



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:13 PM UTC

PDB ID : 3LAK / pdb_00003lak
Title : Crystal structure of HIV-1 reverse transcriptase in complex with N1-heterocycle pyrimidinedione non-nucleoside inhibitor
Authors : Lansdon, E.B.; Mitchell, M.L.
Deposited on : 2010-01-06
Resolution : 2.30 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

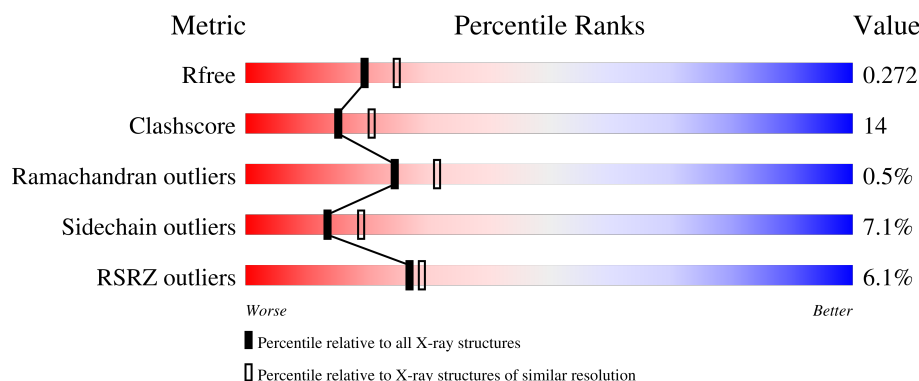
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

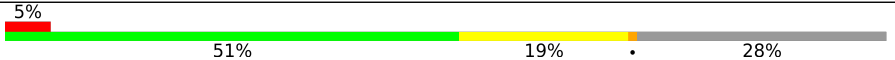
The reported resolution of this entry is 2.30 Å.

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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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](#)

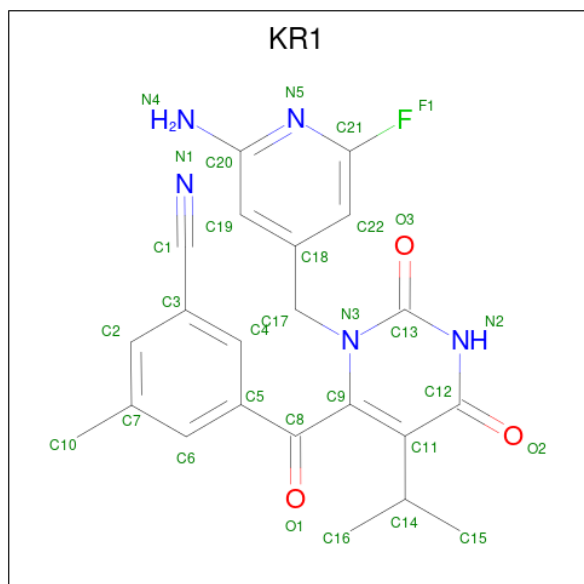
There are 5 unique types of molecules in this entry. The entry contains 8101 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-({3-[(2-amino-6-fluoropyridin-4-yl)methyl]-5-(1-methylethyl)-2,6-dioxo-1,2,3,6-tetrahydropyrimidin-4-yl}carbonyl)-5-methylbenzonitrile (CCD ID: KR1) (formula: C₂₂H₂₀FN₅O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			31	22	1	5	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		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		

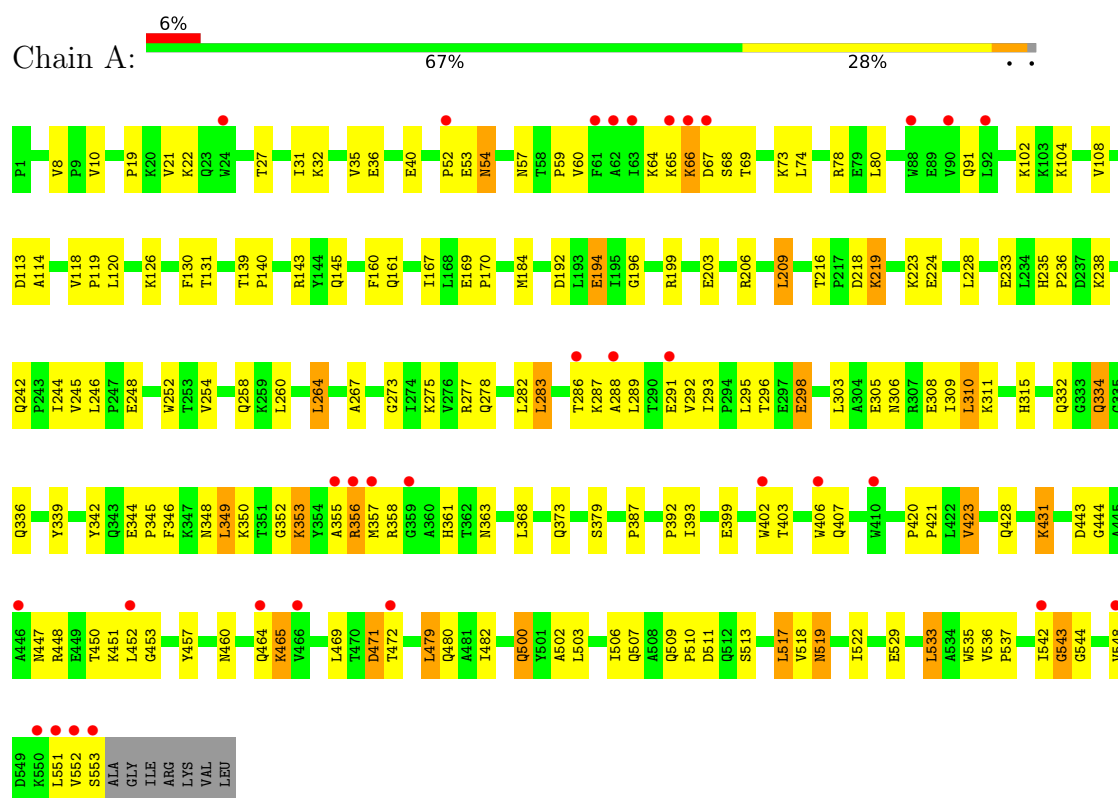
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	110	Total	O	0	0
			110	110		
5	B	97	Total	O	0	0
			97	97		

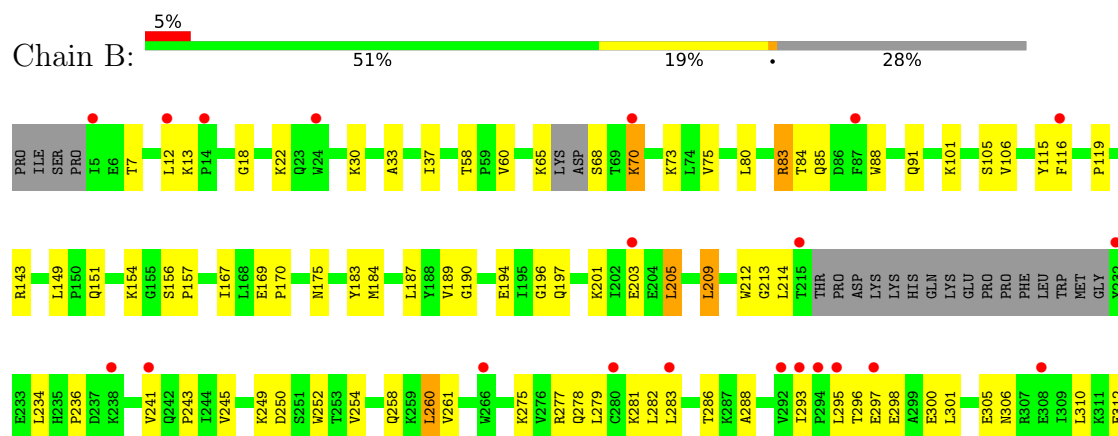
3 Residue-property plots

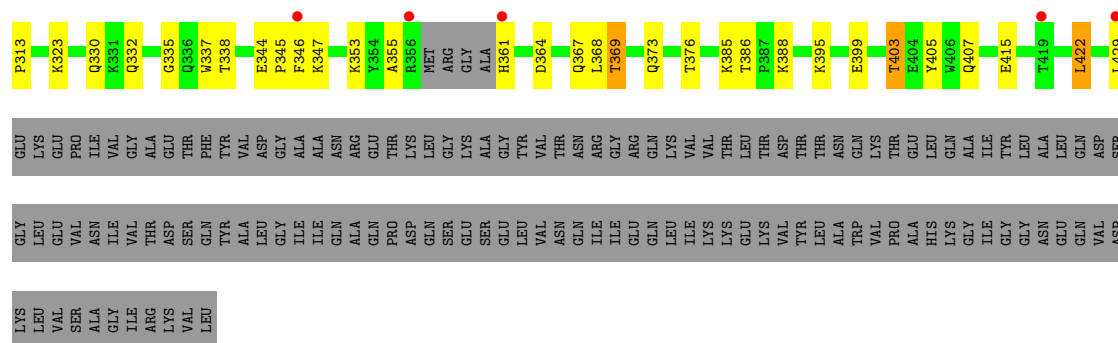
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: HIV Reverse transcriptase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	118.03Å 154.60Å 154.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 2.30 29.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.4 (29.91-2.30) 90.3 (29.91-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.27Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.223 , 0.274 0.221 , 0.272	Depositor DCC
R_{free} test set	2875 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.0	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	0.95	EDS
Total number of atoms	8101	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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, CL, KR1

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	0.41	0/4625	0.74	4/6284 (0.1%)
1	B	0.41	0/3426	0.76	2/4655 (0.0%)
All	All	0.41	0/8051	0.75	6/10939 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	54	ASN	CA-C-N	8.22	128.92	120.04
1	A	54	ASN	C-N-CA	8.22	128.92	120.04
1	A	224	GLU	CA-C-N	5.69	126.24	120.38
1	A	224	GLU	C-N-CA	5.69	126.24	120.38
1	B	18	GLY	CA-C-N	5.06	125.45	119.99
1	B	18	GLY	C-N-CA	5.06	125.45	119.99

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	361	HIS	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	138	0
1	B	3334	0	3365	83	0
2	A	31	0	20	0	0
3	A	20	0	0	0	0
4	B	1	0	0	0	0
5	A	110	0	0	3	0
5	B	97	0	0	4	0
All	All	8101	0	7943	215	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 14.

All (215) 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	1.23	1.08
1:A:66:LYS:HG3	1:A:68:SER:H	1.40	0.87
1:B:296:THR:HG22	1:B:298:GLU:H	1.39	0.86
1:B:209:LEU:HD12	1:B:214:LEU:HD22	1.56	0.85
1:B:194:GLU:HG3	1:B:197:GLN:HG3	1.60	0.84
1:A:393:ILE:HB	1:A:423:VAL:HG13	1.59	0.84
1:B:297:GLU:H	1:B:297:GLU:CD	1.85	0.83
1:B:58:THR:HG23	5:B:563:HOH:O	1.77	0.83
1:B:260:LEU:HD13	1:B:279:LEU:HD21	1.61	0.82
1:A:510:PRO:HG3	5:A:567:HOH:O	1.80	0.80
1:A:64:LYS:HE3	1:A:69:THR:HA	1.64	0.79
1:A:393:ILE:HB	1:A:423:VAL:CG1	2.13	0.79
1:B:373:GLN:HE22	1:B:407:GLN:H	1.32	0.75
1:B:337:TRP:HE1	1:B:367:GLN:HE21	1.32	0.75
1:B:143:ARG:HD3	5:B:627:HOH:O	1.87	0.73
1:A:199:ARG:NH1	1:A:219:LYS:HE2	2.04	0.72
1:B:373:GLN:NE2	1:B:407:GLN:H	1.88	0.72
1:A:298:GLU:H	1:A:298:GLU:CD	1.98	0.71
1:B:12:LEU:HD23	1:B:84:THR:HG22	1.73	0.71
1:A:219:LYS:HB3	1:A:219:LYS:NZ	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:GLU:CD	1:A:194:GLU:H	1.98	0.70
1:A:131:THR:CG2	1:A:143:ARG:HH11	2.05	0.70
1:B:213:GLY:C	1:B:214:LEU:HD12	2.17	0.69
1:B:395:LYS:O	1:B:399:GLU:HG2	1.92	0.69
1:A:503:LEU:HD12	1:A:533:LEU:HD13	1.75	0.69
1:A:66:LYS:HD2	1:A:67:ASP:H	1.58	0.68
1:A:334:GLN:CD	1:A:334:GLN:H	2.02	0.67
1:A:479:LEU:HB3	1:A:517:LEU:HD13	1.77	0.67
1:B:312:GLU:HB3	1:B:313:PRO:HD2	1.76	0.67
1:A:363:ASN:HA	1:A:511:ASP:OD1	1.94	0.67
1:B:376:THR:HG23	1:B:386:THR:HG23	1.78	0.66
1:A:131:THR:HG22	1:A:143:ARG:CG	2.13	0.65
1:B:403:THR:HG21	5:B:596:HOH:O	1.96	0.65
1:B:30:LYS:HD3	5:B:596:HOH:O	1.97	0.64
1:A:356:ARG:CZ	1:A:358:ARG:HD3	2.28	0.64
1:B:252:TRP:CD1	1:B:295:LEU:HD21	2.34	0.62
1:A:27:THR:O	1:A:31:ILE:HG13	1.99	0.62
1:A:66:LYS:HE3	1:A:68:SER:N	2.14	0.62
1:B:115:TYR:HB3	1:B:149:LEU:HB2	1.82	0.61
1:A:57:ASN:OD1	1:A:131:THR:HG23	2.00	0.61
1:A:60:VAL:HG11	1:A:130:PHE:CD2	2.35	0.61
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.16	0.61
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.83	0.61
1:A:108:VAL:HG11	1:A:223:LYS:HB2	1.82	0.61
1:B:254:VAL:O	1:B:258:GLN:HG3	2.02	0.60
1:A:368:LEU:HD22	1:A:423:VAL:HG11	1.84	0.60
1:A:244:ILE:CD1	1:A:267:ALA:HB2	2.32	0.60
1:A:469:LEU:CD1	1:A:480:GLN:HG3	2.32	0.59
1:B:154:LYS:HE2	1:B:184:MET:HE2	1.84	0.59
1:A:513:SER:H	1:A:519:ASN:HD21	1.49	0.58
1:B:154:LYS:CE	1:B:184:MET:HE2	2.34	0.58
1:A:287:LYS:HD2	1:A:293:ILE:HD11	1.84	0.58
1:B:60:VAL:HG12	1:B:75:VAL:HG22	1.85	0.58
1:A:209:LEU:HD23	1:A:216:THR:HG21	1.85	0.58
1:A:510:PRO:HB2	1:A:522:ILE:HD11	1.85	0.58
1:B:282:LEU:HB3	1:B:293:ILE:CD1	2.33	0.57
1:B:65:LYS:HB2	1:B:68:SER:HB2	1.85	0.57
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.86	0.57
1:A:273:GLY:HA2	1:A:332:GLN:NE2	2.20	0.57
1:A:406:TRP:CE3	1:A:407:GLN:HG2	2.40	0.57
1:A:206:ARG:CZ	1:A:218:ASP:HA	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:ILE:HD11	1:B:261:VAL:HG11	1.87	0.57
1:B:282:LEU:HB3	1:B:293:ILE:HD13	1.86	0.56
1:B:296:THR:O	1:B:300:GLU:HG3	2.06	0.56
1:B:429:LEU:N	1:B:429:LEU:HD12	2.21	0.56
1:A:233:GLU:HG2	1:A:235:HIS:NE2	2.21	0.56
1:A:431:LYS:HB2	1:A:431:LYS:NZ	2.21	0.56
1:A:161:GLN:NE2	1:A:184:MET:O	2.38	0.56
1:A:393:ILE:CB	1:A:423:VAL:HG13	2.34	0.56
1:B:183:TYR:CE2	1:B:184:MET:HE3	2.41	0.55
1:B:194:GLU:CG	1:B:197:GLN:HG3	2.34	0.55
1:A:509:GLN:N	1:A:510:PRO:HD3	2.22	0.55
1:A:469:LEU:HD13	1:A:480:GLN:HG3	1.89	0.55
1:A:254:VAL:O	1:A:258:GLN:HG3	2.08	0.54
1:B:388:LYS:HE2	1:B:415:GLU:OE1	2.08	0.54
1:A:254:VAL:HB	1:A:289:LEU:HA	1.90	0.54
1:A:406:TRP:HE3	1:A:407:GLN:HE21	1.56	0.54
1:A:450:THR:O	1:A:451:LYS:HB2	2.07	0.54
1:A:273:GLY:HA2	1:A:332:GLN:HE22	1.73	0.54
1:B:345:PRO:O	1:B:346:PHE:HB2	2.08	0.53
1:B:205:LEU:HD22	1:B:209:LEU:HD22	1.90	0.53
1:A:238:LYS:HD2	1:A:315:HIS:CG	2.44	0.53
1:A:278:GLN:HG3	1:A:298:GLU:HB2	1.91	0.53
1:A:277:ARG:NH1	1:A:334:GLN:HG3	2.24	0.53
1:A:194:GLU:CD	1:A:194:GLU:N	2.65	0.53
1:A:66:LYS:HD2	1:A:67:ASP:N	2.24	0.52
1:B:85:GLN:HA	1:B:88:TRP:NE1	2.24	0.52
1:B:373:GLN:HE22	1:B:407:GLN:N	2.05	0.52
1:B:7:THR:HG22	1:B:119:PRO:HB2	1.92	0.52
1:B:214:LEU:HD12	1:B:214:LEU:N	2.24	0.52
1:A:460:ASN:ND2	1:B:288:ALA:HB2	2.25	0.52
1:A:275:LYS:HG3	5:A:639:HOH:O	2.10	0.52
1:A:233:GLU:HG2	1:A:235:HIS:HE2	1.74	0.52
1:A:542:ILE:HG23	1:B:283:LEU:HD13	1.91	0.51
1:A:228:LEU:HB3	1:A:242:GLN:OE1	2.11	0.51
1:A:342:TYR:HA	1:A:349:LEU:HD23	1.93	0.51
1:B:65:LYS:CB	1:B:68:SER:HB2	2.40	0.51
1:A:513:SER:N	1:A:519:ASN:HD21	2.08	0.51
1:A:503:LEU:CD1	1:A:533:LEU:HD13	2.41	0.50
1:A:356:ARG:NH1	1:A:358:ARG:HD3	2.26	0.50
1:A:392:PRO:O	1:A:423:VAL:HG12	2.11	0.50
1:B:175:ASN:HD21	1:B:201:LYS:NZ	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PRO:HA	1:A:421:PRO:C	2.37	0.49
1:A:518:VAL:O	1:A:522:ILE:HG13	2.12	0.49
1:B:330:GLN:NE2	1:B:338:THR:OG1	2.42	0.49
1:B:297:GLU:CD	1:B:297:GLU:N	2.64	0.49
1:A:289:LEU:HD23	1:A:289:LEU:N	2.27	0.49
1:B:33:ALA:O	1:B:37:ILE:HG13	2.11	0.49
1:A:219:LYS:HB3	1:A:219:LYS:HZ2	1.74	0.49
1:A:464:GLN:O	1:A:465:LYS:HB2	2.12	0.49
1:B:205:LEU:HD22	1:B:209:LEU:CD2	2.42	0.49
1:A:548:VAL:O	1:A:552:VAL:HG22	2.12	0.49
1:B:183:TYR:CE2	1:B:184:MET:HG3	2.48	0.48
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.95	0.48
1:B:13:LYS:HG3	1:B:83:ARG:O	2.12	0.48
1:B:70:LYS:HD2	1:B:70:LYS:N	2.29	0.48
1:A:206:ARG:NH1	1:A:218:ASP:HA	2.28	0.48
1:A:355:ALA:O	1:A:356:ARG:C	2.56	0.48
1:B:169:GLU:HB3	1:B:170:PRO:HD3	1.95	0.48
1:B:277:ARG:O	1:B:281:LYS:HG3	2.13	0.48
1:B:296:THR:HG22	1:B:298:GLU:N	2.18	0.48
1:B:116:PHE:CZ	1:B:151:GLN:NE2	2.82	0.48
1:B:344:GLU:HB2	1:B:347:LYS:HD3	1.96	0.48
1:A:167:ILE:O	1:A:170:PRO:HD2	2.13	0.47
1:A:199:ARG:O	1:A:203:GLU:HG2	2.14	0.47
1:B:209:LEU:HB3	1:B:214:LEU:HB2	1.96	0.47
1:A:8:VAL:O	1:A:10:VAL:HG23	2.14	0.47
1:A:52:PRO:HA	1:A:54:ASN:N	2.29	0.47
1:A:32:LYS:O	1:A:36:GLU:HG3	2.14	0.47
1:A:40:GLU:OE2	1:A:40:GLU:HA	2.15	0.47
1:B:156:SER:N	1:B:157:PRO:HD2	2.30	0.47
1:B:353:LYS:HD3	1:B:429:LEU:CD2	2.44	0.47
1:A:131:THR:CG2	1:A:143:ARG:NH1	2.75	0.46
1:A:536:VAL:HG13	1:A:537:PRO:HD2	1.98	0.46
1:A:66:LYS:HE3	1:A:68:SER:HB2	1.97	0.46
1:A:552:VAL:HG23	1:A:552:VAL:O	2.14	0.46
1:B:241:VAL:O	1:B:243:PRO:HD3	2.16	0.46
1:A:289:LEU:HD23	1:A:289:LEU:H	1.79	0.46
1:A:450:THR:CG2	1:A:452:LEU:HB2	2.46	0.46
1:B:105:SER:O	1:B:190:GLY:HA2	2.16	0.46
1:B:346:PHE:N	1:B:346:PHE:CD1	2.84	0.46
1:A:306:ASN:O	1:A:310:LEU:HD22	2.16	0.46
1:B:429:LEU:HD12	1:B:429:LEU:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:PHE:N	1:B:346:PHE:HD1	2.14	0.46
1:A:245:VAL:HG13	1:A:245:VAL:O	2.15	0.46
1:A:342:TYR:HB3	1:A:348:ASN:HD22	1.81	0.46
1:B:369:THR:HG21	1:B:405:TYR:HB2	1.97	0.45
1:A:542:ILE:O	1:A:543:GLY:C	2.58	0.45
1:B:101:LYS:O	1:B:236:PRO:HB2	2.17	0.45
1:A:126:LYS:HA	1:A:145:GLN:NE2	2.32	0.45
1:A:139:THR:HB	1:A:140:PRO:HD2	1.99	0.45
1:A:286:THR:HG23	1:A:286:THR:O	2.17	0.45
1:A:65:LYS:O	1:A:66:LYS:HG3	2.17	0.45
1:A:502:ALA:O	1:A:506:ILE:HG12	2.17	0.45
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.98	0.45
1:A:31:ILE:O	1:A:35:VAL:HG23	2.17	0.45
1:A:252:TRP:O	1:A:292:VAL:HA	2.17	0.45
1:A:402:TRP:CE3	1:A:403:THR:HG23	2.53	0.44
1:A:447:ASN:HB3	1:A:450:THR:HB	1.99	0.44
1:A:289:LEU:H	1:A:289:LEU:CD2	2.31	0.44
1:A:552:VAL:O	1:A:553:SER:HB3	2.18	0.44
1:A:296:THR:HB	1:A:298:GLU:OE1	2.18	0.44
1:A:406:TRP:CE3	1:A:407:GLN:NE2	2.86	0.44
1:B:116:PHE:HZ	1:B:151:GLN:NE2	2.16	0.44
1:A:363:ASN:HA	1:A:511:ASP:CG	2.42	0.44
1:A:469:LEU:HD11	1:A:480:GLN:HG3	1.99	0.44
1:A:66:LYS:CG	1:A:68:SER:H	2.22	0.43
1:A:21:VAL:HG12	1:A:22:LYS:N	2.32	0.43
1:A:353:LYS:HB3	1:A:353:LYS:HE3	1.59	0.43
1:A:482:ILE:HD12	1:A:502:ALA:HB1	2.00	0.43
1:A:196:GLY:HA3	5:A:618:HOH:O	2.18	0.43
1:A:379:SER:OG	1:A:387:PRO:HD3	2.17	0.43
1:B:115:TYR:HB3	1:B:149:LEU:CB	2.49	0.43
1:A:66:LYS:CG	1:A:67:ASP:N	2.82	0.43
1:A:345:PRO:HA	1:A:346:PHE:HA	1.59	0.42
1:A:443:ASP:OD2	1:A:444:GLY:N	2.51	0.42
1:A:288:ALA:HB3	1:A:291:GLU:HG3	2.01	0.42
1:A:235:HIS:HB3	1:A:236:PRO:CD	2.50	0.42
1:A:544:GLY:HA2	1:B:286:THR:HG22	2.02	0.42
1:A:104:LYS:HB3	1:A:192:ASP:HA	2.01	0.42
1:B:243:PRO:O	1:B:245:VAL:HG13	2.19	0.42
1:B:295:LEU:N	1:B:295:LEU:CD2	2.82	0.42
1:A:450:THR:O	1:A:451:LYS:CB	2.68	0.42
1:A:260:LEU:O	1:A:264:LEU:HD22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.55	0.41
1:A:457:TYR:CD1	1:A:457:TYR:C	2.97	0.41
1:B:278:GLN:HG3	1:B:298:GLU:HB3	2.00	0.41
1:A:431:LYS:HB2	1:A:431:LYS:HZ3	1.85	0.41
1:A:108:VAL:O	1:A:108:VAL:HG13	2.20	0.41
1:A:283:LEU:HD12	1:A:283:LEU:HA	1.82	0.41
1:A:52:PRO:HA	1:A:53:GLU:C	2.46	0.41
1:A:244:ILE:HD12	1:A:267:ALA:HB2	2.02	0.41
1:B:332:GLN:HG3	1:B:338:THR:HG23	2.02	0.41
1:A:102:LYS:HE2	1:A:102:LYS:HB3	1.92	0.41
1:A:118:VAL:HG13	1:A:119:PRO:HD2	2.03	0.41
1:B:154:LYS:HE3	1:B:184:MET:HE2	2.02	0.41
1:A:453:GLY:HA3	1:A:472:THR:HG21	2.03	0.41
1:B:106:VAL:HA	1:B:189:VAL:O	2.21	0.41
1:B:295:LEU:N	1:B:295:LEU:HD22	2.36	0.41
1:B:330:GLN:HE21	1:B:330:GLN:HB2	1.75	0.41
1:A:244:ILE:HD13	1:A:267:ALA:HB2	2.00	0.41
1:B:194:GLU:CD	1:B:196:GLY:H	2.29	0.41
1:B:282:LEU:HB3	1:B:293:ILE:HD11	2.03	0.41
1:B:275:LYS:H	1:B:306:ASN:HD21	1.69	0.40
1:B:335:GLY:O	1:B:355:ALA:HA	2.22	0.40
1:A:19:PRO:HG3	1:A:80:LEU:HB2	2.03	0.40
1:A:305:GLU:O	1:A:309:ILE:HG13	2.21	0.40
1:B:301:LEU:O	1:B:305:GLU:HG3	2.22	0.40
1:A:64:LYS:CE	1:A:69:THR:HA	2.44	0.40
1:A:114:ALA:HB1	1:A:160:PHE:CE1	2.56	0.40
1:A:235:HIS:HB3	1:A:236:PRO:HD2	2.03	0.40
1:A:402:TRP:HE1	1:B:364:ASP:CG	2.28	0.40
1:B:167:ILE:HG12	1:B:212:TRP:CD2	2.56	0.40
1:A:246:LEU:HD22	1:A:260:LEU:HD12	2.02	0.40
1:A:500:GLN:CD	1:B:422:LEU:HD22	2.46	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%)	527 (96%)	19 (3%)	5 (1%)	14	17
1	B	395/560 (70%)	381 (96%)	14 (4%)	0	100	100
All	All	946/1120 (84%)	908 (96%)	33 (4%)	5 (0%)	24	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	356	ARG
1	A	543	GLY
1	A	66	LYS
1	A	465	LYS

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%)	455 (92%)	40 (8%)	11	14
1	B	367/500 (73%)	346 (94%)	21 (6%)	18	27
All	All	862/1000 (86%)	801 (93%)	61 (7%)	13	19

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	74	LEU
1	A	78	ARG
1	A	113	ASP
1	A	120	LEU
1	A	194	GLU
1	A	209	LEU
1	A	219	LYS

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Mol	Chain	Res	Type
1	A	248	GLU
1	A	264	LEU
1	A	282	LEU
1	A	283	LEU
1	A	295	LEU
1	A	298	GLU
1	A	303	LEU
1	A	308	GLU
1	A	310	LEU
1	A	311	LYS
1	A	334	GLN
1	A	344	GLU
1	A	349	LEU
1	A	350	LYS
1	A	353	LYS
1	A	357	MET
1	A	361	HIS
1	A	373	GLN
1	A	399	GLU
1	A	423	VAL
1	A	428	GLN
1	A	431	LYS
1	A	448	ARG
1	A	471	ASP
1	A	479	LEU
1	A	500	GLN
1	A	507	GLN
1	A	517	LEU
1	A	519	ASN
1	A	529	GLU
1	A	533	LEU
1	A	551	LEU
1	B	22	LYS
1	B	70	LYS
1	B	73	LYS
1	B	80	LEU
1	B	83	ARG
1	B	91	GLN
1	B	187	LEU
1	B	203	GLU
1	B	205	LEU
1	B	209	LEU

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Mol	Chain	Res	Type
1	B	234	LEU
1	B	249	LYS
1	B	250	ASP
1	B	260	LEU
1	B	310	LEU
1	B	323	LYS
1	B	368	LEU
1	B	369	THR
1	B	385	LYS
1	B	403	THR
1	B	422	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	A	147	ASN
1	A	174	GLN
1	A	242	GLN
1	A	332	GLN
1	A	336	GLN
1	A	348	ASN
1	A	407	GLN
1	A	487	GLN
1	A	512	GLN
1	A	519	ASN
1	A	524	GLN
1	B	85	GLN
1	B	91	GLN
1	B	137	ASN
1	B	151	GLN
1	B	175	ASN
1	B	197	GLN
1	B	242	GLN
1	B	258	GLN
1	B	306	ASN
1	B	330	GLN
1	B	336	GLN
1	B	340	GLN
1	B	348	ASN
1	B	367	GLN
1	B	373	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](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
2	KR1	A	701	-	33,33,33	2.84	17 (51%)	44,48,48	2.30	12 (27%)
3	SO4	A	562	-	4,4,4	0.37	0	6,6,6	0.11	0
3	SO4	A	564	-	4,4,4	0.39	0	6,6,6	0.09	0
3	SO4	A	563	-	4,4,4	0.39	0	6,6,6	0.05	0
3	SO4	A	561	-	4,4,4	0.36	0	6,6,6	0.21	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	KR1	A	701	-	-	2/18/18/18	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	KR1	C19-C18	6.34	1.50	1.39
2	A	701	KR1	C6-C5	5.74	1.48	1.39
2	A	701	KR1	C21-N5	5.30	1.39	1.31
2	A	701	KR1	C22-C18	4.28	1.46	1.39
2	A	701	KR1	C4-C5	4.19	1.45	1.39
2	A	701	KR1	C2-C3	4.15	1.46	1.39
2	A	701	KR1	C9-C11	4.00	1.42	1.35
2	A	701	KR1	C12-C11	3.59	1.51	1.43
2	A	701	KR1	O2-C12	3.16	1.29	1.23
2	A	701	KR1	C1-N1	2.99	1.21	1.14
2	A	701	KR1	O1-C8	2.94	1.29	1.23
2	A	701	KR1	C9-N3	2.67	1.47	1.40
2	A	701	KR1	C2-C7	2.57	1.43	1.39
2	A	701	KR1	O3-C13	2.28	1.27	1.23
2	A	701	KR1	C14-C11	2.15	1.55	1.52
2	A	701	KR1	C12-N2	2.14	1.42	1.38
2	A	701	KR1	C15-C14	2.09	1.59	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	KR1	C21-N5-C20	6.89	125.65	116.59
2	A	701	KR1	C22-C21-N5	-6.84	120.62	127.23
2	A	701	KR1	F1-C21-N5	4.46	120.00	114.51
2	A	701	KR1	O1-C8-C9	-4.40	112.53	120.35
2	A	701	KR1	C14-C11-C9	3.94	125.84	119.06
2	A	701	KR1	C5-C8-C9	3.78	126.20	119.34
2	A	701	KR1	C18-C22-C21	-3.59	117.02	119.37
2	A	701	KR1	C17-N3-C13	-3.44	113.10	117.05
2	A	701	KR1	C17-N3-C9	3.06	127.52	120.96
2	A	701	KR1	C8-C9-N3	-2.44	111.36	118.26
2	A	701	KR1	O3-C13-N3	-2.33	119.29	122.32
2	A	701	KR1	C5-C4-C3	-2.04	117.91	120.37

There are no chirality outliers.

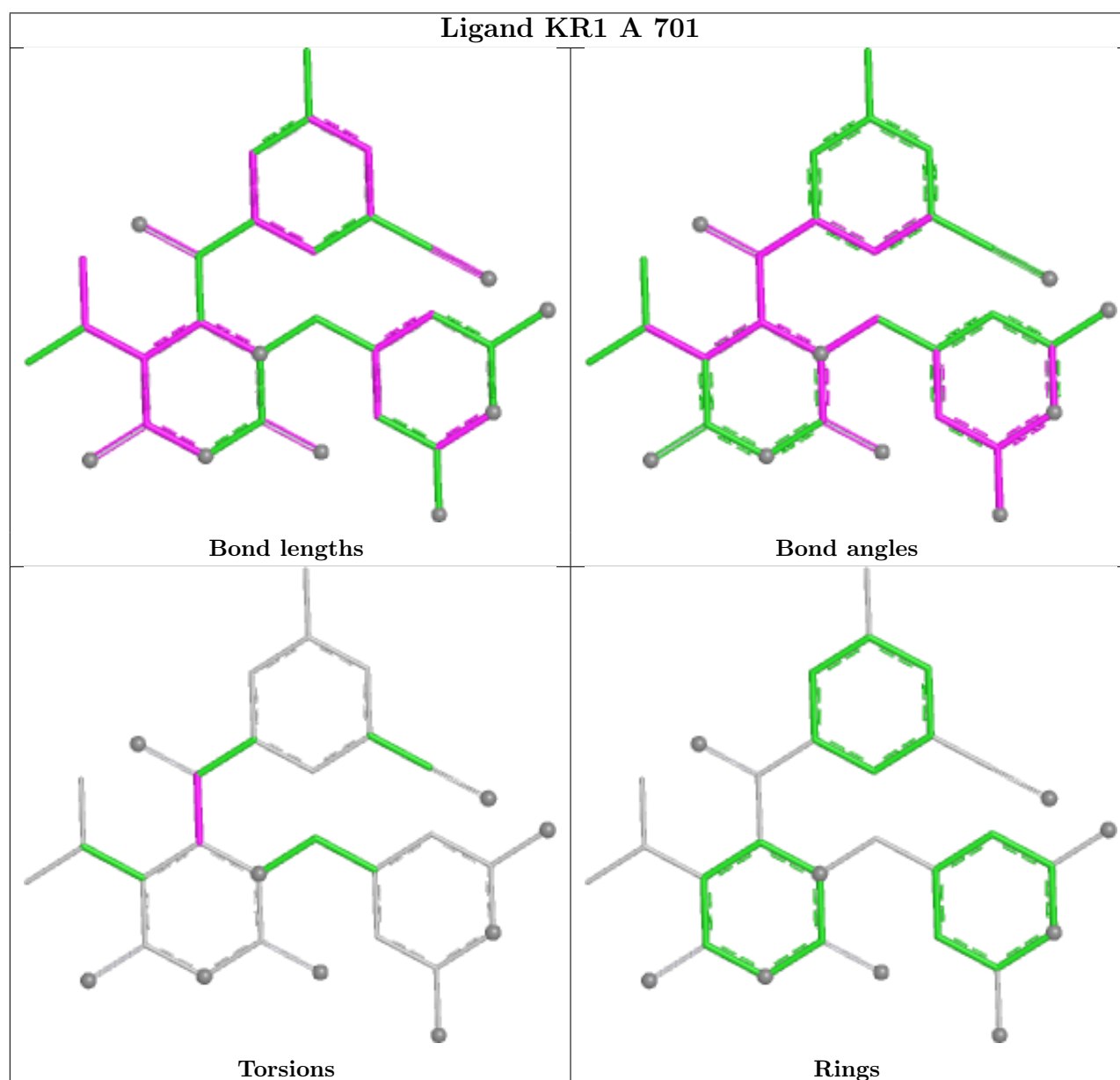
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	KR1	C5-C8-C9-C11
2	A	701	KR1	C5-C8-C9-N3

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	553/560 (98%)	0.38	32 (5%)	29 31	30, 49, 82, 101	0
1	B	403/560 (71%)	0.35	26 (6%)	25 27	26, 47, 82, 95	0
All	All	956/1120 (85%)	0.36	58 (6%)	27 29	26, 48, 82, 101	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	232	TYR	5.0
1	A	551	LEU	4.7
1	A	553	SER	4.7
1	B	5	ILE	4.3
1	B	346	PHE	4.0
1	B	241	VAL	3.7
1	B	361	HIS	3.5
1	A	452	LEU	3.5
1	A	24	TRP	3.4
1	B	24	TRP	3.4
1	A	88	TRP	3.4
1	B	116	PHE	3.4
1	A	552	VAL	3.3
1	B	14	PRO	3.3
1	A	52	PRO	3.2
1	A	406	TRP	3.0
1	A	61	PHE	2.9
1	B	293	ILE	2.9
1	A	291	GLU	2.8
1	B	429	LEU	2.8
1	A	402	TRP	2.7
1	A	66	LYS	2.6
1	A	356	ARG	2.6
1	B	238	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	63	ILE	2.6
1	A	288	ALA	2.6
1	A	65	LYS	2.5
1	A	357	MET	2.5
1	A	446	ALA	2.5
1	A	92	LEU	2.4
1	A	410	TRP	2.4
1	A	548	VAL	2.3
1	A	464	GLN	2.3
1	B	308	GLU	2.3
1	B	87	PHE	2.3
1	B	295	LEU	2.3
1	B	419	THR	2.3
1	A	90	VAL	2.3
1	B	70	LYS	2.3
1	A	472	THR	2.2
1	B	294	PRO	2.2
1	B	266	TRP	2.2
1	A	62	ALA	2.2
1	B	297	GLU	2.1
1	A	286	THR	2.1
1	B	215	THR	2.1
1	B	356	ARG	2.1
1	B	12	LEU	2.1
1	A	355	ALA	2.1
1	A	67	ASP	2.1
1	A	542	ILE	2.1
1	A	466	VAL	2.1
1	A	359	GLY	2.1
1	A	550	LYS	2.0
1	B	280	CYS	2.0
1	B	292	VAL	2.0
1	B	203	GLU	2.0
1	B	283	LEU	2.0

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

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](#)

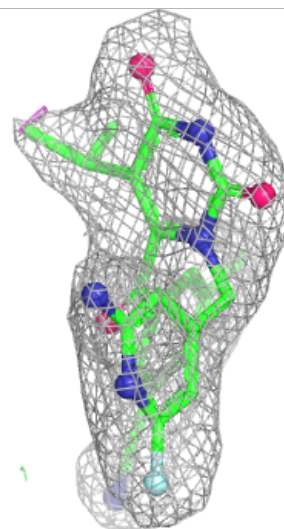
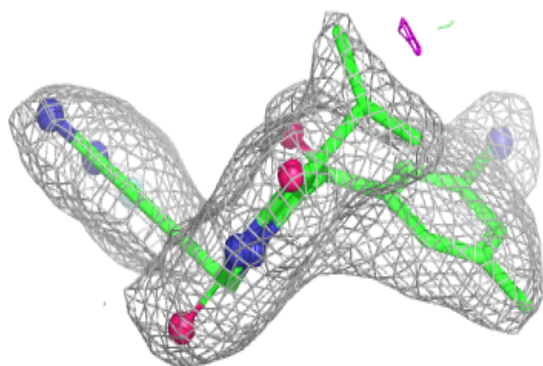
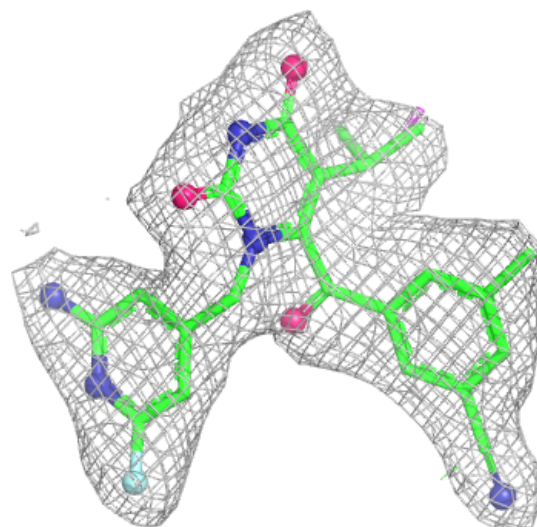
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	564	5/5	0.57	0.14	107,107,108,108	0
3	SO4	A	563	5/5	0.71	0.17	120,120,120,120	0
3	SO4	A	562	5/5	0.89	0.11	58,60,61,64	0
3	SO4	A	561	5/5	0.91	0.12	61,65,67,68	0
2	KR1	A	701	31/31	0.93	0.09	34,41,44,48	0
4	CL	B	561	1/1	0.97	0.22	62,62,62,62	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 KR1 A 701:

$2mF_o-DF_c$ (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.