



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2020 – 12:17 PM EDT

PDB ID : 6UK6  
Title : Crystal structure of human GAC in complex with inhibitor UPGL00018  
Authors : Huang, Q.; Cerione, R.A.  
Deposited on : 2019-10-04  
Resolution : 2.90 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](mailto: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 : 2.14.6  
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) : 2.14.6

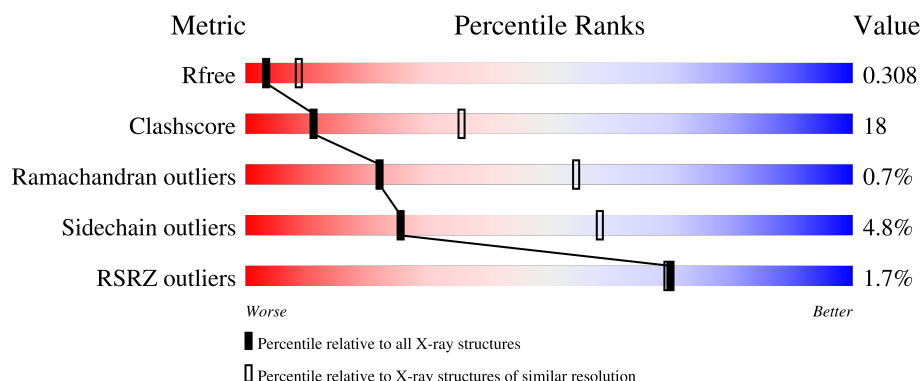
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	527	<div> <div> <div></div> <div>48%</div> <div>26%</div> <div>•</div> <div>23%</div> </div> </div>
1	B	527	<div> <div> <div></div> <div>46%</div> <div>27%</div> <div>•</div> <div>24%</div> </div> </div>
1	C	527	<div> <div> <div></div> <div>48%</div> <div>26%</div> <div>•</div> <div>24%</div> </div> </div>
1	D	527	<div> <div> <div></div> <div>49%</div> <div>23%</div> <div>•</div> <div>25%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12524 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.

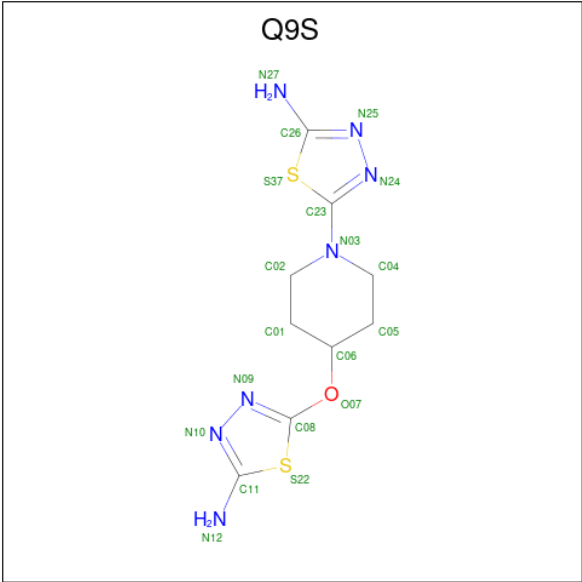
- Molecule 1 is a protein called Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	1	0	0
			3151	2006	532	585	28			
1	B	398	Total	C	N	O	S	1	0	0
			3108	1983	525	572	28			
1	C	402	Total	C	N	O	S	1	0	0
			3128	1988	530	582	28			
1	D	397	Total	C	N	O	S	1	0	0
			3099	1975	524	572	28			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	ALA	VAL	conflict	UNP O94925
B	268	ALA	VAL	conflict	UNP O94925
C	268	ALA	VAL	conflict	UNP O94925
D	268	ALA	VAL	conflict	UNP O94925

- Molecule 2 is 5-{4-[(5-amino-1,3,4-thiadiazol-2-yl)oxy]piperidin-1-yl}-1,3,4-thiadiazol-2-amine (three-letter code: Q9S) (formula: C<sub>9</sub>H<sub>13</sub>N<sub>7</sub>OS<sub>2</sub>) (labeled as "Ligand of Interest" by author).

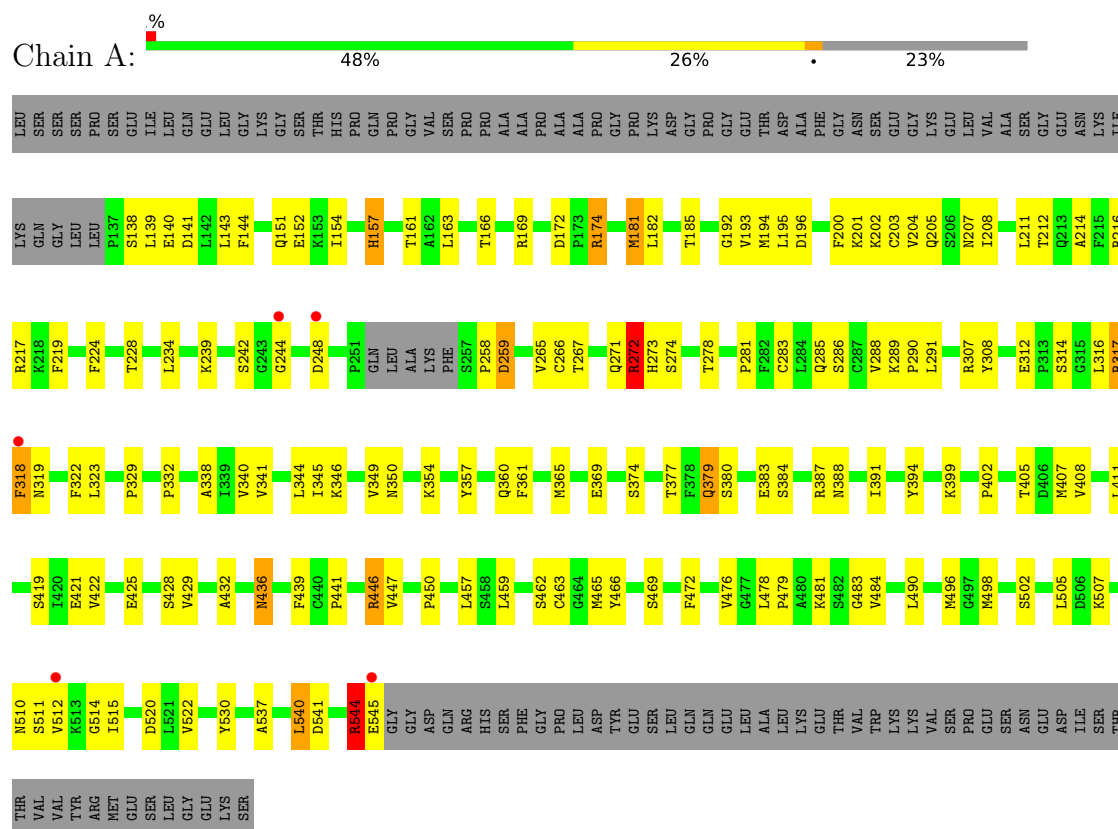


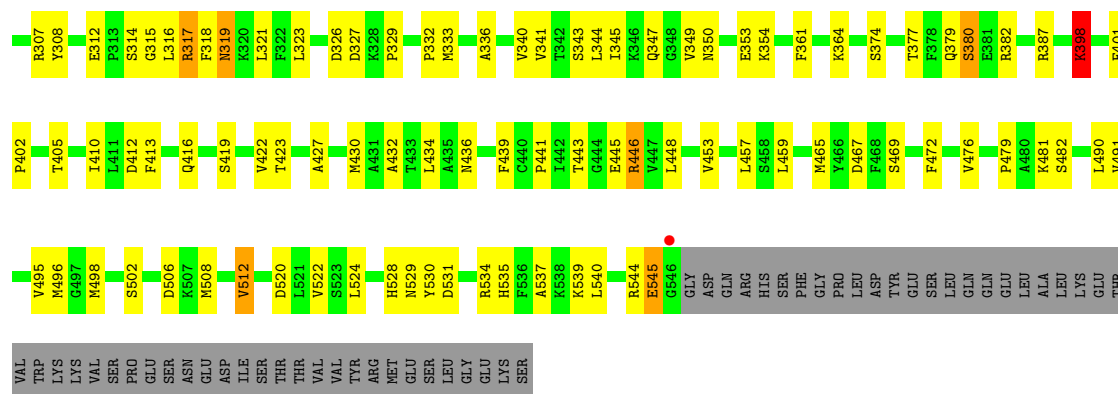
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			19	9	7	1	2		
2	D	1	Total	C	N	O	S	0	0
			19	9	7	1	2		

### 3 Residue-property plots [i](#)

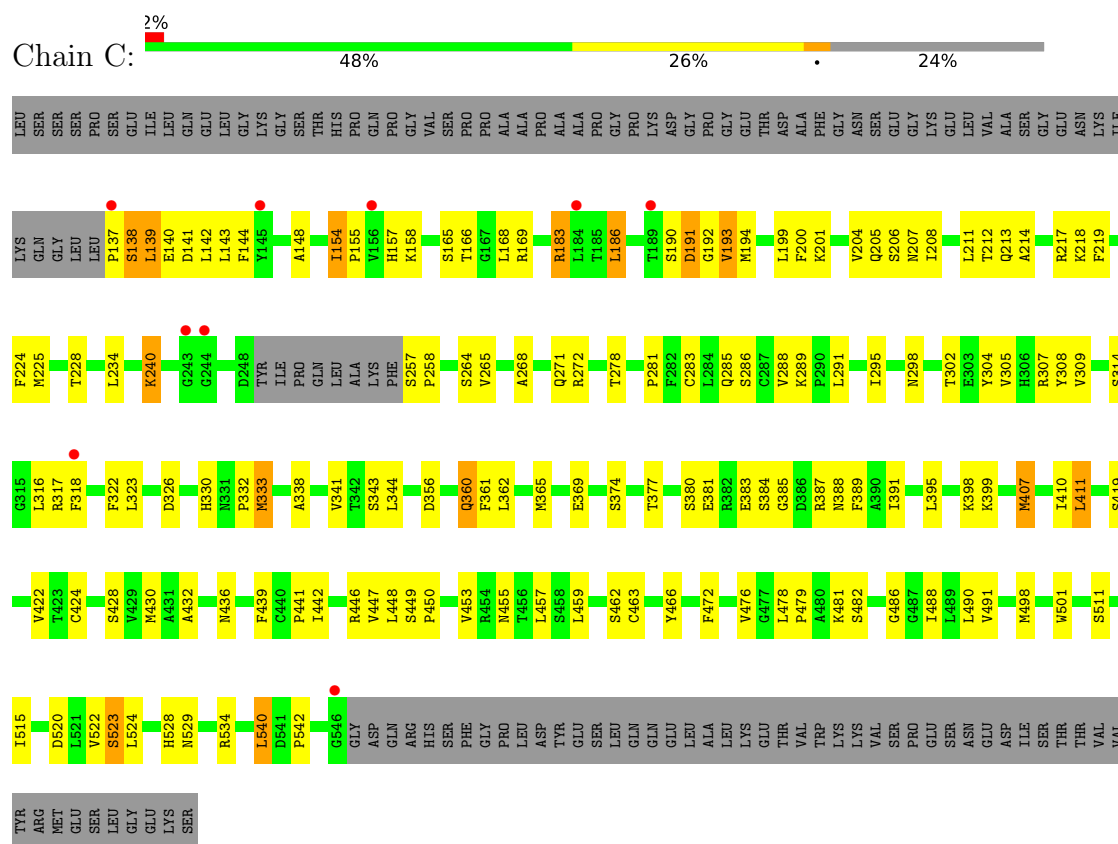
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

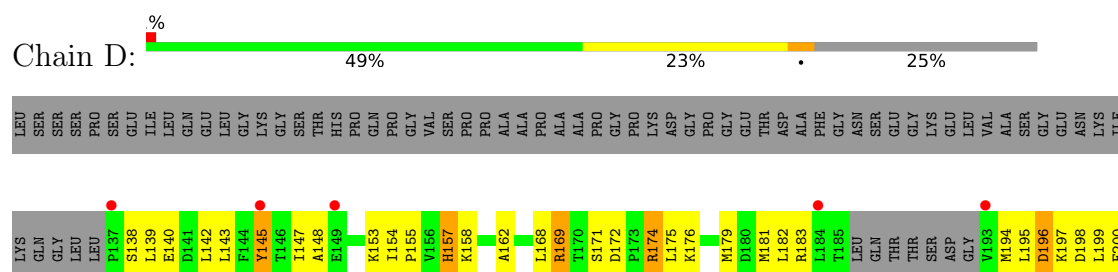


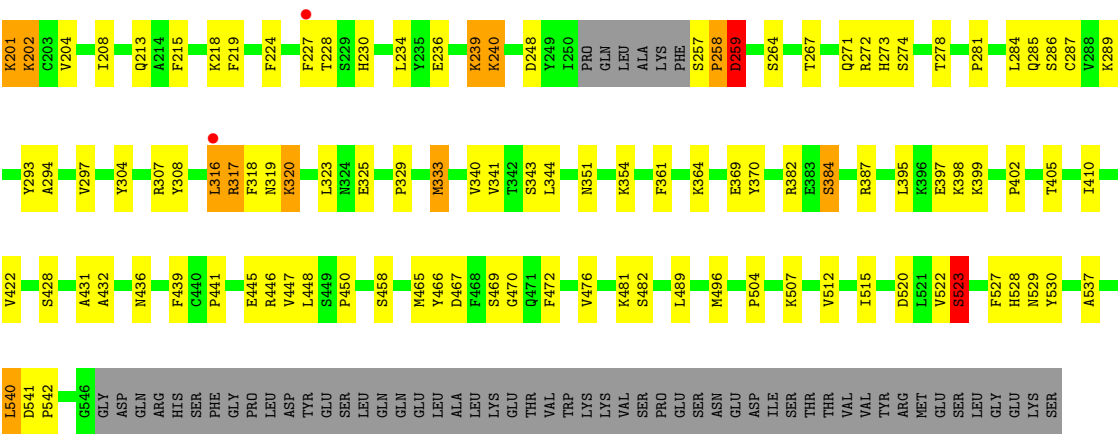


• Molecule 1: Glutaminase kidney isoform, mitochondrial



• Molecule 1: Glutaminase kidney isoform, mitochondrial





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.44Å 138.79Å 179.05Å 90.00° 89.99° 90.00°	Depositor
Resolution (Å)	22.05 – 2.90 22.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (22.05-2.90) 95.7 (22.05-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.89Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.239 , 0.308 0.239 , 0.308	Depositor DCC
$R_{free}$ test set	1603 reflections (2.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	60.8	Xtriage
Anisotropy	1.005	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.40$	Xtriage
Estimated twinning fraction	0.458 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12524	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: Q9S

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	0.62	3/3221 (0.1%)	0.97	21/4347 (0.5%)
1	B	0.59	1/3177 (0.0%)	1.07	24/4284 (0.6%)
1	C	0.56	0/3196	0.93	15/4311 (0.3%)
1	D	0.62	2/3167 (0.1%)	1.15	23/4270 (0.5%)
All	All	0.60	6/12761 (0.0%)	1.03	83/17212 (0.5%)

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	2
1	B	0	3
1	C	0	2
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	ILE	CA-C	-10.62	1.25	1.52
1	A	307	ARG	CG-CD	6.11	1.67	1.51
1	D	145	TYR	CE2-CZ	-5.52	1.31	1.38
1	D	317	ARG	CD-NE	5.48	1.55	1.46
1	B	241	GLN	CA-CB	-5.45	1.42	1.53
1	A	154	ILE	C-O	5.29	1.33	1.23

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	LEU	CB-CG-CD2	-20.77	75.69	111.00
1	D	387	ARG	NE-CZ-NH2	-19.98	110.31	120.30
1	D	317	ARG	NE-CZ-NH1	-18.89	110.86	120.30
1	A	272	ARG	NE-CZ-NH1	-18.18	111.21	120.30
1	D	387	ARG	NE-CZ-NH1	17.95	129.28	120.30
1	B	259	ASP	CB-CG-OD1	16.24	132.92	118.30
1	D	540	LEU	CB-CG-CD2	-13.27	88.45	111.00
1	D	169	ARG	CA-CB-CG	12.38	140.62	113.40
1	C	540	LEU	CB-CG-CD2	-12.15	90.35	111.00
1	B	279	LYS	CD-CE-NZ	11.16	137.37	111.70
1	C	199	LEU	CB-CG-CD2	-10.94	92.40	111.00
1	C	540	LEU	CB-CG-CD1	10.47	128.81	111.00
1	A	182	LEU	CA-CB-CG	10.13	138.60	115.30
1	B	398	LYS	CD-CE-NZ	10.09	134.90	111.70
1	D	317	ARG	NE-CZ-NH2	10.00	125.30	120.30
1	C	154	ILE	CG1-CB-CG2	-9.90	89.62	111.40
1	D	259	ASP	CB-CG-OD1	9.64	126.98	118.30
1	B	199	LEU	CA-CB-CG	9.38	136.88	115.30
1	B	199	LEU	CB-CG-CD1	9.37	126.93	111.00
1	A	217	ARG	NE-CZ-NH2	9.23	124.91	120.30
1	D	540	LEU	CB-CG-CD1	8.81	125.98	111.00
1	D	239	LYS	CB-CG-CD	-8.57	89.33	111.60
1	B	387	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	D	145	TYR	CG-CD2-CE2	8.30	127.94	121.30
1	C	399	LYS	CD-CE-NZ	8.26	130.69	111.70
1	A	307	ARG	CB-CG-CD	8.25	133.05	111.60
1	D	316	LEU	O-C-N	8.20	135.82	122.70
1	A	544	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	B	225	MET	CG-SD-CE	-8.01	87.39	100.20
1	D	169	ARG	CB-CA-C	-8.01	94.39	110.40
1	A	272	ARG	NE-CZ-NH2	7.95	124.28	120.30
1	D	316	LEU	CA-C-N	-7.88	99.86	117.20
1	D	387	ARG	CD-NE-CZ	7.69	134.37	123.60
1	A	217	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	D	145	TYR	CG-CD1-CE1	-7.31	115.45	121.30
1	C	240	LYS	CB-CG-CD	-7.28	92.66	111.60
1	A	272	ARG	CD-NE-CZ	7.24	133.74	123.60
1	B	145	TYR	CB-CG-CD1	-7.23	116.66	121.00
1	B	145	TYR	CB-CG-CD2	7.17	125.30	121.00
1	C	381	GLU	CA-CB-CG	-7.15	97.67	113.40
1	B	259	ASP	N-CA-CB	7.05	123.30	110.60
1	A	154	ILE	O-C-N	-6.98	107.83	121.10
1	B	245	LYS	CB-CG-CD	-6.78	93.96	111.60

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	387	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	272	ARG	CG-CD-NE	6.64	125.75	111.80
1	C	383	GLU	CA-CB-CG	6.61	127.94	113.40
1	D	317	ARG	CB-CG-CD	-6.58	94.48	111.60
1	A	216	ARG	CA-CB-CG	6.56	127.84	113.40
1	A	217	ARG	CG-CD-NE	6.53	125.51	111.80
1	A	272	ARG	CA-CB-CG	-6.49	99.13	113.40
1	B	141	ASP	CB-CG-OD1	6.39	124.05	118.30
1	D	197	LYS	CB-CG-CD	-6.34	95.11	111.60
1	B	176	LYS	CD-CE-NZ	-6.19	97.46	111.70
1	B	387	ARG	CD-NE-CZ	6.05	132.07	123.60
1	C	186	LEU	CA-CB-CG	5.95	128.98	115.30
1	A	540	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	383	GLU	CA-CB-CG	5.84	126.25	113.40
1	C	360	GLN	CB-CA-C	5.68	121.75	110.40
1	D	259	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	D	297	VAL	CG1-CB-CG2	-5.65	101.85	110.90
1	B	225	MET	CB-CG-SD	5.61	129.23	112.40
1	A	318	PHE	CB-CG-CD2	5.57	124.70	120.80
1	A	307	ARG	CG-CD-NE	5.54	123.44	111.80
1	A	216	ARG	CB-CG-CD	5.52	125.94	111.60
1	D	202	LYS	CD-CE-NZ	5.50	124.36	111.70
1	B	245	LYS	CD-CE-NZ	-5.41	99.25	111.70
1	B	141	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	D	240	LYS	CD-CE-NZ	5.36	124.03	111.70
1	C	360	GLN	N-CA-CB	-5.36	100.96	110.60
1	B	524	LEU	CA-CB-CG	5.32	127.53	115.30
1	B	259	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	259	ASP	OD1-CG-OD2	-5.30	113.23	123.30
1	A	544	ARG	CA-CB-CG	5.29	125.03	113.40
1	C	139	LEU	CB-CG-CD2	5.27	119.96	111.00
1	C	398	LYS	CD-CE-NZ	5.27	123.81	111.70
1	D	157	HIS	N-CA-CB	-5.26	101.14	110.60
1	B	512	VAL	CG1-CB-CG2	5.21	119.24	110.90
1	C	139	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	D	399	LYS	CB-CG-CD	-5.16	98.20	111.60
1	A	379	GLN	CA-CB-CG	-5.14	102.09	113.40
1	B	540	LEU	CA-CB-CG	5.10	127.02	115.30
1	A	182	LEU	CB-CG-CD1	-5.03	102.45	111.00
1	C	240	LYS	CG-CD-CE	5.01	126.93	111.90

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	248	ASP	Peptide
1	A	272	ARG	Sidechain
1	B	137	PRO	Peptide
1	B	138	SER	Peptide
1	B	258	PRO	Peptide
1	C	190	SER	Peptide
1	C	191	ASP	Peptide

## 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	3151	0	3122	113	0
1	B	3108	0	3086	120	0
1	C	3128	0	3098	124	0
1	D	3099	0	3070	122	0
2	A	19	0	0	2	0
2	D	19	0	0	0	0
All	All	12524	0	12376	446	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 18.

All (446) 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:272:ARG:NH1	1:A:429:VAL:HG22	1.53	1.24
1:C:139:LEU:CD1	1:C:208:ILE:HG12	1.75	1.16
1:C:139:LEU:HD13	1:C:208:ILE:CG1	1.79	1.12
1:C:139:LEU:HD13	1:C:208:ILE:HG12	1.23	1.07
1:B:535:HIS:HD2	1:C:439:PHE:CD1	1.76	1.03
1:A:346:LYS:HE3	1:A:357:TYR:CG	1.94	1.02
1:A:272:ARG:NH1	1:A:429:VAL:CG2	2.24	1.01
1:A:496:MET:CE	1:A:498:MET:SD	2.49	1.00
1:C:341:VAL:HA	1:C:344:LEU:HD12	1.45	0.99

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:VAL:HA	1:B:344:LEU:HD12	1.43	0.98
1:C:213:GLN:HG2	1:C:218:LYS:HB2	1.47	0.97
1:D:169:ARG:CZ	1:D:272:ARG:NH1	2.30	0.94
1:C:139:LEU:HD12	1:C:140:GLU:N	1.82	0.94
1:A:496:MET:HE2	1:A:498:MET:SD	2.08	0.91
1:D:540:LEU:HD23	1:D:541:ASP:N	1.86	0.91
1:A:181:MET:HE2	1:A:203:CYS:HA	1.54	0.90
1:B:535:HIS:CD2	1:C:439:PHE:CD1	2.60	0.90
1:B:544:ARG:HG3	1:B:545:GLU:H	1.36	0.89
1:A:272:ARG:HH12	1:A:429:VAL:CG2	1.85	0.86
1:C:268:ALA:HB1	1:C:436:ASN:HD22	1.42	0.85
1:D:169:ARG:NH2	1:D:272:ARG:NH1	2.25	0.84
1:D:179:MET:HA	1:D:182:LEU:CD2	2.08	0.83
1:B:318:PHE:HZ	1:C:317:ARG:HG2	1.44	0.81
1:C:424:CYS:O	1:C:428:SER:HB2	1.81	0.81
1:B:148:ALA:HA	1:B:154:ILE:HG21	1.60	0.81
1:B:250:ILE:H	1:B:251:PRO:HD2	1.48	0.79
1:A:266:CYS:HB2	1:A:272:ARG:HE	1.47	0.78
1:A:346:LYS:HE3	1:A:357:TYR:CD1	2.19	0.78
1:B:318:PHE:CZ	1:C:317:ARG:HG2	2.18	0.78
1:D:201:LYS:HE3	1:D:202:LYS:HG3	1.66	0.77
1:A:286:SER:OG	1:A:289:LYS:NZ	2.16	0.77
1:B:143:LEU:HD22	1:B:208:ILE:HD11	1.65	0.77
1:A:341:VAL:HA	1:A:344:LEU:HD12	1.66	0.76
1:C:148:ALA:HA	1:C:154:ILE:HD11	1.66	0.76
1:A:496:MET:HE3	1:A:498:MET:CG	2.16	0.75
1:A:272:ARG:HH11	1:A:429:VAL:HG22	1.51	0.75
1:D:179:MET:HA	1:D:182:LEU:HD22	1.67	0.75
1:B:347:GLN:HE22	1:B:402:PRO:HG2	1.52	0.74
1:C:139:LEU:HD13	1:C:208:ILE:HG13	1.68	0.74
1:D:286:SER:HB2	1:D:289:LYS:HZ3	1.54	0.73
1:D:169:ARG:HG3	1:D:171:SER:OG	1.89	0.73
1:B:495:VAL:HG12	1:B:496:MET:HB2	1.71	0.73
1:D:540:LEU:HD23	1:D:540:LEU:C	2.09	0.73
1:A:169:ARG:NH2	1:A:369:GLU:OE1	2.22	0.72
1:D:139:LEU:HA	1:D:142:LEU:HB2	1.71	0.71
1:B:140:GLU:HA	1:B:208:ILE:HD13	1.73	0.70
1:C:268:ALA:HB1	1:C:436:ASN:ND2	2.06	0.70
1:C:265:VAL:HG12	1:C:498:MET:HG2	1.74	0.70
1:D:402:PRO:O	1:D:405:THR:OG1	2.08	0.70
1:C:264:SER:OG	1:C:278:THR:OG1	2.08	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:535:HIS:HD2	1:C:439:PHE:CE1	2.11	0.68
1:A:174:ARG:O	1:A:207:ASN:ND2	2.26	0.68
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.76	0.68
1:A:496:MET:CE	1:A:498:MET:CG	2.70	0.68
1:C:462:SER:HB2	1:C:463:CYS:SG	2.33	0.68
1:D:341:VAL:HA	1:D:344:LEU:HD12	1.75	0.68
1:A:346:LYS:HE3	1:A:357:TYR:CD2	2.29	0.67
1:B:312:GLU:OE1	1:C:316:LEU:HD11	1.95	0.67
1:D:317:ARG:CG	1:D:317:ARG:HH11	2.07	0.67
1:C:362:LEU:HD22	1:C:430:MET:HE1	1.75	0.67
1:D:286:SER:HG	1:D:466:TYR:HH	0.68	0.67
1:A:286:SER:O	1:A:289:LYS:HG3	1.95	0.66
1:D:319:ASN:ND2	1:D:467:ASP:OD2	2.28	0.66
1:B:529:ASN:ND2	1:C:529:ASN:HD21	1.93	0.66
1:D:447:VAL:HG12	1:D:448:LEU:HG	1.77	0.66
1:B:535:HIS:CD2	1:C:439:PHE:CE1	2.83	0.65
1:C:166:THR:HG21	1:C:214:ALA:HB1	1.78	0.65
1:C:285:GLN:O	1:C:288:VAL:HG12	1.95	0.65
1:B:274:SER:HB3	1:B:278:THR:HG21	1.77	0.65
1:A:407:MET:CE	1:A:411:LEU:HD12	2.27	0.64
1:D:432:ALA:HB1	1:D:441:PRO:HG2	1.78	0.64
1:C:377:THR:HA	1:C:380:SER:HB3	1.79	0.64
1:D:174:ARG:HD3	1:D:174:ARG:H	1.63	0.64
1:B:317:ARG:HG3	1:C:318:PHE:CE2	2.33	0.64
1:A:462:SER:HB2	1:A:463:CYS:SG	2.38	0.63
1:D:155:PRO:HB2	1:D:157:HIS:ND1	2.12	0.63
1:A:407:MET:HE3	1:A:411:LEU:HD12	1.80	0.63
1:A:244:GLY:HA3	1:A:512:VAL:HG21	1.79	0.63
1:A:166:THR:HG21	1:A:214:ALA:HB1	1.81	0.63
1:A:157:HIS:O	1:A:161:THR:HG23	1.99	0.62
1:A:346:LYS:HB3	1:A:354:LYS:HG2	1.82	0.62
1:A:478:LEU:HD13	1:A:490:LEU:HD21	1.82	0.62
1:C:139:LEU:C	1:C:139:LEU:HD12	2.20	0.62
1:D:169:ARG:NH2	1:D:272:ARG:HH12	1.97	0.62
1:C:148:ALA:CA	1:C:154:ILE:HD11	2.30	0.61
1:D:274:SER:HB3	1:D:278:THR:HG21	1.81	0.61
1:D:204:VAL:O	1:D:208:ILE:HB	2.01	0.61
1:A:286:SER:OG	1:A:466:TYR:OH	2.03	0.61
1:A:317:ARG:HB3	1:D:318:PHE:CE2	2.35	0.61
1:C:168:LEU:HD11	1:C:219:PHE:HE2	1.64	0.61
1:B:193:VAL:O	1:B:193:VAL:HG12	2.00	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:ASP:HA	1:C:523:SER:HB3	1.81	0.61
1:C:302:THR:OG1	1:C:455:ASN:OD1	2.18	0.61
1:C:488:ILE:HD11	1:C:511:SER:HB3	1.83	0.61
1:A:537:ALA:HB2	1:D:450:PRO:HG2	1.82	0.60
1:B:148:ALA:HA	1:B:154:ILE:CG2	2.31	0.60
1:A:219:PHE:HB3	1:A:271:GLN:OE1	2.01	0.60
1:A:496:MET:HE3	1:A:498:MET:HG3	1.83	0.60
1:C:144:PHE:O	1:C:148:ALA:N	2.34	0.60
1:D:172:ASP:OD1	1:D:174:ARG:HD3	2.02	0.60
1:D:317:ARG:HG3	1:D:317:ARG:HH11	1.67	0.60
1:D:227:PHE:CZ	1:D:496:MET:HE1	2.37	0.59
1:A:291:LEU:HB3	1:A:365:MET:HE1	1.84	0.59
1:B:529:ASN:HD21	1:C:529:ASN:HD21	1.49	0.59
1:D:155:PRO:HB2	1:D:157:HIS:CE1	2.37	0.59
1:D:140:GLU:HG3	1:D:208:ILE:HD12	1.84	0.59
1:D:181:MET:O	1:D:181:MET:HG3	2.02	0.59
1:B:265:VAL:HG22	1:B:498:MET:HG2	1.85	0.59
1:A:286:SER:HB3	1:A:483:GLY:HA2	1.85	0.59
1:B:314:SER:HB2	1:B:318:PHE:HB2	1.85	0.59
1:A:289:LYS:HD3	1:A:338:ALA:HB2	1.83	0.59
1:C:224:PHE:O	1:C:228:THR:HG23	2.04	0.58
1:A:476:VAL:HA	1:A:522:VAL:HG21	1.85	0.58
1:C:333:MET:HG3	1:C:481:LYS:HD3	1.86	0.58
1:D:171:SER:HA	1:D:176:LYS:NZ	2.19	0.58
1:A:502:SER:O	1:A:511:SER:OG	2.20	0.58
1:A:439:PHE:CZ	1:A:446:ARG:HB2	2.39	0.58
1:D:540:LEU:HD21	1:D:542:PRO:N	2.18	0.58
1:B:439:PHE:CE2	1:B:446:ARG:HB3	2.38	0.58
1:B:145:TYR:HA	1:B:148:ALA:HB3	1.85	0.58
1:A:394:TYR:OH	2:A:601:Q9S:S22	2.58	0.57
1:B:544:ARG:HG3	1:B:545:GLU:N	2.15	0.57
1:D:168:LEU:HD11	1:D:219:PHE:CE2	2.40	0.57
1:D:281:PRO:HB3	1:D:370:TYR:HE2	1.69	0.57
1:B:156:VAL:HG21	1:B:182:LEU:HD11	1.87	0.57
1:B:250:ILE:H	1:B:251:PRO:CD	2.16	0.57
1:B:382:ARG:NH1	1:B:412:ASP:OD2	2.31	0.57
1:C:206:SER:OG	1:C:207:ASN:N	2.38	0.57
1:C:148:ALA:CB	1:C:154:ILE:HD11	2.35	0.57
1:C:264:SER:HG	1:C:278:THR:HG1	1.37	0.57
1:C:476:VAL:HA	1:C:522:VAL:HG11	1.87	0.56
1:C:265:VAL:HG12	1:C:498:MET:HE3	1.87	0.56

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:PHE:CE2	1:D:496:MET:HE1	2.40	0.56
1:C:169:ARG:NH2	1:C:369:GLU:OE2	2.39	0.56
1:A:274:SER:HB3	1:A:278:THR:HG21	1.88	0.56
1:A:365:MET:HG3	1:A:447:VAL:HG11	1.87	0.56
1:A:511:SER:HB3	1:A:514:GLY:H	1.70	0.56
1:D:294:ALA:HB1	1:D:448:LEU:HD22	1.87	0.56
1:D:228:THR:HB	1:D:273:HIS:CE1	2.41	0.56
1:D:540:LEU:HD23	1:D:541:ASP:CA	2.36	0.56
1:C:286:SER:HB2	1:C:466:TYR:OH	2.06	0.56
1:D:139:LEU:HD12	1:D:139:LEU:H	1.70	0.56
1:A:496:MET:HE1	1:A:498:MET:SD	2.43	0.55
1:B:156:VAL:HB	1:B:195:LEU:HD11	1.88	0.55
1:A:496:MET:CE	1:A:498:MET:HG3	2.37	0.55
1:B:529:ASN:HD21	1:C:529:ASN:ND2	2.04	0.55
1:A:388:ASN:HA	1:A:391:ILE:HD12	1.89	0.55
1:B:143:LEU:HD13	1:B:212:THR:HG22	1.89	0.55
1:D:224:PHE:O	1:D:228:THR:HG23	2.07	0.54
1:C:317:ARG:HB3	1:C:318:PHE:HD1	1.71	0.54
1:B:261:TRP:CE3	1:B:502:SER:HB2	2.43	0.54
1:B:196:ASP:OD2	1:B:199:LEU:HD23	2.08	0.54
1:A:151:GLN:HG3	1:A:152:GLU:N	2.23	0.54
1:B:528:HIS:HB3	1:B:531:ASP:OD2	2.07	0.54
1:D:317:ARG:NH1	1:D:320:LYS:NZ	2.56	0.54
1:D:465:MET:H	1:D:469:SER:HB3	1.72	0.53
1:B:522:VAL:HG11	1:B:528:HIS:HB2	1.89	0.53
1:B:535:HIS:CD2	1:C:439:PHE:CG	2.96	0.53
1:C:139:LEU:HD11	1:C:208:ILE:HG12	1.80	0.53
1:A:465:MET:H	1:A:469:SER:HB3	1.73	0.53
1:B:160:ILE:O	1:B:164:LYS:HG3	2.08	0.53
1:C:388:ASN:HA	1:C:391:ILE:HD12	1.90	0.53
1:B:318:PHE:CE2	1:B:321:LEU:HD12	2.43	0.53
1:C:143:LEU:HD22	1:C:200:PHE:HZ	1.74	0.53
1:B:465:MET:H	1:B:469:SER:HB3	1.73	0.53
1:B:354:LYS:HG3	1:B:413:PHE:CE2	2.44	0.53
1:C:168:LEU:HD11	1:C:219:PHE:CE2	2.42	0.53
1:A:316:LEU:O	1:A:316:LEU:HD13	2.09	0.53
1:B:537:ALA:HB2	1:C:450:PRO:HG2	1.91	0.53
1:C:479:PRO:HD2	1:C:491:VAL:O	2.09	0.53
1:C:481:LYS:NZ	1:C:482:SER:O	2.32	0.52
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.90	0.52
1:D:281:PRO:HA	1:D:422:VAL:O	2.09	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:MET:HE2	1:A:408:VAL:HG22	1.92	0.52
1:D:317:ARG:CG	1:D:317:ARG:NH1	2.69	0.52
1:B:162:ALA:HB1	1:B:215:PHE:HE1	1.75	0.52
1:D:201:LYS:CE	1:D:202:LYS:HG3	2.38	0.52
1:D:286:SER:HB2	1:D:289:LYS:NZ	2.22	0.52
1:B:250:ILE:N	1:B:251:PRO:HD2	2.21	0.52
1:D:504:PRO:O	1:D:512:VAL:HG12	2.10	0.52
1:A:436:ASN:ND2	1:A:436:ASN:O	2.42	0.52
1:B:185:THR:HG22	1:B:186:LEU:HD23	1.91	0.52
1:B:427:ALA:HA	1:B:430:MET:CG	2.39	0.52
1:C:219:PHE:HB3	1:C:271:GLN:OE1	2.09	0.52
1:B:434:LEU:HD23	1:B:453:VAL:HG22	1.92	0.51
1:D:140:GLU:HB2	1:D:201:LYS:HG2	1.93	0.51
1:A:316:LEU:O	1:A:319:ASN:ND2	2.42	0.51
1:B:364:LYS:HG2	1:B:445:GLU:OE2	2.11	0.51
1:C:183:ARG:O	1:C:186:LEU:HB3	2.11	0.51
1:A:322:PHE:O	1:A:323:LEU:HD23	2.11	0.51
1:B:139:LEU:H	1:B:139:LEU:HD23	1.76	0.51
1:C:522:VAL:HG21	1:C:528:HIS:HB2	1.93	0.51
1:D:351:ASN:HA	1:D:354:LYS:HG3	1.91	0.51
1:B:185:THR:C	1:B:186:LEU:HD23	2.32	0.50
1:C:338:ALA:HA	1:C:341:VAL:HG22	1.93	0.50
1:D:169:ARG:CZ	1:D:272:ARG:HH11	2.20	0.50
1:C:157:HIS:CD2	1:C:158:LYS:HD3	2.46	0.50
1:D:364:LYS:HB3	1:D:447:VAL:HG22	1.93	0.50
1:B:249:TYR:O	1:B:250:ILE:HG13	2.11	0.50
1:B:186:LEU:HD13	1:B:193:VAL:HG11	1.92	0.50
1:B:156:VAL:CG2	1:B:182:LEU:HD11	2.40	0.50
1:B:377:THR:HA	1:B:380:SER:HB3	1.92	0.50
1:A:202:LYS:HA	1:A:205:GLN:HB2	1.93	0.50
1:B:349:VAL:HG12	1:B:353:GLU:HG3	1.92	0.50
1:B:228:THR:HB	1:B:273:HIS:CE1	2.46	0.50
1:C:332:PRO:HD2	1:C:459:LEU:HD13	1.94	0.50
1:D:148:ALA:HA	1:D:154:ILE:HG22	1.93	0.50
1:D:162:ALA:HB1	1:D:215:PHE:HE1	1.77	0.50
1:A:312:GLU:CD	1:D:316:LEU:HD21	2.32	0.50
1:B:323:LEU:HD13	1:B:327:ASP:HA	1.93	0.50
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.93	0.49
1:C:384:SER:O	1:C:384:SER:OG	2.30	0.49
1:D:304:TYR:HA	1:D:307:ARG:HD2	1.94	0.49
1:A:318:PHE:CE2	1:D:317:ARG:HG2	2.47	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:VAL:CG1	1:A:273:HIS:HB3	2.42	0.49
1:C:478:LEU:HD13	1:C:490:LEU:HD21	1.93	0.49
1:A:224:PHE:O	1:A:228:THR:HG23	2.12	0.49
1:D:472:PHE:CZ	1:D:476:VAL:HG21	2.48	0.49
1:A:425:GLU:O	1:A:428:SER:HB3	2.13	0.49
1:C:447:VAL:HG12	1:C:448:LEU:HG	1.95	0.49
1:A:141:ASP:O	1:A:144:PHE:HB3	2.12	0.49
1:A:139:LEU:HD13	1:A:208:ILE:HG21	1.93	0.49
1:B:530:TYR:OH	1:C:529:ASN:ND2	2.46	0.49
1:A:402:PRO:O	1:A:405:THR:OG1	2.24	0.49
1:B:144:PHE:HE1	1:B:154:ILE:HG12	1.78	0.49
1:D:248:ASP:OD1	1:D:248:ASP:N	2.42	0.49
1:D:523:SER:O	1:D:523:SER:OG	2.31	0.49
1:B:304:TYR:HA	1:B:307:ARG:HD2	1.95	0.49
1:C:139:LEU:CD1	1:C:208:ILE:CG1	2.56	0.49
1:C:139:LEU:HD11	1:C:208:ILE:HG21	1.95	0.49
1:A:143:LEU:HD13	1:A:208:ILE:HD11	1.95	0.48
1:B:467:ASP:HB2	1:B:508:MET:CE	2.43	0.48
1:D:540:LEU:CD2	1:D:542:PRO:N	2.76	0.48
1:A:316:LEU:CD1	1:D:325:GLU:OE1	2.61	0.48
1:C:356:ASP:O	1:C:360:GLN:HB2	2.13	0.48
1:B:379:GLN:HE22	1:B:382:ARG:HH21	1.61	0.48
1:D:431:ALA:HB2	1:D:489:LEU:HD12	1.94	0.48
1:B:522:VAL:CG1	1:B:528:HIS:HB2	2.43	0.48
1:B:239:LYS:HG3	1:B:261:TRP:HD1	1.79	0.48
1:C:191:ASP:HA	1:C:193:VAL:HG13	1.96	0.48
1:A:329:PRO:HG2	1:A:340:VAL:HG21	1.95	0.48
1:B:329:PRO:HG2	1:B:340:VAL:HG21	1.95	0.48
1:A:387:ARG:HH11	1:B:398:LYS:HZ1	1.61	0.48
1:A:317:ARG:HG2	1:D:318:PHE:CZ	2.49	0.48
1:B:239:LYS:HG3	1:B:261:TRP:CD1	2.47	0.48
1:B:432:ALA:HB1	1:B:441:PRO:HG3	1.95	0.48
1:A:195:LEU:HD23	1:A:200:PHE:HA	1.95	0.48
1:A:285:GLN:O	1:A:288:VAL:HG12	2.14	0.48
1:C:457:LEU:HA	1:C:457:LEU:HD23	1.75	0.48
1:A:143:LEU:HD12	1:A:212:THR:HG22	1.96	0.47
1:A:530:TYR:CZ	1:D:529:ASN:ND2	2.82	0.47
1:C:139:LEU:HD11	1:C:140:GLU:OE1	2.14	0.47
1:B:294:ALA:HB1	1:B:448:LEU:HD22	1.97	0.47
1:C:200:PHE:CE1	1:C:204:VAL:HG21	2.49	0.47
1:A:281:PRO:HA	1:A:422:VAL:O	2.13	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ASP:OD2	1:B:259:ASP:C	2.52	0.47
1:C:317:ARG:HB3	1:C:318:PHE:CD1	2.49	0.47
1:C:365:MET:CG	1:C:447:VAL:HG11	2.44	0.47
1:A:479:PRO:HG3	1:D:530:TYR:CE1	2.50	0.47
1:D:143:LEU:O	1:D:147:ILE:HG13	2.15	0.47
1:D:200:PHE:CE2	1:D:204:VAL:HG21	2.50	0.47
1:A:530:TYR:OH	1:D:529:ASN:ND2	2.47	0.47
1:B:283:CYS:HB3	1:B:419:SER:HA	1.95	0.47
1:D:195:LEU:HB3	1:D:199:LEU:HB3	1.96	0.47
1:D:264:SER:HB2	1:D:428:SER:OG	2.14	0.47
1:B:347:GLN:NE2	1:B:402:PRO:HG2	2.25	0.47
1:C:154:ILE:HG22	1:C:155:PRO:O	2.15	0.47
1:A:318:PHE:CD1	1:D:318:PHE:HZ	2.33	0.47
1:B:224:PHE:O	1:B:228:THR:HG23	2.14	0.47
1:C:308:TYR:CD2	1:C:344:LEU:HD21	2.50	0.47
1:D:138:SER:C	1:D:142:LEU:HD13	2.35	0.47
1:A:181:MET:O	1:A:185:THR:HG23	2.16	0.47
1:D:323:LEU:HD21	1:D:395:LEU:CD2	2.45	0.47
1:A:267:THR:HA	1:A:496:MET:HA	1.97	0.46
1:C:138:SER:OG	1:C:141:ASP:OD1	2.31	0.46
1:D:257:SER:N	1:D:258:PRO:HD3	2.30	0.46
1:B:316:LEU:HD12	1:B:319:ASN:HD21	1.81	0.46
1:D:140:GLU:HA	1:D:208:ILE:CD1	2.45	0.46
1:D:439:PHE:CZ	1:D:446:ARG:HB2	2.50	0.46
1:C:387:ARG:HG3	1:C:388:ASN:N	2.31	0.46
1:C:391:ILE:HG22	1:C:395:LEU:HD12	1.97	0.46
1:A:172:ASP:OD1	1:A:174:ARG:HG2	2.15	0.46
1:B:289:LYS:HA	1:B:292:LYS:HE2	1.98	0.46
1:C:268:ALA:CB	1:C:436:ASN:HD22	2.20	0.46
1:D:284:LEU:O	1:D:287:CYS:HB2	2.16	0.46
1:C:165:SER:HB3	1:C:225:MET:HE1	1.97	0.46
1:C:486:GLY:O	1:C:501:TRP:HA	2.16	0.46
1:C:488:ILE:HD11	1:C:511:SER:CB	2.46	0.46
1:D:439:PHE:CE2	1:D:446:ARG:HB2	2.50	0.46
1:B:160:ILE:HG13	1:B:161:THR:N	2.29	0.46
1:B:315:GLY:C	1:B:317:ARG:H	2.19	0.46
1:D:472:PHE:CE1	1:D:476:VAL:HG21	2.49	0.46
1:B:281:PRO:HA	1:B:422:VAL:O	2.16	0.46
1:B:332:PRO:HD2	1:B:459:LEU:HD13	1.98	0.46
1:B:472:PHE:CE1	1:B:476:VAL:HG21	2.51	0.46
1:C:137:PRO:O	1:C:138:SER:HB3	2.16	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:HD22	1:C:200:PHE:CZ	2.50	0.46
1:B:176:LYS:HA	1:B:176:LYS:HD2	1.50	0.46
1:B:140:GLU:HG3	1:B:208:ILE:HG21	1.97	0.46
1:C:365:MET:SD	1:C:448:LEU:HD11	2.56	0.46
1:A:312:GLU:OE1	1:D:470:GLY:HA3	2.16	0.46
1:D:540:LEU:HD21	1:D:542:PRO:CG	2.46	0.46
1:C:472:PHE:CZ	1:C:476:VAL:HG21	2.51	0.45
1:A:484:VAL:HA	1:A:505:LEU:HD11	1.97	0.45
1:A:540:LEU:HD23	1:A:541:ASP:N	2.31	0.45
1:B:156:VAL:HG21	1:B:182:LEU:HD21	1.97	0.45
1:C:387:ARG:O	1:C:391:ILE:HG13	2.16	0.45
1:D:175:LEU:HA	1:D:175:LEU:HD23	1.79	0.45
1:D:319:ASN:N	1:D:319:ASN:OD1	2.45	0.45
1:A:316:LEU:HD12	1:D:325:GLU:OE1	2.16	0.45
1:B:350:ASN:OD1	1:B:353:GLU:HG2	2.15	0.45
1:A:204:VAL:HB	1:A:211:LEU:HD13	1.98	0.45
1:A:332:PRO:HD2	1:A:459:LEU:HD13	1.98	0.45
1:A:472:PHE:CZ	1:A:476:VAL:HG21	2.51	0.45
1:D:169:ARG:HB2	1:D:171:SER:H	1.81	0.45
1:C:322:PHE:O	1:C:323:LEU:HD23	2.16	0.45
1:B:308:TYR:CD2	1:B:344:LEU:HD21	2.52	0.45
1:B:336:ALA:O	1:B:340:VAL:HG23	2.16	0.45
1:C:449:SER:O	1:C:453:VAL:HG12	2.16	0.45
1:D:213:GLN:HE22	1:D:218:LYS:HD3	1.82	0.45
1:C:281:PRO:HA	1:C:422:VAL:O	2.16	0.45
1:C:283:CYS:HB3	1:C:419:SER:HA	1.98	0.45
1:C:200:PHE:O	1:C:204:VAL:HG22	2.17	0.44
1:B:139:LEU:H	1:B:139:LEU:CD2	2.30	0.44
1:A:457:LEU:HA	1:A:457:LEU:HD23	1.67	0.44
1:C:540:LEU:HD12	1:C:542:PRO:HG3	1.98	0.44
1:D:317:ARG:NH1	1:D:320:LYS:HZ1	2.14	0.44
1:A:338:ALA:HA	1:A:341:VAL:HG22	2.00	0.44
1:A:450:PRO:HG2	1:D:537:ALA:HB2	1.98	0.44
1:A:507:LYS:HD3	1:A:507:LYS:HA	1.38	0.44
1:C:234:LEU:HD21	1:C:524:LEU:HD12	1.99	0.44
1:A:192:GLY:C	1:A:194:MET:H	2.20	0.44
1:A:544:ARG:HG3	1:A:545:GLU:OE1	2.18	0.44
1:D:304:TYR:CZ	1:D:308:TYR:HE2	2.36	0.44
1:D:520:ASP:HA	1:D:523:SER:HB3	1.99	0.44
1:A:346:LYS:NZ	1:A:357:TYR:CE1	2.80	0.44
1:D:329:PRO:HG2	1:D:340:VAL:HG11	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:GLN:HG3	1:A:152:GLU:H	1.82	0.44
1:C:204:VAL:HB	1:C:211:LEU:HD13	1.98	0.44
1:A:140:GLU:HG2	1:A:201:LYS:O	2.18	0.43
1:B:427:ALA:HA	1:B:430:MET:HG2	1.99	0.43
1:D:445:GLU:HG3	1:D:446:ARG:N	2.33	0.43
1:B:267:THR:HA	1:B:496:MET:HA	2.00	0.43
1:D:540:LEU:CD2	1:D:542:PRO:CD	2.96	0.43
1:B:481:LYS:NZ	1:B:482:SER:O	2.49	0.43
1:D:213:GLN:NE2	1:D:218:LYS:HD3	2.33	0.43
1:D:267:THR:HA	1:D:496:MET:HA	2.01	0.43
1:A:239:LYS:HG2	1:A:239:LYS:O	2.18	0.43
1:A:346:LYS:CE	1:A:357:TYR:CD2	3.00	0.43
1:B:186:LEU:HD22	1:B:193:VAL:HG13	2.00	0.43
1:B:410:ILE:HA	1:B:410:ILE:HD13	1.91	0.43
1:C:304:TYR:HA	1:C:307:ARG:HD2	2.01	0.43
1:D:196:ASP:CG	1:D:199:LEU:HD23	2.38	0.43
1:B:285:GLN:O	1:B:288:VAL:HG12	2.18	0.43
1:B:479:PRO:HD2	1:B:491:VAL:O	2.18	0.43
1:C:457:LEU:HD11	1:C:491:VAL:HG11	2.01	0.43
1:D:522:VAL:CG1	1:D:528:HIS:HB2	2.48	0.43
1:A:374:SER:HB2	1:A:421:GLU:OE2	2.17	0.43
1:C:318:PHE:CD1	1:C:318:PHE:N	2.86	0.43
1:B:208:ILE:HA	1:B:211:LEU:HB2	2.01	0.43
1:C:272:ARG:NH2	1:C:442:ILE:HG21	2.34	0.43
1:D:431:ALA:HB2	1:D:489:LEU:CD1	2.49	0.43
1:A:465:MET:CE	1:A:510:ASN:HD22	2.32	0.42
1:C:522:VAL:CG2	1:C:528:HIS:HB2	2.49	0.42
1:B:436:ASN:HD21	1:C:534:ARG:NH1	2.17	0.42
1:C:291:LEU:O	1:C:295:ILE:HG13	2.19	0.42
1:D:465:MET:HE2	1:D:515:ILE:HD11	2.01	0.42
1:A:283:CYS:HB3	1:A:419:SER:HA	2.00	0.42
1:B:457:LEU:HA	1:B:457:LEU:HD23	1.82	0.42
1:C:204:VAL:O	1:C:208:ILE:HB	2.20	0.42
1:B:318:PHE:CE1	1:C:318:PHE:CE1	3.07	0.42
1:C:365:MET:HG2	1:C:447:VAL:HG11	2.01	0.42
1:B:318:PHE:CE1	1:C:318:PHE:HE1	2.37	0.42
1:B:349:VAL:CG1	1:B:353:GLU:HG3	2.49	0.42
1:B:430:MET:H	1:B:430:MET:HG2	1.68	0.42
1:B:268:ALA:HB1	1:B:436:ASN:HD22	1.84	0.42
1:B:261:TRP:HE3	1:B:502:SER:HB2	1.82	0.42
1:D:179:MET:O	1:D:183:ARG:HB2	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:317:ARG:HA	1:D:317:ARG:HD2	1.50	0.42
1:A:244:GLY:CA	1:A:512:VAL:HG21	2.49	0.42
1:A:192:GLY:O	1:A:194:MET:N	2.49	0.42
1:B:286:SER:HB3	1:B:289:LYS:HD2	2.01	0.42
1:B:506:ASP:HB3	1:B:512:VAL:HG22	2.02	0.42
1:C:155:PRO:HA	1:C:194:MET:HG2	2.01	0.42
1:C:208:ILE:O	1:C:212:THR:HG23	2.19	0.42
1:C:343:SER:HA	1:C:410:ILE:HD12	2.02	0.42
1:D:138:SER:O	1:D:142:LEU:HD12	2.20	0.42
1:D:236:GLU:O	1:D:239:LYS:HB3	2.20	0.42
1:D:293:TYR:CD2	1:D:333:MET:HE1	2.54	0.42
1:D:540:LEU:HD21	1:D:542:PRO:HG3	2.02	0.42
1:A:407:MET:HE1	1:A:411:LEU:HD12	2.00	0.42
1:A:377:THR:HA	1:A:380:SER:HB2	2.02	0.42
1:C:191:ASP:OD2	1:C:192:GLY:N	2.49	0.42
1:C:289:LYS:HZ2	1:C:289:LYS:HG2	1.75	0.42
1:D:481:LYS:NZ	1:D:482:SER:O	2.50	0.42
1:A:272:ARG:HH11	1:A:429:VAL:CG2	2.21	0.41
2:A:601:Q9S:N27	1:B:323:LEU:HB2	2.35	0.41
1:B:235:TYR:HD1	1:B:263:VAL:HG12	1.84	0.41
1:C:142:LEU:HD23	1:C:142:LEU:HA	1.66	0.41
1:C:387:ARG:HB3	1:D:397:GLU:HG3	2.02	0.41
1:A:224:PHE:CD1	1:A:271:GLN:NE2	2.88	0.41
1:A:308:TYR:CD2	1:A:344:LEU:HD21	2.55	0.41
1:C:457:LEU:HD22	1:C:479:PRO:HB2	2.01	0.41
1:D:527:PHE:HZ	1:D:542:PRO:HG2	1.85	0.41
1:B:204:VAL:O	1:B:208:ILE:N	2.54	0.41
1:C:432:ALA:HB1	1:C:441:PRO:HG2	2.02	0.41
1:A:345:ILE:O	1:A:354:LYS:HD2	2.20	0.41
1:A:432:ALA:HB1	1:A:441:PRO:HG2	2.02	0.41
1:A:515:ILE:HD13	1:A:515:ILE:HA	1.88	0.41
1:B:443:THR:OG1	1:B:445:GLU:HG2	2.21	0.41
1:B:490:LEU:HB3	1:B:498:MET:HB2	2.03	0.41
1:C:407:MET:HE3	1:C:411:LEU:HD11	2.01	0.41
1:D:219:PHE:HB3	1:D:271:GLN:OE1	2.21	0.41
1:C:201:LYS:O	1:C:205:GLN:HB2	2.20	0.41
1:D:155:PRO:HG2	1:D:158:LYS:HB3	2.03	0.41
1:D:208:ILE:HG12	1:D:208:ILE:O	2.20	0.41
1:D:230:HIS:O	1:D:234:LEU:HG	2.21	0.41
1:D:258:PRO:O	1:D:259:ASP:O	2.39	0.41
1:B:439:PHE:CZ	1:B:446:ARG:HB3	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:VAL:HG12	1:A:350:ASN:N	2.35	0.41
1:B:208:ILE:O	1:B:212:THR:HG23	2.21	0.41
1:B:401:PHE:HB3	1:B:405:THR:OG1	2.20	0.41
1:C:305:VAL:O	1:C:309:VAL:HG12	2.21	0.41
1:D:285:GLN:NE2	1:D:285:GLN:HA	2.36	0.41
1:A:290:PRO:HD3	1:A:481:LYS:HG2	2.03	0.41
1:C:515:ILE:HA	1:C:515:ILE:HD13	1.88	0.41
1:A:200:PHE:CE1	1:A:204:VAL:HG21	2.56	0.41
1:B:382:ARG:HD3	1:B:412:ASP:OD2	2.21	0.41
1:C:143:LEU:HD23	1:C:143:LEU:O	2.21	0.41
1:D:194:MET:C	1:D:195:LEU:HD12	2.41	0.41
1:D:465:MET:CE	1:D:515:ILE:HD11	2.51	0.41
1:A:228:THR:HB	1:A:273:HIS:CE1	2.56	0.40
1:B:345:ILE:O	1:B:354:LYS:HE2	2.21	0.40
1:B:279:LYS:HA	1:B:423:THR:HB	2.03	0.40
1:C:385:GLY:O	1:C:389:PHE:HD2	2.04	0.40
1:D:522:VAL:HG11	1:D:528:HIS:HB2	2.03	0.40
1:A:143:LEU:HD23	1:A:143:LEU:O	2.21	0.40
1:B:177:GLU:H	1:B:177:GLU:CD	2.25	0.40
1:B:158:LYS:O	1:B:158:LYS:HG2	2.20	0.40
1:B:534:ARG:NH1	1:C:436:ASN:HD21	2.19	0.40
1:C:407:MET:O	1:C:411:LEU:HD12	2.21	0.40
1:D:272:ARG:NH2	1:D:369:GLU:OE2	2.54	0.40
1:D:384:SER:O	1:D:384:SER:OG	2.35	0.40
1:D:410:ILE:HA	1:D:410:ILE:HD13	1.85	0.40
1:C:314:SER:HB3	1:C:330:HIS:CD2	2.57	0.40
1:D:168:LEU:HD11	1:D:219:PHE:CZ	2.55	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	400/527 (76%)	377 (94%)	20 (5%)	3 (1%)	19	51
1	B	392/527 (74%)	369 (94%)	20 (5%)	3 (1%)	19	51
1	C	398/527 (76%)	375 (94%)	20 (5%)	3 (1%)	19	51
1	D	391/527 (74%)	370 (95%)	19 (5%)	2 (0%)	29	61
All	All	1581/2108 (75%)	1491 (94%)	79 (5%)	11 (1%)	22	54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	259	ASP
1	D	259	ASP
1	A	193	VAL
1	B	545	GLU
1	C	193	VAL
1	D	523	SER
1	B	250	ILE
1	C	138	SER
1	B	138	SER
1	A	258	PRO
1	C	258	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	350/451 (78%)	332 (95%)	18 (5%)	24	56
1	B	344/451 (76%)	328 (95%)	16 (5%)	26	59
1	C	347/451 (77%)	334 (96%)	13 (4%)	34	68
1	D	343/451 (76%)	324 (94%)	19 (6%)	21	53
All	All	1384/1804 (77%)	1318 (95%)	66 (5%)	25	58

All (66) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	138	SER
1	A	157	HIS
1	A	163	LEU
1	A	174	ARG
1	A	181	MET
1	A	196	ASP
1	A	242	SER
1	A	259	ASP
1	A	314	SER
1	A	317	ARG
1	A	360	GLN
1	A	361	PHE
1	A	379	GLN
1	A	384	SER
1	A	399	LYS
1	A	436	ASN
1	A	446	ARG
1	A	544	ARG
1	B	181	MET
1	B	183	ARG
1	B	264	SER
1	B	279	LYS
1	B	317	ARG
1	B	319	ASN
1	B	326	ASP
1	B	333	MET
1	B	343	SER
1	B	361	PHE
1	B	374	SER
1	B	380	SER
1	B	398	LYS
1	B	416	GLN
1	B	446	ARG
1	B	539	LYS
1	C	183	ARG
1	C	217	ARG
1	C	240	LYS
1	C	257	SER
1	C	298	ASN
1	C	326	ASP
1	C	333	MET
1	C	361	PHE
1	C	374	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	407	MET
1	C	411	LEU
1	C	446	ARG
1	C	523	SER
1	D	145	TYR
1	D	153	LYS
1	D	174	ARG
1	D	196	ASP
1	D	198	ASP
1	D	201	LYS
1	D	240	LYS
1	D	258	PRO
1	D	320	LYS
1	D	333	MET
1	D	343	SER
1	D	361	PHE
1	D	382	ARG
1	D	384	SER
1	D	398	LYS
1	D	436	ASN
1	D	458	SER
1	D	507	LYS
1	D	523	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	GLN
1	A	510	ASN
1	A	529	ASN
1	A	532	ASN
1	B	347	GLN
1	B	436	ASN
1	B	461	HIS
1	B	529	ASN
1	B	535	HIS
1	C	207	ASN
1	C	271	GLN
1	C	436	ASN
1	C	461	HIS
1	C	510	ASN
1	D	213	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	461	HIS
1	D	529	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	Q9S	D	601	-	13,21,21	3.54	6 (46%)	8,29,29	1.82	3 (37%)
2	Q9S	A	601	-	13,21,21	3.39	6 (46%)	8,29,29	2.35	4 (50%)

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	Q9S	D	601	-	-	2/4/18/18	0/3/3/3

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Q9S	A	601	-	-	2/4/18/18	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	Q9S	C23-N03	8.51	1.45	1.32
2	A	601	Q9S	C23-N03	7.91	1.44	1.32
2	D	601	Q9S	C02-N03	5.20	1.54	1.46
2	A	601	Q9S	C02-N03	5.01	1.54	1.46
2	A	601	Q9S	C04-N03	4.35	1.53	1.46
2	D	601	Q9S	C04-N03	3.91	1.52	1.46
2	A	601	Q9S	C11-N12	3.79	1.46	1.35
2	D	601	Q9S	O07-C08	3.76	1.41	1.36
2	D	601	Q9S	C26-N27	3.64	1.45	1.35
2	D	601	Q9S	C11-N12	3.63	1.45	1.35
2	A	601	Q9S	C26-N27	3.56	1.45	1.35
2	A	601	Q9S	O07-C08	2.79	1.40	1.36

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	Q9S	C02-C01-C06	3.96	114.67	110.32
2	A	601	Q9S	C01-C02-N03	3.51	118.34	111.10
2	D	601	Q9S	C01-C02-N03	3.46	118.24	111.10
2	D	601	Q9S	C02-C01-C06	3.04	113.66	110.32
2	A	601	Q9S	C04-C05-C06	-2.65	107.40	110.32
2	A	601	Q9S	C05-C06-C01	-2.62	106.69	111.74
2	D	601	Q9S	C05-C06-C01	-2.02	107.83	111.74

There are no chirality outliers.

All (4) torsion outliers are listed below:

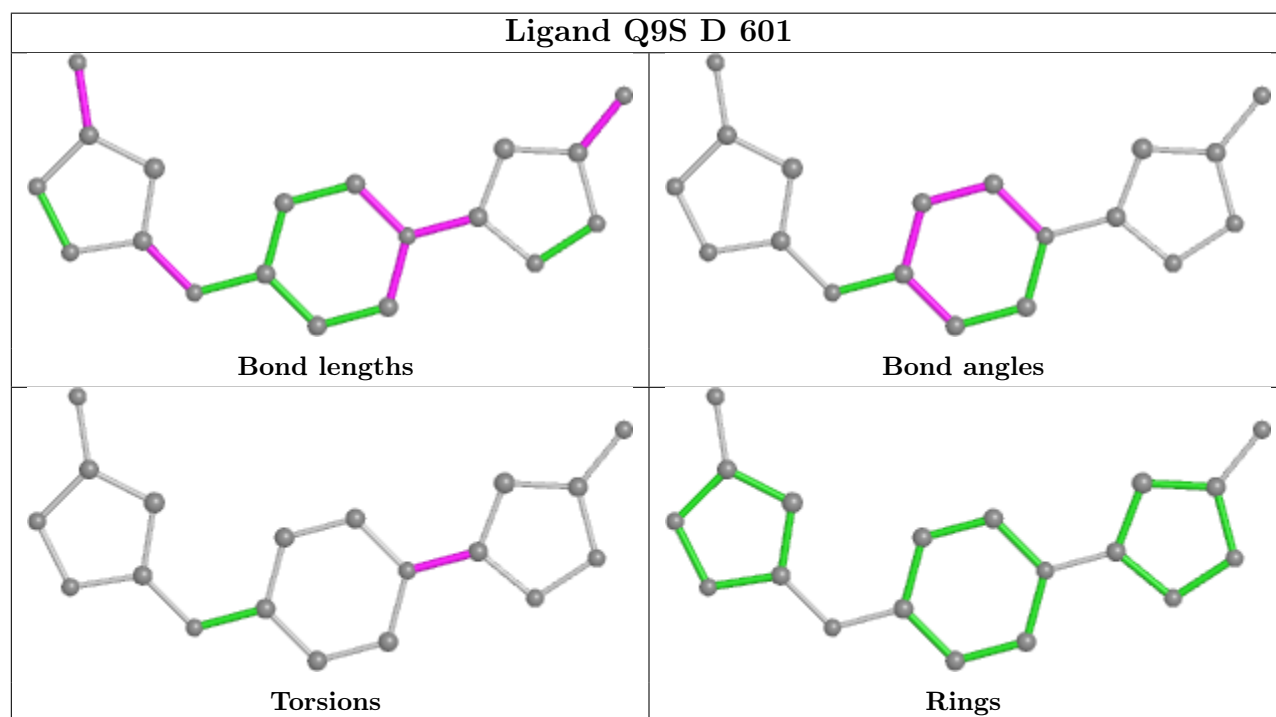
Mol	Chain	Res	Type	Atoms
2	D	601	Q9S	S37-C23-N03-C02
2	D	601	Q9S	S37-C23-N03-C04
2	A	601	Q9S	S37-C23-N03-C02
2	A	601	Q9S	S37-C23-N03-C04

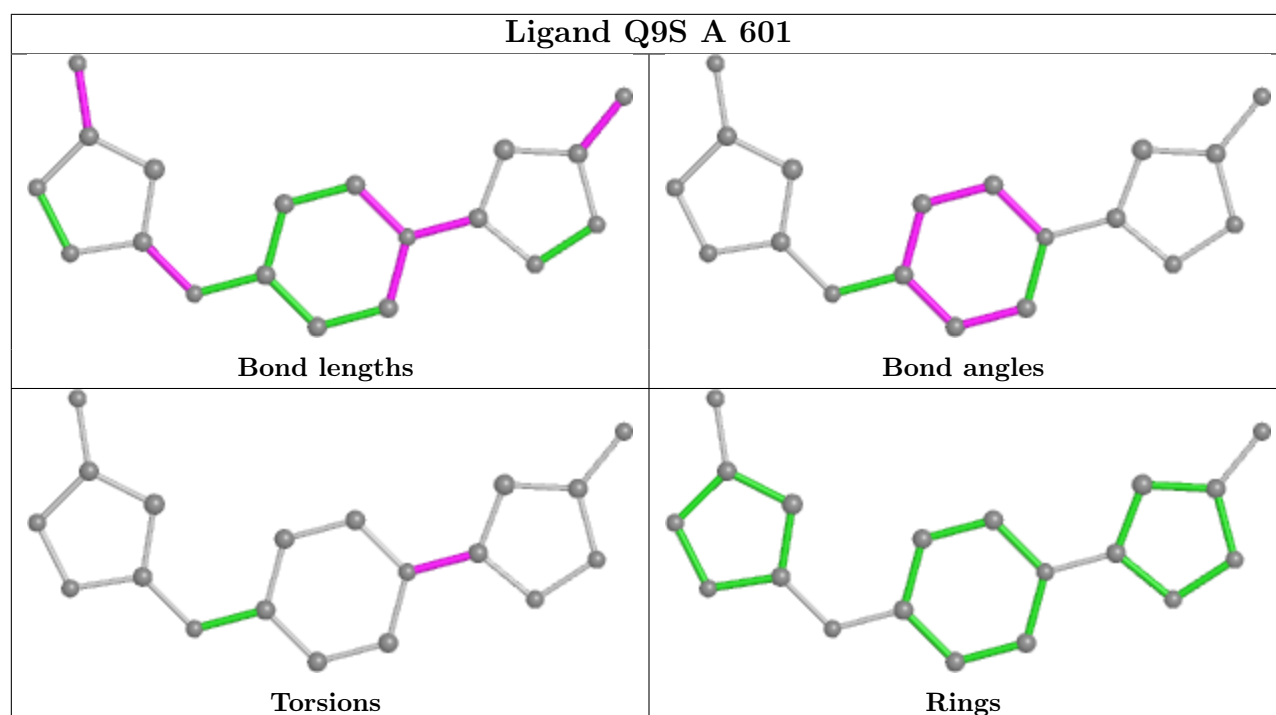
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	Q9S	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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	404/527 (76%)	0.06	5 (1%) 79 79	50, 88, 159, 246	0
1	B	398/527 (75%)	0.06	7 (1%) 68 67	52, 86, 163, 206	0
1	C	402/527 (76%)	0.06	9 (2%) 62 59	46, 88, 160, 230	0
1	D	397/527 (75%)	0.03	7 (1%) 68 67	51, 87, 165, 232	0
All	All	1601/2108 (75%)	0.05	28 (1%) 70 69	46, 87, 163, 246	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	318	PHE	5.6
1	A	545	GLU	5.0
1	B	249	TYR	4.3
1	B	546	GLY	4.0
1	B	152	GLU	3.8
1	C	156	VAL	3.6
1	D	184	LEU	3.5
1	B	150	GLY	3.5
1	C	145	TYR	3.3
1	B	184	LEU	3.2
1	C	137	PRO	3.1
1	C	184	LEU	3.1
1	D	316	LEU	3.0
1	A	244	GLY	2.9
1	D	193	VAL	2.9
1	A	248	ASP	2.8
1	C	189	THR	2.7
1	A	512	VAL	2.6
1	D	145	TYR	2.5
1	D	137	PRO	2.4
1	C	546	GLY	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	318	PHE	2.3
1	B	151	GLN	2.3
1	B	193	VAL	2.2
1	C	244	GLY	2.2
1	C	243	GLY	2.1
1	D	227	PHE	2.1
1	D	149	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

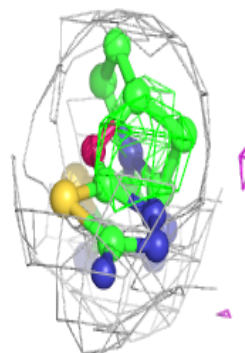
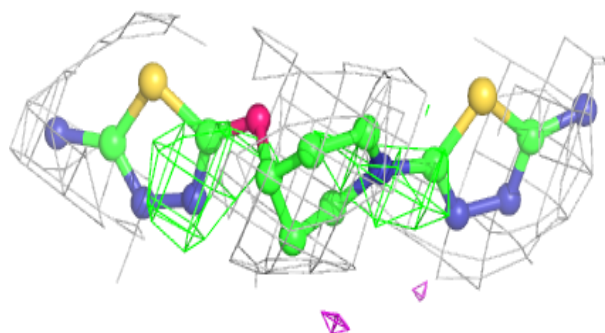
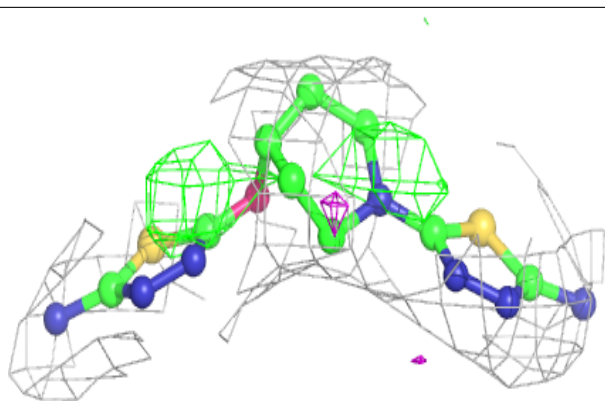
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	Q9S	A	601	19/19	0.95	0.22	58,84,103,110	0
2	Q9S	D	601	19/19	0.96	0.19	48,79,113,117	0

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.

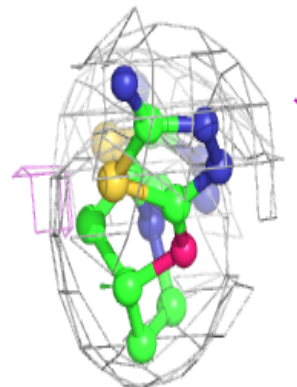
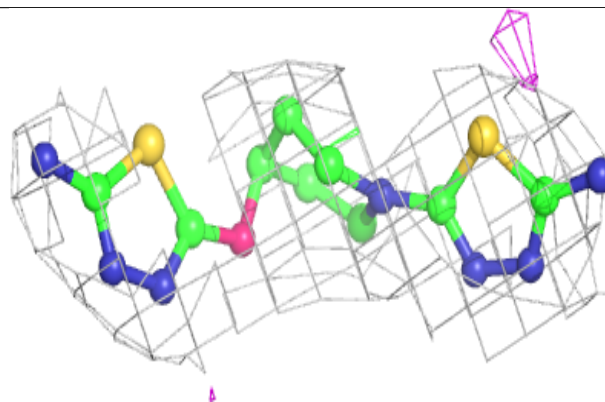
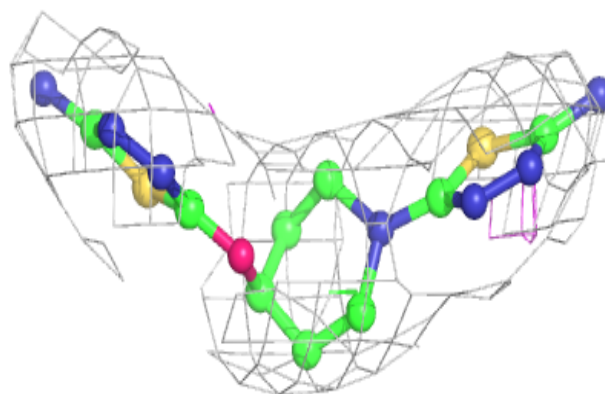


**Electron density around Q9S A 601:**

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

**Electron density around Q9S D 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.