



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 07:34 PM UTC

PDB ID : 1IKX / pdb_00001ikx
Title : K103N Mutant HIV-1 Reverse Transcriptase in Complex with the Inhibitor PNU142721
Authors : Lindberg, J.; Unge, T.
Deposited on : 2001-05-07
Resolution : 2.80 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

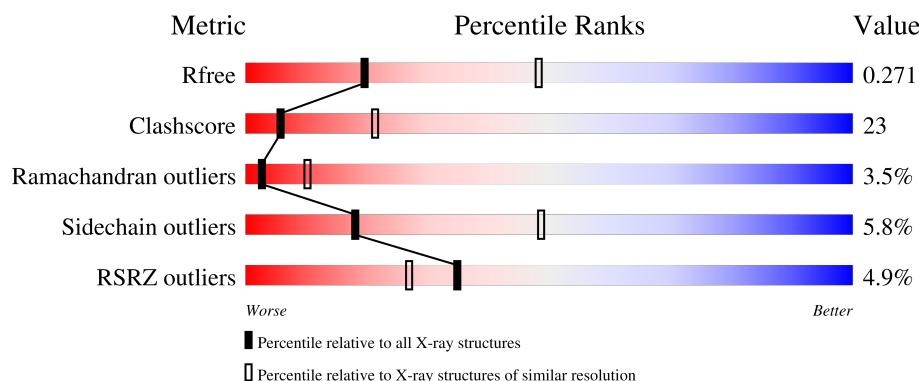
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	
2	B	427	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8132 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 POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	557	Total	C	N	O	S	2	0	0
			4522	2925	754	835	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ASN	LYS	engineered mutation	UNP P03366
A	478	GLN	GLU	engineered mutation	UNP P03366

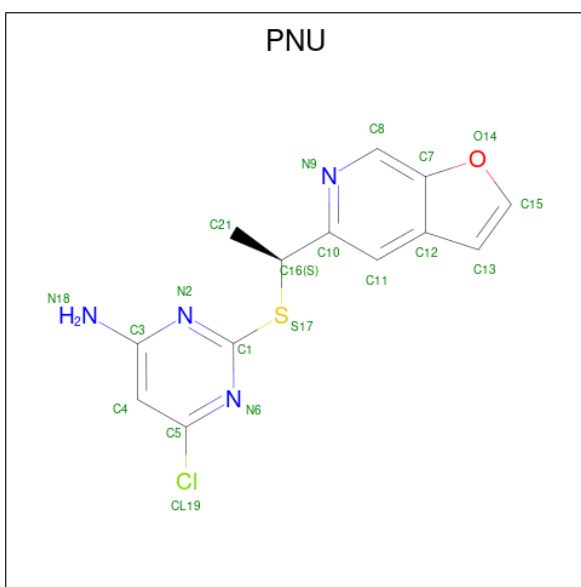
- Molecule 2 is a protein called POL POLYPROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	33	0	0
			3529	2298	584	639	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1103	ASN	LYS	engineered mutation	UNP P03366

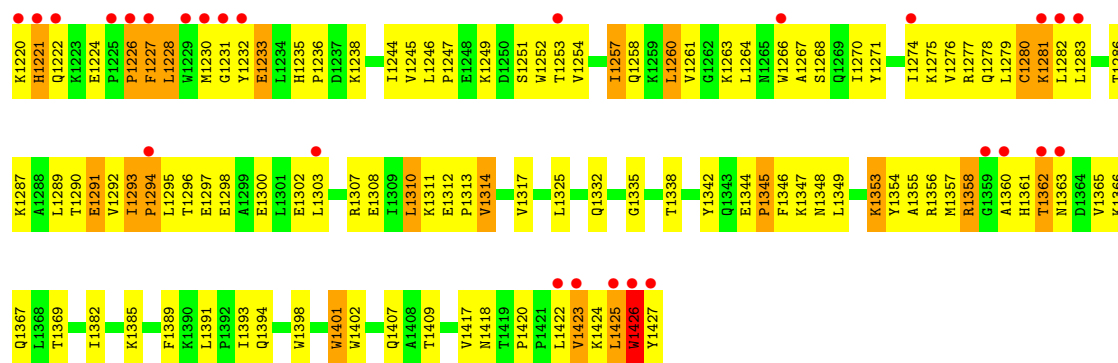
- Molecule 3 is 6-CHLORO-2-(1-FURO[2,3-C]PYRIDIN-5-YL-ETHYLSULFANYL)-PYRIMIDIN-4-YLAMINE (CCD ID: PNU) (formula: C₁₃H₁₁ClN₄OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	S	0	0
			20	13	1	4	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	29	Total	O	0	0
			29	29		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.90Å 156.40Å 156.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.63 – 2.80 23.63 – 2.80	Depositor EDS
% Data completeness (in resolution range)	90.2 (23.63-2.80) 90.2 (23.63-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.210 , 0.274 0.209 , 0.271	Depositor DCC
R_{free} test set	1661 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8132	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: PNU

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	0.44	0/4640	0.93	12/6305 (0.2%)
2	B	0.45	0/3634	0.97	21/4940 (0.4%)
All	All	0.45	0/8274	0.95	33/11245 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	246	LEU	CA-C-N	8.04	129.89	119.84
1	A	246	LEU	C-N-CA	8.04	129.89	119.84
2	B	1349	LEU	N-CA-C	-7.61	103.79	113.23
2	B	1218	ASP	N-CA-C	7.49	121.44	110.59
1	A	382	ILE	N-CA-C	7.43	117.51	110.53
1	A	220	LYS	N-CA-C	-7.16	104.12	112.92
2	B	1382	ILE	N-CA-C	7.04	117.15	110.53
2	B	1401	TRP	N-CA-C	6.75	122.61	113.97
2	B	1151	GLN	N-CA-C	6.29	120.69	112.89
1	A	184	MET	CB-CA-C	-6.28	109.32	116.54
2	B	1310	LEU	N-CA-C	-5.95	102.63	110.43
2	B	1015	GLY	N-CA-C	-5.88	107.13	115.43
1	A	319	TYR	N-CA-C	5.87	119.09	109.76
1	A	51	GLY	CA-C-N	5.83	127.13	119.84
1	A	51	GLY	C-N-CA	5.83	127.13	119.84
2	B	1402	TRP	N-CA-C	5.78	118.32	111.33
1	A	200	THR	N-CA-C	-5.62	105.07	111.14
2	B	1235	HIS	CA-C-N	5.62	125.08	119.24
2	B	1235	HIS	C-N-CA	5.62	125.08	119.24
1	A	348	ASN	N-CA-C	5.61	118.37	110.23
2	B	1227	PHE	N-CA-C	-5.46	104.88	113.02
1	A	493	VAL	N-CA-C	5.45	115.04	108.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1348	ASN	N-CA-C	5.40	118.00	109.96
2	B	1147	ASN	N-CA-C	-5.37	107.10	113.97
2	B	1216	THR	N-CA-C	5.31	118.63	108.97
2	B	1382	ILE	CB-CA-C	-5.29	105.10	112.02
2	B	1245	VAL	N-CA-C	5.26	116.16	108.58
2	B	1389	PHE	N-CA-C	5.20	118.69	109.96
2	B	1391	LEU	N-CA-C	5.12	116.12	109.72
2	B	1233	GLU	N-CA-C	5.12	117.24	108.90
1	A	92	LEU	N-CA-C	-5.12	106.63	112.92
2	B	1175	ASN	CA-C-N	5.10	124.71	119.56
2	B	1175	ASN	C-N-CA	5.10	124.71	119.56

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	4522	0	4572	180	0
2	B	3529	0	3559	201	0
3	A	20	0	11	0	0
4	A	32	0	0	3	0
4	B	29	0	0	3	0
All	All	8132	0	8142	374	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 23.

All (374) 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:131:THR:HG22	1:A:143:ARG:HG2	1.22	1.11
2:B:1275:LYS:HE3	2:B:1277:ARG:HB2	1.41	1.01
1:A:37:ILE:HG22	1:A:41:MET:HE2	1.44	0.99
2:B:1066:LYS:HE2	2:B:1219:LYS:HE3	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:THR:HB	1:A:140:PRO:HD2	1.47	0.95
2:B:1422:LEU:HD23	2:B:1423:VAL:H	1.31	0.93
1:A:278:GLN:HG3	1:A:298:GLU:HB3	1.48	0.93
2:B:1266:TRP:HE1	2:B:1346:PHE:HE2	1.18	0.91
2:B:1226:PRO:HD2	2:B:1228:LEU:HD23	1.56	0.86
2:B:1154:LYS:HE2	2:B:1184:MET:HE2	1.58	0.85
1:A:450:THR:HG22	1:A:452:LEU:HG	1.59	0.84
1:A:485:ALA:O	1:A:489:SER:HB2	1.79	0.82
1:A:54:ASN:HB3	1:A:143:ARG:HH21	1.44	0.82
2:B:1279:LEU:C	2:B:1281:LYS:H	1.86	0.81
2:B:1184:MET:O	2:B:1185:ASP:HB2	1.82	0.80
2:B:1266:TRP:CD1	2:B:1427:TYR:HH	2.01	0.78
2:B:1254:VAL:HG12	2:B:1258:GLN:HE21	1.48	0.78
2:B:1365:VAL:O	2:B:1369:THR:HG23	1.84	0.78
1:A:396:GLU:O	1:A:400:THR:HG22	1.85	0.77
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.64	0.77
1:A:503:LEU:O	1:A:507:GLN:HB2	1.83	0.77
2:B:1007:THR:HG22	2:B:1119:PRO:HG2	1.66	0.76
2:B:1090:VAL:HG23	2:B:1091:GLN:N	2.00	0.75
1:A:450:THR:O	1:A:451:LYS:HB2	1.84	0.73
2:B:1084:THR:HG22	2:B:1088:TRP:HD1	1.52	0.73
2:B:1157:PRO:HG2	2:B:1184:MET:HA	1.68	0.73
2:B:1314:VAL:O	2:B:1317:VAL:HG22	1.88	0.73
2:B:1253:THR:O	2:B:1257:ILE:HG22	1.88	0.73
2:B:1335:GLY:HA3	2:B:1356:ARG:HG3	1.69	0.73
1:A:249:LYS:HD3	1:A:251:SER:O	1.88	0.72
2:B:1282:LEU:H	2:B:1282:LEU:HD12	1.54	0.72
2:B:1109:LEU:HA	2:B:1218:ASP:CG	2.13	0.72
2:B:1154:LYS:HE2	2:B:1184:MET:CE	2.20	0.72
1:A:356:ARG:HG2	1:A:356:ARG:HH11	1.55	0.71
1:A:268:SER:O	1:A:351:THR:HG22	1.90	0.71
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.71	0.70
2:B:1226:PRO:HG2	2:B:1227:PHE:H	1.56	0.70
2:B:1047:ILE:HD12	2:B:1144:TYR:CD1	2.27	0.70
1:A:417:VAL:HG22	1:A:419:THR:HG23	1.74	0.69
2:B:1281:LYS:HB3	2:B:1282:LEU:HD12	1.73	0.69
1:A:466:VAL:CG2	1:A:551:LEU:HD13	2.23	0.69
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.75	0.69
1:A:469:LEU:HD23	1:A:472:THR:HG21	1.74	0.69
2:B:1224:GLU:O	2:B:1226:PRO:HD3	1.93	0.69
2:B:1157:PRO:CG	2:B:1184:MET:HA	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1417:VAL:HG12	2:B:1418:ASN:N	2.08	0.68
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.76	0.68
1:A:435:VAL:HG13	2:B:1290:THR:HG21	1.76	0.68
2:B:1363:ASN:HB3	2:B:1366:LYS:HB2	1.74	0.68
1:A:131:THR:HG22	1:A:143:ARG:CG	2.14	0.68
1:A:466:VAL:HG21	1:A:551:LEU:HD13	1.74	0.67
1:A:441:TYR:O	1:A:548:VAL:HG21	1.94	0.67
1:A:50:ILE:HG13	1:A:51:GLY:H	1.59	0.67
2:B:1184:MET:O	2:B:1184:MET:HG3	1.95	0.67
1:A:131:THR:CG2	1:A:143:ARG:HH11	2.08	0.66
2:B:1059:PRO:HG2	2:B:1076:ASP:HB3	1.76	0.66
2:B:1271:TYR:O	2:B:1274:ILE:HG12	1.96	0.66
2:B:1169:GLU:HB3	2:B:1170:PRO:HD3	1.79	0.65
2:B:1090:VAL:HG23	2:B:1091:GLN:H	1.61	0.65
2:B:1066:LYS:HB2	2:B:1220:LYS:HB3	1.78	0.65
2:B:1001:PRO:HB2	2:B:1117:SER:OG	1.97	0.65
1:A:64:LYS:HD3	1:A:68:SER:OG	1.96	0.65
1:A:542:ILE:HG23	2:B:1283:LEU:HD12	1.79	0.64
2:B:1310:LEU:O	2:B:1311:LYS:HB3	1.96	0.64
1:A:107:THR:HG23	1:A:198:HIS:NE2	2.13	0.64
2:B:1246:LEU:HD12	2:B:1307:ARG:HB3	1.80	0.64
2:B:1112:GLY:C	2:B:1151:GLN:HE21	2.06	0.64
1:A:308:GLU:O	1:A:311:LYS:HG2	1.98	0.63
1:A:409:THR:HG23	4:B:3027:HOH:O	1.98	0.63
2:B:1358:ARG:N	2:B:1358:ARG:HD2	2.14	0.63
1:A:107:THR:HB	1:A:223:LYS:HB3	1.80	0.63
1:A:447:ASN:OD1	1:A:449:GLU:HG2	1.98	0.63
1:A:65:LYS:HZ1	1:A:72:ARG:HD2	1.63	0.62
2:B:1065:LYS:HB3	2:B:1220:LYS:HG3	1.81	0.62
2:B:1356:ARG:NH2	2:B:1362:THR:HA	2.15	0.62
1:A:107:THR:HB	1:A:223:LYS:CB	2.30	0.62
2:B:1230:MET:HE3	2:B:1230:MET:HA	1.81	0.62
2:B:1001:PRO:HB2	2:B:1117:SER:CB	2.30	0.61
1:A:41:MET:HE1	1:A:73:LYS:NZ	2.15	0.61
2:B:1090:VAL:CG2	2:B:1091:GLN:N	2.63	0.61
1:A:223:LYS:HG3	1:A:224:GLU:N	2.14	0.61
2:B:1283:LEU:H	2:B:1283:LEU:HD23	1.65	0.61
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.36	0.61
2:B:1004:PRO:O	2:B:1005:ILE:HB	1.99	0.61
1:A:50:ILE:HG13	1:A:51:GLY:N	2.15	0.61
1:A:303:LEU:O	1:A:307:ARG:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1085:GLN:HA	2:B:1088:TRP:NE1	2.16	0.61
2:B:1072:ARG:HH11	2:B:1072:ARG:HG3	1.65	0.61
2:B:1282:LEU:HD13	2:B:1293:ILE:CG2	2.31	0.61
2:B:1417:VAL:HG12	2:B:1418:ASN:H	1.66	0.61
2:B:1422:LEU:O	2:B:1424:LYS:N	2.34	0.60
2:B:1090:VAL:CG2	2:B:1091:GLN:H	2.13	0.60
1:A:139:THR:HB	1:A:140:PRO:CD	2.27	0.60
2:B:1282:LEU:HD13	2:B:1293:ILE:HG21	1.82	0.60
2:B:1292:VAL:O	2:B:1293:ILE:HD12	2.00	0.60
2:B:1050:ILE:HD12	2:B:1054:ASN:HB3	1.83	0.60
2:B:1264:LEU:HD13	2:B:1276:VAL:HG12	1.83	0.60
1:A:27:THR:O	1:A:31:ILE:HG13	2.02	0.59
1:A:41:MET:HE1	1:A:73:LYS:HZ3	1.67	0.59
2:B:1282:LEU:HD22	2:B:1293:ILE:HG13	1.83	0.59
1:A:218:ASP:HB3	1:A:219:LYS:HD2	1.85	0.59
1:A:324:ASP:O	1:A:343:GLN:HG2	2.02	0.59
2:B:1422:LEU:HD23	2:B:1423:VAL:N	2.12	0.58
2:B:1109:LEU:HA	2:B:1218:ASP:OD1	2.03	0.58
1:A:458:VAL:HG21	1:A:547:GLN:OE1	2.04	0.58
1:A:458:VAL:HB	1:A:548:VAL:HG22	1.85	0.58
1:A:356:ARG:HG2	1:A:356:ARG:NH1	2.19	0.57
2:B:1084:THR:HG22	2:B:1088:TRP:CD1	2.36	0.57
2:B:1282:LEU:HD22	2:B:1293:ILE:HG23	1.86	0.57
2:B:1001:PRO:HD2	2:B:1116:PHE:O	2.05	0.57
2:B:1422:LEU:CD2	2:B:1423:VAL:H	2.13	0.57
1:A:301:LEU:O	1:A:304:ALA:HB3	2.05	0.57
2:B:1409:THR:HB	4:B:3036:HOH:O	2.03	0.57
1:A:65:LYS:HG3	1:A:66:LYS:N	2.20	0.57
2:B:1151:GLN:O	2:B:1185:ASP:OD1	2.23	0.57
2:B:1219:LYS:HG2	2:B:1232:TYR:HB2	1.87	0.57
2:B:1287:LYS:HD3	2:B:1291:GLU:OE2	2.05	0.57
2:B:1263:LYS:HE2	2:B:1425:LEU:HA	1.87	0.56
2:B:1317:VAL:CG1	2:B:1347:LYS:HD2	2.35	0.56
1:A:38:CYS:HA	1:A:41:MET:HE3	1.87	0.56
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.19	0.56
1:A:278:GLN:CG	1:A:298:GLU:HB3	2.31	0.56
2:B:1065:LYS:HD3	2:B:1221:HIS:HB2	1.86	0.56
2:B:1114:ALA:HB2	2:B:1214:LEU:HD22	1.87	0.56
2:B:1142:ILE:HD12	2:B:1142:ILE:H	1.68	0.56
1:A:254:VAL:O	1:A:258:GLN:HG3	2.06	0.56
2:B:1213:GLY:C	2:B:1214:LEU:HD23	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1356:ARG:HE	2:B:1367:GLN:HE22	1.52	0.56
2:B:1066:LYS:O	2:B:1067:ASP:HB2	2.06	0.56
2:B:1109:LEU:HA	2:B:1218:ASP:OD2	2.05	0.56
2:B:1213:GLY:O	2:B:1214:LEU:HD23	2.05	0.56
2:B:1312:GLU:HG3	2:B:1313:PRO:HD2	1.87	0.56
1:A:231:GLY:C	1:A:242:GLN:HG2	2.31	0.56
2:B:1086:ASP:O	2:B:1090:VAL:HG22	2.05	0.56
1:A:20:LYS:HE2	1:A:55:PRO:HB2	1.88	0.55
2:B:1311:LYS:O	2:B:1311:LYS:HG2	2.07	0.55
1:A:194:GLU:HB2	1:A:197:GLN:OE1	2.06	0.55
1:A:221:HIS:C	1:A:223:LYS:H	2.13	0.55
1:A:521:ILE:O	1:A:525:LEU:HG	2.07	0.55
2:B:1270:ILE:O	2:B:1271:TYR:HB2	2.06	0.55
2:B:1214:LEU:O	2:B:1216:THR:HG23	2.07	0.55
2:B:1325:LEU:HD12	2:B:1385:LYS:HG3	1.89	0.55
1:A:222:GLN:O	1:A:222:GLN:HG2	2.07	0.54
1:A:317:VAL:HG23	4:A:3062:HOH:O	2.07	0.54
2:B:1282:LEU:HD12	2:B:1282:LEU:N	2.20	0.54
1:A:357:MET:HG3	1:A:358:ARG:H	1.72	0.54
2:B:1202:ILE:O	2:B:1206:ARG:HG3	2.08	0.54
1:A:497:THR:O	1:A:535:TRP:HA	2.08	0.54
1:A:65:LYS:NZ	1:A:72:ARG:HD2	2.22	0.54
1:A:131:THR:CG2	1:A:143:ARG:HG2	2.15	0.54
2:B:1064:LYS:HD2	2:B:1068:SER:O	2.08	0.54
2:B:1219:LYS:HA	2:B:1232:TYR:HB2	1.89	0.54
1:A:107:THR:HA	1:A:223:LYS:HB2	1.90	0.53
1:A:435:VAL:HG22	2:B:1290:THR:HG23	1.88	0.53
1:A:325:LEU:HD22	1:A:385:LYS:HE3	1.90	0.53
2:B:1066:LYS:HD2	2:B:1407:GLN:HE22	1.73	0.53
1:A:66:LYS:C	1:A:68:SER:H	2.17	0.53
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.24	0.53
1:A:355:ALA:O	1:A:356:ARG:C	2.52	0.53
1:A:361:HIS:CD2	1:A:513:SER:OG	2.62	0.53
1:A:469:LEU:CD2	1:A:472:THR:HG21	2.39	0.53
1:A:458:VAL:CG2	1:A:548:VAL:HG22	2.38	0.53
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.91	0.52
1:A:211:ARG:O	1:A:211:ARG:HG2	2.09	0.52
1:A:277:ARG:HD3	4:A:3019:HOH:O	2.10	0.52
1:A:356:ARG:NH1	1:A:358:ARG:HA	2.25	0.52
1:A:361:HIS:HD2	1:A:513:SER:OG	1.92	0.52
1:A:54:ASN:HB3	1:A:143:ARG:NH2	2.20	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1369:THR:HG22	2:B:1398:TRP:CH2	2.45	0.52
1:A:54:ASN:HD21	1:A:56:TYR:HB2	1.73	0.52
1:A:465:LYS:HG2	1:A:466:VAL:N	2.25	0.52
1:A:54:ASN:O	1:A:56:TYR:N	2.42	0.52
2:B:1222:GLN:HE21	2:B:1228:LEU:HD12	1.75	0.52
2:B:1068:SER:C	2:B:1070:LYS:H	2.18	0.52
1:A:460:ASN:HA	2:B:1286:THR:HG22	1.92	0.51
1:A:410:TRP:CG	1:A:411:ILE:N	2.78	0.51
2:B:1422:LEU:O	2:B:1425:LEU:HG	2.09	0.51
1:A:219:LYS:HD2	1:A:219:LYS:N	2.25	0.51
2:B:1279:LEU:C	2:B:1281:LYS:N	2.57	0.51
2:B:1263:LYS:HA	2:B:1425:LEU:HD22	1.93	0.51
2:B:1276:VAL:HA	2:B:1302:GLU:OE1	2.10	0.51
1:A:469:LEU:HD21	1:A:480:GLN:HG2	1.91	0.51
2:B:1115:TYR:HB3	2:B:1149:LEU:HB2	1.92	0.51
2:B:1417:VAL:CG1	2:B:1418:ASN:N	2.73	0.51
2:B:1065:LYS:HB2	2:B:1068:SER:HB3	1.93	0.50
2:B:1050:ILE:HD12	2:B:1054:ASN:CB	2.40	0.50
2:B:1065:LYS:HE2	2:B:1221:HIS:ND1	2.27	0.50
2:B:1260:LEU:HD11	2:B:1303:LEU:HD13	1.94	0.50
1:A:411:ILE:O	1:A:411:ILE:HG23	2.12	0.50
2:B:1280:CYS:O	2:B:1281:LYS:O	2.29	0.50
2:B:1417:VAL:CG1	2:B:1418:ASN:H	2.24	0.50
1:A:54:ASN:C	1:A:54:ASN:HD22	2.19	0.50
2:B:1282:LEU:HD22	2:B:1293:ILE:CG1	2.42	0.50
1:A:221:HIS:C	1:A:223:LYS:N	2.70	0.50
1:A:356:ARG:HH12	1:A:358:ARG:HA	1.76	0.50
1:A:106:VAL:HG22	1:A:227:PHE:HE2	1.77	0.49
1:A:23:GLN:HG2	1:A:133:PRO:HG3	1.95	0.49
1:A:412:PRO:HG3	2:B:1401:TRP:CZ2	2.47	0.49
2:B:1257:ILE:HG12	2:B:1283:LEU:HD22	1.94	0.49
1:A:108:VAL:C	1:A:109:LEU:HD23	2.37	0.49
1:A:231:GLY:O	1:A:242:GLN:HG2	2.11	0.49
1:A:34:LEU:HD21	1:A:62:ALA:HB2	1.93	0.49
1:A:285:GLY:O	1:A:287:LYS:HG3	2.12	0.49
2:B:1153:TRP:CZ2	2:B:1155:GLY:HA3	2.48	0.49
1:A:305:GLU:O	1:A:308:GLU:HB3	2.13	0.49
1:A:457:TYR:CD1	1:A:457:TYR:C	2.91	0.49
2:B:1010:VAL:HG12	2:B:1011:LYS:N	2.28	0.49
2:B:1257:ILE:CG1	2:B:1283:LEU:HD22	2.43	0.49
2:B:1004:PRO:O	2:B:1005:ILE:CB	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ILE:CG1	1:A:51:GLY:H	2.21	0.48
2:B:1050:ILE:CG2	2:B:1145:GLN:HG2	2.43	0.48
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.94	0.48
2:B:1149:LEU:HB3	2:B:1156:SER:OG	2.14	0.48
1:A:195:ILE:HD11	1:A:199:ARG:NH2	2.28	0.48
2:B:1346:PHE:N	2:B:1346:PHE:CD1	2.82	0.48
1:A:435:VAL:HG22	2:B:1290:THR:CG2	2.44	0.48
1:A:494:ASN:HB3	2:B:1289:LEU:HD12	1.95	0.48
1:A:544:GLY:O	1:A:548:VAL:HG23	2.14	0.48
2:B:1072:ARG:HG3	2:B:1072:ARG:NH1	2.27	0.48
2:B:1264:LEU:HB3	2:B:1276:VAL:HG11	1.96	0.48
1:A:57:ASN:HA	1:A:129:ALA:O	2.14	0.48
2:B:1064:LYS:HZ1	2:B:1069:THR:HA	1.78	0.48
2:B:1226:PRO:CD	2:B:1228:LEU:HD23	2.37	0.48
2:B:1278:GLN:HB3	2:B:1298:GLU:OE2	2.14	0.48
2:B:1296:THR:CG2	2:B:1298:GLU:HG2	2.44	0.48
1:A:42:GLU:OE2	1:A:49:LYS:HG3	2.13	0.47
2:B:1282:LEU:HD22	2:B:1294:PRO:HD2	1.96	0.47
2:B:1296:THR:HG22	2:B:1297:GLU:H	1.78	0.47
1:A:346:PHE:N	1:A:346:PHE:CD2	2.78	0.47
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.97	0.47
2:B:1344:GLU:O	2:B:1347:LYS:HB2	2.15	0.47
2:B:1425:LEU:O	2:B:1426:TRP:C	2.57	0.47
1:A:443:ASP:OD1	1:A:444:GLY:N	2.42	0.47
2:B:1047:ILE:HG22	2:B:1146:TYR:HA	1.96	0.47
2:B:1085:GLN:HA	2:B:1088:TRP:CE2	2.48	0.47
2:B:1254:VAL:O	2:B:1257:ILE:HG23	2.15	0.47
1:A:458:VAL:HG11	1:A:547:GLN:OE1	2.13	0.47
2:B:1244:ILE:HD12	2:B:1310:LEU:HD22	1.97	0.47
2:B:1427:TYR:O	2:B:1427:TYR:CD1	2.68	0.47
1:A:131:THR:CG2	1:A:143:ARG:NH1	2.76	0.47
2:B:1122:GLU:CD	2:B:1122:GLU:H	2.23	0.47
1:A:79:GLU:O	1:A:83:ARG:HD2	2.15	0.46
2:B:1079:GLU:HB2	4:B:3007:HOH:O	2.15	0.46
2:B:1266:TRP:NE1	2:B:1346:PHE:HE2	2.00	0.46
1:A:97:PRO:O	1:A:100:LEU:HB2	2.16	0.46
2:B:1024:TRP:CG	2:B:1025:PRO:HD2	2.50	0.46
2:B:1393:ILE:HG12	2:B:1394:GLN:N	2.30	0.46
2:B:1195:ILE:HG23	2:B:1196:GLY:N	2.30	0.46
1:A:108:VAL:O	1:A:221:HIS:O	2.34	0.46
2:B:1290:THR:O	2:B:1291:GLU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1369:THR:HG22	2:B:1398:TRP:CZ3	2.51	0.46
1:A:454:LYS:O	1:A:552:VAL:HG13	2.16	0.46
2:B:1335:GLY:O	2:B:1355:ALA:HA	2.16	0.46
1:A:479:LEU:HB3	1:A:517:LEU:CD1	2.40	0.46
2:B:1168:LEU:HD13	2:B:1180:ILE:HG21	1.97	0.46
1:A:23:GLN:HE22	1:A:60:VAL:HG22	1.81	0.46
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.56	0.46
1:A:198:HIS:O	1:A:202:ILE:HG12	2.15	0.46
2:B:1209:LEU:HD22	2:B:1214:LEU:HD12	1.98	0.46
2:B:1282:LEU:HD22	2:B:1293:ILE:CG2	2.46	0.46
1:A:65:LYS:HG3	1:A:66:LYS:H	1.80	0.45
2:B:1252:TRP:CD1	2:B:1295:LEU:HD21	2.51	0.45
1:A:202:ILE:O	1:A:205:LEU:HB3	2.16	0.45
2:B:1279:LEU:O	2:B:1281:LYS:N	2.50	0.45
1:A:458:VAL:CB	1:A:548:VAL:HG22	2.46	0.45
1:A:90:VAL:CG1	1:A:161:GLN:HG3	2.46	0.45
2:B:1267:ALA:O	2:B:1270:ILE:O	2.35	0.45
1:A:41:MET:HE1	1:A:73:LYS:CE	2.46	0.45
1:A:361:HIS:HD2	1:A:513:SER:CB	2.30	0.45
1:A:364:ASP:HB3	1:A:423:VAL:HG13	1.98	0.45
1:A:104:LYS:HE2	1:A:194:GLU:OE1	2.16	0.45
2:B:1353:LYS:NZ	2:B:1353:LYS:HB3	2.32	0.45
1:A:23:GLN:CG	1:A:133:PRO:HG3	2.47	0.45
1:A:139:THR:CB	1:A:140:PRO:HD2	2.28	0.45
1:A:210:LEU:C	1:A:212:TRP:H	2.24	0.45
2:B:1066:LYS:HA	2:B:1407:GLN:NE2	2.31	0.45
2:B:1218:ASP:O	2:B:1219:LYS:CB	2.64	0.45
1:A:522:ILE:O	1:A:526:ILE:HG13	2.16	0.44
2:B:1353:LYS:HG2	2:B:1354:TYR:N	2.32	0.44
1:A:67:ASP:O	1:A:68:SER:HB3	2.17	0.44
2:B:1332:GLN:NE2	2:B:1423:VAL:HG13	2.31	0.44
2:B:1120:LEU:O	2:B:1121:ASP:C	2.60	0.44
2:B:1296:THR:O	2:B:1300:GLU:HG2	2.17	0.44
2:B:1426:TRP:O	2:B:1427:TYR:OXT	2.35	0.44
1:A:41:MET:CE	1:A:73:LYS:HZ3	2.31	0.44
2:B:1112:GLY:C	2:B:1151:GLN:NE2	2.75	0.44
2:B:1153:TRP:CE2	2:B:1155:GLY:HA3	2.51	0.44
2:B:1249:LYS:HG2	2:B:1251:SER:H	1.81	0.44
2:B:1286:THR:HG22	2:B:1286:THR:O	2.16	0.44
2:B:1422:LEU:O	2:B:1423:VAL:C	2.61	0.44
2:B:1064:LYS:NZ	2:B:1069:THR:HA	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:C	1:A:196:GLY:N	2.75	0.44
1:A:317:VAL:HG22	1:A:318:TYR:N	2.32	0.43
1:A:54:ASN:ND2	1:A:56:TYR:HB2	2.33	0.43
1:A:57:ASN:OD1	1:A:131:THR:HG23	2.18	0.43
2:B:1103:ASN:ND2	2:B:1179:VAL:CG2	2.82	0.43
2:B:1103:ASN:HD21	2:B:1179:VAL:CG2	2.31	0.43
1:A:69:THR:HG22	1:A:70:LYS:HG3	2.00	0.43
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.49	0.43
2:B:1129:ALA:HA	2:B:1144:TYR:O	2.18	0.43
2:B:1157:PRO:HG3	2:B:1184:MET:HA	1.97	0.43
1:A:39:THR:O	1:A:43:LYS:HG3	2.19	0.43
1:A:181:TYR:HB3	1:A:188:TYR:HB2	2.01	0.43
1:A:433:PRO:HG3	1:A:532:TYR:CE2	2.54	0.43
1:A:553:SER:HA	1:A:557:ARG:CB	2.49	0.43
1:A:410:TRP:CG	1:A:411:ILE:H	2.34	0.43
2:B:1278:GLN:HB2	2:B:1302:GLU:CG	2.49	0.43
2:B:1332:GLN:HE22	2:B:1423:VAL:HG13	1.83	0.43
2:B:1038:CYS:SG	2:B:1132:ILE:HD11	2.59	0.43
1:A:417:VAL:O	1:A:417:VAL:HG13	2.19	0.43
1:A:195:ILE:HG12	1:A:199:ARG:CZ	2.49	0.42
1:A:364:ASP:CB	1:A:423:VAL:HG13	2.49	0.42
1:A:397:THR:O	1:A:400:THR:HG23	2.18	0.42
2:B:1296:THR:HG22	2:B:1297:GLU:N	2.34	0.42
1:A:221:HIS:O	1:A:222:GLN:HB3	2.18	0.42
1:A:539:HIS:O	1:A:540:LYS:HD2	2.19	0.42
2:B:1357:MET:C	2:B:1358:ARG:HD2	2.44	0.42
1:A:20:LYS:HG2	1:A:55:PRO:O	2.19	0.42
1:A:33:ALA:O	1:A:37:ILE:HG13	2.20	0.42
1:A:106:VAL:HG22	1:A:227:PHE:CE2	2.54	0.42
1:A:257:ILE:O	1:A:261:VAL:HG23	2.19	0.42
1:A:351:THR:CG2	1:A:352:GLY:N	2.83	0.42
2:B:1169:GLU:HB3	2:B:1170:PRO:CD	2.49	0.42
2:B:1226:PRO:HD2	2:B:1228:LEU:CD2	2.39	0.42
1:A:94:ILE:HG23	1:A:229:TRP:HH2	1.85	0.42
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.53	0.42
2:B:1226:PRO:CG	2:B:1227:PHE:H	2.28	0.42
2:B:1271:TYR:CG	2:B:1310:LEU:HD23	2.54	0.42
1:A:219:LYS:HD2	1:A:219:LYS:H	1.83	0.42
1:A:298:GLU:H	1:A:298:GLU:CD	2.28	0.42
2:B:1361:HIS:C	2:B:1363:ASN:H	2.27	0.42
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:THR:HG21	1:A:143:ARG:HH11	1.84	0.42
1:A:249:LYS:HB3	4:A:3049:HOH:O	2.19	0.42
2:B:1266:TRP:CD1	2:B:1427:TYR:OH	2.68	0.42
1:A:149:LEU:HA	1:A:150:PRO:HD3	1.90	0.42
2:B:1068:SER:C	2:B:1070:LYS:N	2.77	0.42
2:B:1261:VAL:HG21	2:B:1283:LEU:HD11	2.02	0.42
1:A:339:TYR:CG	1:A:375:ILE:HD11	2.55	0.42
2:B:1153:TRP:CH2	2:B:1155:GLY:HA3	2.55	0.42
2:B:1420:PRO:C	2:B:1422:LEU:H	2.28	0.42
1:A:194:GLU:O	1:A:196:GLY:N	2.53	0.41
2:B:1066:LYS:HD2	2:B:1407:GLN:NE2	2.34	0.41
2:B:1206:ARG:NH1	2:B:1206:ARG:HB3	2.34	0.41
2:B:1312:GLU:HG3	2:B:1313:PRO:CD	2.50	0.41
1:A:550:LYS:C	1:A:552:VAL:H	2.27	0.41
2:B:1353:LYS:CG	2:B:1354:TYR:N	2.83	0.41
2:B:1065:LYS:HB2	2:B:1066:LYS:H	1.74	0.41
1:A:94:ILE:HD13	1:A:94:ILE:HA	1.73	0.41
2:B:1084:THR:O	2:B:1084:THR:CG2	2.68	0.41
2:B:1278:GLN:HB3	2:B:1298:GLU:HB2	2.02	0.41
2:B:1342:TYR:CD1	2:B:1342:TYR:C	2.99	0.41
2:B:1231:GLY:O	2:B:1232:TYR:HB3	2.21	0.41
2:B:1266:TRP:C	2:B:1268:SER:H	2.29	0.41
1:A:210:LEU:C	1:A:212:TRP:N	2.77	0.41
1:A:325:LEU:HD22	1:A:385:LYS:CE	2.51	0.41
1:A:426:TRP:O	1:A:427:TYR:HB3	2.20	0.41
1:A:65:LYS:HZ1	1:A:72:ARG:HH11	1.68	0.41
1:A:66:LYS:C	1:A:68:SER:N	2.78	0.41
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.56	0.41
2:B:1109:LEU:HD23	2:B:1218:ASP:CG	2.45	0.41
2:B:1130:PHE:CZ	2:B:1144:TYR:HB2	2.55	0.41
2:B:1222:GLN:O	2:B:1222:GLN:HG3	2.19	0.41
1:A:246:LEU:HD11	1:A:310:LEU:HD12	2.03	0.41
1:A:473:THR:OG1	1:A:476:LYS:HG3	2.20	0.41
2:B:1002:ILE:HG22	2:B:1003:SER:N	2.36	0.41
2:B:1277:ARG:C	2:B:1279:LEU:H	2.28	0.41
1:A:266:TRP:O	1:A:269:GLN:HG2	2.21	0.40
1:A:357:MET:HG3	1:A:358:ARG:N	2.36	0.40
2:B:1064:LYS:HZ2	2:B:1069:THR:C	2.30	0.40
2:B:1219:LYS:O	2:B:1219:LYS:HD3	2.20	0.40
2:B:1236:PRO:C	2:B:1238:LYS:H	2.29	0.40
1:A:201:LYS:HD3	1:A:201:LYS:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1332:GLN:HG3	2:B:1338:THR:HG23	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	555/560 (99%)	491 (88%)	50 (9%)	14 (2%)	4	16
2	B	425/427 (100%)	367 (86%)	38 (9%)	20 (5%)	2	6
All	All	980/987 (99%)	858 (88%)	88 (9%)	34 (4%)	3	10

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	A	223	LYS
2	B	1005	ILE
2	B	1065	LYS
2	B	1184	MET
2	B	1281	LYS
2	B	1362	THR
2	B	1423	VAL
1	A	18	GLY
1	A	221	HIS
2	B	1004	PRO
2	B	1221	HIS
2	B	1426	TRP
1	A	345	PRO
1	A	356	ARG
2	B	1185	ASP
2	B	1226	PRO

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Mol	Chain	Res	Type
2	B	1291	GLU
2	B	1360	ALA
1	A	50	ILE
1	A	55	PRO
1	A	140	PRO
2	B	1219	LYS
2	B	1280	CYS
2	B	1294	PRO
2	B	1345	PRO
2	B	1069	THR
1	A	556	ILE
2	B	1314	VAL
1	A	466	VAL
1	A	543	GLY
2	B	1247	PRO
1	A	224	GLU
1	A	195	ILE

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	495/500 (99%)	461 (93%)	34 (7%)	14	41
2	B	389/389 (100%)	372 (96%)	17 (4%)	25	59
All	All	884/889 (99%)	833 (94%)	51 (6%)	18	49

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	26	LEU
1	A	29	GLU
1	A	52	PRO
1	A	54	ASN
1	A	79	GLU

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Mol	Chain	Res	Type
1	A	94	ILE
1	A	100	LEU
1	A	101	LYS
1	A	102	LYS
1	A	108	VAL
1	A	109	LEU
1	A	187	LEU
1	A	192	ASP
1	A	219	LYS
1	A	221	HIS
1	A	234	LEU
1	A	247	PRO
1	A	260	LEU
1	A	280	CYS
1	A	297	GLU
1	A	301	LEU
1	A	312	GLU
1	A	325	LEU
1	A	334	GLN
1	A	345	PRO
1	A	351	THR
1	A	400	THR
1	A	402	TRP
1	A	432	GLU
1	A	479	LEU
1	A	488	ASP
1	A	517	LEU
1	A	533	LEU
2	B	1058	THR
2	B	1082	LYS
2	B	1084	THR
2	B	1122	GLU
2	B	1172	LYS
2	B	1218	ASP
2	B	1228	LEU
2	B	1233	GLU
2	B	1257	ILE
2	B	1260	LEU
2	B	1293	ILE
2	B	1308	GLU
2	B	1345	PRO
2	B	1353	LYS

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Mol	Chain	Res	Type
2	B	1358	ARG
2	B	1425	LEU
2	B	1426	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	103	ASN
1	A	136	ASN
1	A	145	GLN
1	A	161	GLN
1	A	182	GLN
1	A	334	GLN
1	A	336	GLN
1	A	361	HIS
1	A	373	GLN
1	A	428	GLN
1	A	474	ASN
1	A	500	GLN
1	A	520	GLN
1	A	524	GLN
2	B	1091	GLN
2	B	1103	ASN
2	B	1147	ASN
2	B	1151	GLN
2	B	1161	GLN
2	B	1197	GLN
2	B	1208	HIS
2	B	1222	GLN
2	B	1255	ASN
2	B	1258	GLN
2	B	1332	GLN
2	B	1367	GLN
2	B	1394	GLN
2	B	1407	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	PNU	A	2000	-	21,22,22	2.78	12 (57%)	27,31,31	3.57	13 (48%)

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	PNU	A	2000	-	-	0/7/8/8	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	PNU	C5-CL19	-8.05	1.57	1.74
3	A	2000	PNU	C5-N6	4.87	1.43	1.33
3	A	2000	PNU	C3-N18	3.01	1.43	1.35
3	A	2000	PNU	O14-C7	2.95	1.41	1.37
3	A	2000	PNU	C10-N9	2.75	1.38	1.34
3	A	2000	PNU	C4-C3	2.67	1.44	1.40
3	A	2000	PNU	C1-N2	2.66	1.38	1.34
3	A	2000	PNU	C12-C13	2.62	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2000	PNU	C4-C5	2.27	1.41	1.38
3	A	2000	PNU	C8-C7	2.07	1.42	1.38
3	A	2000	PNU	C11-C10	2.05	1.43	1.39
3	A	2000	PNU	C1-S17	2.03	1.79	1.76

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	PNU	C5-N6-C1	8.46	121.48	114.15
3	A	2000	PNU	C4-C5-N6	-7.91	116.50	125.47
3	A	2000	PNU	C5-C4-C3	7.05	120.32	115.21
3	A	2000	PNU	C8-N9-C10	7.03	123.03	118.00
3	A	2000	PNU	C7-C8-N9	-4.04	116.86	122.69
3	A	2000	PNU	O14-C15-C13	3.76	115.58	112.49
3	A	2000	PNU	C4-C5-CL19	3.67	123.64	118.92
3	A	2000	PNU	C8-C7-C12	-3.50	121.17	123.15
3	A	2000	PNU	C1-N2-C3	3.28	119.04	115.49
3	A	2000	PNU	C16-C10-N9	3.28	124.33	116.28
3	A	2000	PNU	N18-C3-N2	2.23	120.17	116.59
3	A	2000	PNU	CL19-C5-N6	2.07	119.86	115.45
3	A	2000	PNU	N6-C1-N2	-2.07	123.22	127.00

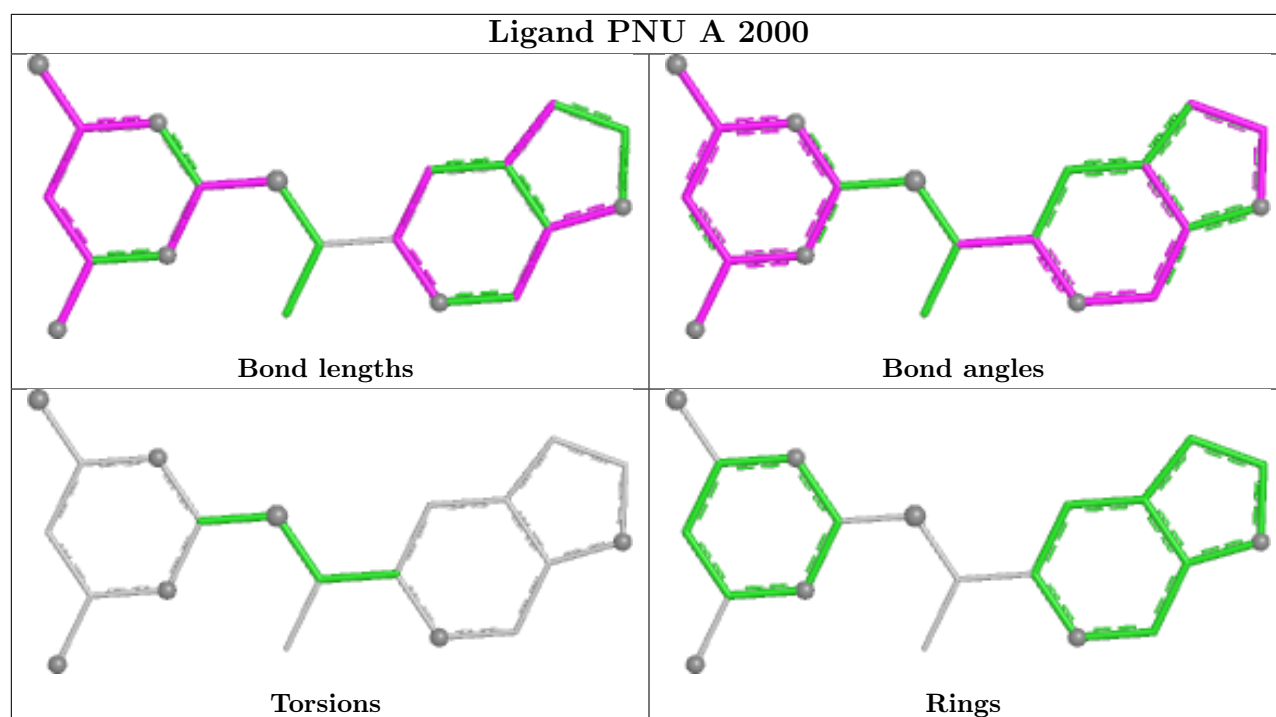
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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, 95th 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	557/560 (99%)	-0.09	11 (1%) 65 56	18, 49, 84, 123	2 (0%)
2	B	427/427 (100%)	0.09	37 (8%) 16 11	19, 46, 118, 166	10 (2%)
All	All	984/987 (99%)	-0.01	48 (4%) 35 27	18, 48, 105, 166	12 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1360	ALA	4.7
2	B	1221	HIS	4.5
2	B	1229	TRP	4.3
2	B	1002	ILE	4.3
2	B	1359	GLY	4.1
2	B	1067	ASP	4.0
2	B	1427	TYR	4.0
1	A	445	ALA	3.8
2	B	1220	LYS	3.7
2	B	1226	PRO	3.7
2	B	1217	PRO	3.5
2	B	1230	MET	3.4
1	A	177	ASP	3.4
2	B	1283	LEU	3.4
2	B	1222	GLN	3.2
2	B	1231	GLY	3.2
2	B	1425	LEU	3.1
1	A	547	GLN	3.0
1	A	446	ALA	3.0
2	B	1363	ASN	2.8
2	B	1423	VAL	2.8
2	B	1225	PRO	2.8
2	B	1218	ASP	2.7
2	B	1422	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	1219	LYS	2.6
2	B	1274	ILE	2.5
2	B	1294	PRO	2.5
1	A	359	GLY	2.5
2	B	1227	PHE	2.5
2	B	1232	TYR	2.4
2	B	1001	PRO	2.4
1	A	53	GLU	2.3
2	B	1266	TRP	2.3
2	B	1426	TRP	2.3
2	B	1281	LYS	2.2
2	B	1362	THR	2.2
2	B	1215	THR	2.2
2	B	1003	SER	2.2
1	A	474	ASN	2.1
1	A	222	GLN	2.1
1	A	61	PHE	2.1
2	B	1214	LEU	2.1
1	A	449	GLU	2.1
2	B	1282	LEU	2.1
2	B	1303	LEU	2.1
1	A	400	THR	2.1
2	B	1216	THR	2.0
2	B	1253	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

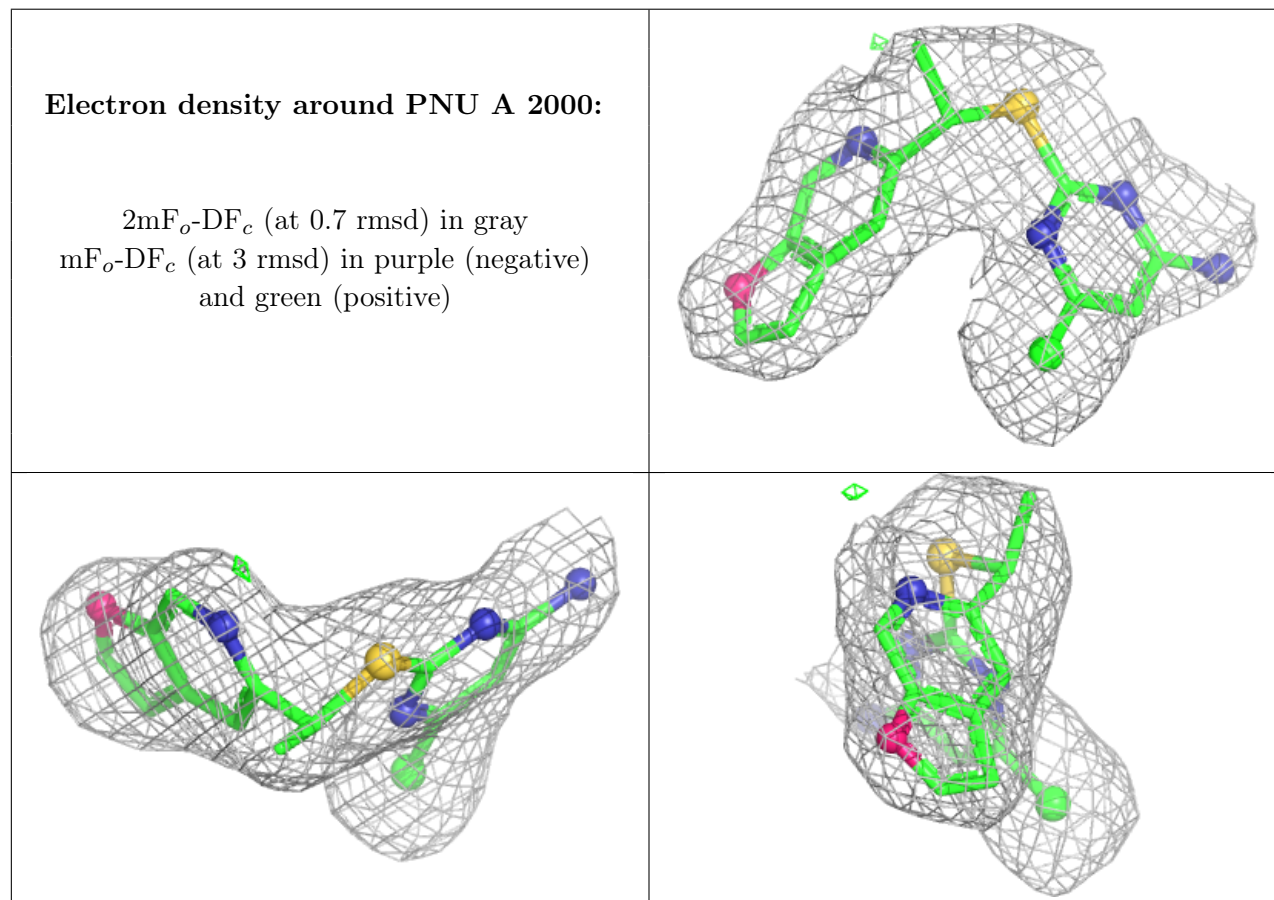
There are no oligosaccharides in this entry.

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, 95th 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($\text{\AA}^2$)	Q<0.9
3	PNU	A	2000	20/20	0.97	0.06	24,28,32,33	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.