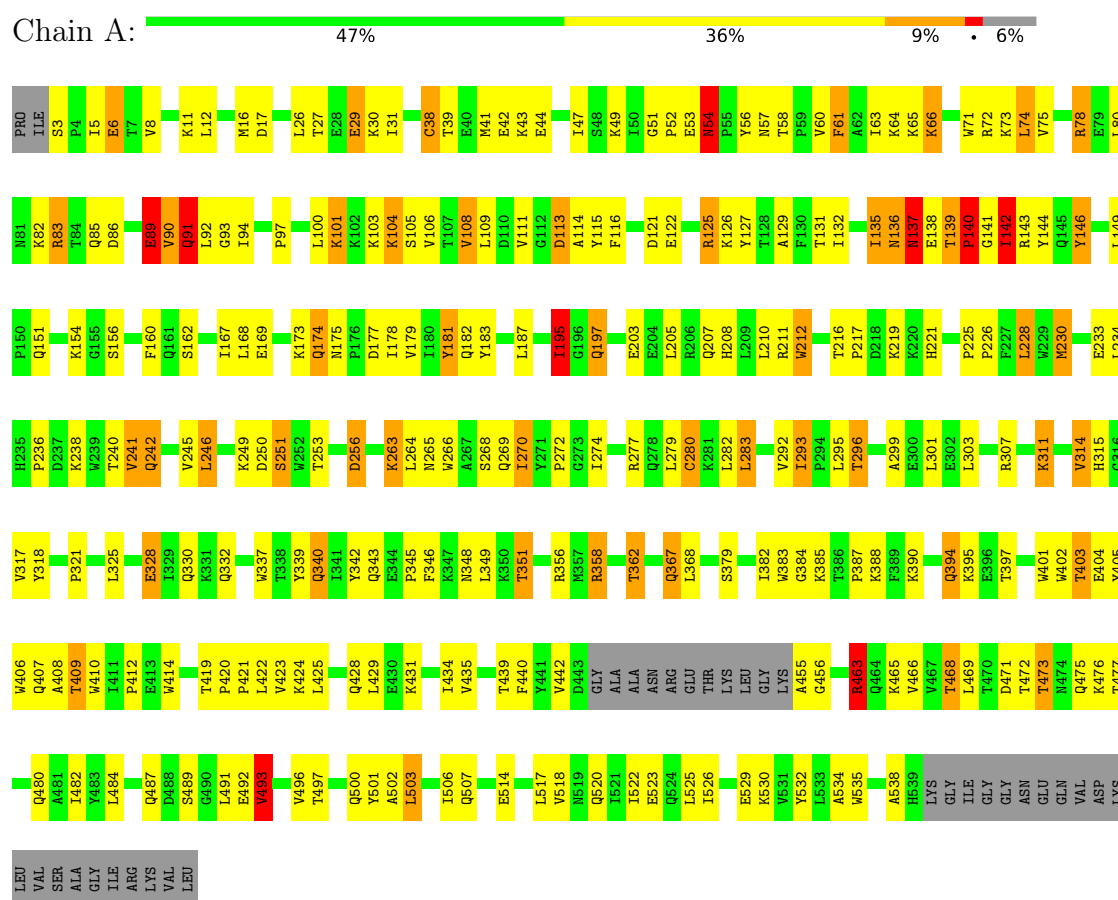
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total 72	O 72	0	0
4	B	59	Total 59	O 59	0	0

3 Residue-property plots

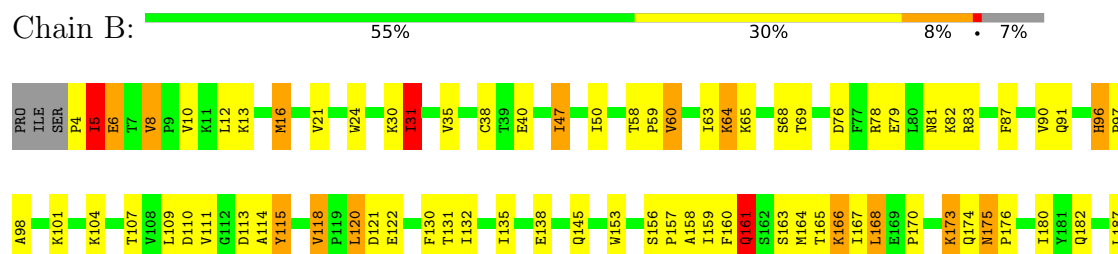
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE



V365	L368	T369	E370	A371	V372	Q373	K374	E378	K385	T386	P387	K388	F389	K390	L391	F392	I393	Q394	W398	W401	W402	T403	I411	V417	N418	T419	P420	V423	Y427	Q428	LEU	GLU	LYS	GLU	PRO	ILE	VAL	GLY	ALA	GLU	THR	PHE									
Y271	R277	C280	K281	R284	G285	T286	K287	A288	L289	I293	P294	L295	E300	L301	E302	L303	V317	Y318	K323	D324	L325	E328	Q334	Q335	Q336	Y339	Y342	Q343	E344	P345	F346	K347	N348	L349	K350	T351	G352	K353	R356	MET	ARG	G359	A360	H361	T362	N363	D364				
Y188	V189	D192	I195	T200	K201	I202	E203	E204	L205	R206	Q207	H208	L209	L210	R211	W212	G213	L214	T215	T216	P217	ASP	LYS	LYS	HIS	GLN	LYS	GLU	PRO	PRO	PHE	LEU	TRP	MET	G231	Y232	E233	L234	W239	T240	V241	Q242	P247	E248	K249	D250	L260	L264	N265	W266	I270

4 Data and refinement statistics

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

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	0.94	6/4423 (0.1%)	1.32	44/6014 (0.7%)
2	B	0.97	6/3478 (0.2%)	1.28	39/4727 (0.8%)
All	All	0.96	12/7901 (0.2%)	1.30	83/10741 (0.8%)

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	388	LYS	CA-C	6.55	1.60	1.52
2	B	5	ILE	CA-CB	6.04	1.62	1.54
1	A	241	VAL	CA-CB	5.84	1.62	1.54
1	A	382	ILE	CA-CB	5.84	1.63	1.54
2	B	31	ILE	CA-CB	5.81	1.61	1.54
2	B	317	VAL	CA-CB	5.75	1.61	1.54
2	B	420	PRO	CA-C	5.74	1.57	1.52
2	B	393	ILE	CA-CB	5.62	1.59	1.55
1	A	274	ILE	CA-CB	5.44	1.59	1.54
1	A	106	VAL	CA-CB	5.29	1.62	1.54
2	B	386	THR	CA-CB	5.25	1.61	1.53
1	A	468	THR	CA-CB	5.00	1.61	1.53

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	538	ALA	N-CA-C	17.04	129.55	110.97
1	A	54	ASN	N-CA-C	-11.69	85.69	108.59
1	A	142	ILE	N-CA-C	8.43	120.31	108.93
1	A	94	ILE	CA-C-N	8.21	128.21	119.76
1	A	94	ILE	C-N-CA	8.21	128.21	119.76
1	A	51	GLY	CA-C-N	8.10	129.97	119.84
1	A	51	GLY	C-N-CA	8.10	129.97	119.84
2	B	96	HIS	CA-C-N	7.64	129.40	119.84
2	B	96	HIS	C-N-CA	7.64	129.40	119.84
2	B	266	TRP	N-CA-C	-7.48	102.27	111.40
1	A	234	LEU	N-CA-C	7.34	120.49	108.52
1	A	80	LEU	N-CA-C	-7.20	103.36	111.14
2	B	6	GLU	N-CA-C	7.12	121.28	109.46
2	B	115	TYR	N-CA-C	7.10	121.57	112.34
2	B	132	ILE	N-CA-C	-7.06	101.13	107.56
2	B	87	PHE	N-CA-C	7.02	120.80	107.75
1	A	104	LYS	N-CA-C	-6.98	103.65	112.93
1	A	473	THR	N-CA-C	-6.96	98.83	109.41
2	B	118	VAL	CA-C-N	6.96	126.88	119.85
2	B	118	VAL	C-N-CA	6.96	126.88	119.85
2	B	401	TRP	N-CA-C	6.92	122.83	113.97
2	B	318	TYR	N-CA-C	6.91	120.66	109.40
2	B	271	TYR	CA-C-N	6.89	126.59	119.56
2	B	271	TYR	C-N-CA	6.89	126.59	119.56
2	B	295	LEU	N-CA-C	6.53	119.70	110.23
1	A	167	ILE	CB-CA-C	-6.52	103.62	111.97
2	B	250	ASP	N-CA-C	-6.49	103.48	111.40
1	A	358	ARG	N-CA-C	-6.47	97.14	108.20
2	B	16	MET	N-CA-C	6.40	119.95	110.48
1	A	135	ILE	N-CA-C	6.40	121.00	112.04
2	B	69	THR	N-CA-C	-6.22	105.33	113.17
2	B	293	ILE	CA-C-N	-6.17	113.15	120.13
2	B	293	ILE	C-N-CA	-6.17	113.15	120.13
2	B	131	THR	CA-C-N	-6.12	118.44	122.60
2	B	131	THR	C-N-CA	-6.12	118.44	122.60
1	A	493	VAL	CB-CA-C	-6.06	101.33	110.55
1	A	101	LYS	N-CA-C	-6.04	100.44	110.17
1	A	314	VAL	CB-CA-C	-5.95	102.69	111.19
1	A	348	ASN	N-CA-C	5.90	118.89	110.10
1	A	93	GLY	N-CA-C	-5.89	102.28	111.00
1	A	397	THR	N-CA-C	-5.87	104.24	111.40
2	B	343	GLN	N-CA-C	-5.80	106.85	114.04
1	A	44	GLU	N-CA-C	-5.79	104.75	113.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	GLY	N-CA-C	-5.73	99.59	113.18
2	B	234	LEU	N-CA-C	5.72	123.00	110.80
1	A	140	PRO	N-CA-C	5.69	124.19	112.47
1	A	349	LEU	N-CA-C	-5.68	104.56	112.45
1	A	463	ARG	N-CA-C	5.66	117.59	110.24
2	B	391	LEU	N-CA-C	5.62	116.74	109.72
1	A	38	CYS	N-CA-C	5.60	118.15	111.71
2	B	24	TRP	N-CA-C	-5.57	103.02	109.93
2	B	293	ILE	N-CA-C	5.55	112.61	107.56
1	A	139	THR	CA-C-N	5.54	126.76	119.84
1	A	139	THR	C-N-CA	5.54	126.76	119.84
2	B	247	PRO	CA-C-N	-5.51	114.81	123.13
2	B	247	PRO	C-N-CA	-5.51	114.81	123.13
2	B	420	PRO	CA-C-N	5.50	125.17	119.56
2	B	420	PRO	C-N-CA	5.50	125.17	119.56
1	A	362	THR	CB-CA-C	-5.44	100.70	111.91
1	A	343	GLN	N-CA-C	-5.43	107.31	114.04
1	A	442	VAL	N-CA-C	5.41	117.36	108.97
2	B	202	ILE	N-CA-C	-5.39	105.59	110.82
2	B	216	THR	N-CA-C	5.37	121.67	109.81
2	B	417	VAL	N-CA-C	5.33	115.32	108.82
1	A	195	ILE	N-CA-C	5.27	120.31	109.34
1	A	456	GLY	N-CA-C	5.23	119.14	110.55
1	A	66	LYS	N-CA-C	5.19	117.43	109.07
1	A	245	VAL	CB-CA-C	-5.19	104.68	110.96
2	B	40	GLU	N-CA-C	-5.18	105.32	110.97
1	A	137	ASN	N-CA-C	5.14	121.74	110.80
1	A	419	THR	CA-C-N	-5.13	115.10	120.38
1	A	419	THR	C-N-CA	-5.13	115.10	120.38
1	A	167	ILE	N-CA-C	5.11	115.33	110.42
1	A	131	THR	N-CA-C	5.10	117.29	109.07
2	B	389	PHE	N-CA-C	5.09	117.43	110.55
2	B	161	GLN	N-CA-C	5.09	117.49	111.33
1	A	293	ILE	CA-C-N	5.07	125.22	119.90
1	A	293	ILE	C-N-CA	5.07	125.22	119.90
1	A	256	ASP	CB-CA-C	-5.07	102.70	110.81
2	B	31	ILE	N-CA-CB	5.07	117.43	110.54
2	B	351	THR	N-CA-C	-5.05	101.39	109.07
1	A	42	GLU	N-CA-C	-5.04	105.91	111.71
2	B	386	THR	N-CA-C	-5.02	103.87	110.39

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	168	0
2	B	3382	0	3410	105	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	267	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 (267) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:334:GLN:C	2:B:360:ALA:HB2	2.22	0.65
2:B:173:LYS:HA	2:B:176:PRO:HG3	1.79	0.65
1:A:332:GLN:O	1:A:332:GLN:HG2	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:89:GLU:CD	1:A:92:LEU:HB2	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:230:MET:HE3	1:A:230:MET:HA	1.87	0.55
2:B:428:GLN:NE2	2:B:428:GLN:HA	2.22	0.55
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:5:ILE:HG13	1:A:6:GLU:N	2.24	0.52
3:A:999:AAP:HM1	2:B:138:GLU:HG2	1.91	0.52
2:B:120:LEU:O	2:B:121:ASP:C	2.51	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
1:A:424:LYS:HG2	1:A:425:LEU:N	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:16:MET:HE2	2:B:83:ARG:HG2	1.95	0.49
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:54:ASN:C	1:A:54:ASN:HD22	2.20	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: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
2:B:166:LYS:HE2	2:B:166:LYS:C	2.39	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
1:A:420:PRO:HA	1:A:421:PRO:C	2.39	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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:HD22	1:A:242:GLN:CD	2.43	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:135:ILE:HG13	1:A:135:ILE:O	2.17	0.43
1:A:137:ASN:ND2	1:A:138:GLU:H	2.17	0.43
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
1:A:225:PRO:HA	1:A:226:PRO:C	2.45	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:406:TRP:CE3	1:A:406:TRP:C	2.97	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
2:B:204:GLU:O	2:B:205:LEU:C	2.63	0.41
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
2:B:12:LEU:O	2:B:13:LYS:C	2.62	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
1:A:342:TYR:CD1	1:A:342:TYR:C	2.99	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
1:A:345:PRO:C	1:A:346:PHE:HD1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:164:MET:HE2	2:B:168:LEU:HD13	2.04	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%)	7	10
2	B	404/440 (92%)	367 (91%)	30 (7%)	7 (2%)	7	10
All	All	925/1000 (92%)	858 (93%)	51 (6%)	16 (2%)	7	10

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

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Mol	Chain	Res	Type
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%)	386 (81%)	88 (19%)	1	2
2	B	372/400 (93%)	323 (87%)	49 (13%)	4	5
All	All	846/899 (94%)	709 (84%)	137 (16%)	2	3

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	29	GLU
1	A	49	LYS
1	A	52	PRO
1	A	53	GLU
1	A	54	ASN
1	A	58	THR
1	A	61	PHE
1	A	74	LEU
1	A	78	ARG
1	A	83	ARG
1	A	89	GLU
1	A	90	VAL
1	A	91	GLN
1	A	97	PRO
1	A	105	SER
1	A	108	VAL
1	A	109	LEU
1	A	122	GLU

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Mol	Chain	Res	Type
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	207	GLN
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	236	PRO
1	A	238	LYS
1	A	242	GLN
1	A	246	LEU
1	A	250	ASP
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	292	VAL
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

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Mol	Chain	Res	Type
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	409	THR
1	A	422	LEU
1	A	423	VAL
1	A	428	GLN
1	A	431	LYS
1	A	434	ILE
1	A	435	VAL
1	A	463	ARG
1	A	468	THR
1	A	471	ASP
1	A	473	THR
1	A	487	GLN
1	A	493	VAL
1	A	496	VAL
1	A	503	LEU
1	A	514	GLU
1	A	525	LEU
2	B	4	PRO
2	B	5	ILE
2	B	8	VAL
2	B	10	VAL
2	B	30	LYS
2	B	31	ILE
2	B	47	ILE
2	B	60	VAL
2	B	63	ILE
2	B	64	LYS
2	B	91	GLN
2	B	107	THR
2	B	109	LEU
2	B	113	ASP
2	B	120	LEU

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Mol	Chain	Res	Type
2	B	122	GLU
2	B	156	SER
2	B	161	GLN
2	B	165	THR
2	B	166	LYS
2	B	168	LEU
2	B	173	LYS
2	B	182	GLN
2	B	189	VAL
2	B	200	THR
2	B	204	GLU
2	B	205	LEU
2	B	210	LEU
2	B	212	TRP
2	B	216	THR
2	B	233	GLU
2	B	240	THR
2	B	242	GLN
2	B	249	LYS
2	B	264	LEU
2	B	265	ASN
2	B	280	CYS
2	B	286	THR
2	B	300	GLU
2	B	301	LEU
2	B	303	LEU
2	B	317	VAL
2	B	325	LEU
2	B	336	GLN
2	B	344	GLU
2	B	368	LEU
2	B	388	LYS
2	B	403	THR
2	B	423	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	57	ASN
1	A	137	ASN
1	A	151	GLN

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Mol	Chain	Res	Type
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	394	GLN
1	A	407	GLN
1	A	474	ASN
1	A	520	GLN
1	A	524	GLN
2	B	57	ASN
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	255	ASN
2	B	269	GLN
2	B	278	GLN
2	B	332	GLN
2	B	334	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	4,7,8	3.63	1 (25%)	1,8,10	10.74	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	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	280	CSD	OD1-SG	7.00	1.54	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	10.74	125.38	105.60

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

There are no oligosaccharides 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	1.07	1 (4%)	30,34,34	1.23	2 (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
3	AAP	A	999	-	-	1/16/16/16	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'	3.19	1.55	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	AAP	C6-C1-C2	3.92	119.33	114.92
3	A	999	AAP	C3-C2-C1	-2.38	119.23	122.38

There are no chirality outliers.

All (1) torsion outliers are listed below:

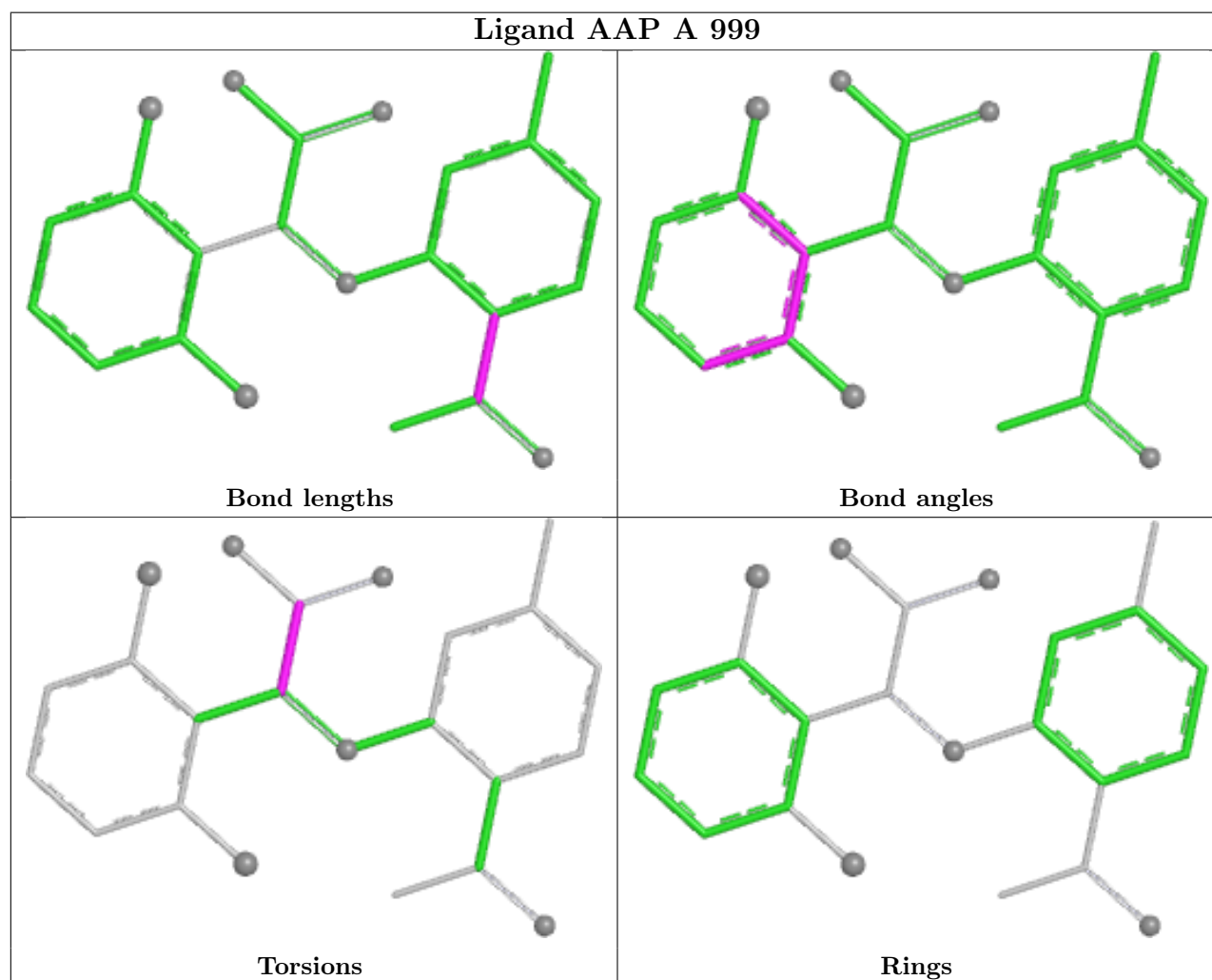
Mol	Chain	Res	Type	Atoms
3	A	999	AAP	O-C-CA-C1

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 than 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.



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.