



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2022 – 02:36 PM EDT

PDB ID : 7REN
Title : Room temperature serial crystal structure of Glutaminase C in complex with inhibitor UPGL-00004
Authors : Milano, S.K.; Finke, A.; Cerione, R.A.
Deposited on : 2021-07-13
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

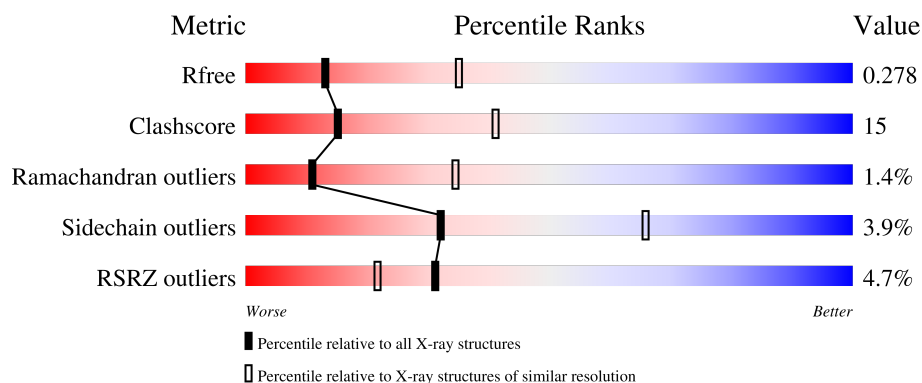
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	539	<div> <div>4%</div> <div> <div></div> <div>51%</div> <div>23%</div> <div>•</div> <div>25%</div> </div> </div>
1	B	539	<div> <div>3%</div> <div> <div></div> <div>49%</div> <div>24%</div> <div>•</div> <div>25%</div> </div> </div>
1	C	539	<div> <div>3%</div> <div> <div></div> <div>54%</div> <div>19%</div> <div>•</div> <div>25%</div> </div> </div>
1	D	539	<div> <div>4%</div> <div> <div></div> <div>47%</div> <div>26%</div> <div>•</div> <div>25%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12675 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 Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	1	0	0
			3148	2003	533	584	28			
1	B	404	Total	C	N	O	S	1	0	0
			3148	2003	533	584	28			
1	C	404	Total	C	N	O	S	1	0	0
			3148	2003	533	584	28			
1	D	404	Total	C	N	O	S	1	0	0
			3148	2003	533	584	28			

There are 48 discrepancies between the modelled and reference sequences:

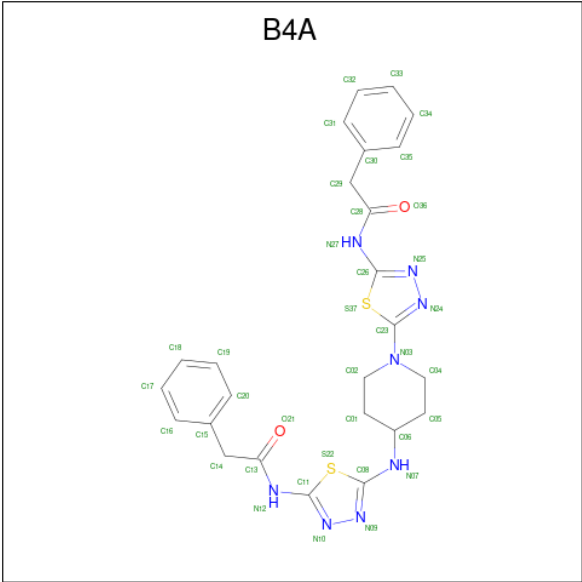
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP O94925
A	61	ARG	-	expression tag	UNP O94925
A	62	GLY	-	expression tag	UNP O94925
A	63	SER	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	UNP O94925
A	66	HIS	-	expression tag	UNP O94925
A	67	HIS	-	expression tag	UNP O94925
A	68	HIS	-	expression tag	UNP O94925
A	69	HIS	-	expression tag	UNP O94925
A	70	GLY	-	expression tag	UNP O94925
A	71	SER	-	expression tag	UNP O94925
B	60	MET	-	initiating methionine	UNP O94925
B	61	ARG	-	expression tag	UNP O94925
B	62	GLY	-	expression tag	UNP O94925
B	63	SER	-	expression tag	UNP O94925
B	64	HIS	-	expression tag	UNP O94925
B	65	HIS	-	expression tag	UNP O94925
B	66	HIS	-	expression tag	UNP O94925
B	67	HIS	-	expression tag	UNP O94925
B	68	HIS	-	expression tag	UNP O94925

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	HIS	-	expression tag	UNP O94925
B	70	GLY	-	expression tag	UNP O94925
B	71	SER	-	expression tag	UNP O94925
C	60	MET	-	initiating methionine	UNP O94925
C	61	ARG	-	expression tag	UNP O94925
C	62	GLY	-	expression tag	UNP O94925
C	63	SER	-	expression tag	UNP O94925
C	64	HIS	-	expression tag	UNP O94925
C	65	HIS	-	expression tag	UNP O94925
C	66	HIS	-	expression tag	UNP O94925
C	67	HIS	-	expression tag	UNP O94925
C	68	HIS	-	expression tag	UNP O94925
C	69	HIS	-	expression tag	UNP O94925
C	70	GLY	-	expression tag	UNP O94925
C	71	SER	-	expression tag	UNP O94925
D	60	MET	-	initiating methionine	UNP O94925
D	61	ARG	-	expression tag	UNP O94925
D	62	GLY	-	expression tag	UNP O94925
D	63	SER	-	expression tag	UNP O94925
D	64	HIS	-	expression tag	UNP O94925
D	65	HIS	-	expression tag	UNP O94925
D	66	HIS	-	expression tag	UNP O94925
D	67	HIS	-	expression tag	UNP O94925
D	68	HIS	-	expression tag	UNP O94925
D	69	HIS	-	expression tag	UNP O94925
D	70	GLY	-	expression tag	UNP O94925
D	71	SER	-	expression tag	UNP O94925

- Molecule 2 is 2-phenyl-N-{5-[4-({5-[(phenylacetyl)amino]-1,3,4-thiadiazol-2-yl}amino)piperidin-1-yl]-1,3,4-thiadiazol-2-yl}acetamide (three-letter code: B4A) (formula: C₂₅H₂₆N₈O₂S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			37	25	8	2	2		
2	C	1	Total	C	N	O	S	0	0
			37	25	8	2	2		

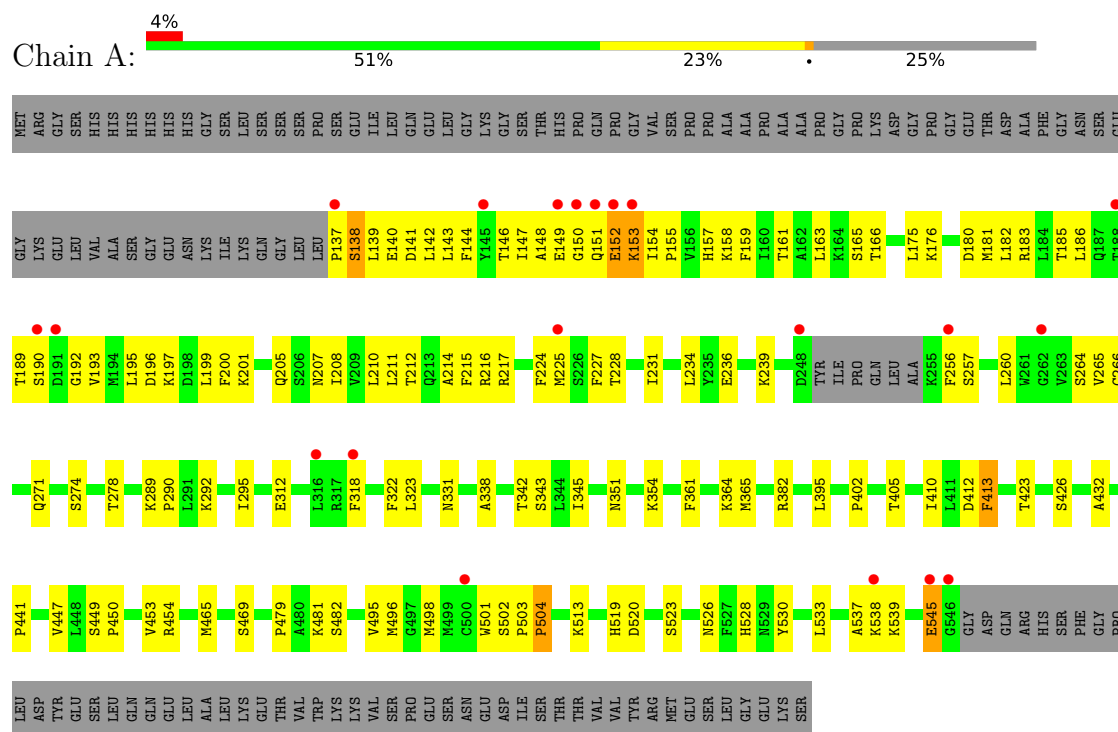
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total	O	0
			3	3	
3	C	3	Total	O	0
			3	3	
3	D	3	Total	O	0
			3	3	

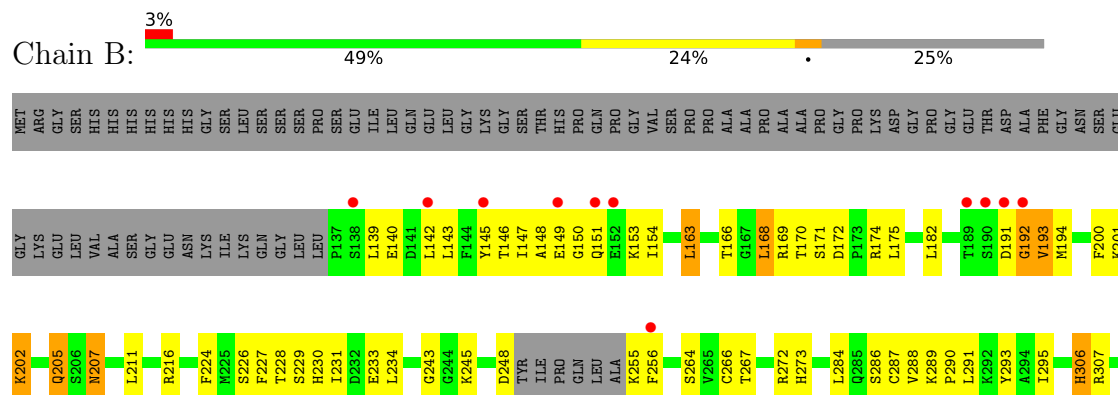
3 Residue-property plots

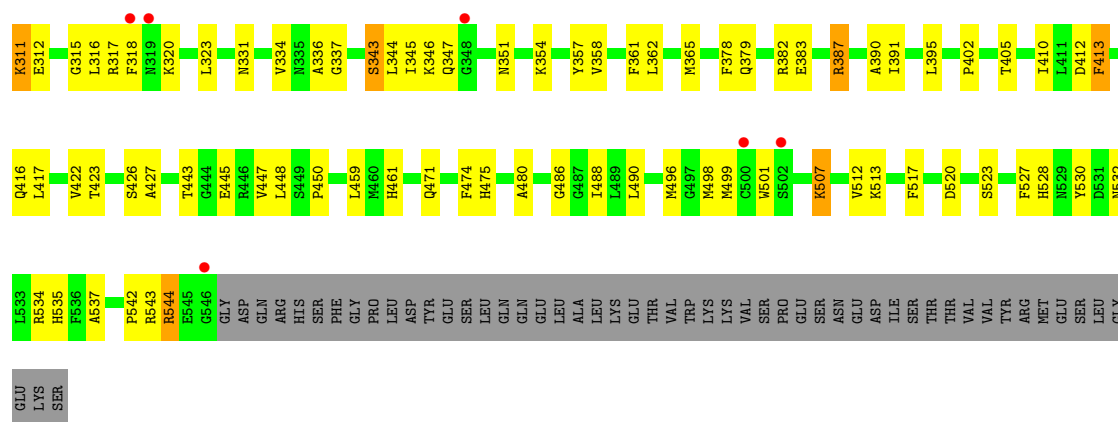
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

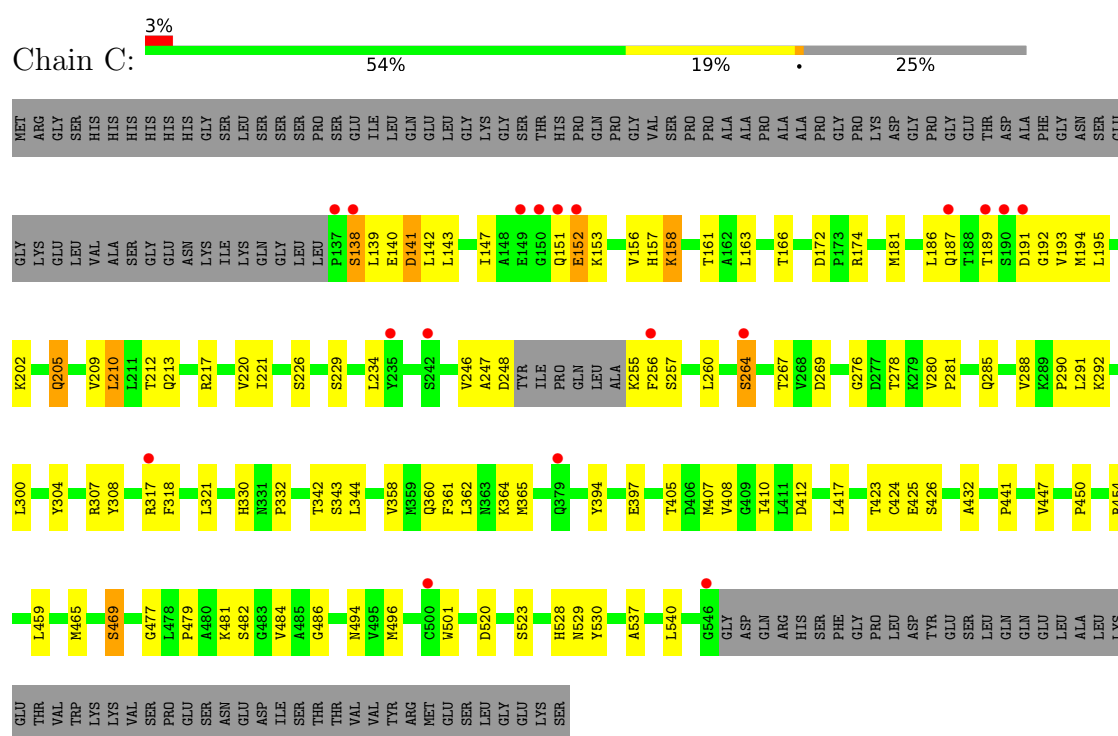


- Molecule 1: Glutaminase kidney isoform, mitochondrial

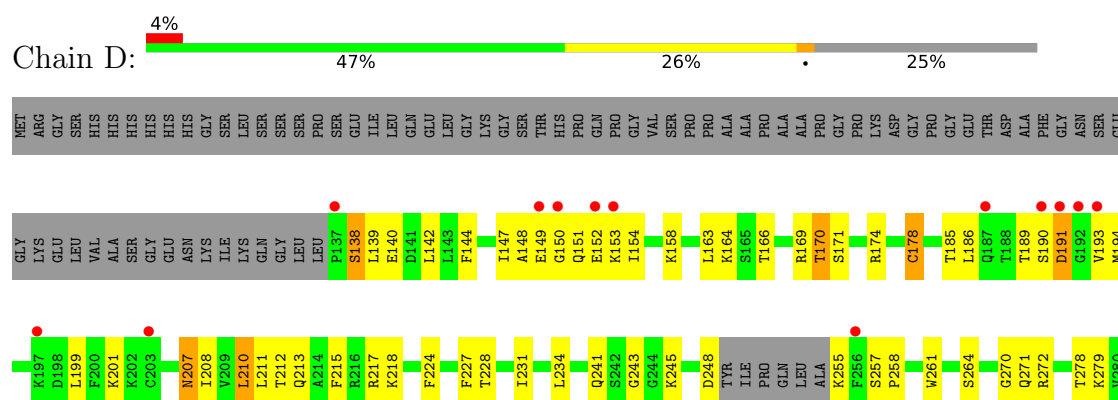




• Molecule 1: Glutaminase kidney isoform, mitochondrial



• Molecule 1: Glutaminase kidney isoform, mitochondrial



LYS	P281	
LYS	Q285	
VAL	T302	
SER	G310	
PRO	K311	
GLU	E312	
SER	P313	
ASN	S314	
GLU	G315	
ASP	L316	
ILE	R317	
SER	F318	
THR	N319	
THR	K320	
THR	L321	
VAL	F322	
VAL	L323	
VAL		
VAL	P329	
VAL	H330	
VAL	N331	
VAL	A336	
VAL	G337	
VAL	A338	
VAL	I339	
VAL	V340	
VAL	V341	
VAL	G348	
VAL	Q360	
VAL	F361	
VAL	K364	
VAL	N365	
VAL	Y370	
VAL	A376	
VAL	R382	
VAL	E383	
VAL	S384	
VAL	R387	
VAL	A390	
VAL	I391	
VAL	C400	
VAL	F401	
VAL	P402	
VAL	E403	
VAL	G404	
VAL	T405	
VAL	D406	
VAL		
VAL	H407	
VAL	L411	
VAL	D412	
VAL		
VAL	C418	
VAL	V422	
VAL	T423	
VAL	C424	
VAL	E425	
VAL	S426	
VAL	L434	
VAL	F439	
VAL		
VAL	R446	
VAL	V447	
VAL	L448	
VAL	S449	
VAL	P450	
VAL	V453	
VAL	R454	
VAL	M455	
VAL	T456	
VAL	L457	
VAL		
VAL	S462	
VAL		
VAL	M465	
VAL	S469	
VAL	G470	
VAL	Q471	
VAL	F472	
VAL	M473	
VAL	F474	
VAL	H475	
VAL	V476	
VAL	G477	
VAL	L478	
VAL	P479	
VAL	A480	
VAL	K481	
VAL	S482	
VAL		
VAL	G487	
VAL	L490	
VAL		
VAL	V495	
VAL	M496	
VAL	G497	
VAL	M498	
VAL	M499	
VAL	C500	
VAL	W501	
VAL	S502	
VAL		
LYS	P503	
LYS	P504	
VAL		
SER	V512	
PRO	K513	
GLU	G514	
SER	I515	
ASN		
GLU	C518	
GLU	H519	
ASP	D520	
ILE	E425	
SER	L521	
SER	V522	
THR	S523	
THR	L524	
VAL	C525	
VAL		
TYR	H528	
ARG	N529	
MET		
GLU	T530	
SER	D531	
LEU	N532	
GLY	L533	
GLY		
LYS	A537	
SER	R538	
	K539	
	L540	
	D541	
	P542	
	R543	
	R544	
	E545	
	G546	
	GLY	
	ASP	
	GLN	
	GLN	
	ARG	
	HIS	
	SER	
	PHE	
	GLY	
	PRO	
	LEU	
	ASP	
	TYR	
	GLU	
	SER	
	LEU	
	GLN	
	GLN	
	LYS	
	GLU	
	LEU	
	ALA	
	LEU	
	LYS	
	GLU	
	THR	
	VAL	
	TRP	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.20Å 138.44Å 177.49Å 90.00° 93.44° 90.00°	Depositor
Resolution (Å)	20.44 – 2.80 20.44 – 2.80	Depositor EDS
% Data completeness (in resolution range)	89.1 (20.44-2.80) 78.6 (20.44-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.37 (at 2.79Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.210 , 0.278 0.210 , 0.278	Depositor DCC
R_{free} test set	2013 reflections (3.26%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12675	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.38% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B4A

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	0.59	1/3217 (0.0%)	0.66	0/4338
1	B	0.49	1/3217 (0.0%)	0.66	1/4338 (0.0%)
1	C	0.48	0/3217	0.65	1/4338 (0.0%)
1	D	0.46	0/3217	0.67	2/4338 (0.0%)
All	All	0.51	2/12868 (0.0%)	0.66	4/17352 (0.0%)

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	1
1	B	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	504	PRO	N-CD	-20.09	1.19	1.47
1	B	266	CYS	CB-SG	5.05	1.90	1.82

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	502	SER	N-CA-C	-6.16	94.36	111.00
1	C	210	LEU	CA-CB-CG	5.69	128.38	115.30
1	D	210	LEU	CA-CB-CG	5.56	128.08	115.30
1	B	168	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	GLN	Peptide
1	B	306	HIS	Peptide
1	B	320	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	3148	0	3117	97	0
1	B	3148	0	3117	104	0
1	C	3148	0	3116	86	0
1	D	3148	0	3117	111	0
2	B	37	0	0	2	0
2	C	37	0	0	2	0
3	A	3	0	0	2	0
3	C	3	0	0	2	0
3	D	3	0	0	7	0
All	All	12675	0	12467	376	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 (376) 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:C:255:LYS:HA	3:C:703:HOH:O	1.26	1.32
2:C:601:B4A:N09	2:C:601:B4A:N10	1.60	1.19
2:B:601:B4A:N24	2:B:601:B4A:N25	1.60	1.16
1:D:255:LYS:HA	3:D:601:HOH:O	1.47	1.11
1:A:195:LEU:HD23	1:A:199:LEU:HG	1.08	1.08
1:A:195:LEU:CD2	1:A:199:LEU:HG	1.96	0.93
1:A:195:LEU:HD23	1:A:199:LEU:CG	1.98	0.92
1:D:255:LYS:CA	3:D:601:HOH:O	2.08	0.88
1:D:525:CYS:HB2	3:D:602:HOH:O	1.72	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:525:CYS:SG	3:D:602:HOH:O	2.32	0.85
1:D:525:CYS:CB	3:D:602:HOH:O	2.25	0.84
1:D:481:LYS:NZ	1:D:482:SER:O	2.11	0.83
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.61	0.82
1:B:532:ASN:HD22	1:B:535:HIS:H	1.23	0.82
1:B:174:ARG:O	1:B:207:ASN:ND2	2.12	0.82
1:B:163:LEU:O	1:B:166:THR:HG22	1.80	0.81
1:D:189:THR:HG22	1:D:190:SER:H	1.46	0.81
1:A:351:ASN:HB3	3:A:602:HOH:O	1.81	0.80
1:B:316:LEU:HD21	1:D:312:GLU:OE1	1.81	0.80
1:A:537:ALA:HB2	1:C:450:PRO:HG2	1.63	0.79
1:C:394:TYR:CZ	2:C:601:B4A:N09	2.52	0.77
1:A:165:SER:HA	1:A:225:MET:CE	2.17	0.75
1:A:152:GLU:OE1	1:A:153:LYS:HB2	1.87	0.74
1:B:148:ALA:HB2	1:B:154:ILE:HG12	1.67	0.74
1:D:387:ARG:H	1:D:387:ARG:HD2	1.53	0.74
1:A:265:VAL:HG22	1:A:498:MET:HG2	1.70	0.73
1:A:163:LEU:O	1:A:166:THR:HG22	1.87	0.73
1:B:532:ASN:ND2	1:B:535:HIS:H	1.87	0.73
1:A:143:LEU:HD12	1:A:200:PHE:HZ	1.54	0.72
1:C:481:LYS:NZ	1:C:482:SER:O	2.22	0.72
1:B:346:LYS:NZ	1:B:357:TYR:CD1	2.57	0.72
1:A:142:LEU:O	1:A:146:THR:OG1	2.08	0.71
1:D:423:THR:HG23	1:D:426:SER:H	1.55	0.70
1:B:543:ARG:C	1:B:544:ARG:HD2	2.12	0.69
1:B:143:LEU:O	1:B:147:ILE:HD12	1.93	0.69
1:A:189:THR:HB	1:A:193:VAL:HG22	1.76	0.68
1:A:217:ARG:NH2	1:A:545:GLU:OE2	2.27	0.68
1:C:163:LEU:O	1:C:166:THR:HG22	1.93	0.68
1:B:346:LYS:NZ	1:B:357:TYR:CE1	2.61	0.68
1:C:138:SER:HB3	1:C:141:ASP:HB2	1.75	0.68
1:C:343:SER:HA	1:C:410:ILE:HD12	1.76	0.68
1:D:144:PHE:HE1	1:D:154:ILE:HG12	1.59	0.68
1:B:153:LYS:HB3	1:B:194:MET:HB3	1.75	0.67
1:D:213:GLN:HB2	1:D:218:LYS:HB2	1.75	0.67
1:D:279:LYS:HE2	1:D:425:GLU:OE2	1.94	0.67
1:D:147:ILE:O	1:D:158:LYS:NZ	2.26	0.67
1:A:165:SER:HA	1:A:225:MET:HE2	1.76	0.66
1:D:178:CYS:HB3	1:D:207:ASN:ND2	2.09	0.66
1:A:503:PRO:N	1:A:504:PRO:HD2	2.10	0.66
1:C:191:ASP:HB3	1:C:193:VAL:HB	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:LEU:HD11	1:A:212:THR:HG21	1.78	0.65
1:A:351:ASN:CB	3:A:602:HOH:O	2.38	0.65
1:B:387:ARG:HD3	1:B:387:ARG:H	1.61	0.65
1:A:481:LYS:NZ	1:A:482:SER:O	2.30	0.65
1:A:323:LEU:HD21	1:A:395:LEU:HD21	1.79	0.64
1:B:382:ARG:NH1	1:B:412:ASP:OD1	2.29	0.64
1:A:143:LEU:HD12	1:A:200:PHE:CZ	2.32	0.64
1:B:423:THR:HG23	1:B:426:SER:H	1.62	0.63
1:C:202:LYS:HA	1:C:205:GLN:HG2	1.81	0.63
1:C:174:ARG:HB3	3:C:701:HOH:O	1.98	0.63
1:B:316:LEU:HD22	1:B:316:LEU:H	1.64	0.63
1:D:434:LEU:HB3	1:D:457:LEU:HD11	1.80	0.63
1:A:175:LEU:HD21	1:A:210:LEU:HD23	1.80	0.63
1:A:450:PRO:HG2	1:C:537:ALA:HB2	1.81	0.63
1:B:267:THR:HA	1:B:496:MET:HA	1.79	0.63
1:B:498:MET:HE1	1:B:517:PHE:HE1	1.62	0.63
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.80	0.62
1:C:278:THR:O	1:C:425:GLU:HG3	2.00	0.61
1:A:274:SER:HB3	1:A:278:THR:HG21	1.82	0.61
1:B:498:MET:HE1	1:B:517:PHE:CE1	2.34	0.61
1:B:530:TYR:OH	1:D:479:PRO:HD3	2.00	0.61
1:C:304:TYR:HE2	1:C:344:LEU:HD22	1.66	0.61
1:B:422:VAL:HG21	1:B:427:ALA:HB2	1.82	0.61
1:C:285:GLN:HG3	1:C:484:VAL:HG23	1.83	0.61
1:D:270:GLY:O	1:D:272:ARG:HG2	2.00	0.61
1:D:360:GLN:O	1:D:364:LYS:HG3	2.00	0.60
1:A:533:LEU:H	1:C:494:ASN:HD21	1.50	0.60
1:D:148:ALA:O	1:D:150:GLY:N	2.35	0.60
1:B:148:ALA:O	1:B:150:GLY:N	2.34	0.60
1:C:156:VAL:HG23	1:C:195:LEU:HD11	1.83	0.60
1:D:336:ALA:HA	1:D:391:ILE:HG21	1.84	0.60
1:D:465:MET:H	1:D:469:SER:HB3	1.66	0.60
1:B:379:GLN:O	1:B:383:GLU:HG2	2.02	0.60
1:C:397:GLU:HG3	1:D:387:ARG:HB3	1.83	0.60
1:C:407:MET:HE3	1:C:408:VAL:HG22	1.83	0.60
1:D:382:ARG:NH2	1:D:412:ASP:OD1	2.35	0.60
1:A:165:SER:HA	1:A:225:MET:HE3	1.83	0.59
1:B:286:SER:HB3	1:B:289:LYS:HD2	1.84	0.59
1:D:423:THR:HG22	1:D:426:SER:HB3	1.84	0.59
1:B:346:LYS:NZ	1:B:357:TYR:CG	2.70	0.59
1:B:317:ARG:HG2	1:D:318:PHE:CE1	2.38	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:VAL:O	1:B:337:GLY:N	2.35	0.59
1:D:138:SER:O	1:D:142:LEU:HG	2.03	0.59
1:D:169:ARG:HD3	1:D:170:THR:H	1.68	0.59
1:C:365:MET:HG3	1:C:447:VAL:HG11	1.85	0.59
1:D:224:PHE:O	1:D:228:THR:HG23	2.03	0.58
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.85	0.58
1:A:176:LYS:O	1:A:180:ASP:N	2.34	0.58
1:B:507:LYS:H	1:B:507:LYS:HD2	1.68	0.58
1:D:474:PHE:HD2	1:D:475:HIS:CD2	2.20	0.58
1:B:293:TYR:OH	1:B:306:HIS:NE2	2.26	0.58
1:D:365:MET:HG3	1:D:447:VAL:HG11	1.84	0.58
1:B:450:PRO:HG2	1:D:537:ALA:HB2	1.84	0.58
1:D:522:VAL:HG21	1:D:528:HIS:HB2	1.85	0.58
1:B:226:SER:O	1:B:229:SER:OG	2.18	0.58
1:D:189:THR:HG22	1:D:190:SER:N	2.17	0.57
1:B:139:LEU:HA	1:B:142:LEU:HG	1.84	0.57
1:B:528:HIS:CG	1:D:454:ARG:HD2	2.39	0.57
1:D:495:VAL:HG12	1:D:496:MET:HG2	1.86	0.57
1:B:486:GLY:O	1:B:501:TRP:HA	2.04	0.56
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.85	0.56
1:A:465:MET:H	1:A:469:SER:HB3	1.69	0.56
1:B:343:SER:HA	1:B:410:ILE:HD12	1.88	0.56
1:D:255:LYS:C	3:D:601:HOH:O	2.36	0.56
1:C:477:GLY:O	1:C:529:ASN:HB2	2.05	0.56
1:D:139:LEU:HA	1:D:142:LEU:HD12	1.87	0.56
1:B:201:LYS:O	1:B:205:GLN:HB2	2.05	0.56
1:A:338:ALA:O	1:A:342:THR:HG23	2.06	0.56
1:A:382:ARG:NH2	1:A:412:ASP:OD2	2.38	0.56
1:C:423:THR:H	1:C:426:SER:HB3	1.71	0.56
1:D:211:LEU:O	1:D:215:PHE:HD2	1.89	0.56
1:A:454:ARG:HD2	1:C:528:HIS:CD2	2.41	0.56
1:D:403:GLU:CD	1:D:403:GLU:H	2.09	0.56
1:A:154:ILE:HG22	1:A:155:PRO:O	2.06	0.56
1:B:387:ARG:H	1:B:387:ARG:CD	2.17	0.56
1:D:512:VAL:HG13	1:D:513:LYS:H	1.71	0.56
1:B:480:ALA:HB2	1:B:490:LEU:HD12	1.87	0.56
1:C:143:LEU:HD21	1:C:212:THR:HG22	1.88	0.55
1:D:163:LEU:O	1:D:166:THR:HG22	2.07	0.55
1:C:288:VAL:HG21	1:C:417:LEU:O	2.06	0.55
1:A:530:TYR:OH	1:C:479:PRO:HD3	2.07	0.55
1:A:343:SER:HA	1:A:410:ILE:HD12	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:TYR:O	1:D:426:SER:HB2	2.06	0.55
1:A:147:ILE:HG12	1:A:158:LYS:NZ	2.22	0.54
1:B:346:LYS:NZ	1:B:357:TYR:CZ	2.75	0.54
1:A:140:GLU:HG2	1:A:205:GLN:HG3	1.87	0.54
1:A:141:ASP:OD2	1:A:201:LYS:NZ	2.40	0.54
1:B:512:VAL:HG13	1:B:513:LYS:H	1.73	0.54
1:C:172:ASP:OD1	1:C:174:ARG:HD3	2.07	0.54
1:C:248:ASP:OD1	1:C:248:ASP:N	2.38	0.54
1:C:358:VAL:HG21	1:C:417:LEU:HD21	1.89	0.54
1:D:407:MET:SD	1:D:411:LEU:HD11	2.47	0.54
1:B:427:ALA:HB3	1:B:499:MET:HG2	1.90	0.54
1:B:139:LEU:H	1:B:139:LEU:HD23	1.73	0.54
2:B:601:B4A:C19	1:C:317:ARG:HD2	2.37	0.54
1:D:261:TRP:HA	1:D:501:TRP:O	2.08	0.54
1:B:224:PHE:O	1:B:228:THR:HG23	2.08	0.54
1:B:230:HIS:HA	1:B:233:GLU:HB2	1.89	0.54
1:C:174:ARG:HB2	1:C:210:LEU:HD21	1.89	0.53
1:A:312:GLU:O	1:A:331:ASN:HB3	2.08	0.53
1:C:140:GLU:N	1:C:140:GLU:OE1	2.40	0.53
1:D:329:PRO:HG2	1:D:340:VAL:HG21	1.89	0.53
1:C:191:ASP:CB	1:C:193:VAL:HB	2.39	0.53
1:B:534:ARG:HD2	1:B:535:HIS:NE2	2.24	0.53
1:A:147:ILE:HD11	1:A:159:PHE:HA	1.90	0.53
1:B:193:VAL:HG22	1:B:194:MET:H	1.74	0.53
1:C:143:LEU:N	1:C:143:LEU:HD22	2.24	0.53
1:D:302:THR:HG22	1:D:455:ASN:ND2	2.24	0.53
1:A:502:SER:OG	1:A:513:LYS:NZ	2.35	0.52
1:B:312:GLU:OE1	1:D:316:LEU:CD2	2.57	0.52
1:B:312:GLU:OE1	1:D:316:LEU:HD21	2.09	0.52
1:C:226:SER:O	1:C:229:SER:OG	2.26	0.52
1:B:537:ALA:HB2	1:D:450:PRO:HG2	1.90	0.52
1:A:533:LEU:H	1:C:494:ASN:ND2	2.07	0.52
1:A:318:PHE:HE2	1:C:317:ARG:HB2	1.74	0.52
1:A:227:PHE:O	1:A:231:ILE:HG12	2.09	0.52
1:D:447:VAL:HG12	1:D:448:LEU:HG	1.92	0.51
1:B:544:ARG:HD2	1:B:544:ARG:N	2.25	0.51
1:C:151:GLN:HG2	1:C:152:GLU:H	1.75	0.51
1:B:143:LEU:HD12	1:B:146:THR:HB	1.93	0.51
1:B:405:THR:HG22	1:B:410:ILE:HG13	1.93	0.51
1:A:519:HIS:O	1:A:523:SER:OG	2.10	0.51
1:A:528:HIS:CG	1:C:454:ARG:HD2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:GLN:HG2	1:C:152:GLU:N	2.26	0.51
1:B:243:GLY:O	1:B:512:VAL:HG11	2.10	0.51
1:B:387:ARG:O	1:B:390:ALA:HB3	2.11	0.51
1:B:354:LYS:HB3	1:B:413:PHE:CZ	2.45	0.50
1:A:224:PHE:O	1:A:228:THR:HG23	2.11	0.50
1:B:143:LEU:HG	1:B:147:ILE:HD11	1.92	0.50
1:B:284:LEU:HB3	1:B:287:CYS:HB2	1.94	0.50
1:A:292:LYS:HA	1:A:295:ILE:HD12	1.92	0.50
1:B:228:THR:HB	1:B:273:HIS:CE1	2.47	0.50
1:D:140:GLU:HG3	1:D:208:ILE:HG12	1.93	0.50
1:A:182:LEU:O	1:A:186:LEU:HG	2.12	0.50
1:C:486:GLY:O	1:C:501:TRP:HA	2.12	0.50
1:D:189:THR:HB	1:D:191:ASP:H	1.76	0.50
1:B:402:PRO:O	1:B:405:THR:OG1	2.31	0.49
1:A:181:MET:O	1:A:185:THR:HG23	2.13	0.49
1:D:313:PRO:HG3	1:D:462:SER:HB2	1.94	0.49
1:D:320:LYS:HG3	1:D:321:LEU:HD12	1.94	0.49
1:D:465:MET:HG3	1:D:472:PHE:CG	2.48	0.49
1:A:479:PRO:HG3	1:C:530:TYR:CE1	2.47	0.49
1:C:304:TYR:CE2	1:C:344:LEU:HD22	2.47	0.49
1:D:518:CYS:O	1:D:522:VAL:HG12	2.13	0.49
1:D:217:ARG:HH22	1:D:545:GLU:CG	2.26	0.49
1:B:474:PHE:HD2	1:B:475:HIS:CD2	2.31	0.49
1:D:519:HIS:O	1:D:523:SER:OG	2.19	0.49
1:B:336:ALA:HA	1:B:391:ILE:HG21	1.95	0.48
1:C:209:VAL:O	1:C:213:GLN:HG3	2.12	0.48
1:D:482:SER:HA	1:D:487:GLY:O	2.13	0.48
1:B:143:LEU:HG	1:B:147:ILE:CD1	2.43	0.48
1:A:158:LYS:O	1:A:158:LYS:HG2	2.11	0.48
1:A:186:LEU:HD22	1:A:193:VAL:HB	1.95	0.48
1:B:532:ASN:HD22	1:B:535:HIS:N	2.02	0.48
1:B:291:LEU:O	1:B:295:ILE:HG13	2.13	0.48
1:A:260:LEU:HD13	1:A:501:TRP:CH2	2.49	0.48
1:C:153:LYS:HD2	1:C:194:MET:HB2	1.95	0.48
1:C:358:VAL:O	1:C:362:LEU:HG	2.14	0.48
1:D:449:SER:O	1:D:453:VAL:HG23	2.13	0.48
1:A:365:MET:HG3	1:A:447:VAL:HG11	1.96	0.47
1:A:256:PHE:HB3	1:A:257:SER:H	1.56	0.47
1:B:346:LYS:NZ	1:B:357:TYR:CD2	2.82	0.47
1:D:521:LEU:HD12	3:D:602:HOH:O	2.14	0.47
1:C:276:GLY:O	1:C:278:THR:HG23	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:VAL:HG13	1:C:221:ILE:HG13	1.97	0.47
1:B:166:THR:HG23	1:B:168:LEU:H	1.80	0.47
1:A:289:LYS:HA	1:A:292:LYS:HE2	1.96	0.47
1:A:354:LYS:HB3	1:A:413:PHE:CZ	2.50	0.47
1:A:449:SER:O	1:A:453:VAL:HG23	2.14	0.47
1:D:185:THR:HG21	1:D:199:LEU:HD11	1.97	0.47
1:C:405:THR:HG22	1:C:410:ILE:HG13	1.97	0.47
1:B:288:VAL:HG21	1:B:417:LEU:O	2.15	0.46
1:C:307:ARG:HB2	1:C:308:TYR:CE1	2.51	0.46
1:C:143:LEU:CD2	1:C:212:THR:HG22	2.45	0.46
1:D:174:ARG:H	1:D:174:ARG:HG3	1.50	0.46
1:D:541:ASP:OD1	1:D:543:ARG:HD3	2.15	0.46
1:A:152:GLU:CD	1:A:153:LYS:HB2	2.36	0.46
1:B:228:THR:HB	1:B:273:HIS:ND1	2.31	0.46
1:D:217:ARG:HH22	1:D:545:GLU:HG3	1.79	0.46
1:D:387:ARG:O	1:D:390:ALA:HB3	2.15	0.46
1:A:423:THR:HG23	1:A:426:SER:H	1.79	0.46
1:B:172:ASP:HB3	1:B:175:LEU:HG	1.96	0.46
1:B:311:LYS:HE3	1:D:471:GLN:HG3	1.98	0.46
1:C:189:THR:HB	1:C:191:ASP:OD1	2.15	0.46
1:C:332:PRO:HD2	1:C:459:LEU:HD13	1.96	0.46
1:D:178:CYS:HB3	1:D:207:ASN:HD22	1.80	0.46
1:B:207:ASN:O	1:B:211:LEU:HB2	2.16	0.46
1:A:152:GLU:OE1	1:A:153:LYS:HE2	2.15	0.46
1:A:260:LEU:HD13	1:A:501:TRP:HH2	1.81	0.46
1:B:315:GLY:O	1:B:318:PHE:N	2.44	0.46
1:C:153:LYS:HB2	1:C:194:MET:HE1	1.97	0.46
1:C:300:LEU:HD22	1:C:304:TYR:CE2	2.50	0.46
1:B:346:LYS:O	1:B:354:LYS:HE3	2.15	0.45
1:D:227:PHE:O	1:D:231:ILE:HG12	2.15	0.45
1:A:318:PHE:CE2	1:C:317:ARG:HB2	2.51	0.45
1:D:302:THR:HG22	1:D:455:ASN:HD21	1.81	0.45
1:A:140:GLU:HG3	1:A:208:ILE:HG12	1.98	0.45
1:D:164:LYS:HE2	1:D:169:ARG:NH1	2.32	0.45
1:D:257:SER:HA	1:D:258:PRO:HD3	1.78	0.45
1:A:138:SER:OG	1:A:141:ASP:HB2	2.16	0.45
1:A:454:ARG:HD2	1:C:528:HIS:CG	2.52	0.45
1:B:543:ARG:O	1:B:544:ARG:HD2	2.17	0.45
1:A:354:LYS:HD3	1:A:413:PHE:CE2	2.51	0.45
1:D:139:LEU:HD21	1:D:212:THR:HG21	1.99	0.45
1:D:504:PRO:O	1:D:512:VAL:HG12	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:MET:HG2	1:C:202:LYS:O	2.16	0.45
1:B:227:PHE:CZ	1:B:231:ILE:HD11	2.51	0.45
1:B:245:LYS:HA	1:B:245:LYS:HD2	1.80	0.45
1:C:192:GLY:N	1:C:193:VAL:HB	2.32	0.45
1:D:243:GLY:O	1:D:512:VAL:HG11	2.17	0.45
1:B:527:PHE:CZ	1:B:542:PRO:HG2	2.52	0.44
1:A:154:ILE:HG23	1:A:158:LYS:NZ	2.32	0.44
1:D:387:ARG:O	1:D:391:ILE:HG13	2.17	0.44
1:D:422:VAL:HB	1:D:426:SER:OG	2.17	0.44
1:A:351:ASN:HA	1:A:354:LYS:HB2	2.00	0.44
1:A:143:LEU:HD13	1:A:143:LEU:O	2.17	0.44
1:A:197:LYS:O	1:A:201:LYS:HE2	2.18	0.44
1:B:140:GLU:OE1	1:B:140:GLU:N	2.47	0.44
1:C:432:ALA:HB1	1:C:441:PRO:HG3	1.98	0.44
1:A:266:CYS:HA	1:A:271:GLN:O	2.17	0.44
1:B:378:PHE:CE1	1:B:416:GLN:HG3	2.52	0.44
1:B:512:VAL:HG13	1:B:513:LYS:N	2.32	0.44
1:C:220:VAL:N	1:C:269:ASP:OD2	2.36	0.44
1:D:317:ARG:NE	1:D:317:ARG:HA	2.32	0.44
1:C:264:SER:HB2	1:C:424:CYS:HB3	1.99	0.44
1:D:512:VAL:HG13	1:D:513:LYS:N	2.33	0.44
1:A:148:ALA:C	1:A:150:GLY:H	2.21	0.43
1:A:190:SER:O	1:A:190:SER:OG	2.28	0.43
1:B:443:THR:OG1	1:B:445:GLU:HG2	2.18	0.43
1:D:302:THR:CG2	1:D:455:ASN:HD21	2.31	0.43
1:B:202:LYS:HA	1:B:205:GLN:HB2	2.00	0.43
1:C:157:HIS:O	1:C:161:THR:HG23	2.18	0.43
1:C:417:LEU:HD23	1:C:417:LEU:HA	1.69	0.43
1:D:281:PRO:HA	1:D:422:VAL:O	2.18	0.43
1:A:364:LYS:HB3	1:A:447:VAL:HG22	2.00	0.43
1:B:365:MET:HG3	1:B:447:VAL:HG11	2.01	0.43
1:A:323:LEU:HD21	1:A:395:LEU:CD2	2.48	0.43
1:B:507:LYS:H	1:B:507:LYS:CD	2.29	0.43
1:B:293:TYR:CE2	1:B:459:LEU:HD12	2.53	0.43
1:C:292:LYS:HD3	1:C:342:THR:OG1	2.18	0.43
1:A:503:PRO:N	1:A:504:PRO:CD	2.78	0.43
1:C:143:LEU:O	1:C:147:ILE:HG13	2.18	0.43
1:A:147:ILE:HG12	1:A:158:LYS:HZ1	1.82	0.43
1:A:166:THR:HG21	1:A:214:ALA:HB1	2.01	0.43
1:D:186:LEU:HA	1:D:193:VAL:HG21	1.99	0.43
1:D:323:LEU:HD11	1:D:400:CYS:SG	2.58	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:THR:CG2	1:D:426:SER:H	2.25	0.43
1:A:180:ASP:OD1	1:A:183:ARG:NH2	2.50	0.43
1:D:189:THR:HB	1:D:191:ASP:HB2	2.00	0.43
1:A:495:VAL:HG12	1:A:496:MET:HB3	2.01	0.43
1:B:317:ARG:HA	1:B:317:ARG:HD2	1.85	0.43
1:C:360:GLN:O	1:C:364:LYS:HG3	2.19	0.43
1:D:338:ALA:O	1:D:341:VAL:HG12	2.18	0.43
1:B:312:GLU:O	1:B:331:ASN:HB3	2.19	0.43
1:D:531:ASP:OD2	1:D:539:LYS:NZ	2.51	0.43
1:A:530:TYR:CE1	1:C:479:PRO:HG3	2.53	0.42
1:B:354:LYS:HD3	1:B:413:PHE:CE2	2.54	0.42
1:C:246:VAL:HG12	1:C:247:ALA:H	1.84	0.42
1:A:137:PRO:O	1:A:138:SER:HB3	2.18	0.42
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.86	0.42
1:C:260:LEU:HB3	1:C:501:TRP:CZ3	2.54	0.42
1:C:280:VAL:HA	1:C:281:PRO:HD3	1.89	0.42
1:B:345:ILE:O	1:B:354:LYS:HE2	2.19	0.42
1:D:423:THR:N	1:D:426:SER:OG	2.48	0.42
1:A:322:PHE:O	1:A:323:LEU:HD23	2.18	0.42
1:B:289:LYS:N	1:B:290:PRO:HD2	2.34	0.42
1:D:169:ARG:C	1:D:171:SER:H	2.23	0.42
1:C:139:LEU:HB2	1:C:140:GLU:OE1	2.19	0.42
1:C:290:PRO:HD3	1:C:481:LYS:HD3	2.01	0.42
1:D:139:LEU:O	1:D:139:LEU:HD23	2.20	0.42
1:A:236:GLU:O	1:A:239:LYS:HB3	2.20	0.42
1:B:169:ARG:O	1:B:171:SER:N	2.52	0.42
1:B:216:ARG:HD3	1:B:216:ARG:HA	1.89	0.42
1:D:525:CYS:HB3	1:D:540:LEU:O	2.20	0.42
1:A:144:PHE:HD1	1:A:154:ILE:HD11	1.85	0.42
1:C:291:LEU:H	1:C:291:LEU:HG	1.66	0.42
1:A:402:PRO:O	1:A:405:THR:OG1	2.22	0.41
1:B:201:LYS:O	1:B:201:LYS:HG2	2.19	0.41
1:B:346:LYS:HD3	1:B:346:LYS:HA	1.93	0.41
1:C:158:LYS:HA	1:C:158:LYS:HD2	1.66	0.41
1:D:278:THR:O	1:D:423:THR:OG1	2.34	0.41
1:D:320:LYS:H	1:D:320:LYS:HG2	1.63	0.41
1:A:289:LYS:N	1:A:290:PRO:HD2	2.34	0.41
1:B:488:ILE:O	1:B:499:MET:HA	2.20	0.41
1:C:256:PHE:HB3	1:C:257:SER:H	1.76	0.41
1:D:545:GLU:OE1	1:D:545:GLU:N	2.52	0.41
1:A:432:ALA:HB1	1:A:441:PRO:HG3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ARG:C	1:B:171:SER:H	2.23	0.41
1:D:140:GLU:HB2	1:D:201:LYS:HG3	2.01	0.41
1:D:522:VAL:CG2	1:D:528:HIS:HB2	2.50	0.41
1:A:157:HIS:O	1:A:161:THR:HG23	2.21	0.41
1:A:292:LYS:HD2	1:A:342:THR:HG22	2.02	0.41
1:B:317:ARG:HG2	1:D:318:PHE:CZ	2.55	0.41
1:C:465:MET:H	1:C:469:SER:CB	2.34	0.41
1:D:271:GLN:H	1:D:271:GLN:HG3	1.67	0.41
1:B:358:VAL:O	1:B:362:LEU:HG	2.21	0.41
1:C:465:MET:H	1:C:469:SER:HB2	1.85	0.41
1:D:310:GLY:O	1:D:331:ASN:HA	2.20	0.41
1:B:323:LEU:HD21	1:B:395:LEU:HD21	2.01	0.41
1:D:164:LYS:HE2	1:D:169:ARG:CZ	2.51	0.41
1:B:344:LEU:HA	1:B:347:GLN:HE21	1.85	0.41
1:A:526:ASN:HA	1:A:539:LYS:HE3	2.02	0.41
1:C:138:SER:O	1:C:142:LEU:HG	2.21	0.41
1:C:267:THR:HA	1:C:496:MET:HA	2.03	0.41
1:C:318:PHE:CD1	1:C:321:LEU:HD13	2.56	0.41
1:D:439:PHE:CE2	1:D:446:ARG:HB3	2.56	0.41
1:D:477:GLY:O	1:D:529:ASN:HB2	2.20	0.41
1:D:285:GLN:OE1	1:D:418:CYS:HB3	2.20	0.41
1:A:140:GLU:HG2	1:A:205:GLN:CG	2.49	0.40
1:C:152:GLU:HB2	1:C:153:LYS:H	1.60	0.40
1:C:257:SER:O	1:C:260:LEU:HD12	2.21	0.40
1:D:480:ALA:HB2	1:D:490:LEU:HD12	2.03	0.40
1:C:186:LEU:HD12	1:C:186:LEU:O	2.22	0.40
1:D:151:GLN:OE1	1:D:153:LYS:O	2.39	0.40
1:A:216:ARG:HD2	1:A:216:ARG:HA	1.79	0.40
1:B:413:PHE:O	1:B:417:LEU:HD13	2.20	0.40
1:B:448:LEU:HA	1:B:448:LEU:HD23	1.79	0.40
1:A:211:LEU:O	1:A:215:PHE:HD2	2.04	0.40
1:A:479:PRO:HD3	1:C:530:TYR:OH	2.21	0.40
1:B:192:GLY:HA3	1:B:193:VAL:HA	1.92	0.40
1:D:490:LEU:HB3	1:D:498:MET:HB2	2.02	0.40
1:D:528:HIS:HB3	1:D:531:ASP:OD2	2.22	0.40
1:A:139:LEU:HA	1:A:142:LEU:HG	2.04	0.40
1:C:187:GLN:C	1:C:189:THR:H	2.24	0.40
1:D:402:PRO:O	1:D:405:THR:OG1	2.24	0.40
1:D:515:ILE:HD13	1:D:515:ILE:HA	1.94	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	400/539 (74%)	361 (90%)	34 (8%)	5 (1%)	12	36
1	B	400/539 (74%)	358 (90%)	34 (8%)	8 (2%)	7	24
1	C	400/539 (74%)	358 (90%)	39 (10%)	3 (1%)	19	49
1	D	400/539 (74%)	358 (90%)	35 (9%)	7 (2%)	8	28
All	All	1600/2156 (74%)	1435 (90%)	142 (9%)	23 (1%)	11	34

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	B	149	GLU
1	B	191	ASP
1	C	152	GLU
1	C	330	HIS
1	D	138	SER
1	D	149	GLU
1	A	152	GLU
1	A	345	ILE
1	D	152	GLU
1	A	192	GLY
1	B	256	PHE
1	C	138	SER
1	D	170	THR
1	D	191	ASP
1	D	241	GLN
1	A	149	GLU
1	B	170	THR
1	B	351	ASN
1	B	461	HIS
1	D	376	ALA
1	B	192	GLY
1	B	193	VAL

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	349/462 (76%)	341 (98%)	8 (2%)	50 82
1	B	349/462 (76%)	328 (94%)	21 (6%)	19 48
1	C	349/462 (76%)	339 (97%)	10 (3%)	42 76
1	D	349/462 (76%)	334 (96%)	15 (4%)	29 62
All	All	1396/1848 (76%)	1342 (96%)	54 (4%)	32 66

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	LYS
1	A	196	ASP
1	A	207	ASN
1	A	264	SER
1	A	361	PHE
1	A	413	PHE
1	A	538	LYS
1	A	545	GLU
1	B	145	TYR
1	B	151	GLN
1	B	163	LEU
1	B	200	PHE
1	B	202	LYS
1	B	205	GLN
1	B	207	ASN
1	B	248	ASP
1	B	255	LYS
1	B	264	SER
1	B	272	ARG
1	B	307	ARG
1	B	311	LYS
1	B	343	SER
1	B	361	PHE
1	B	387	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	413	PHE
1	B	471	GLN
1	B	507	LYS
1	B	523	SER
1	B	544	ARG
1	C	141	ASP
1	C	158	LYS
1	C	205	GLN
1	C	217	ARG
1	C	264	SER
1	C	361	PHE
1	C	412	ASP
1	C	469	SER
1	C	523	SER
1	C	540	LEU
1	D	178	CYS
1	D	194	MET
1	D	207	ASN
1	D	210	LEU
1	D	245	LYS
1	D	248	ASP
1	D	264	SER
1	D	317	ARG
1	D	318	PHE
1	D	361	PHE
1	D	384	SER
1	D	387	ARG
1	D	446	ARG
1	D	502	SER
1	D	544	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	532	ASN
1	C	151	GLN
1	C	213	GLN
1	C	494	ASN
1	D	207	ASN
1	D	455	ASN

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 monosaccharides 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	B4A	C	601	-	32,41,41	3.77	8 (25%)	35,55,55	1.87	8 (22%)
2	B4A	B	601	-	32,41,41	3.65	8 (25%)	35,55,55	1.78	8 (22%)

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	B4A	C	601	-	-	5/16/34/34	1/5/5/5
2	B4A	B	601	-	-	4/16/34/34	1/5/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	B4A	N25-N24	11.89	1.60	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	B4A	N10-N09	11.76	1.60	1.37
2	C	601	B4A	N25-N24	11.59	1.60	1.37
2	B	601	B4A	N10-N09	11.26	1.59	1.37
2	C	601	B4A	C23-N03	8.54	1.45	1.32
2	B	601	B4A	C23-N03	7.73	1.44	1.32
2	C	601	B4A	C11-N12	5.10	1.45	1.36
2	C	601	B4A	C26-N27	4.56	1.44	1.36
2	C	601	B4A	C28-N27	4.53	1.45	1.35
2	B	601	B4A	C28-N27	4.48	1.45	1.35
2	B	601	B4A	C26-N27	4.42	1.44	1.36
2	B	601	B4A	C11-N12	4.36	1.44	1.36
2	C	601	B4A	C13-N12	4.10	1.44	1.35
2	B	601	B4A	C13-N12	3.92	1.44	1.35
2	B	601	B4A	O21-C13	-2.49	1.18	1.23
2	C	601	B4A	O21-C13	-2.09	1.19	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	B4A	C11-N12-C13	-5.72	114.09	129.54
2	C	601	B4A	C26-N27-C28	-5.54	114.59	129.54
2	B	601	B4A	C08-N07-C06	-4.69	115.52	124.26
2	C	601	B4A	C05-C06-N07	-4.24	103.99	110.60
2	C	601	B4A	C01-C06-N07	-3.97	104.41	110.60
2	C	601	B4A	C08-N07-C06	-3.85	117.08	124.26
2	B	601	B4A	O21-C13-N12	-3.59	117.08	123.63
2	B	601	B4A	C14-C13-N12	2.93	120.83	114.77
2	B	601	B4A	C02-C01-C06	2.93	115.64	110.50
2	C	601	B4A	O36-C28-N27	-2.76	118.60	123.63
2	C	601	B4A	C29-C28-N27	2.68	120.31	114.77
2	C	601	B4A	C11-N12-C13	-2.57	122.60	129.54
2	B	601	B4A	C05-C06-N07	-2.34	106.95	110.60
2	B	601	B4A	C01-C02-N03	-2.30	106.36	111.10
2	B	601	B4A	C26-N27-C28	-2.27	123.42	129.54
2	C	601	B4A	O21-C13-N12	-2.02	119.93	123.63

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	B4A	S37-C23-N03-C02
2	B	601	B4A	S37-C23-N03-C04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	601	B4A	S37-C23-N03-C04
2	B	601	B4A	O36-C28-C29-C30
2	C	601	B4A	C13-C14-C15-C20
2	C	601	B4A	C13-C14-C15-C16
2	C	601	B4A	O36-C28-C29-C30
2	B	601	B4A	N27-C28-C29-C30
2	C	601	B4A	N27-C28-C29-C30

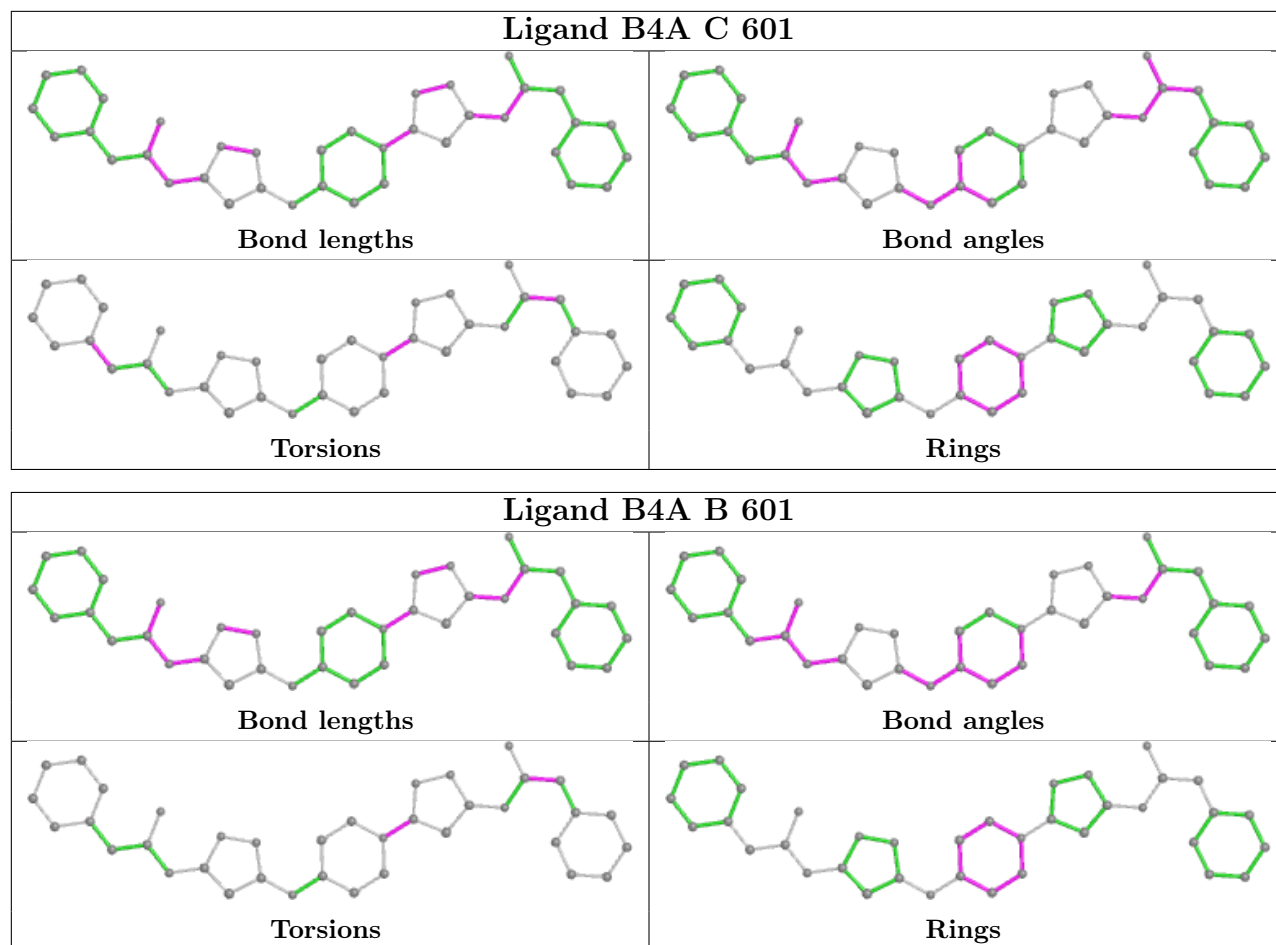
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	601	B4A	C01-C02-C04-C05-C06-N03
2	B	601	B4A	C01-C02-C04-C05-C06-N03

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	B4A	2	0
2	B	601	B4A	2	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

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	404/539 (74%)	0.01	20 (4%) 28 19	48, 78, 139, 245	0
1	B	404/539 (74%)	-0.04	17 (4%) 36 26	45, 77, 141, 245	0
1	C	404/539 (74%)	-0.03	18 (4%) 33 23	45, 78, 144, 243	0
1	D	404/539 (74%)	0.02	21 (5%) 27 18	45, 78, 149, 228	0
All	All	1616/2156 (74%)	-0.01	76 (4%) 31 22	45, 78, 147, 245	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	190	SER	11.4
1	C	190	SER	9.0
1	D	137	PRO	6.7
1	C	150	GLY	6.5
1	A	137	PRO	6.2
1	C	189	THR	6.0
1	D	500	CYS	4.6
1	A	190	SER	4.4
1	B	152	GLU	4.4
1	D	191	ASP	4.0
1	A	500	CYS	3.8
1	B	192	GLY	3.8
1	D	256	PHE	3.7
1	A	150	GLY	3.5
1	C	137	PRO	3.5
1	B	500	CYS	3.5
1	D	192	GLY	3.5
1	A	153	LYS	3.5
1	B	318	PHE	3.4
1	B	546	GLY	3.4
1	D	190	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	318	PHE	3.3
1	B	138	SER	3.3
1	A	191	ASP	3.3
1	C	191	ASP	3.3
1	A	318	PHE	3.2
1	D	538	LYS	3.1
1	B	145	TYR	3.0
1	D	150	GLY	3.0
1	B	189	THR	2.9
1	C	138	SER	2.9
1	C	256	PHE	2.9
1	D	149	GLU	2.8
1	D	537	ALA	2.8
1	B	151	GLN	2.8
1	D	348	GLY	2.8
1	D	315	GLY	2.8
1	C	317	ARG	2.7
1	A	316	LEU	2.7
1	D	316	LEU	2.7
1	C	500	CYS	2.7
1	C	546	GLY	2.7
1	B	149	GLU	2.7
1	B	191	ASP	2.7
1	B	348	GLY	2.6
1	A	248	ASP	2.5
1	C	151	GLN	2.5
1	A	149	GLU	2.5
1	D	203	CYS	2.5
1	D	152	GLU	2.5
1	A	225	MET	2.4
1	A	256	PHE	2.4
1	A	188	THR	2.4
1	D	187	GLN	2.3
1	D	533	LEU	2.3
1	A	152	GLU	2.3
1	A	151	GLN	2.3
1	B	319	ASN	2.2
1	B	142	LEU	2.2
1	C	149	GLU	2.2
1	A	262	GLY	2.2
1	D	197	LYS	2.2
1	B	502	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	152	GLU	2.1
1	C	264	SER	2.1
1	C	242	SER	2.1
1	A	145	TYR	2.1
1	C	187	GLN	2.1
1	B	256	PHE	2.1
1	C	235	TYR	2.1
1	A	538	LYS	2.1
1	D	153	LYS	2.1
1	D	193	VAL	2.1
1	A	546	GLY	2.1
1	C	379	GLN	2.0
1	A	545	GLU	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 monosaccharides in this entry.

6.4 Ligands [i](#)

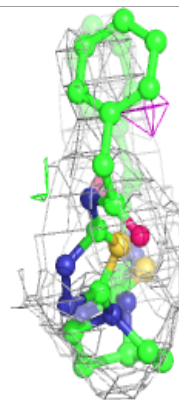
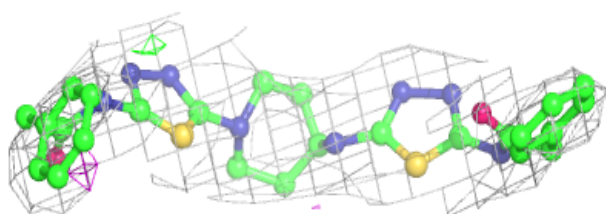
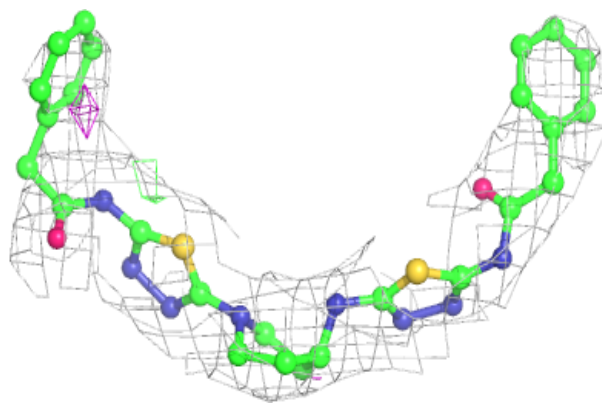
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	B4A	B	601	37/37	0.85	0.27	78,99,117,121	0
2	B4A	C	601	37/37	0.86	0.22	59,103,118,120	0

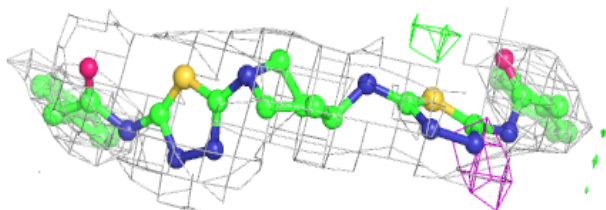
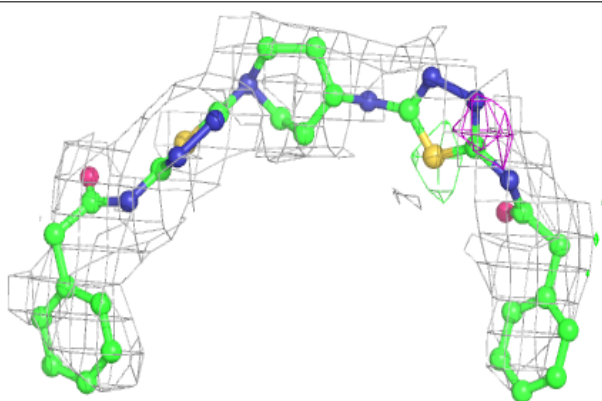
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around B4A B 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 B4A C 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.