



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:00 PM UTC

PDB ID : 1KYN / pdb_00001kyn
Title : Cathepsin-G
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Gordon, P.; Maryanoff, B.E.
Deposited on : 2002-02-05
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 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

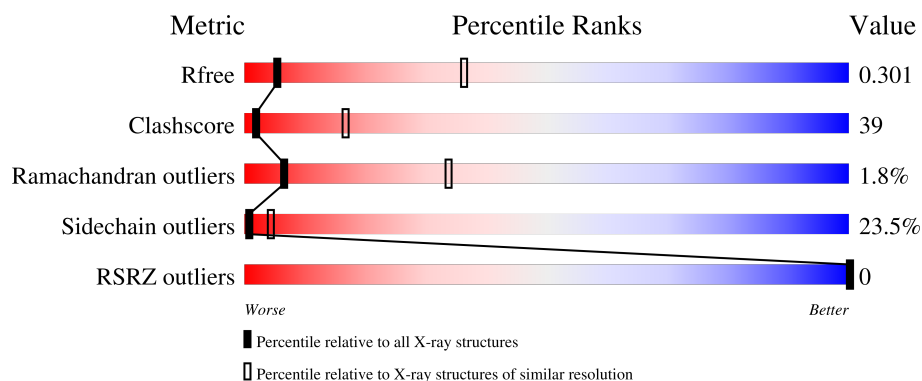
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	235	
1	B	235	

2 Entry composition [i](#)

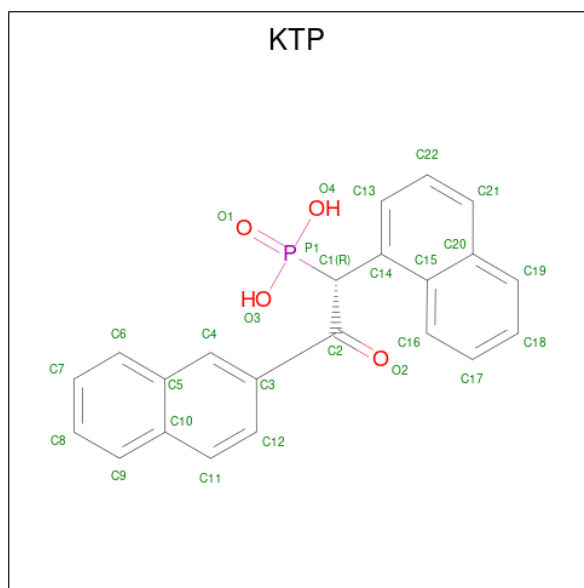
There are 2 unique types of molecules in this entry. The entry contains 3607 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 cathepsin G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1774	1090	366	308	10			
1	B	225	Total	C	N	O	S	0	0	0
			1779	1092	367	310	10			

- Molecule 2 is (2-NAPHTHALEN-2-YL-1-NAPHTHALEN-1-YL-2-OXO-ETHYL)-PHOSPHONIC ACID (CCD ID: KTP) (formula: C₂₂H₁₇O₄P).

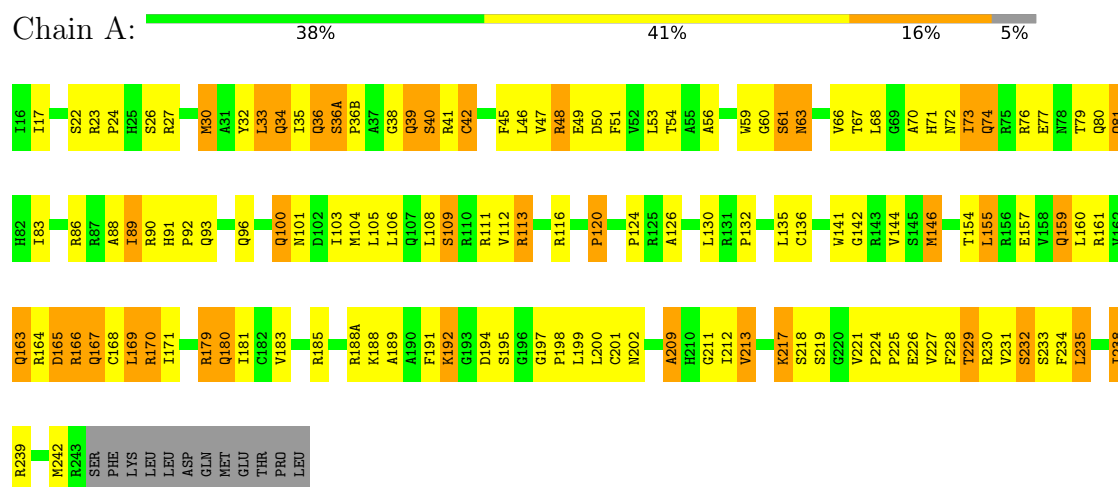


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			27	22	4	1		
2	B	1	Total	C	O	P	0	0
			27	22	4	1		

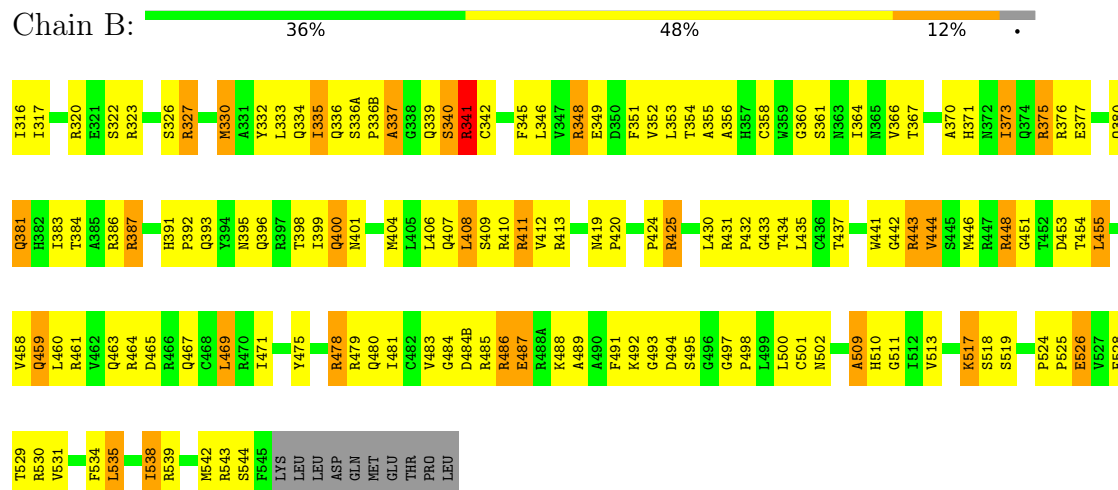
3 Residue-property plots

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: cathepsin G



• Molecule 1: cathepsin G



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	59.44Å 59.44Å 130.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.86 – 3.50 14.86 – 3.50	Depositor EDS
% Data completeness (in resolution range)	72.6 (14.86-3.50) 72.6 (14.86-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.01Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.258 , 0.328 0.222 , 0.301	Depositor DCC
R_{free} test set	453 reflections (6.41%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 8.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	0.220 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3607	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9853e-03.*

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: KTP

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	0.30	0/1808	0.72	0/2440
1	B	0.29	0/1813	0.72	0/2446
All	All	0.29	0/3621	0.72	0/4886

There are no bond length outliers.

There are no bond angle outliers.

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	1774	0	1782	125	0
1	B	1779	0	1781	147	0
2	A	27	0	15	6	0
2	B	27	0	15	7	0
All	All	3607	0	3593	279	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 39.

All (279) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:601:KTP:C2	2:A:601:KTP:C1	1.77	1.62
2:B:701:KTP:C2	2:B:701:KTP:C1	1.78	1.55
1:A:36(B):PRO:HG3	1:A:63:ASN:N	1.76	1.00
1:A:36(B):PRO:HG3	1:A:63:ASN:H	1.32	0.94
1:A:166:ARG:HH11	1:A:170:ARG:HD3	1.32	0.94
1:A:36(B):PRO:HB2	1:A:61:SER:H	1.37	0.88
2:B:701:KTP:C2	2:B:701:KTP:HC1	2.01	0.88
1:B:392:PRO:HB2	1:B:393:GLN:HE21	1.39	0.88
2:A:601:KTP:C2	2:A:601:KTP:HC1	2.05	0.87
1:B:335:ILE:HD11	1:B:337:ALA:HA	1.56	0.87
1:B:481:ILE:HG12	1:B:530:ARG:HH21	1.39	0.86
1:B:336(A):SER:HB2	1:B:339:GLN:H	1.40	0.86
1:A:35:ILE:HD11	1:A:42:CYS:HB2	1.59	0.85
1:A:36(A):SER:OG	1:A:36(B):PRO:HD3	1.77	0.84
1:B:443:ARG:HH11	1:B:492:LYS:HG2	1.41	0.83
1:B:335:ILE:HG21	1:B:364:ILE:HG12	1.59	0.82
1:A:180:GLN:HG2	1:A:227:VAL:HG13	1.60	0.82
1:B:336(A):SER:HB2	1:B:339:GLN:N	1.95	0.82
1:B:377:GLU:HB2	1:B:380:GLN:HG3	1.60	0.81
1:B:336:GLN:H	1:B:340:SER:HA	1.46	0.80
1:A:35:ILE:HD12	1:A:35:ILE:H	1.48	0.78
1:B:400:GLN:HG2	1:B:479:ARG:HH21	1.50	0.77
1:A:36:GLN:HA	1:A:39:GLN:HA	1.66	0.77
1:B:345:PHE:HB3	1:B:498:PRO:HG3	1.68	0.75
1:A:93:GLN:HB2	1:A:101:ASN:ND2	2.01	0.74
1:B:443:ARG:NH1	1:B:492:LYS:HG2	2.02	0.74
1:A:45:PHE:HB3	1:A:198:PRO:HG3	1.70	0.73
1:B:393:GLN:HB2	1:B:401:ASN:ND2	2.02	0.73
1:B:336:GLN:HB2	1:B:341:ARG:N	2.04	0.73
1:B:393:GLN:HB2	1:B:401:ASN:HD22	1.52	0.73
1:B:478:ARG:HB2	1:B:478:ARG:CZ	2.16	0.73
1:A:36(B):PRO:CB	1:A:61:SER:H	2.01	0.72
1:B:413:ARG:O	1:B:413:ARG:HG3	1.88	0.71
1:A:168:CYS:HA	1:A:171:ILE:HD12	1.71	0.71
1:B:481:ILE:HG12	1:B:530:ARG:HE	1.54	0.71
1:A:36(B):PRO:HB2	1:A:61:SER:N	2.06	0.71
1:B:336:GLN:H	1:B:340:SER:CA	2.04	0.70
1:B:481:ILE:HG12	1:B:530:ARG:NH2	2.07	0.70
1:A:36(B):PRO:HB2	1:A:61:SER:OG	1.92	0.69
1:A:93:GLN:HB2	1:A:101:ASN:HD22	1.57	0.68
1:B:400:GLN:HG2	1:B:479:ARG:NH2	2.08	0.68
1:A:63:ASN:C	1:A:63:ASN:HD22	2.01	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ILE:HG12	1:B:360:GLY:HA3	1.77	0.67
1:B:333:LEU:HD11	1:B:354:THR:HG21	1.75	0.67
1:B:335:ILE:O	1:B:335:ILE:HG23	1.94	0.67
1:B:432:PRO:HG2	1:B:464:ARG:HG2	1.75	0.67
1:B:433:GLY:HA2	1:B:461:ARG:HD2	1.77	0.66
1:B:425:ARG:H	1:B:425:ARG:HD2	1.60	0.65
1:A:91:HIS:ND1	1:A:92:PRO:HD2	2.11	0.65
1:B:471:ILE:HD11	1:B:485:ARG:HH22	1.62	0.65
1:B:322:SER:HB2	1:B:455:LEU:HD23	1.78	0.64
1:A:36(B):PRO:HB2	1:A:61:SER:CB	2.27	0.64
1:A:238:ILE:O	1:A:242:MET:HG3	1.98	0.64
1:B:346:LEU:HD21	1:B:412:VAL:HG21	1.80	0.63
1:A:141:TRP:CE2	1:A:155:LEU:HB2	2.33	0.62
1:B:489:ALA:HB1	1:B:526:GLU:OE2	1.99	0.62
1:A:46:LEU:HD21	1:A:112:VAL:HG21	1.82	0.62
1:A:218:SER:HA	2:A:601:KTP:HC11	1.81	0.62
1:B:336(A):SER:CB	1:B:339:GLN:H	2.13	0.61
1:A:166:ARG:HD3	1:A:170:ARG:HD3	1.82	0.61
1:B:330:MET:HG3	1:B:455:LEU:HD11	1.83	0.61
1:A:72:ASN:C	1:A:72:ASN:HD22	2.09	0.61
1:B:435:LEU:HD11	1:B:459:GLN:HB3	1.82	0.61
1:A:197:GLY:O	1:A:213:VAL:HG23	2.02	0.60
1:A:59:TRP:CD1	1:A:90:ARG:HE	2.20	0.60
1:A:36(B):PRO:CG	1:A:61:SER:N	2.65	0.59
1:B:355:ALA:O	1:B:404:MET:HE2	2.01	0.59
1:B:348:ARG:HB2	1:B:351:PHE:HB2	1.84	0.59
1:A:36(B):PRO:CG	1:A:63:ASN:N	2.60	0.58
1:B:435:LEU:HB2	1:B:461:ARG:HH12	1.68	0.58
1:A:142:GLY:HA3	1:A:194:ASP:OD1	2.03	0.58
1:B:333:LEU:HD21	1:B:406:LEU:CD1	2.32	0.58
1:B:335:ILE:N	1:B:340:SER:HA	2.17	0.58
1:B:460:LEU:HD21	1:B:489:ALA:HA	1.84	0.58
1:B:333:LEU:HD22	1:B:364:ILE:HG21	1.84	0.58
1:A:86:ARG:HB2	1:A:109:SER:HA	1.85	0.58
1:A:126:ALA:HA	1:A:235:LEU:HD23	1.84	0.57
1:B:493:GLY:H	2:B:701:KTP:P1	2.27	0.57
1:B:539:ARG:O	1:B:543:ARG:HG2	2.04	0.57
1:A:124:PRO:HD3	1:A:209:ALA:O	2.04	0.57
1:B:481:ILE:HG12	1:B:530:ARG:NE	2.19	0.57
1:B:332:TYR:CD2	1:B:373:ILE:HG21	2.40	0.57
1:B:471:ILE:HD11	1:B:485:ARG:NH2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36(B):PRO:CB	1:A:61:SER:N	2.66	0.57
1:B:463:GLN:NE2	1:B:484(B):ASP:HA	2.21	0.56
1:B:467:GLN:HE21	1:B:485:ARG:HH21	1.53	0.56
1:B:497:GLY:O	1:B:513:VAL:HG23	2.06	0.56
1:A:32:TYR:CD1	1:A:73:ILE:HG21	2.42	0.55
2:A:601:KTP:C2	2:A:601:KTP:C14	2.77	0.55
1:B:336:GLN:N	1:B:340:SER:HA	2.19	0.55
1:B:431:ARG:HH21	1:B:431:ARG:HG3	1.72	0.55
1:B:475:TYR:HA	1:B:480:GLN:OE1	2.07	0.55
1:B:489:ALA:HB1	1:B:526:GLU:CD	2.32	0.55
1:A:38:GLY:C	1:A:39:GLN:HG3	2.30	0.55
1:A:180:GLN:HG2	1:A:227:VAL:CG1	2.36	0.55
1:A:130:LEU:HD21	1:A:201:CYS:SG	2.48	0.54
1:A:36(A):SER:HG	1:A:36(B):PRO:HD3	1.73	0.54
1:B:333:LEU:HD21	1:B:406:LEU:HD13	1.87	0.54
1:B:336(A):SER:HB3	1:B:336(B):PRO:HD2	1.87	0.54
2:B:701:KTP:C2	2:B:701:KTP:C14	2.80	0.54
1:B:345:PHE:CD1	1:B:498:PRO:HB3	2.42	0.54
1:B:481:ILE:HG23	1:B:530:ARG:HH21	1.73	0.54
1:A:36(B):PRO:CG	1:A:63:ASN:H	2.13	0.53
1:B:484(B):ASP:HB3	1:B:487:GLU:HG3	1.89	0.53
1:B:501:CYS:O	1:B:502:ASN:HB2	2.09	0.53
1:A:36(B):PRO:CG	1:A:61:SER:H	2.19	0.53
1:B:349:GLU:HB3	1:B:411:ARG:HG3	1.90	0.53
1:A:36:GLN:HG2	1:A:39:GLN:CA	2.38	0.53
1:B:370:ALA:HB2	1:B:380:GLN:HG2	1.89	0.53
1:B:356:ALA:HA	1:B:404:MET:HB3	1.91	0.52
1:B:341:ARG:HH12	1:B:442:GLY:HA2	1.74	0.52
1:B:442:GLY:HA3	1:B:494:ASP:OD1	2.10	0.52
1:B:486:ARG:HB2	1:B:486:ARG:CZ	2.39	0.52
1:A:181:ILE:HG12	1:A:230:ARG:HE	1.75	0.52
1:A:217:LYS:C	1:A:219:SER:H	2.18	0.52
1:A:189:ALA:HB1	1:A:226:GLU:OE2	2.09	0.52
1:B:316:ILE:O	1:B:444:VAL:HA	2.10	0.52
1:A:59:TRP:HA	1:A:104:MET:HE1	1.92	0.51
1:B:345:PHE:CB	1:B:498:PRO:HG3	2.40	0.51
1:A:32:TYR:CG	1:A:73:ILE:HG21	2.46	0.51
1:A:36(A):SER:CB	1:A:36(B):PRO:HD3	2.41	0.51
1:A:67:THR:HA	1:A:81:GLN:O	2.10	0.51
1:B:354:THR:HG21	1:B:406:LEU:HD11	1.93	0.51
1:A:88:ALA:HA	1:A:106:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:THR:HA	1:B:381:GLN:O	2.11	0.51
1:B:441:TRP:CE2	1:B:455:LEU:HB2	2.45	0.51
1:A:161:ARG:HH12	1:A:163:GLN:HA	1.75	0.51
1:A:201:CYS:O	1:A:202:ASN:HB2	2.11	0.51
1:B:517:LYS:C	1:B:519:SER:H	2.18	0.51
1:A:48:ARG:HB2	1:A:51:PHE:HB2	1.92	0.50
1:B:317:ILE:O	1:B:488:LYS:HA	2.12	0.50
1:B:323:ARG:HB3	1:B:326:SER:HB3	1.93	0.50
1:B:492:LYS:HZ3	2:B:701:KTP:HC1	1.76	0.50
1:A:159:GLN:O	1:A:160:LEU:HD23	2.11	0.50
1:A:50:ASP:HB3	1:A:111:ARG:HD3	1.92	0.50
1:B:375:ARG:HH11	1:B:375:ARG:HG2	1.76	0.50
1:B:492:LYS:HZ3	2:B:701:KTP:HC13	1.76	0.50
1:B:481:ILE:CG1	1:B:530:ARG:HE	2.22	0.50
1:B:387:ARG:NH2	1:B:407:GLN:HE22	2.10	0.50
1:B:483:VAL:HG12	1:B:484:GLY:N	2.27	0.50
1:B:346:LEU:HG	1:B:348:ARG:O	2.11	0.49
1:A:36:GLN:HG2	1:A:39:GLN:HA	1.93	0.49
1:A:46:LEU:O	1:A:120:PRO:HA	2.12	0.49
1:A:113:ARG:O	1:A:113:ARG:HG3	2.12	0.49
1:A:23:ARG:HB3	1:A:26:SER:HB3	1.95	0.49
1:A:45:PHE:CB	1:A:198:PRO:HG3	2.41	0.49
1:A:212:ILE:HD11	1:A:231:VAL:HG22	1.94	0.49
1:A:89:ILE:O	1:A:104:MET:HG3	2.12	0.49
1:A:92:PRO:HB2	1:A:93:GLN:HE21	1.77	0.49
1:A:56:ALA:HA	1:A:104:MET:CB	2.42	0.49
1:B:346:LEU:HD12	1:B:352:VAL:HG22	1.95	0.49
1:B:543:ARG:HG3	1:B:544:SER:N	2.27	0.49
1:A:36:GLN:HG2	1:A:39:GLN:C	2.38	0.49
1:A:36(B):PRO:HG3	1:A:63:ASN:CA	2.43	0.48
1:B:481:ILE:CG1	1:B:530:ARG:HH21	2.20	0.48
1:B:327:ARG:O	1:B:330:MET:HB2	2.14	0.48
1:B:492:LYS:NZ	2:B:701:KTP:HC1	2.28	0.48
1:A:35:ILE:O	1:A:36(B):PRO:HD2	2.13	0.48
1:B:334:GLN:C	1:B:340:SER:HB2	2.39	0.48
1:A:165:ASP:O	1:A:169:LEU:HB2	2.14	0.48
1:B:346:LEU:O	1:B:420:PRO:HA	2.14	0.48
1:B:399:ILE:HG22	1:B:399:ILE:O	2.13	0.48
1:B:408:LEU:N	1:B:408:LEU:HD23	2.29	0.48
1:A:27:ARG:O	1:A:30:MET:HB2	2.13	0.48
1:B:465:ASP:O	1:B:469:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36(B):PRO:HG2	1:A:61:SER:N	2.29	0.48
1:A:56:ALA:HA	1:A:104:MET:HB3	1.96	0.48
1:B:335:ILE:HD11	1:B:337:ALA:CA	2.35	0.48
1:B:481:ILE:HD11	1:B:530:ARG:HA	1.96	0.48
1:B:513:VAL:HG22	1:B:528:PHE:CE2	2.49	0.47
1:A:45:PHE:CD1	1:A:198:PRO:HB3	2.49	0.47
1:B:356:ALA:HA	1:B:404:MET:CB	2.44	0.47
1:B:430:LEU:HD11	1:B:434:THR:HG21	1.95	0.47
1:B:349:GLU:O	1:B:412:VAL:HG22	2.14	0.47
1:B:424:PRO:HD3	1:B:509:ALA:O	2.14	0.47
1:B:481:ILE:HG12	1:B:530:ARG:CZ	2.45	0.47
1:B:336:GLN:HG3	1:B:341:ARG:O	2.15	0.47
1:B:383:ILE:HG12	1:B:410:ARG:CZ	2.45	0.47
1:A:238:ILE:HG22	1:A:239:ARG:N	2.28	0.47
1:B:349:GLU:HB3	1:B:411:ARG:CG	2.45	0.47
1:A:211:GLY:HA2	1:A:229:THR:O	2.15	0.46
1:B:335:ILE:CA	1:B:340:SER:HA	2.45	0.46
1:A:70:ALA:HA	1:A:77:GLU:OE1	2.16	0.46
1:A:191:PHE:CG	1:A:192:LYS:N	2.83	0.46
1:B:511:GLY:HA2	1:B:529:THR:O	2.15	0.46
1:B:538:ILE:HG22	1:B:539:ARG:N	2.29	0.46
1:A:36(B):PRO:HB2	1:A:61:SER:CA	2.45	0.46
1:A:45:PHE:CD1	1:A:45:PHE:N	2.83	0.46
1:A:70:ALA:HB2	1:A:80:GLN:HG2	1.97	0.46
1:B:345:PHE:CZ	1:B:353:LEU:HD23	2.51	0.46
1:B:383:ILE:HG12	1:B:410:ARG:NE	2.31	0.46
1:A:63:ASN:C	1:A:63:ASN:ND2	2.68	0.46
1:A:36:GLN:CA	1:A:39:GLN:HA	2.41	0.46
1:A:17:ILE:HD11	1:A:191:PHE:CG	2.51	0.46
1:A:51:PHE:CD1	1:A:105:LEU:HD22	2.51	0.46
1:A:217:LYS:C	1:A:219:SER:N	2.74	0.46
1:B:386:ARG:HB2	1:B:409:SER:HA	1.97	0.46
1:B:517:LYS:C	1:B:519:SER:N	2.74	0.46
1:B:383:ILE:CD1	1:B:412:VAL:HG12	2.46	0.45
1:B:479:ARG:HD2	1:B:534:PHE:CZ	2.52	0.45
1:B:491:PHE:CG	1:B:492:LYS:N	2.84	0.45
1:A:49:GLU:OE1	1:A:120:PRO:HG3	2.16	0.45
1:B:340:SER:O	1:B:341:ARG:HB2	2.16	0.45
1:B:391:HIS:ND1	1:B:392:PRO:HD2	2.31	0.45
1:B:498:PRO:HA	1:B:511:GLY:O	2.17	0.45
1:A:217:LYS:O	2:A:601:KTP:HC9	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:ASN:HD22	1:A:74:GLN:H	1.65	0.44
1:A:77:GLU:O	1:A:80:GLN:HB2	2.17	0.44
1:A:188(A):ARG:C	1:A:188:LYS:HG2	2.42	0.44
1:A:72:ASN:C	1:A:72:ASN:ND2	2.76	0.44
1:B:336:GLN:NE2	1:B:341:ARG:HB3	2.32	0.44
1:B:463:GLN:HG3	1:B:484:GLY:O	2.18	0.44
1:A:198:PRO:HA	1:A:211:GLY:O	2.18	0.44
1:A:100:GLN:HG2	1:A:179:ARG:NH2	2.33	0.44
1:B:371:HIS:O	1:B:454:THR:HA	2.18	0.44
1:A:179:ARG:HB3	1:A:234:PHE:CZ	2.52	0.44
1:B:510:HIS:O	1:B:531:VAL:HG23	2.18	0.44
1:B:538:ILE:HG23	1:B:542:MET:HE2	1.99	0.43
1:A:70:ALA:HB2	1:A:80:GLN:CG	2.48	0.43
1:A:71:HIS:O	1:A:154:THR:HA	2.18	0.43
1:B:335:ILE:O	1:B:335:ILE:CG2	2.66	0.43
1:A:30:MET:HE3	1:A:141:TRP:CZ3	2.53	0.43
1:A:72:ASN:ND2	1:A:74:GLN:H	2.16	0.43
1:B:481:ILE:HG23	1:B:530:ARG:NH2	2.33	0.43
1:A:132:PRO:HG3	1:A:164:ARG:HA	2.00	0.43
1:A:213:VAL:HG22	1:A:228:PHE:CE2	2.54	0.43
1:A:224:PRO:HA	1:A:225:PRO:C	2.44	0.43
1:A:33:LEU:HD11	1:A:54:THR:HG21	2.01	0.43
1:A:35:ILE:HD13	1:A:40:SER:O	2.19	0.43
1:A:100:GLN:O	1:A:101:ASN:HB2	2.19	0.43
1:B:335:ILE:HA	1:B:339:GLN:O	2.19	0.42
1:B:524:PRO:HA	1:B:525:PRO:C	2.43	0.42
1:A:46:LEU:HG	1:A:48:ARG:O	2.19	0.42
1:A:167:GLN:O	1:A:171:ILE:HG13	2.19	0.42
1:A:232:SER:HA	1:A:235:LEU:HD22	1.99	0.42
1:B:458:VAL:HG22	1:B:459:GLN:N	2.33	0.42
1:B:345:PHE:CZ	1:B:353:LEU:HB3	2.54	0.42
1:B:395:ASN:ND2	1:B:398:THR:HG23	2.34	0.42
1:B:336(A):SER:HB3	1:B:336(B):PRO:CD	2.49	0.42
1:B:345:PHE:CD1	1:B:345:PHE:N	2.87	0.42
1:A:35:ILE:O	1:A:35:ILE:HG22	2.20	0.42
1:A:146:MET:HE2	1:A:146:MET:HB2	1.84	0.42
1:B:432:PRO:HG3	1:B:464:ARG:HA	2.01	0.42
1:A:81:GLN:HB3	1:A:83:ILE:HD11	2.02	0.42
1:A:68:LEU:HD22	1:A:68:LEU:N	2.34	0.42
1:A:72:ASN:HD21	1:A:74:GLN:HB2	1.84	0.42
1:B:358:CYS:C	1:B:404:MET:HE1	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:483:VAL:HG12	1:B:484:GLY:H	1.84	0.42
1:A:33:LEU:HD11	1:A:106:LEU:HD11	2.01	0.41
1:B:443:ARG:HD2	1:B:492:LYS:HB3	2.02	0.41
1:B:471:ILE:HG21	1:B:517:LYS:HE3	2.00	0.41
1:A:83:ILE:HB	1:A:108:LEU:HD13	2.01	0.41
1:B:375:ARG:HG2	1:B:375:ARG:NH1	2.34	0.41
1:A:36(B):PRO:HG2	1:A:60:GLY:HA3	2.02	0.41
1:A:53:LEU:HD21	1:A:103:ILE:HD11	2.02	0.41
1:A:124:PRO:O	1:A:235:LEU:HD21	2.20	0.41
1:B:392:PRO:CB	1:B:393:GLN:HE21	2.22	0.41
1:B:535:LEU:HA	1:B:535:LEU:HD13	1.84	0.41
1:B:351:PHE:CZ	1:B:542:MET:HA	2.55	0.41
1:B:373:ILE:H	1:B:373:ILE:HG13	1.26	0.41
1:A:136:CYS:HB2	1:A:199:LEU:HD11	2.03	0.41
1:A:34:GLN:C	1:A:36:GLN:H	2.27	0.41
2:A:601:KTP:HC13	2:A:601:KTP:O3	2.21	0.41
1:A:23:ARG:O	1:A:24:PRO:C	2.64	0.41
1:B:317:ILE:HG13	1:B:491:PHE:HB2	2.03	0.41
1:A:22:SER:OG	1:A:157:GLU:HG2	2.20	0.40
1:B:383:ILE:HG21	1:B:408:LEU:HB3	2.03	0.40
1:B:448:ARG:HD3	1:B:451:GLY:H	1.85	0.40
1:A:146:MET:SD	1:A:191:PHE:HZ	2.44	0.40
1:A:50:ASP:OD2	1:A:111:ARG:NH1	2.55	0.40
1:A:141:TRP:CH2	1:A:155:LEU:HD13	2.55	0.40
1:B:317:ILE:HD11	1:B:491:PHE:CG	2.57	0.40
1:B:400:GLN:O	1:B:401:ASN:HB2	2.22	0.40
1:B:431:ARG:HA	1:B:432:PRO:HD3	1.95	0.40
1:B:460:LEU:HB3	1:B:483:VAL:HG12	2.03	0.40
1:B:431:ARG:HH21	1:B:431:ARG:CG	2.35	0.40
1:A:22:SER:HB2	1:A:155:LEU:HD23	2.02	0.40
1:A:132:PRO:HG2	1:A:164:ARG:HG2	2.02	0.40
1:B:336:GLN:H	1:B:340:SER:N	2.20	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	221/235 (94%)	187 (85%)	30 (14%)	4 (2%)	6	34
1	B	223/235 (95%)	187 (84%)	32 (14%)	4 (2%)	6	34
All	All	444/470 (94%)	374 (84%)	62 (14%)	8 (2%)	6	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36(A)	SER
1	B	335	ILE
1	B	337	ALA
1	A	209	ALA
1	B	341	ARG
1	B	509	ALA
1	A	36	GLN
1	A	120	PRO

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	189/202 (94%)	140 (74%)	49 (26%)	0	3
1	B	189/202 (94%)	149 (79%)	40 (21%)	1	6
All	All	378/404 (94%)	289 (76%)	89 (24%)	1	4

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	33	LEU
1	A	34	GLN
1	A	39	GLN

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Mol	Chain	Res	Type
1	A	40	SER
1	A	41	ARG
1	A	42	CYS
1	A	47	VAL
1	A	48	ARG
1	A	61	SER
1	A	63	ASN
1	A	66	VAL
1	A	73	ILE
1	A	74	GLN
1	A	76	ARG
1	A	79	THR
1	A	81	GLN
1	A	89	ILE
1	A	96	GLN
1	A	100	GLN
1	A	109	SER
1	A	113	ARG
1	A	116	ARG
1	A	135	LEU
1	A	144	VAL
1	A	146	MET
1	A	155	LEU
1	A	159	GLN
1	A	163	GLN
1	A	165	ASP
1	A	166	ARG
1	A	167	GLN
1	A	169	LEU
1	A	170	ARG
1	A	179	ARG
1	A	180	GLN
1	A	183	VAL
1	A	185	ARG
1	A	192	LYS
1	A	195	SER
1	A	200	LEU
1	A	213	VAL
1	A	217	LYS
1	A	221	VAL
1	A	229	THR
1	A	232	SER

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Mol	Chain	Res	Type
1	A	233	SER
1	A	235	LEU
1	A	238	ILE
1	B	320	ARG
1	B	327	ARG
1	B	330	MET
1	B	340	SER
1	B	341	ARG
1	B	342	CYS
1	B	348	ARG
1	B	361	SER
1	B	366	VAL
1	B	373	ILE
1	B	375	ARG
1	B	376	ARG
1	B	381	GLN
1	B	384	THR
1	B	387	ARG
1	B	396	GLN
1	B	400	GLN
1	B	408	LEU
1	B	411	ARG
1	B	419	ASN
1	B	425	ARG
1	B	437	THR
1	B	443	ARG
1	B	444	VAL
1	B	446	MET
1	B	448	ARG
1	B	453	ASP
1	B	455	LEU
1	B	459	GLN
1	B	469	LEU
1	B	478	ARG
1	B	486	ARG
1	B	487	GLU
1	B	495	SER
1	B	500	LEU
1	B	517	LYS
1	B	518	SER
1	B	526	GLU
1	B	535	LEU

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Mol	Chain	Res	Type
1	B	538	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	63	ASN
1	A	72	ASN
1	A	82	HIS
1	A	93	GLN
1	A	95	ASN
1	A	96	GLN
1	A	101	ASN
1	A	159	GLN
1	A	163	GLN
1	A	167	GLN
1	A	210	HIS
1	B	371	HIS
1	B	393	GLN
1	B	400	GLN
1	B	419	ASN
1	B	459	GLN
1	B	463	GLN
1	B	467	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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
2	KTP	B	701	-	28,30,30	2.87	19 (67%)	36,44,44	3.76	5 (13%)
2	KTP	A	601	-	28,30,30	2.67	20 (71%)	36,44,44	2.34	3 (8%)

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	KTP	B	701	-	-	6/18/18/18	0/4/4/4
2	KTP	A	601	-	-	1/18/18/18	0/4/4/4

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	KTP	P1-C1	5.32	1.91	1.82
2	B	701	KTP	P1-O3	4.75	1.62	1.54
2	B	701	KTP	C3-C2	4.71	1.56	1.49
2	B	701	KTP	C14-C15	4.68	1.51	1.43
2	A	601	KTP	P1-C1	4.59	1.90	1.82
2	A	601	KTP	P1-O3	4.30	1.61	1.54
2	A	601	KTP	C3-C2	4.11	1.55	1.49
2	B	701	KTP	C12-C3	3.99	1.45	1.39
2	B	701	KTP	P1-O4	3.97	1.61	1.54
2	A	601	KTP	P1-O4	3.88	1.61	1.54
2	A	601	KTP	C12-C3	3.69	1.45	1.39
2	A	601	KTP	C18-C19	3.57	1.44	1.36
2	B	701	KTP	C15-C20	3.40	1.49	1.43
2	B	701	KTP	C17-C16	3.35	1.43	1.36
2	B	701	KTP	O2-C2	-3.33	1.17	1.22
2	A	601	KTP	C17-C16	3.29	1.43	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	KTP	O2-C2	-3.24	1.18	1.22
2	B	701	KTP	C18-C19	3.03	1.43	1.36
2	A	601	KTP	C14-C15	3.00	1.48	1.43
2	A	601	KTP	C22-C21	2.98	1.43	1.36
2	A	601	KTP	C8-C9	2.96	1.43	1.36
2	B	701	KTP	C8-C9	2.72	1.42	1.36
2	B	701	KTP	C8-C7	2.67	1.44	1.38
2	A	601	KTP	C15-C20	2.66	1.47	1.43
2	A	601	KTP	C13-C14	2.63	1.42	1.37
2	A	601	KTP	C8-C7	2.62	1.44	1.38
2	B	701	KTP	C22-C21	2.55	1.42	1.36
2	A	601	KTP	C11-C12	2.54	1.42	1.36
2	A	601	KTP	C18-C17	2.43	1.43	1.38
2	B	701	KTP	C10-C5	2.38	1.47	1.42
2	B	701	KTP	C18-C17	2.31	1.43	1.38
2	A	601	KTP	C7-C6	2.29	1.41	1.36
2	B	701	KTP	C13-C14	2.28	1.41	1.37
2	B	701	KTP	C7-C6	2.26	1.41	1.36
2	A	601	KTP	C10-C5	2.18	1.47	1.42
2	B	701	KTP	C11-C12	2.14	1.41	1.36
2	A	601	KTP	C22-C13	2.13	1.42	1.38
2	A	601	KTP	C4-C3	2.13	1.41	1.37
2	B	701	KTP	C4-C3	2.04	1.41	1.37

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	KTP	O2-C2-C3	-14.42	102.78	120.70
2	B	701	KTP	O4-P1-O1	-13.67	79.19	113.45
2	A	601	KTP	O2-C2-C3	-12.44	105.24	120.70
2	B	701	KTP	O4-P1-O3	-7.52	87.18	107.58
2	B	701	KTP	O1-P1-C1	4.43	128.80	114.03
2	A	601	KTP	O3-P1-O1	-3.71	104.15	113.45
2	B	701	KTP	C13-C14-C1	-3.42	115.17	121.68
2	A	601	KTP	O4-P1-O1	-3.06	105.77	113.45

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	701	KTP	C2-C1-P1-O3
2	B	701	KTP	C14-C1-P1-O4

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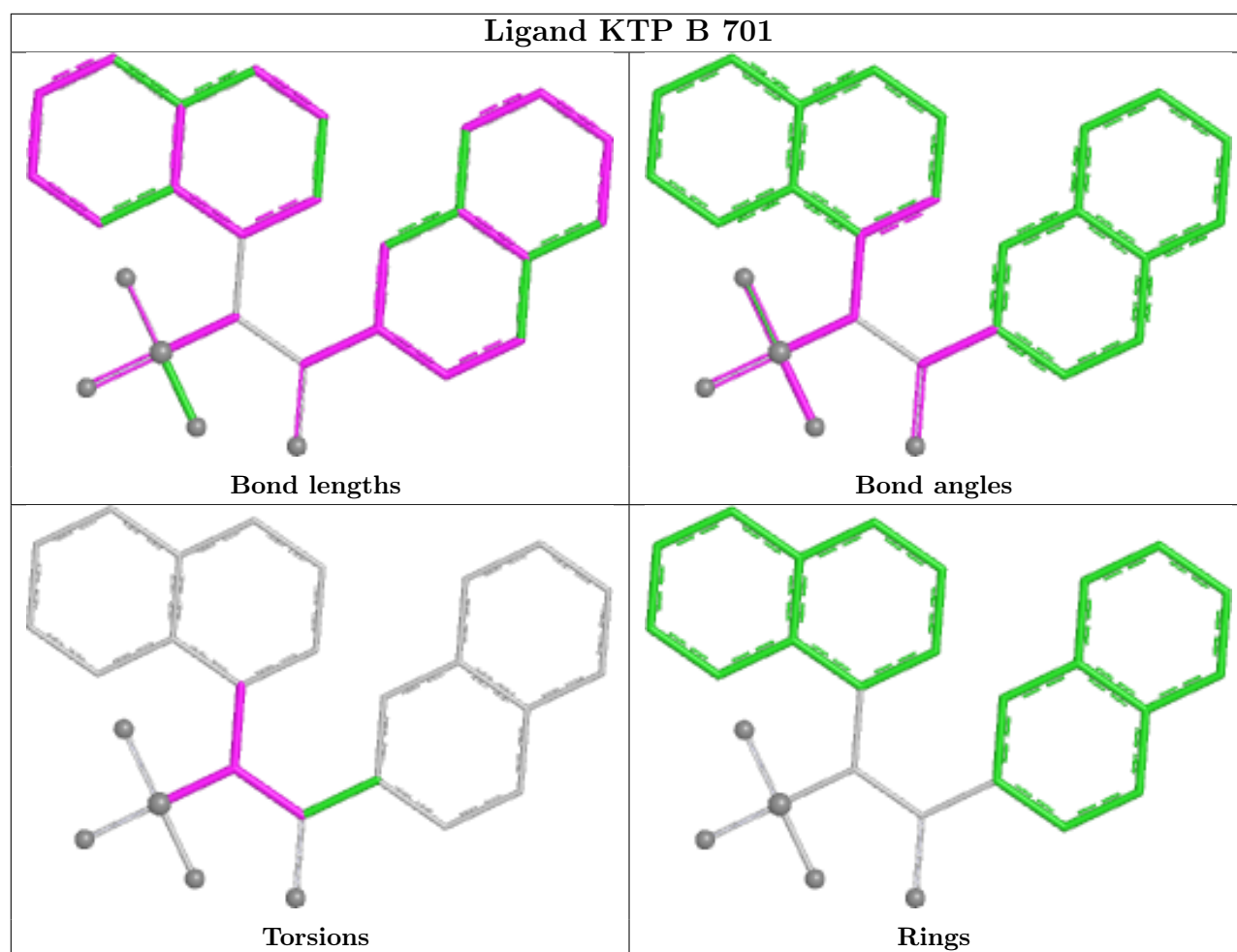
Mol	Chain	Res	Type	Atoms
2	B	701	KTP	C14-C1-P1-O3
2	B	701	KTP	C2-C1-P1-O4
2	B	701	KTP	P1-C1-C14-C15
2	B	701	KTP	C14-C1-C2-C3
2	A	601	KTP	P1-C1-C2-O2

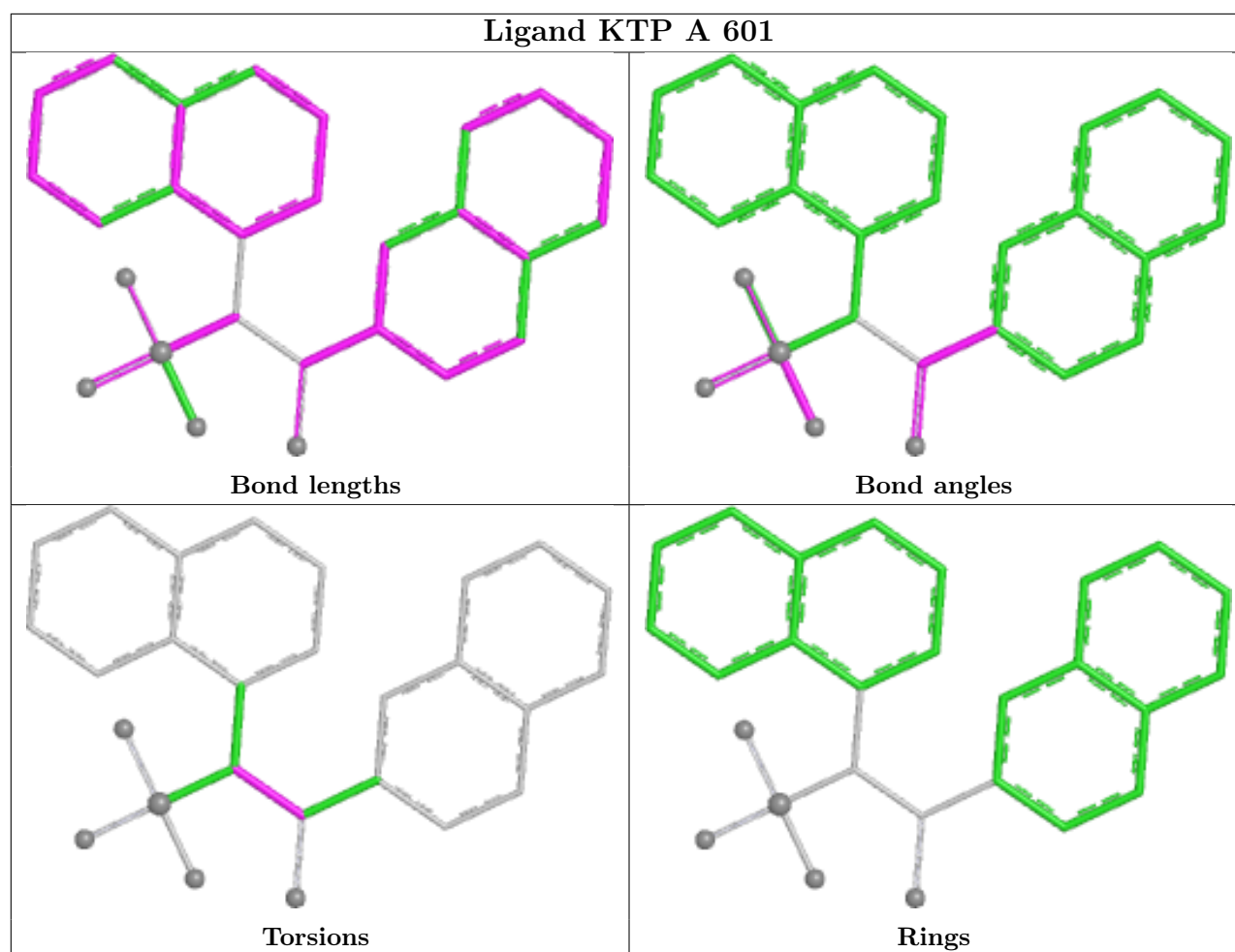
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	KTP	7	0
2	A	601	KTP	6	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	223/235 (94%)	-1.39	0 100 100	26, 26, 26, 26	0
1	B	225/235 (95%)	-1.37	0 100 100	26, 26, 26, 26	0
All	All	448/470 (95%)	-1.38	0 100 100	26, 26, 26, 26	0

There are no RSRZ outliers to report.

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](#)

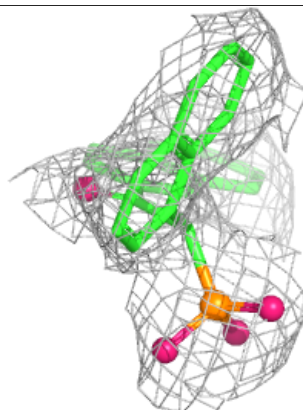
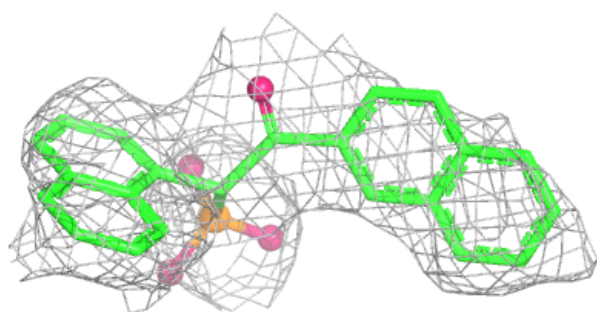
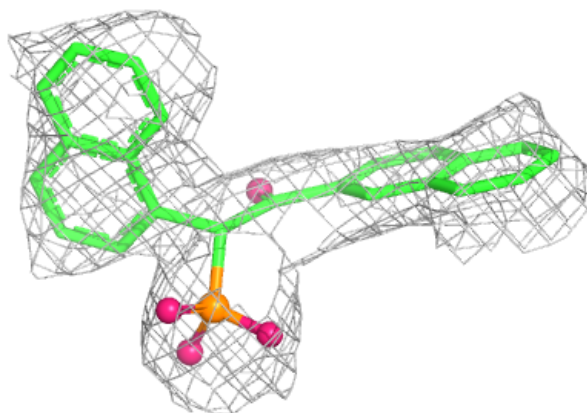
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	KTP	A	601	27/27	0.99	0.03	26,26,26,26	0
2	KTP	B	701	27/27	0.99	0.04	26,26,26,26	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.

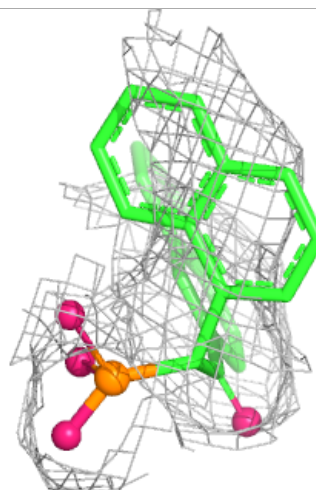
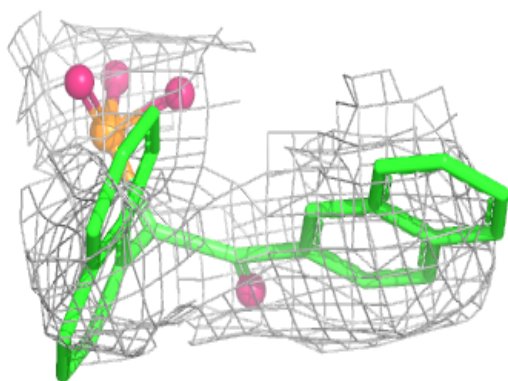
Electron density around KTP A 601:

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



Electron density around KTP B 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.