



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:24 PM UTC

PDB ID : 9MD7 / pdb_00009md7
Title : Hip1 complex with inhibitor #1 (Hip1-1) via Ser228
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Deposited on : 2024-12-05
Resolution : 2.72 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

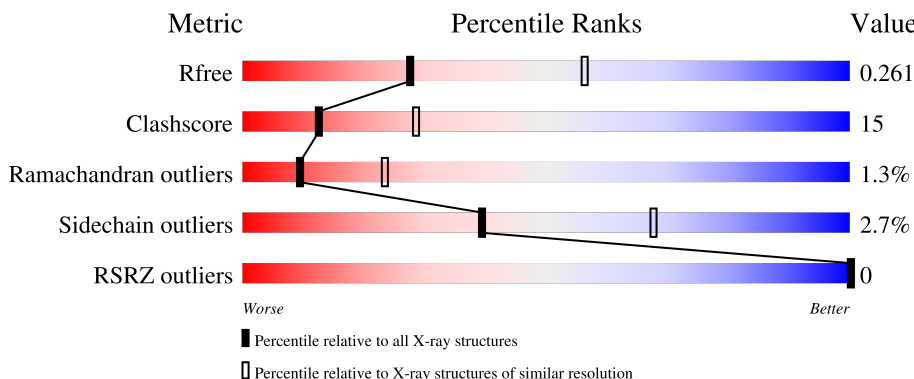
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	486	 62% 32% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3545 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.

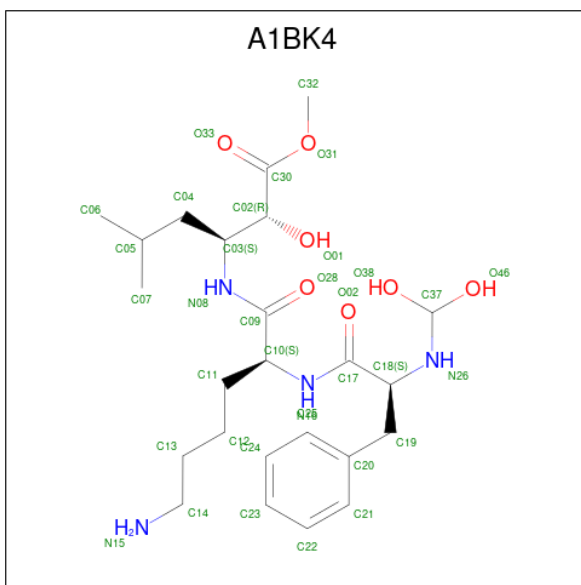
- Molecule 1 is a protein called Protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	464	3508	2192	621	679	16	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	GLY	-	expression tag	UNP A0A654TLU9
A	36	PRO	-	expression tag	UNP A0A654TLU9
A	37	LEU	-	expression tag	UNP A0A654TLU9
A	38	GLY	-	expression tag	UNP A0A654TLU9
A	39	SER	-	expression tag	UNP A0A654TLU9
A	40	PRO	-	expression tag	UNP A0A654TLU9
A	41	GLU	-	expression tag	UNP A0A654TLU9
A	42	PHE	-	expression tag	UNP A0A654TLU9

- Molecule 2 is N-(dihydroxymethyl)-L-phenylalanyl-N-[(2R,3S)-2-hydroxy-1-methoxy-5-methyl-1-oxohexan-3-yl]-L-lysineamide (CCD ID: A1BK4) (formula: C₂₄H₄₀N₄O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	24	4	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		

- Molecule 1: Protease

H445	S843	S235	E113	GLY
A446	P344	A236	S114	PR0
P450	N345	L237	GL15	GLY
	L346	E240	I116	SER
V453	H349	F241	E117	SER
F454	L351			GLU
F455	D352	R244	F123	PHE
V456	G353	V245	Q124	GLU
V457	G354	R246	T125	PR0
L354	L354	A247	L126	PR0
S458	S355	M248	P127	LVS
V459	E356	L249	K128	LEV
T460	L357	L250	E132	GLY
	V357		R133	GLN
Y468	L358	N257	R133	P49
Q477	N360		V137	V50
	R361	P260	F138	E51
L483	T364	E261	F139	C55
T484	L365	E262	D140	R56
F485	L365	A263	G143	SER
D486	A369	E264		SER
G487	D370	L265	S146	ASN
T488		R266		PR0
Q489	M373	C282	P149	VAL
V492	R374	A283	W152	LVS
	R375	K284	P166	LVS
S498	G379	C288	P166	P65
		R289	D169	L69
E502	N382	L290		
T505	N383		E179	K72
Y507	A390	V298	N180	D78
L508	I391	E299	E181	Y79
L509		V300	T182	D80
G510	V394	Y301	K183	R81
G511	D395		C189	P82
T512	Q396	V305		
		D306		
P515	I406	P307	L198	L89
S516	D407	L308		A90
G517		V309	V201	L91
A518	R410	P314	G202	R93
L519	R411		T203	
	K423	S317	L210	A96
G520				
	D427	R321	I213	D99
		S331	A216	K100
F435				I101
W436		V335	K221	G102
P437	P437	G336		T106
V438	V438	T337	L225	N107
P439	P439	I338		P108
P440	P440	M339	L225	G109
T441	T441	A340	S228	G110
S442	S442	L341	Y229	P111
		Y242		C112

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.33Å 104.33Å 129.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.37 – 2.72 48.37 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.37-2.72) 99.7 (48.37-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.219 , 0.259 0.221 , 0.261	Depositor DCC
R_{free} test set	2011 reflections (9.00%)	wwPDB-VP
Wilson B-factor (Å ²)	57.1	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.166 for -h,-k,l	Xtriage
Reported twinning fraction	0.210 for -h,-k,l	Depositor
Outliers	0 of 22305 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3545	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1BK4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	1/3590 (0.0%)	0.53	1/4894 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	SER	CB-OG	-11.01	1.20	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	SER	CA-CB-OG	9.21	129.51	111.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3508	0	3395	106	0
2	A	35	0	0	0	0
3	A	2	0	0	0	0
All	All	3545	0	3395	106	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 15.

All (106) 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:101:ILE:HD12	1:A:133:ARG:HB3	1.71	0.72
1:A:249:ILE:HG23	1:A:456:VAL:HB	1.71	0.71
1:A:169:ASP:HB2	1:A:314:PRO:HB2	1.76	0.68
1:A:210:LEU:HA	1:A:213:ILE:HD12	1.78	0.66
1:A:180:ASN:HA	1:A:183:LYS:HE3	1.77	0.65
1:A:260:PRO:HB3	1:A:396:GLN:HE22	1.60	0.65
1:A:406:ILE:HD13	1:A:427:ASP:HA	1.81	0.63
1:A:179:GLU:HB3	1:A:435:PHE:HZ	1.66	0.60
1:A:240:GLU:HB3	1:A:241:PHE:CD1	2.36	0.60
1:A:498:SER:O	1:A:502:GLU:HG3	2.02	0.59
1:A:108:PRO:HG2	1:A:113:GLU:HB3	1.85	0.59
1:A:344:PRO:HD3	1:A:489:GLN:HB3	1.82	0.59
1:A:90:ALA:HB3	1:A:140:ASP:HB2	1.84	0.58
1:A:72:LYS:HA	1:A:89:LEU:O	2.03	0.57
1:A:353:GLY:HA3	1:A:365:LEU:HG	1.86	0.57
1:A:78:ASP:HB3	1:A:81:ARG:HB2	1.87	0.56
1:A:301:TYR:O	1:A:305:VAL:HG22	2.06	0.55
1:A:353:GLY:O	1:A:356:GLU:HB2	2.06	0.55
1:A:262:GLU:HB3	1:A:266:ARG:NH1	2.21	0.55
1:A:369:ALA:O	1:A:373:MET:HG2	2.06	0.55
1:A:410:ARG:HH21	1:A:411:ARG:HG2	1.71	0.55
1:A:260:PRO:HB3	1:A:396:GLN:NE2	2.21	0.55
1:A:460:THR:HG23	1:A:485:PHE:HD2	1.72	0.55
1:A:331:SER:O	1:A:335:VAL:HG23	2.08	0.54
1:A:109:GLY:O	1:A:113:GLU:HB2	2.09	0.52
1:A:340:ALA:HA	1:A:346:LEU:HB2	1.92	0.51
1:A:179:GLU:HB3	1:A:435:PHE:CZ	2.45	0.51
1:A:410:ARG:NH2	1:A:411:ARG:HG2	2.26	0.51
1:A:93:ARG:HG3	1:A:137:VAL:HG22	1.91	0.51
1:A:133:ARG:HG3	1:A:509:ILE:HD13	1.91	0.50
1:A:356:GLU:HB3	1:A:361:ARG:O	2.12	0.50
1:A:241:PHE:HB3	1:A:244:ARG:HB2	1.93	0.49
1:A:260:PRO:O	1:A:264:GLU:HG3	2.11	0.49
1:A:307:PRO:C	1:A:309:VAL:H	2.21	0.49
1:A:350:LEU:O	1:A:354:LEU:HG	2.13	0.49
1:A:257:ASN:HB2	1:A:446:ALA:HA	1.95	0.49
1:A:321:ARG:HH22	1:A:361:ARG:NE	2.11	0.49
1:A:395:ASP:O	1:A:442:SER:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASP:O	1:A:82:PRO:HD3	2.13	0.48
1:A:106:ILE:HA	1:A:225:LEU:O	2.12	0.48
1:A:69:LEU:HB2	1:A:93:ARG:HB3	1.96	0.48
1:A:50:VAL:HG21	1:A:216:ALA:HB1	1.96	0.47
1:A:298:VAL:O	1:A:301:TYR:HB3	2.14	0.47
1:A:360:ASN:O	1:A:361:ARG:HG2	2.14	0.47
1:A:96:ALA:HB1	1:A:132:GLU:O	2.15	0.47
1:A:248:MET:HE3	1:A:250:LEU:HD21	1.96	0.47
1:A:115:GLY:HA3	1:A:139:PHE:O	2.15	0.46
1:A:390:ALA:HA	1:A:436:TRP:CZ2	2.50	0.46
1:A:458:VAL:HG22	1:A:483:LEU:HB3	1.96	0.46
1:A:166:PRO:HD3	1:A:317:SER:HB2	1.97	0.46
1:A:349:HIS:O	1:A:364:THR:HG21	2.15	0.46
1:A:374:ARG:HB3	1:A:382:ASN:HD21	1.80	0.46
1:A:455:THR:HA	1:A:507:TYR:OH	2.16	0.46
1:A:111:PRO:HB3	1:A:229:TYR:CE2	2.51	0.45
1:A:69:LEU:O	1:A:92:ILE:HA	2.16	0.45
1:A:237:TYR:CE1	1:A:241:PHE:HB2	2.51	0.45
1:A:394:VAL:HA	1:A:440:PRO:HA	1.99	0.45
1:A:515:PRO:HG2	1:A:518:ALA:HB2	1.98	0.45
1:A:507:TYR:HA	1:A:512:THR:N	2.32	0.45
1:A:179:GLU:HA	1:A:182:THR:OG1	2.16	0.44
1:A:357:LEU:HD23	1:A:361:ARG:O	2.17	0.44
1:A:241:PHE:O	1:A:245:VAL:HG23	2.18	0.44
1:A:407:ASP:O	1:A:411:ARG:HG3	2.17	0.44
1:A:257:ASN:HB2	1:A:477:GLN:HE22	1.83	0.44
1:A:370:ASP:O	1:A:374:ARG:N	2.50	0.44
1:A:459:SER:HB3	1:A:468:TYR:HD1	1.81	0.44
1:A:460:THR:HG23	1:A:485:PHE:CD2	2.51	0.44
1:A:354:LEU:O	1:A:358:VAL:HG23	2.17	0.44
1:A:357:LEU:HD23	1:A:357:LEU:HA	1.77	0.44
1:A:126:LEU:HD12	1:A:126:LEU:HA	1.80	0.43
1:A:99:ASP:O	1:A:133:ARG:HA	2.18	0.43
1:A:107:ASN:ND2	1:A:108:PRO:HD2	2.33	0.43
1:A:143:GLY:HA2	1:A:149:PRO:O	2.19	0.43
1:A:152:TRP:CH2	1:A:383:ASN:HB3	2.53	0.43
1:A:445:HIS:O	1:A:445:HIS:HD2	2.01	0.43
1:A:128:LYS:O	1:A:132:GLU:HG3	2.18	0.43
1:A:198:LEU:O	1:A:201:VAL:HG22	2.19	0.42
1:A:247:ALA:HB1	1:A:507:TYR:CE2	2.54	0.42
1:A:51:GLU:H	1:A:51:GLU:HG2	1.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:TYR:CE1	1:A:484:THR:HG23	2.55	0.42
1:A:505:THR:HA	1:A:508:LEU:HB2	2.00	0.42
1:A:126:LEU:HD12	1:A:127:PRO:HD2	2.02	0.42
1:A:289:PRO:HG2	1:A:354:LEU:HD12	2.02	0.42
1:A:290:LEU:HA	1:A:300:VAL:HG11	2.02	0.42
1:A:515:PRO:HD2	1:A:518:ALA:HB2	2.01	0.42
1:A:375:ARG:CZ	1:A:379:GLY:HA2	2.49	0.42
1:A:353:GLY:HA2	1:A:356:GLU:OE2	2.20	0.42
1:A:179:GLU:H	1:A:179:GLU:HG3	1.67	0.41
1:A:114:SER:O	1:A:117:GLU:HB2	2.20	0.41
1:A:337:THR:O	1:A:341:LEU:HG	2.20	0.41
1:A:108:PRO:CG	1:A:113:GLU:HB3	2.50	0.41
1:A:460:THR:HG22	1:A:487:GLY:O	2.19	0.41
1:A:117:GLU:CD	1:A:374:ARG:HH22	2.29	0.41
1:A:123:PHE:HD2	1:A:124:GLN:OE1	2.04	0.41
1:A:221:LYS:HB3	1:A:246:ARG:N	2.35	0.41
1:A:246:ARG:O	1:A:453:VAL:HG21	2.21	0.41
1:A:282:CYS:O	1:A:288:CYS:HB2	2.21	0.41
1:A:423:LYS:HE3	1:A:423:LYS:HB3	1.86	0.41
1:A:507:TYR:O	1:A:511:GLY:HA2	2.21	0.41
1:A:436:TRP:HD1	1:A:438:VAL:O	2.03	0.41
1:A:445:HIS:CD2	1:A:445:HIS:C	2.99	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.76	0.41
1:A:100:LYS:HE3	1:A:102:GLY:HA2	2.04	0.40
1:A:340:ALA:HB3	1:A:350:LEU:HD22	2.02	0.40
1:A:284:LYS:HB2	1:A:284:LYS:HE2	1.90	0.40
1:A:338:ILE:HG22	1:A:342:TYR:HE2	1.86	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	460/486 (95%)	419 (91%)	35 (8%)	6 (1%)	9 23

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	492	VAL
1	A	117	GLU
1	A	189	CYS
1	A	352	ASP
1	A	450	PRO
1	A	437	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	371/390 (95%)	361 (97%)	10 (3%)	39 68

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	CYS
1	A	146	SER
1	A	203	THR
1	A	235	SER
1	A	240	GLU
1	A	350	LEU
1	A	391	ILE
1	A	442	SER
1	A	459	SER
1	A	516	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	180	ASN
1	A	184	GLN
1	A	205	ASN
1	A	445	HIS

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	A1BK4	A	601	1	35,35,35	1.16	4 (11%)	40,45,45	1.22	6 (15%)

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	A1BK4	A	601	1	-	11/41/43/43	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	A1BK4	O01-C02	-2.80	1.36	1.42
2	A	601	A1BK4	C19-C20	-2.62	1.45	1.51
2	A	601	A1BK4	C17-N16	2.59	1.39	1.34
2	A	601	A1BK4	C37-N26	2.43	1.48	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	A1BK4	O31-C30-O33	-2.83	118.34	123.85
2	A	601	A1BK4	C04-C03-N08	2.79	113.78	110.20
2	A	601	A1BK4	C10-N16-C17	2.25	126.48	121.65
2	A	601	A1BK4	O01-C02-C30	2.13	116.31	110.33
2	A	601	A1BK4	C11-C10-N16	-2.09	106.77	110.91
2	A	601	A1BK4	O28-C09-N08	-2.01	119.35	122.96

There are no chirality outliers.

All (11) torsion outliers are listed below:

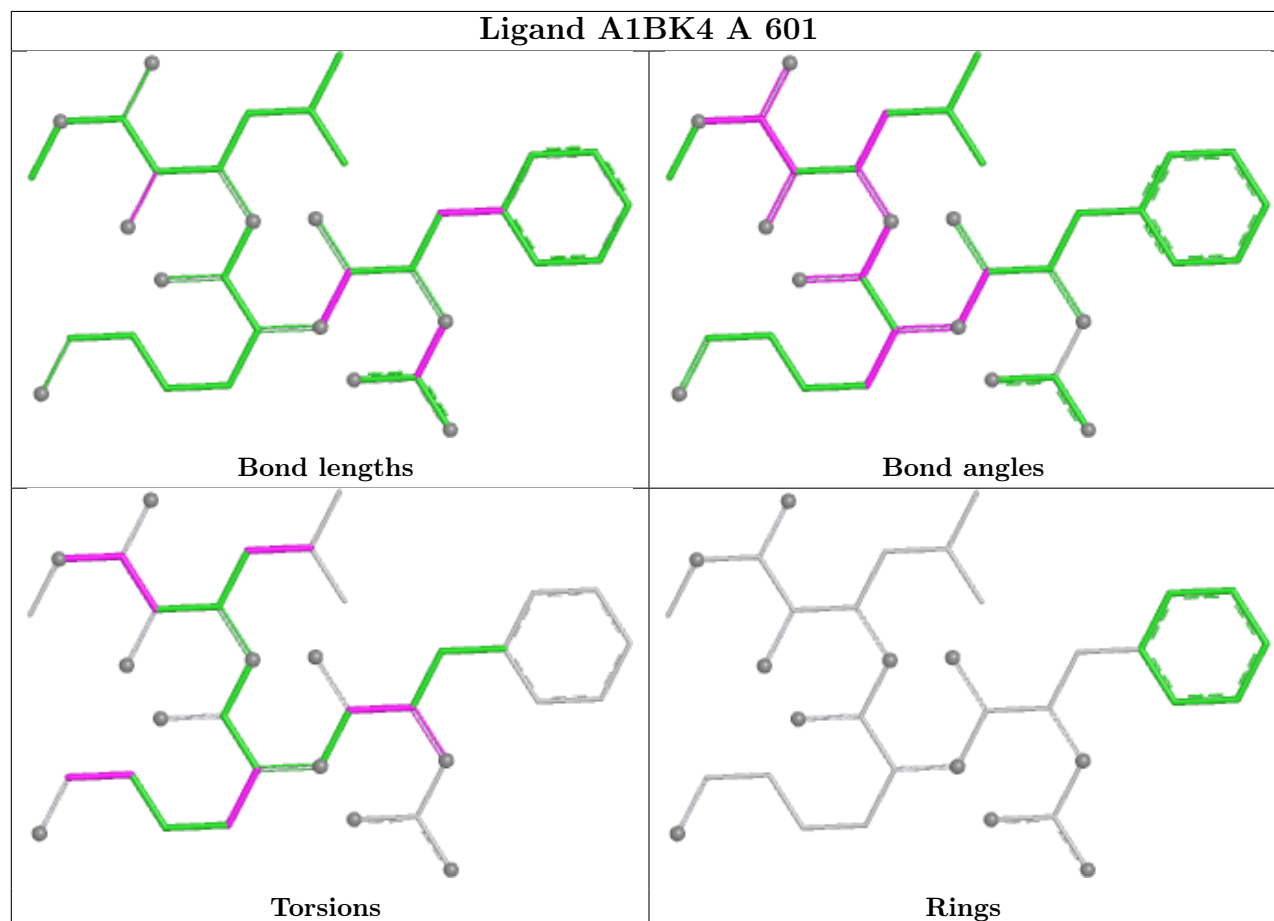
Mol	Chain	Res	Type	Atoms
2	A	601	A1BK4	C09-C10-C11-C12
2	A	601	A1BK4	N16-C10-C11-C12
2	A	601	A1BK4	C02-C30-O31-C32
2	A	601	A1BK4	C19-C18-N26-C37
2	A	601	A1BK4	C03-C04-C05-C07
2	A	601	A1BK4	O33-C30-O31-C32
2	A	601	A1BK4	O02-C17-C18-N26
2	A	601	A1BK4	N16-C17-C18-N26
2	A	601	A1BK4	C17-C18-N26-C37
2	A	601	A1BK4	C12-C13-C14-N15
2	A	601	A1BK4	C03-C02-C30-O31

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 [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	464/486 (95%)	-1.28	0 100 100	45, 59, 83, 125	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](#)

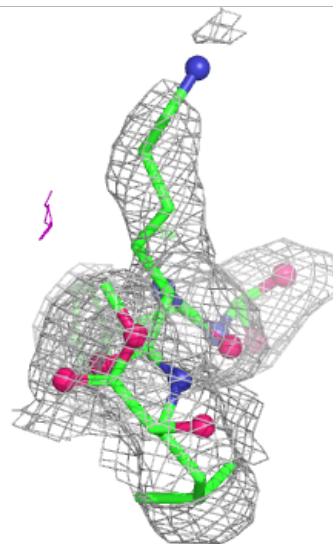
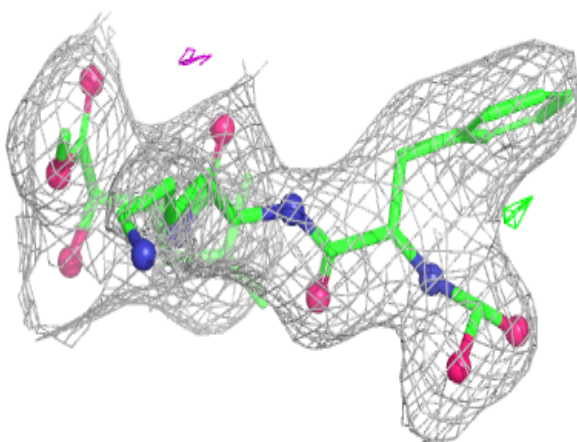
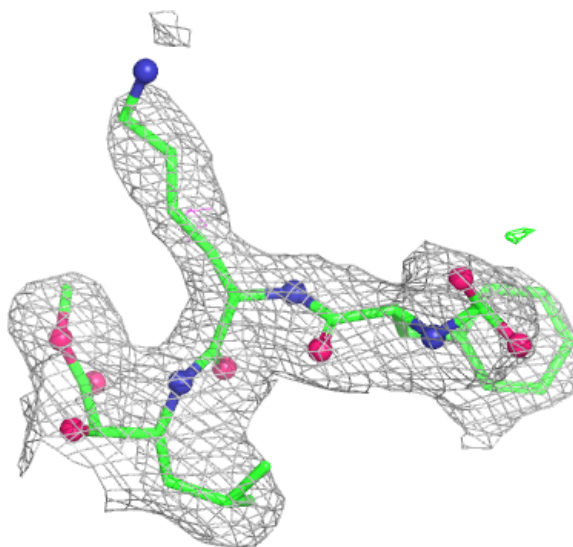
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	A1BK4	A	601	35/35	0.99	0.04	50,52,55,57	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 A1BK4 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.