Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2022 – 08:52 PM EST

PDB ID	:	1JLA
Title	:	CRYSTAL STRUCTURE OF Y181C MUTANT HIV-1 REVERSE TRANSCRIPTASE IN COMPLEX WITH TNK-651
Authors	:	Ren, J.; Nichols, C.; Bird, L.; Chamberlain, P.; Weaver, K.; Short, S.; Stuart, D.I.; Stammers, D.K.
Deposited on	:	2001-07-16
Resolution	:	2.50 Å(reported)

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

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

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

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

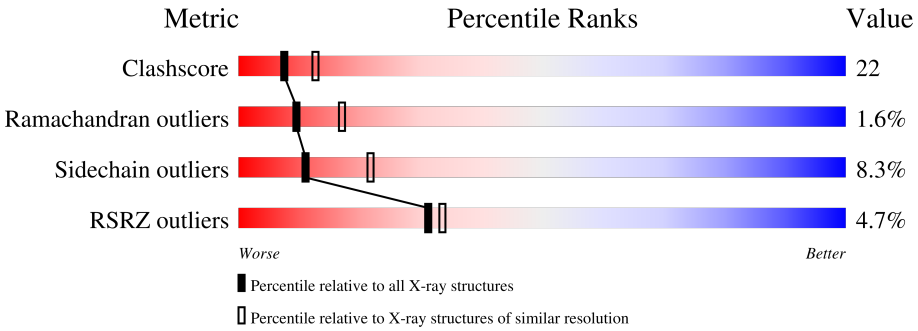
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 2.50 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	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 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.

Mol	Chain	Length	Quality of chain
1	A	560	5% 53% 37% 6%
2	B	440	4% 58% 30% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7894 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 RT A-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	547	Total	C	N	O	S	0	0	0
			4458	2883	743	823	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	CYS	TYR	engineered mutation	UNP P04585
A	280	CSD	CYS	modified residue	UNP P04585

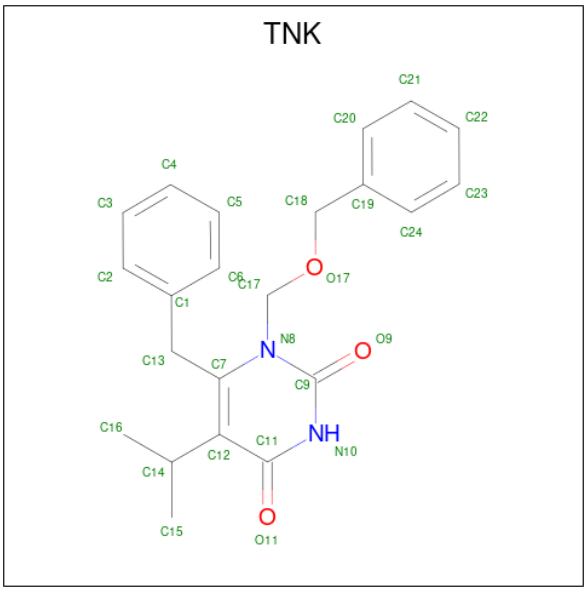
- Molecule 2 is a protein called HIV-1 RT B-chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	408	Total	C	N	O	S	0	0	0
			3363	2181	560	614	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	181	CYS	TYR	engineered mutation	UNP P04585

- Molecule 3 is 6-BENZYL-1-BENZYLOXYMETHYL-5-ISOPROPYL URACIL (three-letter code: TNK) (formula: $C_{22}H_{24}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 27 22 2 3	0	0

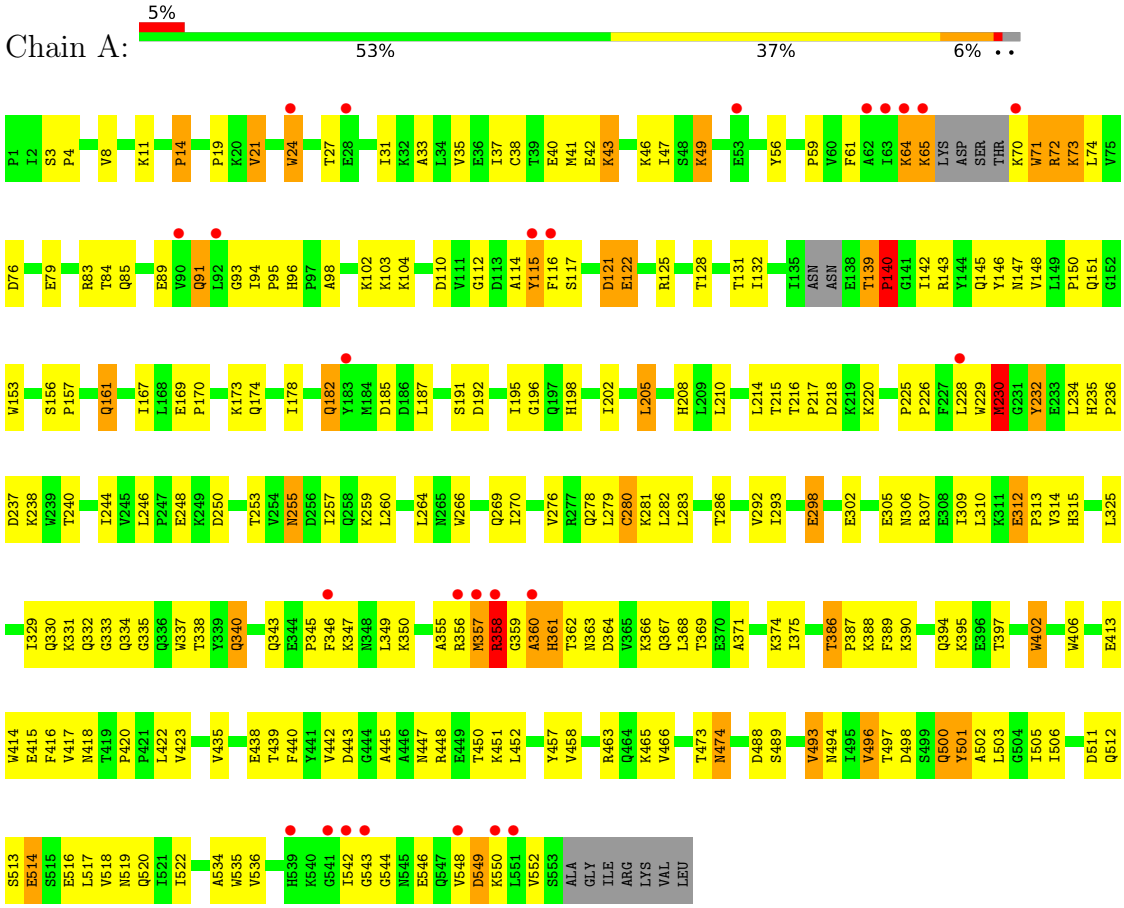
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	30	Total O 30 30	0	0
4	B	16	Total O 16 16	0	0

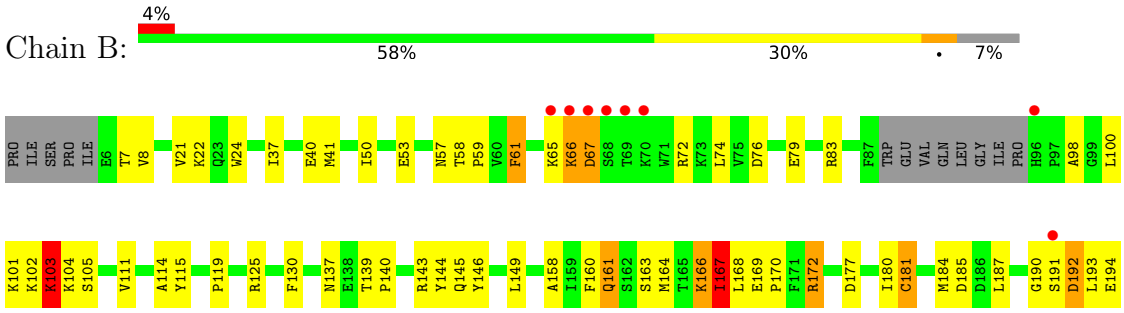
3 Residue-property plots (i)

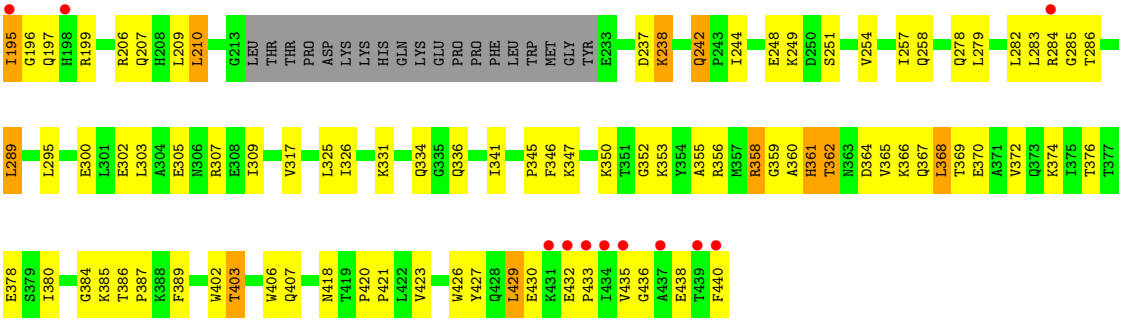
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: HIV-1 RT A-chain



• Molecule 2: HIV-1 RT B-chain




I195 G196 Q197 H198 R199 R206 Q207 H208 L209 L210 G213 LEU THR THR PRO ASP LYS LYS HIS GLN LYS GLU PRO PRO PHE LEU TRP MET GLY TYR E233 D237 K238 Q242 P243 I244 E248 K249 D250 S251 V254 I257 Q258 Q278 L279 L282 L283 R284 G285 T286
L289 L295 E300 L301 E302 L303 A304 E305 N306 R307 E308 I309 V317 L325 I326 K331 Q334 G335 Q336 I341 P345 F346 K347 K350 T351 G352 K353 Y354 A355 R356 M357 R358 G359 A360 H361 T362 N363 D364 V365 K366 Q367 L368 T369 E370 A371 V372 Q373 K374 I375 T376 T377
E378 S379 I380 G384 K385 T386 P387 K388 F389 W402 T403 W406 Q407 N418 T419 P420 P421 L422 V423 W426 Y427 Q428 L429 E430 K431 E432 P433 I434 V435 G436 A437 E438 T439 F440

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	140.40Å 111.20Å 73.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.50 29.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.90-2.50) 98.6 (29.90-2.50)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.39 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.273 0.200 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 75.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7894	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.40	0/4564	0.66	0/6198
2	B	0.40	0/3454	0.66	1/4686 (0.0%)
All	All	0.40	0/8018	0.66	1/10884 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	438	GLU	N-CA-C	5.26	125.19	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4458	0	4510	223	0
2	B	3363	0	3393	139	0
3	A	27	0	24	2	0
4	A	30	0	0	4	0
4	B	16	0	0	2	0
All	All	7894	0	7927	349	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 22.

All (349) 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)
2:B:242:GLN:HE22	2:B:352:GLY:HA2	1.17	1.06
2:B:167:ILE:HD11	2:B:209:LEU:HD23	1.41	0.99
1:A:360:ALA:HA	1:A:514:GLU:HG2	1.49	0.95
2:B:193:LEU:HB3	2:B:197:GLN:HB3	1.54	0.90
1:A:70:LYS:HG3	1:A:71:TRP:H	1.36	0.90
2:B:242:GLN:NE2	2:B:352:GLY:HA2	1.88	0.88
2:B:353:LYS:HE3	2:B:430:GLU:HB3	1.57	0.87
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.54	0.87
1:A:139:THR:HB	1:A:140:PRO:HD2	1.55	0.86
2:B:7:THR:HG22	2:B:119:PRO:HG2	1.56	0.86
1:A:46:LYS:HD2	1:A:116:PHE:HB3	1.61	0.80
2:B:167:ILE:HD11	2:B:209:LEU:CD2	2.11	0.80
1:A:279:LEU:HD23	1:A:302:GLU:OE1	1.83	0.78
2:B:65:LYS:HD3	2:B:72:ARG:HD2	1.65	0.78
1:A:70:LYS:HG3	1:A:71:TRP:N	1.98	0.78
2:B:195:ILE:HG23	2:B:196:GLY:H	1.49	0.78
2:B:358:ARG:H	2:B:358:ARG:HD3	1.49	0.78
1:A:31:ILE:O	1:A:35:VAL:HG23	1.85	0.77
1:A:366:LYS:O	1:A:369:THR:HB	1.84	0.76
1:A:122:GLU:HA	1:A:125:ARG:HG3	1.67	0.75
1:A:244:ILE:HD12	1:A:244:ILE:N	2.00	0.75
1:A:43:LYS:HE3	1:A:43:LYS:HA	1.69	0.75
2:B:79:GLU:O	2:B:83:ARG:HG3	1.87	0.74
1:A:115:TYR:OH	1:A:157:PRO:HA	1.88	0.74
1:A:335:GLY:HA2	1:A:367:GLN:OE1	1.89	0.73
2:B:172:ARG:HD3	2:B:180:ILE:HD12	1.69	0.73
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.87	0.72
2:B:167:ILE:CD1	2:B:209:LEU:HD23	2.17	0.71
1:A:244:ILE:HD12	1:A:244:ILE:H	1.56	0.71
1:A:70:LYS:CG	1:A:71:TRP:H	2.05	0.70
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.73	0.70
2:B:207:GLN:HA	2:B:210:LEU:HD22	1.73	0.70
1:A:356:ARG:NH1	1:A:358:ARG:HA	2.07	0.69
1:A:257:ILE:HD12	1:A:293:ILE:HD12	1.75	0.69
2:B:426:TRP:O	2:B:429:LEU:HB2	1.92	0.68
1:A:246:LEU:HD21	1:A:310:LEU:HD12	1.76	0.68
1:A:345:PRO:O	1:A:346:PHE:HB3	1.92	0.68
1:A:139:THR:HB	1:A:140:PRO:CD	2.23	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:ARG:O	2:B:210:LEU:HD13	1.94	0.67
2:B:365:VAL:O	2:B:369:THR:HG23	1.95	0.67
2:B:104:LYS:HG2	2:B:237:ASP:OD2	1.94	0.67
1:A:511:ASP:OD1	1:A:512:GLN:HG3	1.94	0.67
2:B:66:LYS:NZ	2:B:407:GLN:HB2	2.10	0.67
1:A:543:GLY:HA3	2:B:285:GLY:H	1.60	0.67
1:A:335:GLY:HA3	1:A:356:ARG:HE	1.59	0.66
1:A:458:VAL:CG2	1:A:548:VAL:HG22	2.25	0.65
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.32	0.65
1:A:448:ARG:NH1	1:A:473:THR:HB	2.12	0.65
1:A:65:LYS:HD3	1:A:65:LYS:N	2.11	0.65
1:A:248:GLU:HG3	4:A:1024:HOH:O	1.97	0.65
2:B:139:THR:HG22	2:B:140:PRO:O	1.97	0.64
2:B:161:GLN:HE21	2:B:161:GLN:HA	1.63	0.64
1:A:278:GLN:O	1:A:282:LEU:HD13	1.98	0.64
2:B:254:VAL:O	2:B:258:GLN:HG3	1.99	0.63
1:A:96:HIS:HD2	1:A:98:ALA:HB3	1.64	0.62
1:A:331:LYS:HE2	1:A:333:GLY:O	1.99	0.62
1:A:402:TRP:CH2	2:B:362:THR:HA	2.35	0.61
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.82	0.61
2:B:366:LYS:O	2:B:370:GLU:HG3	1.99	0.61
1:A:458:VAL:HB	1:A:548:VAL:HG22	1.81	0.61
2:B:163:SER:O	2:B:167:ILE:HG23	2.01	0.61
2:B:238:LYS:HD2	2:B:238:LYS:O	2.00	0.61
2:B:317:VAL:HG22	2:B:347:LYS:HD2	1.81	0.61
1:A:114:ALA:HA	1:A:117:SER:OG	2.01	0.60
1:A:70:LYS:NZ	1:A:72:ARG:NH1	2.49	0.60
1:A:131:THR:HG1	1:A:143:ARG:HH11	1.46	0.60
2:B:195:ILE:HG23	2:B:196:GLY:N	2.15	0.59
1:A:357:MET:O	1:A:357:MET:HG2	2.02	0.59
1:A:457:TYR:HA	1:A:548:VAL:HG11	1.83	0.59
1:A:516:GLU:O	1:A:520:GLN:HG3	2.03	0.58
1:A:49:LYS:NZ	1:A:49:LYS:HB3	2.17	0.58
1:A:546:GLU:OE1	2:B:284:ARG:HG2	2.04	0.58
1:A:302:GLU:HA	1:A:305:GLU:OE1	2.03	0.58
2:B:58:THR:HG23	2:B:76:ASP:O	2.03	0.58
1:A:334:GLN:NE2	1:A:512:GLN:HG2	2.18	0.58
2:B:50:ILE:CG2	2:B:145:GLN:HB3	2.33	0.58
1:A:70:LYS:HZ1	1:A:72:ARG:NH1	2.02	0.57
2:B:368:LEU:O	2:B:372:VAL:HG23	2.03	0.57
1:A:359:GLY:O	1:A:361:HIS:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:210:LEU:HD13	2:B:210:LEU:H	1.69	0.57
1:A:178:ILE:HD13	1:A:191:SER:HB3	1.87	0.57
2:B:358:ARG:H	2:B:358:ARG:CD	2.16	0.57
2:B:358:ARG:HD3	2:B:358:ARG:N	2.20	0.57
1:A:195:ILE:HG13	1:A:196:GLY:N	2.19	0.57
1:A:33:ALA:HB2	1:A:71:TRP:CD1	2.39	0.56
2:B:66:LYS:O	2:B:67:ASP:CB	2.52	0.56
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.87	0.56
2:B:376:THR:CG2	2:B:386:THR:HG22	2.36	0.56
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.86	0.56
1:A:218:ASP:OD2	1:A:220:LYS:HB2	2.06	0.56
1:A:443:ASP:OD2	1:A:549:ASP:HA	2.06	0.56
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.87	0.56
2:B:57:ASN:HD22	2:B:143:ARG:HH11	1.54	0.56
1:A:548:VAL:O	1:A:552:VAL:HG22	2.06	0.56
1:A:226:PRO:HB3	1:A:235:HIS:CD2	2.41	0.56
2:B:66:LYS:HZ3	2:B:407:GLN:HB2	1.69	0.56
1:A:114:ALA:HB1	1:A:214:LEU:HD22	1.88	0.55
1:A:489:SER:HB2	1:A:493:VAL:HG13	1.89	0.55
1:A:544:GLY:HA2	2:B:286:THR:HG22	1.88	0.55
1:A:448:ARG:HE	1:A:474:ASN:HB2	1.71	0.55
1:A:161:GLN:HE22	2:B:140:PRO:HG2	1.72	0.55
1:A:228:LEU:HD12	1:A:228:LEU:N	2.22	0.55
1:A:390:LYS:NZ	1:A:415:GLU:OE2	2.40	0.55
2:B:103:LYS:HD2	2:B:192:ASP:OD1	2.06	0.55
1:A:71:TRP:HA	1:A:71:TRP:CE3	2.43	0.54
1:A:543:GLY:HA3	2:B:283:LEU:O	2.07	0.54
1:A:270:ILE:HD11	1:A:314:VAL:HB	1.88	0.54
2:B:248:GLU:HA	2:B:307:ARG:HH22	1.71	0.54
2:B:433:PRO:CG	2:B:436:GLY:HA2	2.37	0.54
1:A:356:ARG:HD2	1:A:356:ARG:C	2.28	0.54
2:B:361:HIS:CE1	4:B:1010:HOH:O	2.60	0.54
1:A:65:LYS:HD3	1:A:65:LYS:H	1.72	0.54
1:A:42:GLU:OE1	1:A:49:LYS:HE2	2.08	0.53
2:B:345:PRO:O	2:B:346:PHE:HB2	2.08	0.53
1:A:114:ALA:O	1:A:117:SER:HB2	2.08	0.53
1:A:445:ALA:HB3	1:A:552:VAL:O	2.08	0.53
2:B:50:ILE:HG21	2:B:145:GLN:HB3	1.89	0.53
2:B:350:LYS:HE3	2:B:378:GLU:OE2	2.09	0.53
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.89	0.53
1:A:89:GLU:HA	1:A:91:GLN:NE2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:HIS:O	1:A:202:ILE:HD13	2.08	0.53
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.89	0.53
1:A:458:VAL:CB	1:A:548:VAL:HG22	2.38	0.53
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.91	0.53
1:A:448:ARG:CZ	1:A:474:ASN:H	2.22	0.53
1:A:116:PHE:CZ	1:A:151:GLN:HG2	2.44	0.53
2:B:103:LYS:HG3	2:B:191:SER:C	2.28	0.53
1:A:283:LEU:O	1:A:286:THR:HG23	2.08	0.53
1:A:544:GLY:HA2	2:B:286:THR:CG2	2.38	0.53
2:B:66:LYS:O	2:B:67:ASP:HB2	2.08	0.52
1:A:19:PRO:O	1:A:56:TYR:HB3	2.10	0.52
1:A:337:TRP:N	1:A:337:TRP:CD1	2.78	0.52
2:B:195:ILE:O	2:B:199:ARG:HG3	2.10	0.52
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.90	0.52
2:B:172:ARG:NH1	2:B:180:ILE:HB	2.24	0.52
1:A:122:GLU:HA	1:A:125:ARG:CG	2.38	0.52
1:A:502:ALA:O	1:A:506:ILE:HG13	2.10	0.52
1:A:64:LYS:HG2	1:A:70:LYS:O	2.09	0.51
1:A:229:TRP:HB3	1:A:234:LEU:HD21	1.91	0.51
1:A:125:ARG:HD3	1:A:147:ASN:HA	1.92	0.51
1:A:276:VAL:O	1:A:280:CSD:HB3	2.10	0.51
1:A:543:GLY:HA2	1:A:546:GLU:HG2	1.92	0.51
2:B:167:ILE:HD12	2:B:167:ILE:O	2.11	0.51
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.26	0.51
2:B:433:PRO:HB2	2:B:436:GLY:N	2.25	0.51
1:A:49:LYS:HA	1:A:143:ARG:O	2.11	0.51
1:A:466:VAL:HG13	1:A:552:VAL:HG12	1.92	0.50
2:B:406:TRP:C	2:B:407:GLN:HG2	2.30	0.50
1:A:448:ARG:HH21	1:A:474:ASN:HB3	1.77	0.50
2:B:61:PHE:CE1	2:B:74:LEU:HD23	2.46	0.50
2:B:244:ILE:HG21	2:B:426:TRP:CZ2	2.46	0.50
1:A:49:LYS:HB3	1:A:49:LYS:HZ3	1.75	0.50
1:A:260:LEU:O	1:A:264:LEU:HD23	2.12	0.50
1:A:357:MET:O	1:A:358:ARG:C	2.48	0.50
1:A:235:HIS:HB2	1:A:238:LYS:O	2.11	0.50
1:A:240:THR:HG22	1:A:315:HIS:HB3	1.94	0.50
1:A:513:SER:HB3	1:A:519:ASN:OD1	2.11	0.50
2:B:139:THR:HG23	2:B:140:PRO:HD2	1.93	0.50
1:A:389:PHE:HB2	1:A:414:TRP:HB3	1.94	0.50
1:A:395:LYS:HG2	1:A:414:TRP:CH2	2.47	0.49
2:B:98:ALA:O	2:B:101:LYS:HG2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:TYR:HD2	1:A:501:TYR:O	1.96	0.49
1:A:102:LYS:O	1:A:103:LYS:HD3	2.12	0.49
1:A:161:GLN:HE22	2:B:140:PRO:CG	2.26	0.49
2:B:65:LYS:HD3	2:B:72:ARG:HH11	1.77	0.49
2:B:406:TRP:O	2:B:407:GLN:HG2	2.13	0.49
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.28	0.49
1:A:260:LEU:HD23	1:A:279:LEU:HD12	1.94	0.49
2:B:61:PHE:N	2:B:61:PHE:CD2	2.80	0.49
2:B:172:ARG:HH11	2:B:180:ILE:HB	1.78	0.49
2:B:103:LYS:HG2	2:B:190:GLY:C	2.33	0.49
1:A:417:VAL:O	1:A:417:VAL:HG13	2.13	0.49
1:A:65:LYS:HG2	1:A:65:LYS:O	2.13	0.48
1:A:332:GLN:HG3	1:A:338:THR:HG23	1.94	0.48
2:B:103:LYS:HG2	2:B:191:SER:N	2.28	0.48
1:A:182:GLN:HG2	1:A:187:LEU:HD12	1.94	0.48
1:A:489:SER:HB2	1:A:493:VAL:CG1	2.43	0.48
1:A:8:VAL:HG13	2:B:53:GLU:OE1	2.14	0.48
1:A:161:GLN:NE2	2:B:140:PRO:HG2	2.29	0.48
1:A:225:PRO:HA	1:A:226:PRO:C	2.34	0.48
2:B:166:LYS:O	2:B:168:LEU:N	2.46	0.48
2:B:356:ARG:HG3	2:B:356:ARG:HH11	1.78	0.48
1:A:246:LEU:CD2	1:A:310:LEU:HD12	2.42	0.48
1:A:494:ASN:HB3	2:B:289:LEU:HD22	1.94	0.48
1:A:544:GLY:O	1:A:548:VAL:HG23	2.14	0.48
2:B:100:LEU:HD22	2:B:181:CYS:HB3	1.95	0.48
2:B:376:THR:O	2:B:380:ILE:HG13	2.13	0.47
1:A:215:THR:HG22	1:A:216:THR:N	2.29	0.47
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.49	0.47
2:B:103:LYS:HG3	2:B:191:SER:O	2.14	0.47
2:B:66:LYS:HG3	2:B:407:GLN:CD	2.35	0.47
2:B:282:LEU:HD13	2:B:295:LEU:HD23	1.97	0.47
1:A:232:TYR:N	1:A:232:TYR:CD1	2.83	0.47
1:A:450:THR:O	1:A:451:LYS:HB2	2.14	0.47
2:B:435:VAL:HG23	2:B:436:GLY:H	1.80	0.47
2:B:161:GLN:HE21	2:B:161:GLN:CA	2.26	0.46
1:A:42:GLU:OE2	1:A:49:LYS:HG2	2.15	0.46
1:A:497:THR:O	1:A:535:TRP:HA	2.15	0.46
1:A:498:ASP:HA	1:A:536:VAL:O	2.15	0.46
2:B:317:VAL:CG2	2:B:347:LYS:HD2	2.44	0.46
1:A:450:THR:HB	1:A:452:LEU:HD23	1.97	0.46
1:A:355:ALA:O	1:A:356:ARG:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:HH12	1:A:358:ARG:HA	1.80	0.46
1:A:359:GLY:O	1:A:360:ALA:C	2.54	0.46
1:A:500:GLN:HE21	1:A:500:GLN:HA	1.80	0.46
2:B:278:GLN:HB2	2:B:302:GLU:OE1	2.16	0.46
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.16	0.46
1:A:458:VAL:HB	1:A:548:VAL:CG2	2.44	0.46
2:B:423:VAL:O	2:B:427:TYR:HD2	1.99	0.46
1:A:278:GLN:HE22	1:A:281:LYS:HE2	1.81	0.46
1:A:314:VAL:HG23	1:A:314:VAL:O	2.16	0.46
2:B:65:LYS:O	2:B:67:ASP:N	2.47	0.46
1:A:278:GLN:NE2	1:A:278:GLN:HA	2.31	0.45
1:A:110:ASP:HB3	1:A:217:PRO:HB3	1.98	0.45
1:A:170:PRO:O	1:A:174:GLN:HG3	2.16	0.45
1:A:418:ASN:O	1:A:420:PRO:HD3	2.16	0.45
2:B:433:PRO:HG3	2:B:436:GLY:HA2	1.97	0.45
1:A:438:GLU:OE2	1:A:463:ARG:NH2	2.43	0.45
2:B:249:LYS:HG2	2:B:251:SER:O	2.17	0.45
1:A:270:ILE:HG12	1:A:314:VAL:HG21	1.99	0.45
1:A:496:VAL:HA	1:A:534:ALA:O	2.16	0.45
1:A:546:GLU:O	1:A:550:LYS:CD	2.65	0.45
3:A:999:TNK:H6	3:A:999:TNK:H162	1.99	0.45
2:B:359:GLY:HA2	2:B:361:HIS:CE1	2.52	0.45
2:B:361:HIS:HE1	4:B:1010:HOH:O	2.00	0.45
2:B:380:ILE:O	2:B:384:GLY:HA2	2.17	0.45
1:A:346:PHE:CD2	1:A:347:LYS:HD2	2.51	0.44
1:A:489:SER:CB	1:A:493:VAL:HG11	2.47	0.44
2:B:158:ALA:O	2:B:161:GLN:HB3	2.18	0.44
1:A:139:THR:CB	1:A:140:PRO:CD	2.91	0.44
1:A:518:VAL:O	1:A:522:ILE:HG13	2.17	0.44
2:B:376:THR:HG23	2:B:386:THR:HG22	2.00	0.44
2:B:402:TRP:CE2	2:B:403:THR:HG22	2.51	0.44
1:A:41:MET:HE2	1:A:47:ILE:HG23	2.00	0.44
2:B:210:LEU:H	2:B:210:LEU:CD1	2.30	0.44
1:A:65:LYS:HE3	1:A:70:LYS:N	2.32	0.44
1:A:244:ILE:N	1:A:244:ILE:CD1	2.71	0.44
1:A:390:LYS:NZ	1:A:415:GLU:CD	2.71	0.44
2:B:161:GLN:HA	2:B:161:GLN:NE2	2.32	0.44
2:B:305:GLU:O	2:B:309:ILE:HG13	2.18	0.44
2:B:435:VAL:HG23	2:B:436:GLY:N	2.32	0.44
1:A:269:GLN:NE2	4:A:1023:HOH:O	2.50	0.44
1:A:544:GLY:C	1:A:546:GLU:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:546:GLU:O	1:A:550:LYS:CG	2.65	0.44
1:A:71:TRP:HA	1:A:71:TRP:HE3	1.82	0.44
1:A:457:TYR:CD1	1:A:457:TYR:C	2.91	0.44
2:B:66:LYS:HG2	2:B:407:GLN:NE2	2.32	0.44
2:B:257:ILE:HG21	2:B:283:LEU:CD1	2.48	0.44
1:A:132:ILE:HB	1:A:142:ILE:HB	1.99	0.44
1:A:148:VAL:O	1:A:150:PRO:HD3	2.18	0.44
2:B:114:ALA:HB1	2:B:160:PHE:CZ	2.52	0.44
2:B:242:GLN:HE22	2:B:352:GLY:CA	2.07	0.44
2:B:336:GLN:HE21	2:B:355:ALA:CB	2.31	0.44
1:A:122:GLU:HA	1:A:125:ARG:CD	2.47	0.43
3:A:999:TNK:H153	3:A:999:TNK:H132	2.00	0.43
2:B:242:GLN:N	2:B:242:GLN:OE1	2.51	0.43
1:A:325:LEU:HD23	1:A:325:LEU:HA	1.73	0.43
1:A:253:THR:O	1:A:257:ILE:HG13	2.18	0.43
2:B:21:VAL:HB	2:B:59:PRO:HD3	2.00	0.43
1:A:270:ILE:HG13	1:A:270:ILE:O	2.18	0.43
2:B:210:LEU:CD1	2:B:210:LEU:N	2.81	0.43
1:A:8:VAL:O	1:A:121:ASP:HB2	2.17	0.43
1:A:253:THR:HG22	1:A:292:VAL:HG22	2.01	0.43
1:A:388:LYS:HD2	1:A:413:GLU:OE1	2.18	0.43
1:A:502:ALA:HA	1:A:505:ILE:HD12	2.00	0.43
2:B:130:PHE:CZ	2:B:144:TYR:HB2	2.54	0.43
2:B:356:ARG:HG3	2:B:356:ARG:NH1	2.34	0.43
1:A:332:GLN:CG	1:A:338:THR:HG23	2.49	0.43
1:A:416:PHE:HE1	1:A:422:LEU:HD22	1.83	0.43
1:A:500:GLN:HE21	1:A:500:GLN:CA	2.32	0.43
2:B:125:ARG:HG2	2:B:146:TYR:O	2.19	0.43
1:A:89:GLU:HA	1:A:91:GLN:HE22	1.84	0.43
1:A:115:TYR:C	1:A:117:SER:H	2.22	0.43
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.84	0.43
1:A:546:GLU:O	1:A:550:LYS:HD3	2.18	0.43
1:A:435:VAL:HG12	4:A:1016:HOH:O	2.19	0.42
1:A:79:GLU:O	1:A:83:ARG:HG2	2.19	0.42
1:A:330:GLN:NE2	1:A:340:GLN:OE1	2.51	0.42
2:B:257:ILE:HG21	2:B:283:LEU:HD13	2.00	0.42
1:A:83:ARG:HG2	1:A:83:ARG:HH11	1.85	0.42
1:A:270:ILE:HG13	1:A:314:VAL:HG11	2.02	0.42
2:B:37:ILE:O	2:B:41:MET:HG3	2.19	0.42
2:B:325:LEU:HD22	2:B:385:LYS:HG3	2.02	0.42
1:A:61:PHE:N	1:A:74:LEU:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:VAL:HG23	1:A:548:VAL:HG22	2.00	0.42
2:B:326:ILE:O	2:B:341:ILE:HA	2.19	0.42
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.89	0.42
2:B:420:PRO:HB2	2:B:423:VAL:HG23	2.00	0.42
1:A:332:GLN:HG3	1:A:338:THR:CG2	2.49	0.42
2:B:432:GLU:HB3	2:B:433:PRO:HD2	2.00	0.42
1:A:439:THR:HG21	2:B:289:LEU:HD13	2.00	0.42
1:A:84:THR:HG22	1:A:85:GLN:N	2.34	0.42
2:B:66:LYS:HZ2	2:B:407:GLN:HB2	1.81	0.42
1:A:27:THR:O	1:A:31:ILE:HG13	2.20	0.42
2:B:279:LEU:HG	2:B:302:GLU:OE1	2.20	0.42
1:A:24:TRP:HB2	1:A:61:PHE:CE1	2.55	0.42
2:B:184:MET:HB3	2:B:185:ASP:H	1.66	0.42
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.60	0.41
1:A:145:GLN:HG2	1:A:146:TYR:N	2.35	0.41
1:A:278:GLN:HG3	1:A:298:GLU:HB3	2.01	0.41
1:A:21:VAL:HG13	1:A:59:PRO:HD3	2.01	0.41
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.21	0.41
1:A:229:TRP:CB	1:A:234:LEU:HD21	2.50	0.41
1:A:244:ILE:HB	1:A:310:LEU:HD13	2.02	0.41
1:A:65:LYS:HE2	1:A:70:LYS:HG2	2.02	0.41
1:A:71:TRP:O	1:A:72:ARG:HD3	2.20	0.41
1:A:73:LYS:C	1:A:73:LYS:HD2	2.41	0.41
1:A:122:GLU:HA	1:A:125:ARG:NE	2.36	0.41
1:A:232:TYR:HB3	1:A:240:THR:O	2.21	0.41
1:A:306:ASN:HA	1:A:309:ILE:HG22	2.01	0.41
1:A:458:VAL:HG23	1:A:548:VAL:HG13	2.01	0.41
1:A:465:LYS:CE	1:A:488:ASP:OD1	2.69	0.41
1:A:229:TRP:O	1:A:230:MET:C	2.59	0.41
1:A:402:TRP:CD1	1:A:402:TRP:C	2.94	0.41
1:A:552:VAL:O	1:A:552:VAL:HG23	2.20	0.41
2:B:278:GLN:HB2	2:B:302:GLU:CD	2.40	0.41
1:A:11:LYS:O	1:A:85:GLN:HB3	2.21	0.41
1:A:47:ILE:HA	1:A:145:GLN:O	2.21	0.41
2:B:65:LYS:HE3	2:B:65:LYS:HB2	1.84	0.41
2:B:102:LYS:HB2	2:B:102:LYS:HE2	1.68	0.41
2:B:360:ALA:HB1	2:B:367:GLN:HG3	2.02	0.41
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.55	0.41
1:A:37:ILE:O	1:A:40:GLU:HB3	2.19	0.41
1:A:205:LEU:O	1:A:208:HIS:HB3	2.21	0.41
1:A:3:SER:HA	1:A:4:PRO:HD3	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.51	0.41
1:A:362:THR:HB	1:A:363:ASN:H	1.66	0.41
1:A:503:LEU:HG	2:B:421:PRO:HG2	2.03	0.41
2:B:139:THR:HG23	2:B:140:PRO:CD	2.51	0.41
1:A:500:GLN:HA	1:A:500:GLN:NE2	2.36	0.41
2:B:242:GLN:NE2	2:B:430:GLU:OE1	2.54	0.41
2:B:358:ARG:CD	2:B:358:ARG:N	2.83	0.41
1:A:93:GLY:O	2:B:137:ASN:CB	2.69	0.40
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.01	0.40
2:B:22:LYS:HE3	2:B:22:LYS:HB2	1.92	0.40
1:A:70:LYS:CG	1:A:71:TRP:N	2.66	0.40
1:A:364:ASP:HB3	1:A:423:VAL:HG13	2.03	0.40
1:A:255:ASN:O	1:A:259:LYS:HG3	2.21	0.40
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.56	0.40
1:A:94:ILE:HA	1:A:95:PRO:HD3	1.93	0.40
1:A:125:ARG:O	1:A:128:THR:OG1	2.30	0.40
1:A:371:ALA:O	1:A:375:ILE:HG13	2.21	0.40
1:A:386:THR:HA	1:A:387:PRO:HD3	1.87	0.40
2:B:244:ILE:HD13	2:B:244:ILE:HA	1.95	0.40
2:B:331:LYS:NZ	2:B:364:ASP:OD1	2.34	0.40
1:A:112:GLY:CA	1:A:185:ASP:HB3	2.52	0.40
1:A:167:ILE:O	1:A:170:PRO:HD2	2.22	0.40
1:A:350:LYS:NZ	4:A:1013:HOH:O	2.50	0.40
2:B:244:ILE:HD13	2:B:430:GLU:HG3	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	540/560 (96%)	485 (90%)	46 (8%)	9 (2%)	9 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	402/440 (91%)	366 (91%)	30 (8%)	6 (2%)	10 18
All	All	942/1000 (94%)	851 (90%)	76 (8%)	15 (2%)	9 17

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	PRO
2	B	67	ASP
1	A	230	MET
1	A	360	ALA
1	A	542	ILE
1	A	14	PRO
1	A	361	HIS
2	B	166	LYS
1	A	358	ARG
2	B	66	LYS
2	B	167	ILE
1	A	122	GLU
2	B	103	LYS
1	A	121	ASP
2	B	195	ILE

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	488/499 (98%)	446 (91%)	42 (9%)	10 20
2	B	370/400 (92%)	341 (92%)	29 (8%)	12 24
All	All	858/899 (95%)	787 (92%)	71 (8%)	11 22

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PRO

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Mol	Chain	Res	Type
1	A	21	VAL
1	A	24	TRP
1	A	43	LYS
1	A	49	LYS
1	A	64	LYS
1	A	65	LYS
1	A	71	TRP
1	A	72	ARG
1	A	73	LYS
1	A	91	GLN
1	A	115	TYR
1	A	139	THR
1	A	140	PRO
1	A	161	GLN
1	A	173	LYS
1	A	182	GLN
1	A	205	LEU
1	A	210	LEU
1	A	230	MET
1	A	232	TYR
1	A	237	ASP
1	A	250	ASP
1	A	255	ASN
1	A	266	TRP
1	A	298	GLU
1	A	312	GLU
1	A	340	GLN
1	A	357	MET
1	A	358	ARG
1	A	368	LEU
1	A	374	LYS
1	A	386	THR
1	A	402	TRP
1	A	474	ASN
1	A	493	VAL
1	A	496	VAL
1	A	500	GLN
1	A	501	TYR
1	A	514	GLU
1	A	517	LEU
1	A	549	ASP
2	B	8	VAL

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Mol	Chain	Res	Type
2	B	24	TRP
2	B	40	GLU
2	B	61	PHE
2	B	103	LYS
2	B	105	SER
2	B	161	GLN
2	B	164	MET
2	B	167	ILE
2	B	172	ARG
2	B	177	ASP
2	B	181	CYS
2	B	192	ASP
2	B	194	GLU
2	B	210	LEU
2	B	238	LYS
2	B	242	GLN
2	B	289	LEU
2	B	300	GLU
2	B	303	LEU
2	B	334	GLN
2	B	358	ARG
2	B	361	HIS
2	B	362	THR
2	B	368	LEU
2	B	374	LYS
2	B	403	THR
2	B	429	LEU
2	B	440	PHE

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	91	GLN
1	A	96	HIS
1	A	151	GLN
1	A	161	GLN
1	A	174	GLN
1	A	242	GLN
1	A	255	ASN
1	A	278	GLN
1	A	334	GLN
1	A	418	ASN

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Mol	Chain	Res	Type
1	A	474	ASN
1	A	487	GLN
1	A	500	GLN
1	A	545	ASN
2	B	57	ASN
2	B	137	ASN
2	B	147	ASN
2	B	161	GLN
2	B	174	GLN
2	B	182	GLN
2	B	207	GLN
2	B	208	HIS
2	B	242	GLN
2	B	334	GLN
2	B	336	GLN
2	B	361	HIS
2	B	407	GLN
2	B	418	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	1.11	0	1,8,10	6.98	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	6.98	118.81	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	TNK	A	999	-	29,29,29	1.70	3 (10%)	32,39,39	0.93	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	TNK	A	999	-	-	4/14/14/14	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	TNK	C7-C12	6.28	1.42	1.35
3	A	999	TNK	C13-C7	2.95	1.54	1.50
3	A	999	TNK	C14-C12	2.06	1.54	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	999	TNK	C1-C13-C7	2.95	120.90	114.71
3	A	999	TNK	C14-C12-C7	2.46	126.67	120.21

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	TNK	O17-C17-N8-C9
3	A	999	TNK	N8-C17-O17-C18
3	A	999	TNK	O17-C17-N8-C7
3	A	999	TNK	C19-C18-O17-C17

There are no ring outliers.

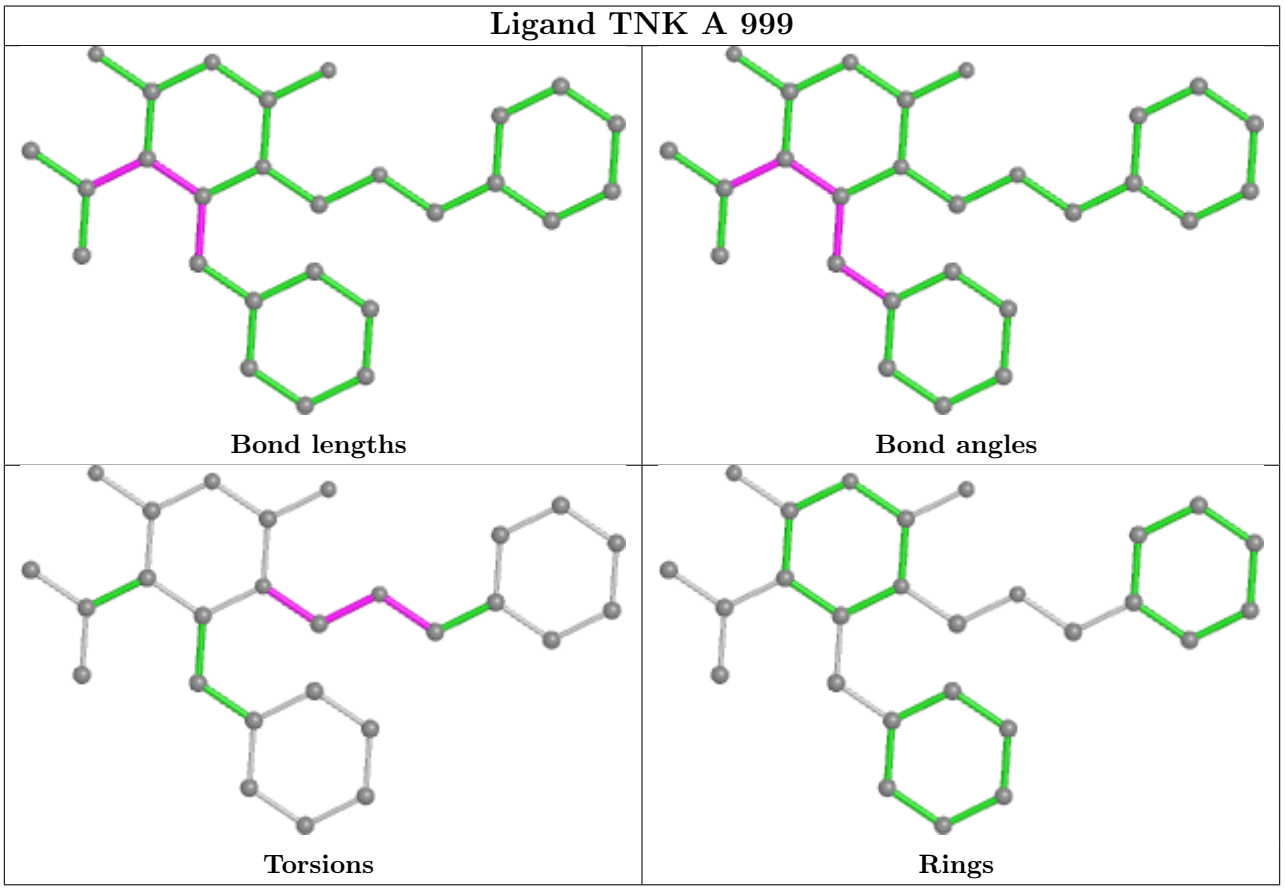
1 monomer is involved in 2 short contacts:

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	546/560 (97%)	-0.17	26 (4%)	30	32	21, 55, 113, 139	0
2	B	408/440 (92%)	-0.15	19 (4%)	31	33	23, 52, 106, 150	0
All	All	954/1000 (95%)	-0.16	45 (4%)	31	33	21, 53, 111, 150	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	435	VAL	6.9
1	A	90	VAL	5.7
2	B	67	ASP	5.6
1	A	115	TYR	5.3
2	B	440	PHE	5.2
1	A	358	ARG	5.1
2	B	437	ALA	5.0
1	A	92	LEU	4.8
2	B	434	ILE	4.2
2	B	195	ILE	4.0
1	A	550	LYS	4.0
1	A	357	MET	4.0
2	B	433	PRO	4.0
2	B	65	LYS	3.7
1	A	28	GLU	3.4
2	B	69	THR	3.3
2	B	70	LYS	3.3
2	B	68	SER	3.2
1	A	70	LYS	3.2
1	A	53	GLU	3.1
1	A	542	ILE	3.1
1	A	65	LYS	3.0
1	A	548	VAL	2.9
2	B	439	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	284	ARG	2.8
2	B	66	LYS	2.8
1	A	541	GLY	2.7
1	A	63	ILE	2.6
1	A	551	LEU	2.6
1	A	64	LYS	2.4
1	A	360	ALA	2.4
2	B	432	GLU	2.4
1	A	543	GLY	2.4
1	A	24	TRP	2.4
1	A	539	HIS	2.4
2	B	431	LYS	2.3
1	A	116	PHE	2.3
1	A	183	TYR	2.2
2	B	198	HIS	2.1
2	B	96	HIS	2.1
1	A	62	ALA	2.1
1	A	346	PHE	2.1
1	A	356	ARG	2.0
2	B	191	SER	2.0
1	A	228	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSD	A	280	8/9	0.95	0.12	51,55,64,69	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

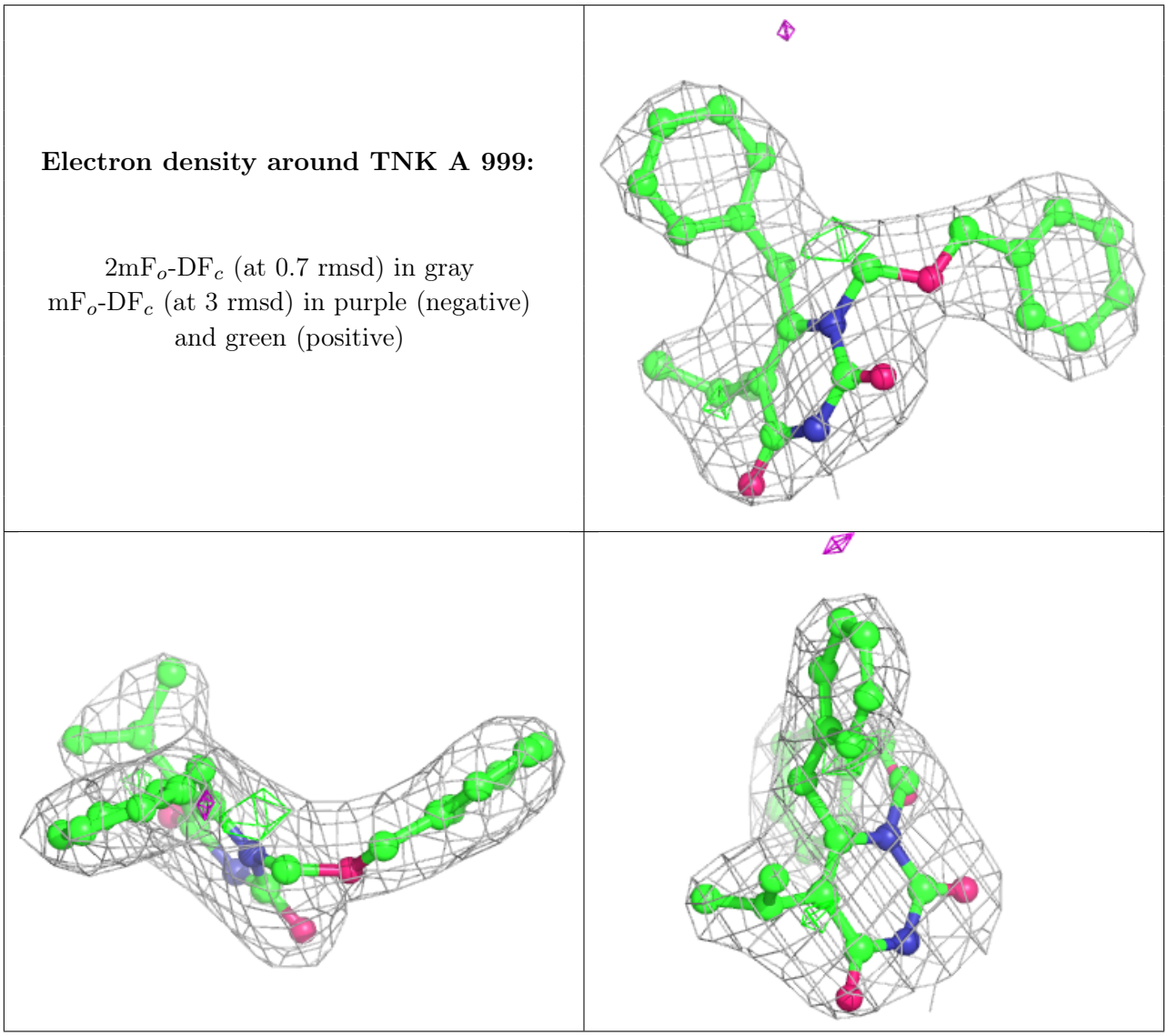
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TNK	A	999	27/27	0.95	0.15	28,40,51,54	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TNK A 999:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.