



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 12:17 PM UTC

PDB ID : 3LAM / pdb_00003lam
Title : Crystal structure of HIV-1 reverse transcriptase in complex with N1-propyl pyrimidinedione non-nucleoside inhibitor
Authors : Lansdon, E.B.; Mitchell, M.L.
Deposited on : 2010-01-06
Resolution : 2.76 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

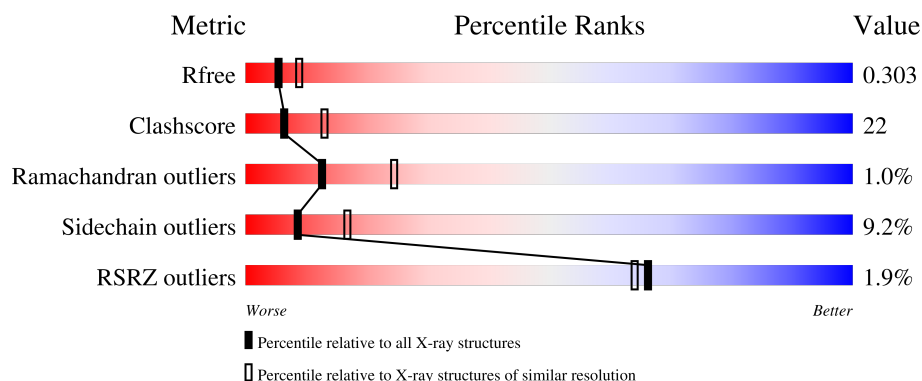
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

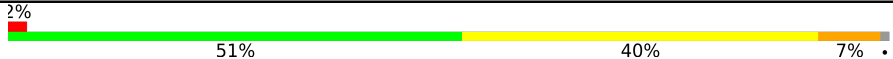
The reported resolution of this entry is 2.76 Å.

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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	
1	B	560	

2 Entry composition [i](#)

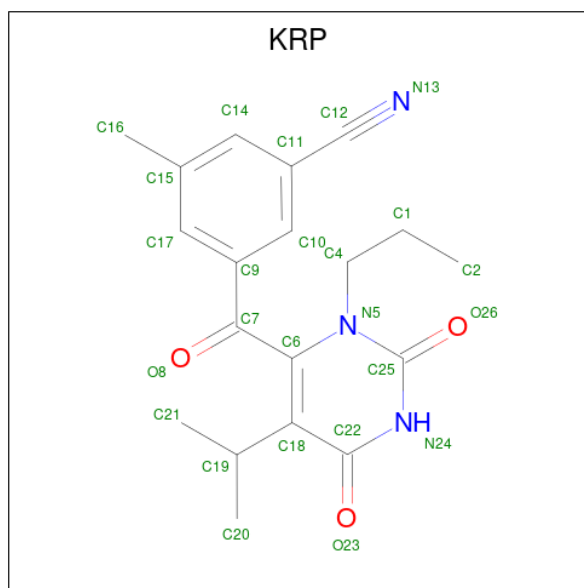
There are 4 unique types of molecules in this entry. The entry contains 7995 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Reverse transcriptase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4508	2914	752	834	8			
1	B	403	Total	C	N	O	S	0	0	0
			3334	2173	550	605	6			

- Molecule 2 is 3-methyl-5-{[5-(1-methylethyl)-2,6-dioxo-3-propyl-1,2,3,6-tetrahydropyrimidin-4-yl]carbonyl}benzonitrile (CCD ID: KRP) (formula: C₁₉H₂₁N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	19	3	3		

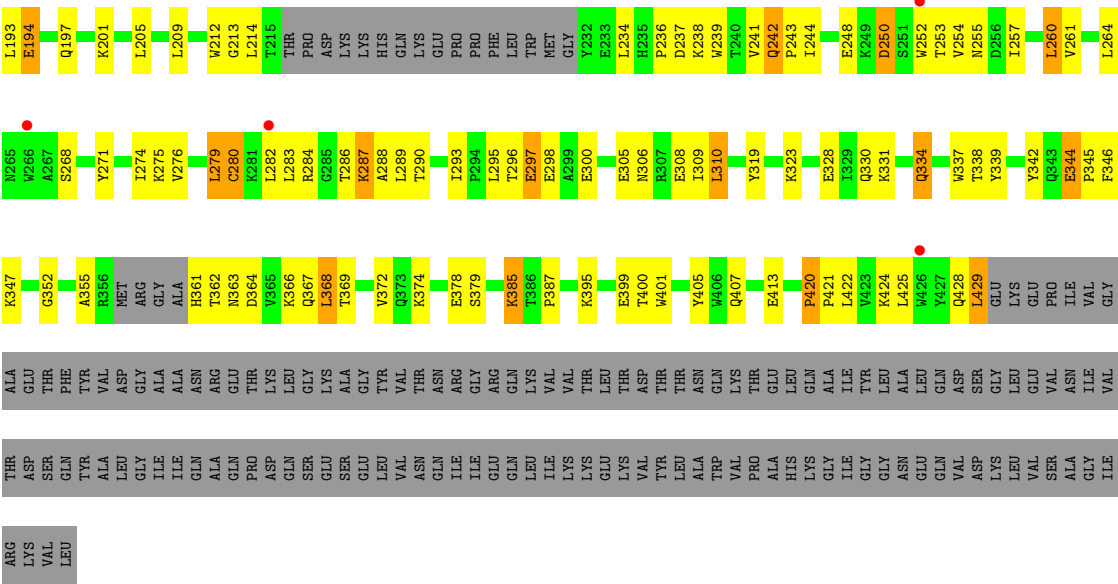
- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	45	Total	O	0	0
			45	45		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	119.64Å 154.47Å 153.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.76 29.91 – 2.76	Depositor EDS
% Data completeness (in resolution range)	93.3 (29.91-2.76) 93.5 (29.91-2.76)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.81 (at 2.77Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.231 , 0.280 (Not available) , 0.303	Depositor DCC
R_{free} test set	1716 reflections (4.71%)	wwPDB-VP
Wilson B-factor (Å ²)	69.0	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.9	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	7995	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: SO4, KRP

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	0.47	1/4625 (0.0%)	0.85	9/6284 (0.1%)
1	B	0.46	0/3426	0.85	8/4655 (0.2%)
All	All	0.46	1/8051 (0.0%)	0.85	17/10939 (0.2%)

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	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	VAL	CA-CB	6.04	1.58	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	SER	CA-C-N	7.94	127.58	119.56
1	A	3	SER	C-N-CA	7.94	127.58	119.56
1	B	18	GLY	CA-C-N	7.36	127.63	119.90
1	B	18	GLY	C-N-CA	7.36	127.63	119.90
1	A	54	ASN	CA-C-N	6.26	127.40	120.45
1	A	54	ASN	C-N-CA	6.26	127.40	120.45
1	A	67	ASP	N-CA-C	-5.93	107.02	114.56
1	B	184	MET	CB-CA-C	-5.93	109.75	116.63
1	A	320	ASP	CA-C-N	5.75	125.42	119.56
1	A	320	ASP	C-N-CA	5.75	125.42	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	LYS	CA-C-N	5.51	125.34	119.28
1	A	13	LYS	C-N-CA	5.51	125.34	119.28
1	B	355	ALA	N-CA-C	5.42	117.42	109.24
1	B	420	PRO	CA-C-N	5.40	126.59	119.84
1	B	420	PRO	C-N-CA	5.40	126.59	119.84
1	B	132	ILE	CA-C-N	5.36	125.35	120.21
1	B	132	ILE	C-N-CA	5.36	125.35	120.21

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	52	PRO	Peptide
1	A	65	LYS	Peptide
1	A	66	LYS	Peptide

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	4508	0	4558	223	0
1	B	3334	0	3365	137	0
2	A	25	0	21	4	0
3	A	20	0	0	0	0
3	B	5	0	0	0	0
4	A	58	0	0	3	0
4	B	45	0	0	2	0
All	All	7995	0	7944	350	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 (350) 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:337:TRP:HE1	1:A:367:GLN:NE2	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:LEU:HB3	1:B:293:ILE:HD13	1.46	0.93
1:A:472:THR:HG23	1:A:476:LYS:HB2	1.51	0.92
1:A:228:LEU:HD12	1:A:228:LEU:H	1.32	0.91
1:A:547:GLN:H	1:A:547:GLN:HE21	1.22	0.86
1:A:547:GLN:HE21	1:A:547:GLN:N	1.73	0.86
1:B:344:GLU:HB3	1:B:347:LYS:HD3	1.59	0.85
1:B:13:LYS:HE3	1:B:85:GLN:HG3	1.57	0.84
1:B:296:THR:HG22	1:B:298:GLU:H	1.44	0.83
1:A:41:MET:HE1	1:A:73:LYS:HZ2	1.45	0.81
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.61	0.81
1:B:194:GLU:HG3	1:B:197:GLN:HG3	1.61	0.81
1:A:257:ILE:O	1:A:261:VAL:HG23	1.81	0.80
1:A:278:GLN:HB3	1:A:299:ALA:HA	1.64	0.79
1:A:278:GLN:HG3	1:A:298:GLU:HB2	1.63	0.79
1:A:40:GLU:O	1:A:44:GLU:HG2	1.84	0.78
1:B:60:VAL:HG12	1:B:75:VAL:HG22	1.66	0.76
1:B:282:LEU:HB3	1:B:293:ILE:CD1	2.15	0.76
1:B:58:THR:HG23	4:B:563:HOH:O	1.84	0.76
1:A:41:MET:HE1	1:A:73:LYS:NZ	2.01	0.75
1:A:298:GLU:H	1:A:298:GLU:CD	1.93	0.75
1:B:61:PHE:CZ	1:B:74:LEU:HD23	2.22	0.75
1:A:181:TYR:CE2	1:A:183:TYR:HB2	2.21	0.74
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.23	0.74
1:B:297:GLU:H	1:B:297:GLU:CD	1.93	0.74
1:B:61:PHE:CE2	1:B:74:LEU:HD23	2.23	0.73
1:A:175:ASN:HB3	1:A:178:ILE:HD12	1.71	0.72
1:B:296:THR:O	1:B:300:GLU:HG3	1.90	0.72
1:A:337:TRP:HE1	1:A:367:GLN:HE21	1.37	0.71
1:B:276:VAL:HG12	1:B:280:CYS:SG	2.30	0.71
1:A:445:ALA:O	1:A:477:THR:HG21	1.91	0.70
1:A:518:VAL:O	1:A:522:ILE:HG13	1.92	0.70
1:B:86:ASP:O	1:B:90:VAL:HG22	1.91	0.70
1:B:279:LEU:HD23	1:B:282:LEU:HD12	1.73	0.69
1:B:20:LYS:HE2	1:B:55:PRO:HB2	1.76	0.68
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.76	0.67
1:A:450:THR:CG2	1:A:452:LEU:HB2	2.24	0.67
1:A:244:ILE:HD12	1:A:267:ALA:HB2	1.76	0.67
1:B:13:LYS:CE	1:B:85:GLN:HG3	2.25	0.66
1:B:296:THR:HG22	1:B:298:GLU:N	2.09	0.66
1:A:3:SER:OG	1:A:5:ILE:HG22	1.96	0.66
1:A:175:ASN:HD21	1:A:201:LYS:HE2	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:GLU:HG3	1:B:139:THR:HG23	1.77	0.65
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.77	0.65
1:A:472:THR:HG23	1:A:476:LYS:CB	2.26	0.64
1:A:450:THR:HG22	1:A:452:LEU:HB2	1.79	0.64
1:B:369:THR:HG21	1:B:405:TYR:HB2	1.78	0.64
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.27	0.64
1:A:228:LEU:H	1:A:228:LEU:CD1	2.07	0.64
1:B:253:THR:O	1:B:257:ILE:HG12	1.97	0.64
1:A:335:GLY:HA2	1:A:367:GLN:HE22	1.63	0.63
1:A:155:GLY:O	1:A:159:ILE:HG13	1.98	0.62
1:A:181:TYR:CZ	1:A:183:TYR:HB2	2.33	0.62
1:A:228:LEU:HD12	1:A:228:LEU:N	2.09	0.62
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.33	0.62
1:A:354:TYR:HD1	1:A:374:LYS:HD3	1.64	0.62
1:B:194:GLU:CG	1:B:197:GLN:HG3	2.29	0.62
1:B:337:TRP:HE1	1:B:367:GLN:HE21	1.47	0.62
1:A:305:GLU:O	1:A:309:ILE:HG13	2.00	0.61
1:A:447:ASN:HB3	1:A:450:THR:HB	1.81	0.61
1:A:105:SER:O	1:A:190:GLY:HA2	2.00	0.61
1:B:252:TRP:HB3	1:B:257:ILE:HD11	1.82	0.61
1:A:233:GLU:CD	1:A:235:HIS:HE2	2.08	0.61
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.31	0.60
1:A:44:GLU:HB2	1:A:46:LYS:HG2	1.83	0.60
1:A:37:ILE:HG23	1:A:41:MET:HE3	1.84	0.60
1:B:334:GLN:HE21	1:B:334:GLN:N	1.99	0.60
1:A:27:THR:O	1:A:31:ILE:HG13	2.02	0.60
1:B:169:GLU:HB3	1:B:170:PRO:HD3	1.83	0.60
1:A:494:ASN:N	1:A:494:ASN:HD22	1.99	0.59
1:B:81:ASN:CG	1:B:154:LYS:HG3	2.27	0.59
1:B:237:ASP:C	1:B:239:TRP:H	2.10	0.59
1:B:284:ARG:O	1:B:287:LYS:HE3	2.02	0.59
1:A:65:LYS:O	1:A:68:SER:HB3	2.03	0.59
1:B:101:LYS:HG2	4:B:573:HOH:O	2.02	0.58
1:A:230:MET:HA	1:A:230:MET:HE2	1.84	0.58
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.86	0.58
1:A:106:VAL:HG21	2:A:561:KRP:H2B	1.86	0.57
1:A:407:GLN:HA	1:A:407:GLN:NE2	2.19	0.57
1:B:50:ILE:CG2	1:B:145:GLN:HG2	2.35	0.57
1:B:395:LYS:O	1:B:399:GLU:HG3	2.03	0.57
1:A:183:TYR:CE2	1:A:184:MET:HG3	2.39	0.57
1:A:194:GLU:H	1:A:194:GLU:CD	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:TRP:CE2	1:B:154:LYS:HD2	2.40	0.57
1:A:52:PRO:HA	1:A:54:ASN:N	2.20	0.57
1:A:392:PRO:O	1:A:423:VAL:HG12	2.04	0.57
1:B:422:LEU:N	1:B:422:LEU:HD22	2.20	0.57
1:A:536:VAL:HG13	1:A:537:PRO:HD2	1.86	0.56
1:A:552:VAL:O	1:A:553:SER:HB3	2.04	0.56
1:B:213:GLY:C	1:B:214:LEU:HD12	2.30	0.56
1:B:260:LEU:HD22	1:B:264:LEU:CD1	2.35	0.56
1:B:306:ASN:O	1:B:310:LEU:HD22	2.05	0.56
1:A:60:VAL:HG12	1:A:61:PHE:N	2.20	0.56
1:A:295:LEU:HB2	1:A:300:GLU:OE2	2.05	0.56
1:B:65:LYS:C	1:B:407:GLN:HE21	2.13	0.56
1:B:319:TYR:OH	1:B:385:LYS:HE2	2.05	0.56
1:A:89:GLU:HG3	1:A:92:LEU:HD11	1.87	0.56
1:B:361:HIS:C	1:B:363:ASN:H	2.13	0.56
1:A:454:LYS:HD3	1:A:553:SER:H	1.71	0.56
1:A:105:SER:HB3	1:A:198:HIS:CG	2.40	0.56
1:A:424:LYS:HD2	1:A:426:TRP:CH2	2.41	0.56
1:B:175:ASN:HD21	1:B:201:LYS:NZ	2.04	0.56
1:A:175:ASN:ND2	1:A:201:LYS:HE2	2.19	0.56
1:B:295:LEU:HD22	1:B:295:LEU:N	2.21	0.56
1:A:273:GLY:HA2	1:A:332:GLN:NE2	2.20	0.55
1:A:480:GLN:HG2	1:A:517:LEU:HD11	1.88	0.55
1:A:343:GLN:HG3	1:A:349:LEU:HD11	1.87	0.55
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.88	0.55
1:B:24:TRP:HH2	1:B:61:PHE:CE1	2.25	0.55
1:A:343:GLN:HG3	1:A:349:LEU:CD1	2.37	0.55
1:B:275:LYS:H	1:B:306:ASN:HD21	1.54	0.55
1:A:273:GLY:C	1:A:332:GLN:HE22	2.14	0.55
1:A:520:GLN:HA	1:A:523:GLU:HG2	1.90	0.54
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.22	0.54
1:A:60:VAL:HG21	1:A:130:PHE:HD2	1.72	0.54
1:B:72:ARG:HG2	1:B:73:LYS:N	2.23	0.54
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.38	0.54
1:B:345:PRO:O	1:B:346:PHE:HB2	2.08	0.54
1:B:260:LEU:HD22	1:B:264:LEU:HD11	1.90	0.54
1:A:40:GLU:OE2	1:A:40:GLU:HA	2.08	0.53
1:A:298:GLU:HA	1:A:301:LEU:HD12	1.90	0.53
1:A:229:TRP:HB2	2:A:561:KRP:N13	2.23	0.53
1:A:420:PRO:HA	1:A:421:PRO:C	2.33	0.53
1:B:11:LYS:HG2	1:B:12:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.09	0.53
1:A:433:PRO:HB2	1:B:290:THR:HG22	1.90	0.53
1:B:47:ILE:HD12	1:B:144:TYR:CD1	2.44	0.53
1:A:434:ILE:HB	1:A:494:ASN:HD21	1.74	0.52
1:B:241:VAL:O	1:B:243:PRO:HD3	2.09	0.52
1:B:257:ILE:HB	1:B:283:LEU:HD21	1.92	0.52
1:B:149:LEU:HD13	1:B:156:SER:HA	1.92	0.52
1:B:151:GLN:HB3	1:B:185:ASP:OD2	2.10	0.52
1:B:368:LEU:O	1:B:372:VAL:HG23	2.09	0.52
1:B:429:LEU:N	1:B:429:LEU:HD12	2.23	0.52
1:A:90:VAL:HG23	1:A:161:GLN:HG2	1.92	0.52
1:A:89:GLU:HG3	1:A:92:LEU:HD21	1.92	0.52
1:B:242:GLN:HB2	1:B:352:GLY:HA2	1.90	0.52
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.92	0.51
1:A:289:LEU:HD12	1:A:290:THR:N	2.25	0.51
1:A:407:GLN:HA	1:A:407:GLN:HE21	1.76	0.51
1:B:24:TRP:CH2	1:B:61:PHE:CD1	2.98	0.51
1:B:331:LYS:O	1:B:424:LYS:HE3	2.09	0.51
1:A:39:THR:O	1:A:43:LYS:HG2	2.10	0.51
1:A:77:PHE:O	1:A:78:ARG:C	2.53	0.51
1:A:64:LYS:O	1:A:66:LYS:HA	2.11	0.51
1:A:324:ASP:OD1	1:A:388:LYS:HE2	2.08	0.51
1:B:395:LYS:HG2	1:B:399:GLU:OE1	2.10	0.51
1:B:37:ILE:O	1:B:41:MET:HG2	2.10	0.51
1:B:344:GLU:CB	1:B:347:LYS:HD3	2.37	0.51
1:A:402:TRP:CD1	1:A:402:TRP:C	2.89	0.51
1:B:88:TRP:CZ2	1:B:154:LYS:HD2	2.46	0.51
1:B:112:GLY:HA3	1:B:151:GLN:HE21	1.75	0.50
1:A:168:LEU:HD22	1:A:180:ILE:HD13	1.93	0.50
1:A:171:PHE:CE2	1:A:205:LEU:HD23	2.46	0.50
1:A:376:THR:O	1:A:380:ILE:HG12	2.11	0.50
1:A:433:PRO:CG	1:B:255:ASN:ND2	2.74	0.50
1:A:473:THR:H	1:A:476:LYS:HD2	1.75	0.50
1:B:271:TYR:O	1:B:274:ILE:HG12	2.11	0.50
1:A:500:GLN:OE1	1:B:422:LEU:HD23	2.11	0.50
1:A:278:GLN:HG3	1:A:298:GLU:C	2.36	0.50
1:B:61:PHE:CD1	1:B:61:PHE:N	2.79	0.50
1:A:5:ILE:HG12	1:A:6:GLU:O	2.11	0.50
1:A:308:GLU:O	1:A:311:LYS:HB2	2.12	0.50
1:A:356:ARG:HG3	1:A:357:MET:H	1.76	0.50
1:B:425:LEU:O	1:B:428:GLN:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASN:HB3	1:B:289:LEU:HD12	1.93	0.50
1:B:379:SER:OG	1:B:387:PRO:HD3	2.12	0.49
1:A:271:TYR:HB3	1:A:274:ILE:HD11	1.95	0.49
1:A:450:THR:HG21	1:A:452:LEU:HB2	1.94	0.49
1:B:115:TYR:HB3	1:B:149:LEU:HB2	1.94	0.49
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.94	0.49
1:B:346:PHE:N	1:B:346:PHE:HD1	2.11	0.49
1:A:337:TRP:NE1	1:A:367:GLN:HE21	2.06	0.49
1:B:328:GLU:O	1:B:339:TYR:HA	2.12	0.49
1:A:194:GLU:CD	1:A:194:GLU:N	2.71	0.49
1:B:120:LEU:O	1:B:121:ASP:C	2.55	0.49
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.27	0.48
1:B:33:ALA:O	1:B:37:ILE:HG13	2.13	0.48
1:B:346:PHE:N	1:B:346:PHE:CD1	2.81	0.48
1:A:460:ASN:ND2	1:B:288:ALA:HB2	2.28	0.48
1:A:500:GLN:HE22	1:B:421:PRO:HD2	1.79	0.48
1:B:154:LYS:HG2	1:B:184:MET:SD	2.53	0.48
1:B:330:GLN:NE2	1:B:338:THR:OG1	2.44	0.48
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.54	0.48
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.94	0.48
1:A:544:GLY:HA3	1:B:286:THR:HG22	1.96	0.48
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.95	0.48
1:B:110:ASP:C	1:B:110:ASP:OD1	2.56	0.48
1:A:183:TYR:CD2	1:A:184:MET:HG3	2.49	0.48
1:A:296:THR:HB	1:A:298:GLU:OE1	2.13	0.48
1:A:108:VAL:HG12	1:A:188:TYR:HD2	1.79	0.48
1:B:305:GLU:O	1:B:309:ILE:HG13	2.13	0.48
1:A:89:GLU:OE2	1:A:89:GLU:HA	2.13	0.48
1:B:24:TRP:CZ3	1:B:61:PHE:CD1	3.02	0.48
1:B:163:SER:O	1:B:167:ILE:HG13	2.13	0.48
1:A:406:TRP:HE3	1:A:407:GLN:NE2	2.12	0.47
1:B:193:LEU:CD1	1:B:201:LYS:HG3	2.44	0.47
1:A:175:ASN:HD21	1:A:201:LYS:CE	2.25	0.47
1:B:194:GLU:H	1:B:197:GLN:HE21	1.61	0.47
1:A:54:ASN:O	1:A:143:ARG:NH2	2.48	0.47
1:B:252:TRP:HB3	1:B:257:ILE:CD1	2.44	0.47
1:B:175:ASN:HD21	1:B:201:LYS:HZ2	1.62	0.47
1:A:48:SER:O	1:A:144:TYR:HA	2.15	0.47
1:A:438:GLU:HG3	1:A:461:ARG:HD2	1.97	0.47
1:A:483:TYR:O	1:A:487:GLN:HG3	2.15	0.47
1:A:545:ASN:O	1:A:549:ASP:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:SER:C	1:A:515:SER:H	2.21	0.47
1:A:542:ILE:HG23	1:B:283:LEU:CD1	2.45	0.47
1:B:24:TRP:CH2	1:B:61:PHE:CE1	3.02	0.47
1:B:65:LYS:C	1:B:407:GLN:HB2	2.39	0.47
1:B:374:LYS:HE3	1:B:378:GLU:OE2	2.15	0.47
1:A:139:THR:HB	1:A:140:PRO:HD2	1.97	0.47
1:B:257:ILE:HG23	1:B:279:LEU:HD22	1.97	0.46
1:B:12:LEU:HD23	1:B:84:THR:HG22	1.97	0.46
1:A:97:PRO:HG2	1:A:232:TYR:CD1	2.51	0.46
1:A:199:ARG:HA	1:A:202:ILE:HB	1.96	0.46
1:A:354:TYR:CD1	1:A:374:LYS:HD3	2.47	0.46
1:A:278:GLN:CG	1:A:298:GLU:HB2	2.41	0.46
1:A:431:LYS:HB2	1:A:431:LYS:NZ	2.31	0.46
1:B:305:GLU:O	1:B:308:GLU:HB3	2.15	0.46
1:A:345:PRO:HA	1:A:346:PHE:HA	1.54	0.46
1:A:542:ILE:O	1:A:543:GLY:O	2.34	0.46
1:B:77:PHE:CE1	1:B:80:LEU:HD12	2.51	0.45
1:A:168:LEU:HD22	1:A:180:ILE:CD1	2.47	0.45
1:A:230:MET:O	1:A:230:MET:HG3	2.17	0.45
1:A:271:TYR:O	1:A:274:ILE:HG12	2.15	0.45
1:B:254:VAL:HG13	1:B:283:LEU:HD22	1.98	0.45
1:B:46:LYS:HZ3	1:B:116:PHE:HD2	1.64	0.45
1:A:2:ILE:O	1:A:3:SER:C	2.59	0.45
1:A:542:ILE:O	1:A:543:GLY:C	2.58	0.45
1:B:363:ASN:HB3	1:B:366:LYS:HB3	1.99	0.45
1:A:104:LYS:HD2	1:A:192:ASP:O	2.17	0.45
1:A:278:GLN:HB3	1:A:299:ALA:CA	2.42	0.45
1:B:72:ARG:HG2	1:B:73:LYS:H	1.81	0.45
1:B:420:PRO:HA	1:B:421:PRO:HD3	1.77	0.45
1:A:156:SER:N	1:A:157:PRO:HD2	2.31	0.45
1:A:227:PHE:O	1:A:228:LEU:C	2.58	0.45
1:B:101:LYS:O	1:B:236:PRO:HB2	2.17	0.45
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.47	0.44
1:A:281:LYS:HD2	1:A:284:ARG:CZ	2.47	0.44
1:A:463:ARG:NH2	1:A:488:ASP:O	2.48	0.44
1:A:32:LYS:O	1:A:36:GLU:HG3	2.16	0.44
1:A:208:HIS:O	1:A:212:TRP:HD1	2.00	0.44
1:B:82:LYS:HE3	1:B:413:GLU:OE1	2.17	0.44
1:A:19:PRO:O	1:A:20:LYS:HG3	2.18	0.44
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.99	0.44
1:A:249:LYS:HE2	1:A:256:ASP:CG	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:GLN:O	1:A:465:LYS:HB2	2.16	0.44
1:B:236:PRO:O	1:B:239:TRP:HB2	2.18	0.44
1:B:250:ASP:OD2	1:B:250:ASP:N	2.51	0.44
1:A:53:GLU:O	1:A:55:PRO:HD3	2.17	0.44
1:A:298:GLU:CD	1:A:298:GLU:N	2.71	0.44
1:A:393:ILE:HG23	1:A:393:ILE:O	2.17	0.44
1:A:319:TYR:O	1:A:321:PRO:HD3	2.17	0.44
1:B:160:PHE:O	1:B:160:PHE:CD2	2.71	0.44
1:A:509:GLN:N	1:A:510:PRO:HD3	2.33	0.43
1:B:77:PHE:CD1	1:B:80:LEU:HD12	2.53	0.43
1:A:37:ILE:CG2	1:A:41:MET:HE3	2.46	0.43
1:A:129:ALA:HA	1:A:144:TYR:O	2.17	0.43
1:A:283:LEU:HA	1:A:283:LEU:HD12	1.59	0.43
1:B:108:VAL:HG22	1:B:188:TYR:CD2	2.53	0.43
1:B:187:LEU:HD12	1:B:187:LEU:HA	1.85	0.43
1:B:257:ILE:HG23	1:B:279:LEU:CD2	2.48	0.43
1:A:282:LEU:HD11	1:A:296:THR:HG23	1.99	0.43
1:A:60:VAL:HG12	1:A:61:PHE:H	1.83	0.43
1:A:66:LYS:HE3	1:A:66:LYS:HB2	1.74	0.43
1:A:233:GLU:HG2	1:A:235:HIS:NE2	2.33	0.43
1:A:275:LYS:HE3	1:A:332:GLN:HG2	2.00	0.43
1:A:399:GLU:O	1:A:403:THR:HG23	2.19	0.43
1:B:237:ASP:C	1:B:239:TRP:N	2.75	0.43
1:A:233:GLU:CG	1:A:235:HIS:HE2	2.31	0.43
1:A:356:ARG:HG3	1:A:357:MET:N	2.33	0.43
1:A:52:PRO:HA	1:A:54:ASN:H	1.83	0.43
1:B:167:ILE:HG12	1:B:212:TRP:CD2	2.54	0.43
1:B:260:LEU:HD13	1:B:279:LEU:CD1	2.48	0.43
1:A:253:THR:HA	1:A:292:VAL:HA	2.00	0.43
1:B:104:LYS:HG3	1:B:192:ASP:OD1	2.19	0.43
1:A:171:PHE:CD2	1:A:205:LEU:HD23	2.54	0.43
1:A:330:GLN:NE2	1:A:338:THR:HG23	2.34	0.43
1:A:542:ILE:HD11	1:B:261:VAL:HG11	2.00	0.43
1:B:425:LEU:HD12	1:B:428:GLN:NE2	2.33	0.43
1:B:429:LEU:HD12	1:B:429:LEU:H	1.84	0.43
1:A:7:THR:HG22	1:A:119:PRO:HB2	2.01	0.42
1:B:65:LYS:HD3	1:B:72:ARG:HH11	1.84	0.42
1:B:244:ILE:HB	1:B:310:LEU:HG	2.01	0.42
1:A:386:THR:HG22	4:A:571:HOH:O	2.18	0.42
1:A:81:ASN:O	1:A:82:LYS:C	2.61	0.42
1:A:260:LEU:HD23	1:A:279:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LYS:HD3	1:A:414:TRP:CZ2	2.55	0.42
1:A:479:LEU:HD12	1:A:479:LEU:HA	1.77	0.42
1:B:72:ARG:NH2	1:B:151:GLN:HE22	2.17	0.42
1:B:108:VAL:HG22	1:B:188:TYR:CE2	2.55	0.42
1:A:478:GLU:O	1:A:482:ILE:HG13	2.20	0.42
1:A:289:LEU:HD12	1:A:289:LEU:C	2.45	0.42
1:A:104:LYS:HD2	1:A:192:ASP:C	2.45	0.42
1:A:278:GLN:HB2	1:A:302:GLU:CD	2.45	0.42
1:A:457:TYR:HA	1:A:548:VAL:HG21	2.00	0.42
1:A:181:TYR:HH	1:A:183:TYR:HB2	1.85	0.42
1:A:269:GLN:HA	1:A:351:THR:O	2.19	0.42
1:A:329:ILE:HD11	1:A:375:ILE:HD12	2.02	0.42
1:B:180:ILE:HA	1:B:188:TYR:O	2.20	0.42
1:A:175:ASN:ND2	1:A:201:LYS:CE	2.82	0.41
1:A:233:GLU:HG2	1:A:235:HIS:CD2	2.55	0.41
1:A:245:VAL:O	1:A:245:VAL:HG13	2.20	0.41
1:B:425:LEU:CD1	1:B:428:GLN:NE2	2.83	0.41
1:A:310:LEU:HD12	1:A:310:LEU:HA	1.92	0.41
1:B:361:HIS:C	1:B:363:ASN:N	2.79	0.41
1:B:400:THR:HB	1:B:401:TRP:CD1	2.56	0.41
1:A:13:LYS:HB3	1:A:14:PRO:HD2	2.02	0.41
1:A:301:LEU:O	1:A:304:ALA:HB3	2.19	0.41
1:A:350:LYS:HE2	1:A:350:LYS:HB2	1.85	0.41
1:B:88:TRP:CD1	1:B:154:LYS:HB2	2.56	0.41
1:A:249:LYS:HE2	1:A:256:ASP:OD1	2.21	0.41
1:A:303:LEU:O	1:A:307:ARG:HB2	2.19	0.41
1:A:409:THR:O	1:B:364:ASP:HB2	2.20	0.41
1:A:457:TYR:CD1	1:A:457:TYR:C	2.99	0.41
1:A:547:GLN:H	1:A:547:GLN:NE2	2.03	0.41
1:A:208:HIS:O	1:A:208:HIS:HD2	2.04	0.41
1:B:342:TYR:CD2	1:B:342:TYR:C	2.99	0.41
1:A:271:TYR:HA	1:A:272:PRO:HD3	1.91	0.41
1:A:406:TRP:CE3	1:A:407:GLN:NE2	2.89	0.41
1:A:73:LYS:NZ	1:A:73:LYS:HB3	2.35	0.41
1:A:401:TRP:O	1:A:402:TRP:C	2.62	0.41
1:A:426:TRP:HB3	1:A:526:ILE:CD1	2.50	0.41
1:A:77:PHE:O	1:A:79:GLU:N	2.54	0.41
1:A:125:ARG:NH1	1:A:147:ASN:HB3	2.35	0.41
1:A:208:HIS:CD2	1:A:208:HIS:C	2.98	0.41
1:A:225:PRO:HA	1:A:226:PRO:C	2.45	0.41
1:A:233:GLU:HG2	1:A:235:HIS:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:VAL:O	1:A:552:VAL:HG23	2.21	0.41
1:B:8:VAL:HA	1:B:9:PRO:HD3	1.95	0.41
1:B:46:LYS:NZ	1:B:116:PHE:HD2	2.19	0.41
1:B:103:LYS:HE3	1:B:179:VAL:HG23	2.03	0.41
1:A:108:VAL:HG12	1:A:188:TYR:CD2	2.56	0.41
1:A:12:LEU:HB3	1:A:83:ARG:O	2.21	0.40
1:A:235:HIS:O	2:A:561:KRP:H1	2.21	0.40
1:A:287:LYS:NZ	1:A:291:GLU:HG2	2.36	0.40
1:A:534:ALA:HA	4:A:609:HOH:O	2.21	0.40
1:B:103:LYS:HA	1:B:103:LYS:HD3	1.91	0.40
1:A:437:ALA:O	4:A:577:HOH:O	2.22	0.40
1:A:543:GLY:C	1:A:545:ASN:H	2.28	0.40
1:B:72:ARG:HH21	1:B:151:GLN:HE22	1.70	0.40
1:B:111:VAL:HG11	1:B:187:LEU:HD22	2.02	0.40
1:A:175:ASN:HD22	1:A:178:ILE:HD12	1.86	0.40
1:A:219:LYS:HE3	1:A:219:LYS:HB3	1.87	0.40
1:A:407:GLN:HE21	1:A:407:GLN:CA	2.33	0.40
1:A:179:VAL:HG23	2:A:561:KRP:H21A	2.03	0.40
1:A:171:PHE:CZ	1:A:205:LEU:HD23	2.55	0.40
1:A:536:VAL:HG13	1:A:537:PRO:CD	2.51	0.40
1:B:268:SER:HA	1:B:274:ILE:HG13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/560 (98%)	497 (90%)	48 (9%)	6 (1%)	11	22
1	B	395/560 (70%)	367 (93%)	25 (6%)	3 (1%)	16	30
All	All	946/1120 (84%)	864 (91%)	73 (8%)	9 (1%)	12	24

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	A	27	THR
1	A	543	GLY
1	A	68	SER
1	B	238	LYS
1	B	362	THR
1	A	465	LYS
1	A	3	SER
1	B	242	GLN

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%)	447 (90%)	48 (10%)	8	15
1	B	367/500 (73%)	336 (92%)	31 (8%)	10	19
All	All	862/1000 (86%)	783 (91%)	79 (9%)	8	17

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ILE
1	A	64	LYS
1	A	66	LYS
1	A	72	ARG
1	A	73	LYS
1	A	90	VAL
1	A	94	ILE
1	A	120	LEU
1	A	126	LYS
1	A	138	GLU
1	A	161	GLN
1	A	195	ILE
1	A	205	LEU
1	A	209	LEU

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Mol	Chain	Res	Type
1	A	230	MET
1	A	238	LYS
1	A	248	GLU
1	A	264	LEU
1	A	282	LEU
1	A	283	LEU
1	A	298	GLU
1	A	300	GLU
1	A	303	LEU
1	A	308	GLU
1	A	310	LEU
1	A	311	LYS
1	A	341	ILE
1	A	344	GLU
1	A	356	ARG
1	A	373	GLN
1	A	402	TRP
1	A	407	GLN
1	A	411	ILE
1	A	423	VAL
1	A	431	LYS
1	A	451	LYS
1	A	466	VAL
1	A	472	THR
1	A	479	LEU
1	A	482	ILE
1	A	494	ASN
1	A	497	THR
1	A	500	GLN
1	A	517	LEU
1	A	529	GLU
1	A	533	LEU
1	A	536	VAL
1	A	547	GLN
1	B	11	LYS
1	B	24	TRP
1	B	48	SER
1	B	73	LYS
1	B	80	LEU
1	B	82	LYS
1	B	83	ARG
1	B	85	GLN

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Mol	Chain	Res	Type
1	B	89	GLU
1	B	90	VAL
1	B	91	GLN
1	B	138	GLU
1	B	165	THR
1	B	194	GLU
1	B	205	LEU
1	B	209	LEU
1	B	234	LEU
1	B	248	GLU
1	B	250	ASP
1	B	260	LEU
1	B	279	LEU
1	B	280	CYS
1	B	287	LYS
1	B	297	GLU
1	B	310	LEU
1	B	323	LYS
1	B	334	GLN
1	B	344	GLU
1	B	368	LEU
1	B	385	LYS
1	B	429	LEU

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	145	GLN
1	A	175	ASN
1	A	208	HIS
1	A	221	HIS
1	A	258	GLN
1	A	330	GLN
1	A	332	GLN
1	A	340	GLN
1	A	348	ASN
1	A	367	GLN
1	A	407	GLN
1	A	428	GLN
1	A	447	ASN
1	A	500	GLN
1	A	547	GLN

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Mol	Chain	Res	Type
1	B	151	GLN
1	B	175	ASN
1	B	182	GLN
1	B	197	GLN
1	B	255	ASN
1	B	258	GLN
1	B	306	ASN
1	B	330	GLN
1	B	334	GLN
1	B	336	GLN
1	B	340	GLN
1	B	348	ASN
1	B	367	GLN
1	B	407	GLN

5.3.3 RNA [i](#)

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](#)

6 ligands are 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	SO4	A	565	-	4,4,4	0.36	0	6,6,6	0.11	0
3	SO4	A	563	-	4,4,4	0.38	0	6,6,6	0.16	0
2	KRP	A	561	-	26,26,26	3.19	13 (50%)	33,37,37	1.50	6 (18%)
3	SO4	B	561	-	4,4,4	0.44	0	6,6,6	0.06	0
3	SO4	A	564	-	4,4,4	0.37	0	6,6,6	0.04	0
3	SO4	A	562	-	4,4,4	0.38	0	6,6,6	0.18	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	KRP	A	561	-	-	2/17/17/17	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	561	KRP	C22-C18	6.44	1.57	1.43
2	A	561	KRP	C17-C9	5.93	1.48	1.39
2	A	561	KRP	C4-N5	4.79	1.58	1.47
2	A	561	KRP	C6-C18	4.64	1.43	1.35
2	A	561	KRP	C10-C9	4.63	1.46	1.39
2	A	561	KRP	C19-C18	4.37	1.58	1.52
2	A	561	KRP	C17-C15	4.17	1.45	1.39
2	A	561	KRP	C10-C11	3.76	1.46	1.39
2	A	561	KRP	C9-C7	3.36	1.55	1.49
2	A	561	KRP	C6-C7	3.36	1.56	1.47
2	A	561	KRP	C14-C15	3.10	1.43	1.39
2	A	561	KRP	C6-N5	3.06	1.48	1.40
2	A	561	KRP	C14-C11	2.77	1.44	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	561	KRP	C19-C18-C6	3.52	125.13	119.06
2	A	561	KRP	C18-C22-N24	3.38	120.10	116.10
2	A	561	KRP	C9-C7-C6	2.67	124.19	119.34
2	A	561	KRP	O26-C25-N24	-2.41	117.05	121.49
2	A	561	KRP	N24-C25-N5	2.22	119.43	115.45
2	A	561	KRP	O8-C7-C6	-2.16	116.51	120.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

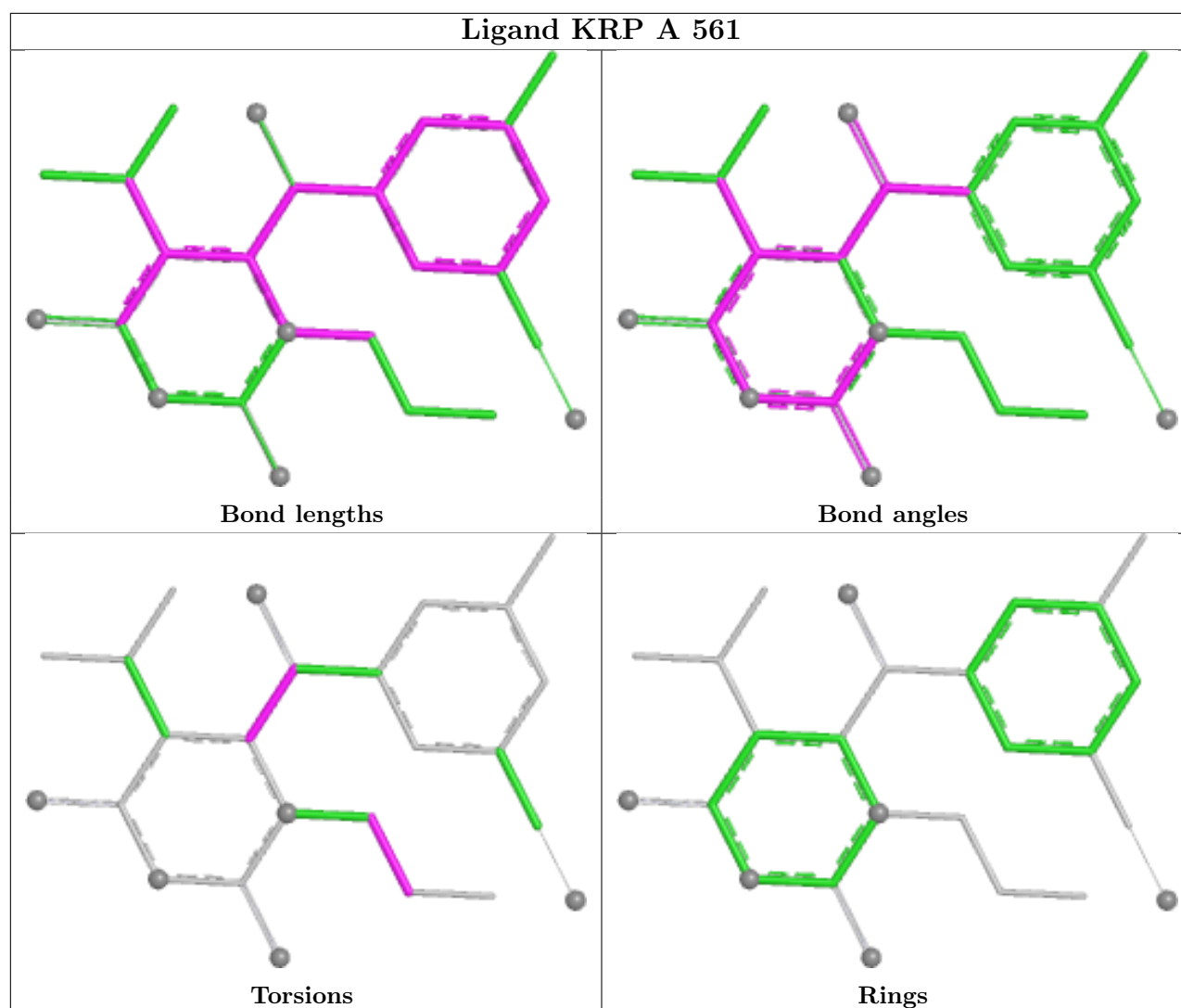
Mol	Chain	Res	Type	Atoms
2	A	561	KRP	C2-C1-C4-N5
2	A	561	KRP	N5-C6-C7-C9

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	561	KRP	4	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 [i](#)

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

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	553/560 (98%)	0.19	10 (1%) 67 65	38, 70, 103, 121	0
1	B	403/560 (71%)	0.03	8 (1%) 65 63	35, 63, 104, 122	0
All	All	956/1120 (85%)	0.12	18 (1%) 66 64	35, 68, 104, 122	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	TYR	4.0
1	B	88	TRP	3.6
1	A	247	PRO	3.0
1	A	551	LEU	2.9
1	A	291	GLU	2.8
1	A	52	PRO	2.8
1	B	87	PHE	2.7
1	B	266	TRP	2.5
1	A	195	ILE	2.5
1	A	402	TRP	2.5
1	A	92	LEU	2.4
1	B	252	TRP	2.3
1	A	246	LEU	2.2
1	B	282	LEU	2.2
1	A	222	GLN	2.1
1	B	5	ILE	2.1
1	B	69	THR	2.0
1	B	426	TRP	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](#)

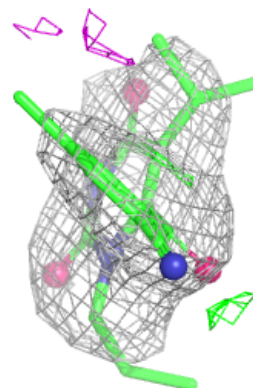
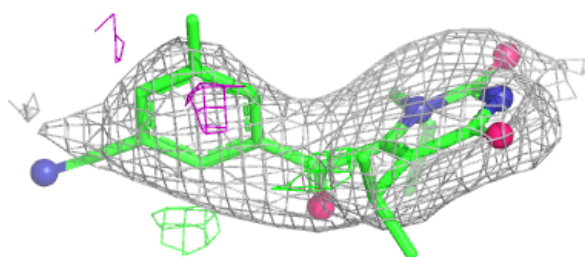
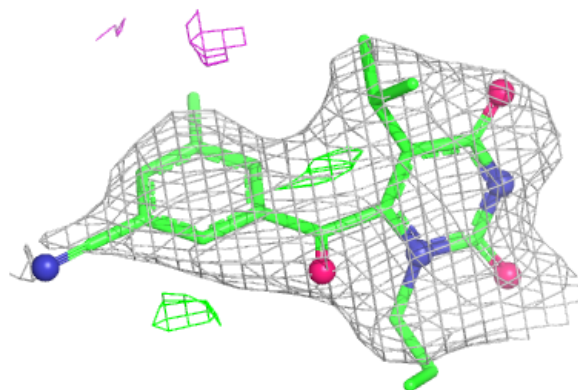
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	A	565	5/5	0.74	0.09	132,134,134,134	0
3	SO4	A	564	5/5	0.78	0.19	165,165,165,166	0
3	SO4	A	563	5/5	0.86	0.09	91,91,94,96	0
3	SO4	B	561	5/5	0.88	0.14	107,107,107,108	0
3	SO4	A	562	5/5	0.89	0.10	83,85,86,87	0
2	KRP	A	561	25/25	0.91	0.16	73,76,79,80	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 KRP A 561:

$2mF_o-DF_c$ (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.