



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:29 AM UTC

PDB ID : 6UL9 / pdb_00006ul9
Title : Crystal structure of human GAC in complex with inhibitor UPGL00023
Authors : Huang, Q.Q.; Cerione, R.A.
Deposited on : 2019-10-07
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

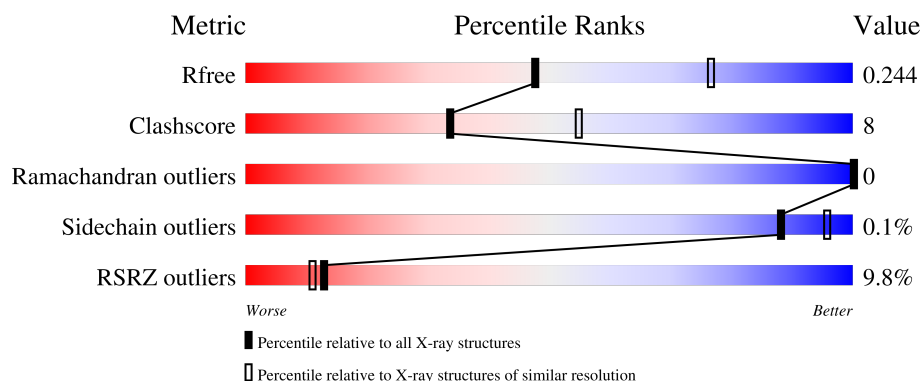
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	527	8% 64% 12% • 24%
1	B	527	8% 63% 14% 22%
1	C	527	8% 66% 11% 22%
1	D	527	6% 66% 12% 22%

2 Entry composition [i](#)

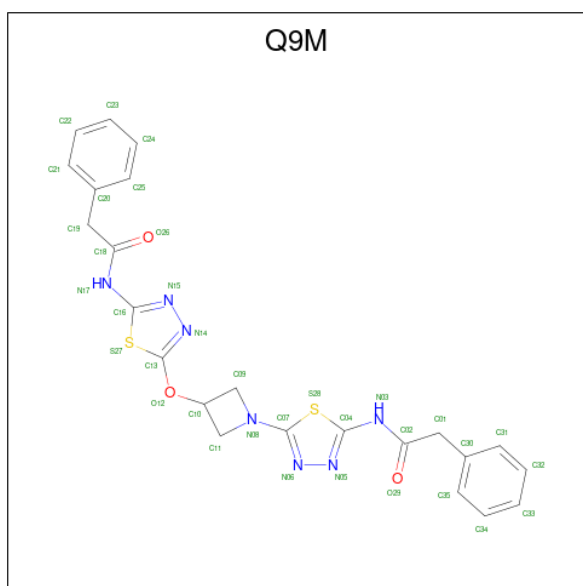
There are 3 unique types of molecules in this entry. The entry contains 13389 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	402	Total	C	N	O	S	1	0	0
			3135	1996	530	581	28			
1	B	409	Total	C	N	O	S	1	0	0
			3192	2036	539	589	28			
1	C	410	Total	C	N	O	S	1	0	0
			3196	2038	540	590	28			
1	D	409	Total	C	N	O	S	1	0	0
			3192	2036	539	589	28			

- Molecule 2 is 2-phenyl-N-{5-[(1-{5-[(phenylacetyl)amino]-1,3,4-thiadiazol-2-yl}azetidin-3-yl)oxy]-1,3,4-thiadiazol-2-yl}acetamide (CCD ID: Q9M) (formula: C₂₃H₂₁N₇O₃S₂) (labeled as "Ligand of Interest" by depositor).



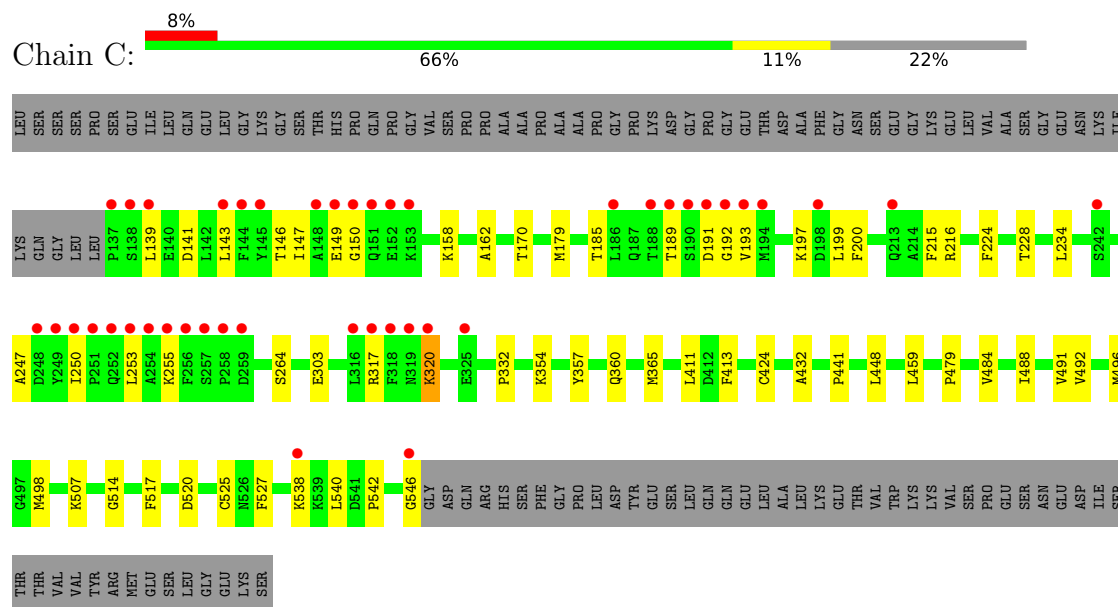
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	S	0	0
			35	23	7	3	2		

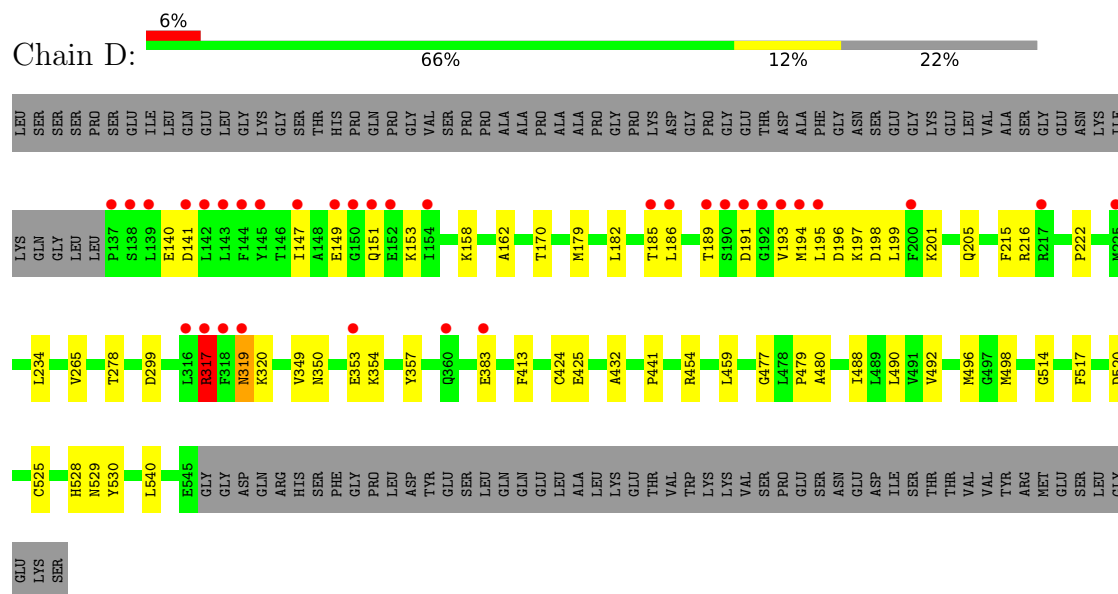
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	160	Total	O	0	0
			160	160		
3	B	156	Total	O	0	0
			156	156		
3	C	133	Total	O	0	0
			133	133		
3	D	155	Total	O	0	0
			155	155		

- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.88Å 138.24Å 176.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.94 – 2.50 48.94 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.94-2.50) 99.2 (48.94-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.192 , 0.244 0.193 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (2.40%)	wwPDB-VP
Wilson B-factor (Å ²)	25.5	Xtriage
Anisotropy	0.591	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13389	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.1778e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: Q9M

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	0.43	0/3204	0.73	9/4323 (0.2%)
1	B	0.40	0/3264	0.65	1/4406 (0.0%)
1	C	0.39	0/3268	0.69	5/4411 (0.1%)
1	D	0.37	0/3264	0.63	2/4406 (0.0%)
All	All	0.40	0/13000	0.67	17/17546 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	THR	CA-C-N	-8.87	107.92	122.65
1	A	185	THR	C-N-CA	-8.87	107.92	122.65
1	C	538	LYS	CD-CE-NZ	-8.35	85.20	111.90
1	A	176	LYS	CA-CB-CG	-8.23	97.63	114.10
1	D	383	GLU	CA-CB-CG	7.63	129.36	114.10
1	A	176	LYS	CB-CG-CD	6.29	125.76	111.30
1	C	538	LYS	CB-CG-CD	-6.09	97.28	111.30
1	A	202	LYS	CA-CB-CG	6.07	126.24	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	GLY	N-CA-C	5.95	123.05	114.67
1	A	325	GLU	N-CA-CB	-5.81	101.28	110.28
1	C	320	LYS	CG-CD-CE	-5.53	98.58	111.30
1	C	149	GLU	CA-CB-CG	5.39	124.88	114.10
1	A	320	LYS	CA-CB-CG	5.33	124.77	114.10
1	A	190	SER	CA-C-N	-5.22	115.05	122.41
1	A	190	SER	C-N-CA	-5.22	115.05	122.41
1	B	205	GLN	CA-CB-CG	5.10	124.31	114.10
1	D	317	ARG	CA-CB-CG	-5.04	104.02	114.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	ARG	Peptide
1	B	317	ARG	Peptide
1	C	317	ARG	Peptide
1	D	317	ARG	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	3135	0	3106	46	2
1	B	3192	0	3171	66	1
1	C	3196	0	3174	37	1
1	D	3192	0	3171	53	0
2	B	35	0	0	2	0
2	D	35	0	0	1	1
3	A	160	0	0	3	0
3	B	156	0	0	2	1
3	C	133	0	0	1	0
3	D	155	0	0	3	0
All	All	13389	0	12622	196	3

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 8.

All (196) 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:B:139:LEU:O	1:B:143:LEU:HD13	1.28	1.32
1:D:151:GLN:HE22	1:D:194:MET:HE1	1.17	1.08
1:A:186:LEU:HD22	1:A:193:VAL:HG21	1.35	1.07
1:C:185:THR:O	1:C:189:THR:OG1	1.87	0.91
1:B:139:LEU:O	1:B:143:LEU:CD1	2.21	0.87
1:D:350:ASN:ND2	1:D:353:GLU:OE2	2.10	0.85
1:D:151:GLN:NE2	1:D:194:MET:HE1	1.92	0.84
1:D:141:ASP:CG	1:D:197:LYS:HE2	2.04	0.82
1:B:143:LEU:HD21	1:B:212:THR:OG1	1.84	0.78
1:A:147:ILE:O	1:A:158:LYS:NZ	2.18	0.76
1:A:186:LEU:HD22	1:A:193:VAL:CG2	2.15	0.75
1:B:143:LEU:HD22	1:B:208:ILE:HD11	1.67	0.75
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.69	0.75
1:D:317:ARG:HD2	1:D:320:LYS:HE3	1.70	0.73
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.72	0.72
1:B:189:THR:HG22	1:C:255:LYS:HD3	1.72	0.71
1:A:186:LEU:CD2	1:A:193:VAL:HG21	2.19	0.69
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.73	0.69
1:A:319:ASN:ND2	3:A:603:HOH:O	2.26	0.69
1:B:529:ASN:OD1	1:D:529:ASN:ND2	2.25	0.68
1:C:146:THR:HG21	1:C:216:ARG:NH1	2.08	0.68
1:B:151:GLN:HG3	1:B:152:GLU:N	2.10	0.67
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.76	0.66
1:D:153:LYS:HB2	1:D:194:MET:HE2	1.78	0.66
1:B:162:ALA:O	1:B:165:SER:HB3	1.95	0.66
1:C:498:MET:HE1	1:C:517:PHE:CE1	2.31	0.66
1:D:182:LEU:O	1:D:186:LEU:HD12	1.95	0.66
1:C:146:THR:HG21	1:C:216:ARG:HH12	1.61	0.65
1:D:151:GLN:HE22	1:D:194:MET:CE	2.03	0.65
1:B:265:VAL:HG22	1:B:498:MET:HE2	1.79	0.64
1:B:153:LYS:HB2	1:B:194:MET:HE2	1.81	0.63
1:B:349:VAL:O	1:B:354:LYS:HE3	1.98	0.63
1:D:317:ARG:HA	1:D:319:ASN:OD1	1.99	0.62
1:A:496:MET:CE	1:A:498:MET:HE3	2.32	0.60
1:B:398:LYS:NZ	3:B:705:HOH:O	2.33	0.59
1:B:181:MET:HE2	1:B:202:LYS:HG2	1.84	0.58
1:A:176:LYS:HD3	1:A:180:ASP:OD2	2.03	0.58
1:A:199:LEU:O	1:A:202:LYS:HB3	2.04	0.58
1:B:245:LYS:HD2	1:B:246:VAL:O	2.04	0.58
1:C:488:ILE:HD12	1:C:514:GLY:HA3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ARG:NH1	1:A:545:GLU:OE2	2.35	0.56
1:D:265:VAL:HG22	1:D:498:MET:HE3	1.87	0.56
1:D:195:LEU:HD23	1:D:199:LEU:HG	1.88	0.55
1:A:225:MET:HE3	1:A:225:MET:HA	1.88	0.55
1:A:244:GLY:C	1:A:245:LYS:HG2	2.32	0.55
1:D:299:ASP:OD2	1:D:357:TYR:OH	2.17	0.55
1:B:201:LYS:O	1:B:205:GLN:HB3	2.07	0.55
1:A:303:GLU:H	1:A:303:GLU:CD	2.15	0.54
1:B:151:GLN:HG3	1:B:152:GLU:H	1.72	0.54
1:C:498:MET:HE1	1:C:517:PHE:HE1	1.73	0.54
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.73	0.54
1:B:530:TYR:CE1	1:D:479:PRO:HG3	2.43	0.54
1:A:477:GLY:O	1:A:529:ASN:HB2	2.08	0.53
1:B:232:ASP:O	1:B:236:GLU:HG2	2.08	0.53
1:B:422:VAL:HG21	1:B:427:ALA:HB2	1.91	0.53
1:B:525:CYS:HA	1:B:540:LEU:O	2.09	0.53
1:B:252:GLN:O	1:B:255:LYS:HG2	2.08	0.53
1:B:528:HIS:CD2	1:D:454:ARG:HD2	2.44	0.53
1:A:488:ILE:HD12	1:A:514:GLY:HA3	1.91	0.53
1:C:507:LYS:H	1:C:507:LYS:HE2	1.74	0.53
1:D:147:ILE:O	1:D:158:LYS:HE2	2.08	0.52
1:D:216:ARG:HA	1:D:216:ARG:HE	1.74	0.52
1:A:285:GLN:HA	1:A:418:CYS:HB3	1.91	0.52
1:B:162:ALA:HB1	1:B:215:PHE:HE1	1.74	0.52
1:B:432:ALA:HB1	1:B:441:PRO:HG2	1.91	0.52
1:B:319:ASN:O	3:B:702:HOH:O	2.18	0.51
1:B:477:GLY:O	1:B:529:ASN:HB2	2.10	0.51
1:C:141:ASP:OD2	1:C:197:LYS:HD2	2.10	0.51
1:D:141:ASP:OD1	1:D:197:LYS:HE2	2.10	0.51
1:D:195:LEU:CD2	1:D:199:LEU:HG	2.39	0.50
1:B:143:LEU:N	1:B:143:LEU:HD12	2.26	0.50
1:B:479:PRO:HG3	1:D:530:TYR:CE1	2.46	0.50
1:D:349:VAL:O	1:D:354:LYS:HE3	2.09	0.50
1:A:316:LEU:HD21	3:A:720:HOH:O	2.11	0.50
1:B:316:LEU:O	1:B:319:ASN:ND2	2.44	0.50
1:B:488:ILE:HD12	1:B:514:GLY:HA3	1.93	0.49
1:A:265:VAL:HG22	1:A:498:MET:HE2	1.95	0.49
1:D:196:ASP:OD1	1:D:198:ASP:HB2	2.11	0.49
1:A:265:VAL:HG22	1:A:498:MET:HG2	1.95	0.49
1:A:181:MET:HE2	1:A:202:LYS:HG3	1.93	0.49
1:D:265:VAL:CG2	1:D:498:MET:HE3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:THR:O	1:D:189:THR:HB	2.13	0.49
1:D:201:LYS:O	1:D:205:GLN:HB2	2.13	0.48
1:A:247:ALA:HB2	1:A:484:VAL:HG22	1.94	0.48
1:A:317:ARG:HA	1:A:319:ASN:OD1	2.12	0.48
1:C:303:GLU:H	1:C:303:GLU:CD	2.21	0.48
1:A:384:SER:OG	3:A:601:HOH:O	2.20	0.48
1:D:162:ALA:HB1	1:D:215:PHE:HE1	1.79	0.48
1:D:153:LYS:NZ	3:D:706:HOH:O	2.36	0.48
1:A:265:VAL:CG2	1:A:498:MET:HE2	2.44	0.48
1:B:265:VAL:CG2	1:B:498:MET:HE2	2.43	0.48
1:A:257:SER:OG	1:A:259:ASP:OD2	2.32	0.48
1:B:204:VAL:HG23	1:B:208:ILE:HD13	1.96	0.48
1:C:147:ILE:O	1:C:158:LYS:NZ	2.29	0.48
1:B:153:LYS:CB	1:B:194:MET:HE2	2.42	0.47
1:D:477:GLY:O	1:D:529:ASN:HB2	2.14	0.47
1:B:496:MET:CE	1:B:498:MET:HE3	2.44	0.47
1:A:156:VAL:HG11	1:A:186:LEU:HD11	1.96	0.47
1:D:432:ALA:HB1	1:D:441:PRO:HG2	1.95	0.47
1:B:245:LYS:HB3	1:B:245:LYS:HE3	1.63	0.47
1:C:492:VAL:HG21	1:C:496:MET:HE2	1.96	0.47
1:D:425:GLU:OE2	3:D:701:HOH:O	2.20	0.47
1:A:506:ASP:HB3	1:A:512:VAL:HG22	1.97	0.47
1:C:162:ALA:HB1	1:C:215:PHE:HE1	1.80	0.47
1:C:189:THR:HA	1:C:191:ASP:OD1	2.14	0.47
1:D:216:ARG:HA	1:D:216:ARG:NE	2.30	0.47
1:B:316:LEU:HD23	1:B:316:LEU:HA	1.68	0.46
1:A:176:LYS:O	1:A:176:LYS:HG2	1.88	0.46
1:B:156:VAL:HG21	1:B:186:LEU:HD21	1.97	0.46
1:C:357:TYR:O	1:C:360:GLN:HG3	2.16	0.46
1:C:479:PRO:HD2	1:C:491:VAL:O	2.16	0.46
1:C:332:PRO:HD2	1:C:459:LEU:HD13	1.97	0.46
1:A:140:GLU:OE1	1:A:205:GLN:HG2	2.16	0.46
1:B:374:SER:HB2	1:B:421:GLU:OE2	2.16	0.45
1:D:140:GLU:OE1	1:D:140:GLU:N	2.36	0.45
1:A:192:GLY:HA3	1:A:193:VAL:HA	1.58	0.45
2:B:601:Q9M:N05	2:B:601:Q9M:O29	2.48	0.45
1:C:192:GLY:HA3	1:C:193:VAL:HA	1.53	0.45
1:C:354:LYS:HB3	1:C:413:PHE:CZ	2.52	0.45
1:B:140:GLU:OE1	1:B:140:GLU:N	2.40	0.45
1:B:289:LYS:HA	1:B:292:LYS:HE2	1.97	0.45
1:A:379:GLN:O	1:A:382:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:193:VAL:HG23	1:D:193:VAL:O	2.16	0.45
1:B:454:ARG:HD2	1:D:528:HIS:CD2	2.52	0.45
1:C:507:LYS:H	1:C:507:LYS:CE	2.30	0.45
1:B:507:LYS:H	1:B:507:LYS:HE2	1.83	0.44
1:B:181:MET:HE1	1:B:202:LYS:HE2	2.00	0.44
1:C:432:ALA:HB1	1:C:441:PRO:HG2	1.98	0.44
1:D:195:LEU:HD23	1:D:199:LEU:CG	2.47	0.44
1:D:222:PRO:HG3	3:D:745:HOH:O	2.18	0.44
2:D:601:Q9M:C25	2:D:601:Q9M:O26	2.64	0.44
1:B:192:GLY:HA3	1:B:193:VAL:HA	1.63	0.44
1:C:247:ALA:HB2	1:C:484:VAL:HG22	1.99	0.44
1:A:148:ALA:O	1:A:149:GLU:HB2	2.17	0.44
1:C:143:LEU:HD23	1:C:200:PHE:HZ	1.82	0.44
1:C:224:PHE:O	1:C:228:THR:HG23	2.18	0.44
1:B:281:PRO:HA	1:B:422:VAL:O	2.18	0.43
1:D:149:GLU:O	1:D:149:GLU:HG3	2.18	0.43
1:A:289:LYS:HA	1:A:292:LYS:HE2	1.99	0.43
1:B:246:VAL:HG22	1:B:503:PRO:HB2	2.00	0.43
1:B:317:ARG:HA	1:B:319:ASN:OD1	2.18	0.43
1:B:544:ARG:HA	1:B:544:ARG:HD3	1.52	0.43
1:D:480:ALA:HB2	1:D:490:LEU:HD12	2.00	0.43
1:D:488:ILE:HD12	1:D:514:GLY:HA3	1.99	0.43
1:B:194:MET:HE2	1:B:194:MET:HB3	1.80	0.43
1:B:317:ARG:HE	2:B:601:Q9M:C22	2.32	0.43
1:C:527:PHE:CZ	1:C:542:PRO:HG2	2.54	0.43
1:D:317:ARG:HD2	1:D:320:LYS:CE	2.45	0.42
1:D:496:MET:HE3	1:D:498:MET:SD	2.59	0.42
1:A:350:ASN:OD1	1:A:350:ASN:N	2.48	0.42
1:C:255:LYS:HB3	1:C:255:LYS:HE3	1.82	0.42
1:C:546:GLY:HA2	3:C:635:HOH:O	2.19	0.42
1:B:249:TYR:CD1	1:B:250:ILE:HG23	2.54	0.42
1:B:332:PRO:C	1:B:333:MET:HE2	2.43	0.42
1:D:278:THR:HA	1:D:424:CYS:HB2	2.01	0.42
1:D:525:CYS:HA	1:D:540:LEU:O	2.18	0.42
1:A:149:GLU:CD	1:A:158:LYS:HE3	2.44	0.42
1:D:492:VAL:HG21	1:D:496:MET:HE2	2.02	0.42
1:B:278:THR:HA	1:B:424:CYS:HB2	2.01	0.42
1:D:194:MET:HE2	1:D:194:MET:HB3	1.76	0.42
1:C:250:ILE:HG13	1:C:253:LEU:HD12	2.01	0.42
1:A:354:LYS:HB3	1:A:413:PHE:CZ	2.54	0.42
1:C:170:THR:O	1:C:179:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:LEU:HD23	1:A:411:LEU:HA	1.86	0.42
1:B:507:LYS:HE2	1:B:507:LYS:HB2	1.78	0.42
1:A:148:ALA:O	1:A:151:GLN:HB3	2.20	0.41
1:B:209:VAL:O	1:B:213:GLN:HB2	2.20	0.41
1:B:528:HIS:CG	1:D:454:ARG:HD2	2.54	0.41
1:D:354:LYS:HB3	1:D:413:PHE:CZ	2.55	0.41
1:A:224:PHE:O	1:A:228:THR:HG23	2.20	0.41
1:D:191:ASP:OD1	1:D:191:ASP:N	2.42	0.41
1:D:498:MET:HE1	1:D:517:PHE:CZ	2.55	0.41
1:B:299:ASP:OD2	1:B:357:TYR:OH	2.37	0.41
1:B:216:ARG:HA	1:B:216:ARG:HD2	1.65	0.41
1:B:379:GLN:O	1:B:382:ARG:HG2	2.20	0.41
1:B:454:ARG:HD2	1:D:528:HIS:CG	2.54	0.41
1:C:264:SER:OG	1:C:424:CYS:HB3	2.20	0.41
1:A:228:THR:HB	1:A:273:HIS:CD2	2.56	0.41
1:C:365:MET:HE2	1:C:448:LEU:HD11	2.03	0.41
1:A:153:LYS:HB3	1:A:194:MET:HB3	2.02	0.41
1:A:281:PRO:HA	1:A:422:VAL:O	2.20	0.41
1:B:332:PRO:HD2	1:B:459:LEU:HD13	2.03	0.41
1:B:507:LYS:H	1:B:507:LYS:CE	2.34	0.41
1:C:139:LEU:HD23	1:C:139:LEU:HA	1.90	0.41
1:A:432:ALA:HB1	1:A:441:PRO:HG2	2.02	0.40
1:A:496:MET:HE1	1:A:498:MET:HE3	2.02	0.40
1:B:156:VAL:HG12	1:B:193:VAL:HG23	2.02	0.40
1:C:191:ASP:OD1	1:C:191:ASP:N	2.30	0.40
1:C:525:CYS:HA	1:C:540:LEU:O	2.20	0.40
1:B:208:ILE:HD12	1:B:208:ILE:HA	1.75	0.40
1:D:170:THR:O	1:D:179:MET:HG3	2.20	0.40
1:A:186:LEU:CD2	1:A:193:VAL:CG2	2.89	0.40
1:D:459:LEU:HD23	1:D:459:LEU:HA	1.84	0.40
1:B:182:LEU:HD23	1:B:182:LEU:HA	1.94	0.40
1:C:199:LEU:HD12	1:C:199:LEU:HA	1.86	0.40
1:C:411:LEU:HD23	1:C:411:LEU:HA	1.94	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:LYS:CE	2:D:601:Q9M:N17[4_445]	1.44	0.76
1:C:320:LYS:NZ	3:B:705:HOH:O[2_555]	1.97	0.23
1:A:307:ARG:NH2	1:B:259:ASP:OD1[1_455]	2.10	0.10

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	398/527 (76%)	388 (98%)	10 (2%)	0	100	100
1	B	407/527 (77%)	396 (97%)	11 (3%)	0	100	100
1	C	408/527 (77%)	397 (97%)	11 (3%)	0	100	100
1	D	407/527 (77%)	397 (98%)	10 (2%)	0	100	100
All	All	1620/2108 (77%)	1578 (97%)	42 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	348/452 (77%)	348 (100%)	0	100	100
1	B	354/452 (78%)	354 (100%)	0	100	100
1	C	354/452 (78%)	354 (100%)	0	100	100
1	D	354/452 (78%)	353 (100%)	1 (0%)	86	94
All	All	1410/1808 (78%)	1409 (100%)	1 (0%)	88	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	319	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	347	GLN
1	A	368	ASN
1	A	475	HIS
1	A	516	HIS
1	B	368	ASN
1	C	157	HIS
1	C	347	GLN
1	C	475	HIS
1	C	516	HIS
1	C	529	ASN
1	D	151	GLN
1	D	157	HIS
1	D	368	ASN
1	D	471	GLN
1	D	516	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](#)

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	Q9M	B	601	-	39,39,39	2.63	13 (33%)	48,53,53	4.87	25 (52%)
2	Q9M	D	601	-	39,39,39	2.28	10 (25%)	48,53,53	6.34	27 (56%)

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	Q9M	B	601	-	-	8/18/32/32	0/5/5/5
2	Q9M	D	601	-	-	3/18/32/32	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	Q9M	C11-C10	-6.88	1.41	1.53
2	D	601	Q9M	C11-C10	-6.43	1.41	1.53
2	B	601	Q9M	C04-N03	5.83	1.46	1.38
2	D	601	Q9M	C04-N03	5.29	1.46	1.38
2	B	601	Q9M	C16-N17	5.01	1.45	1.38
2	D	601	Q9M	C02-N03	5.00	1.46	1.37
2	B	601	Q9M	C07-N08	4.82	1.45	1.34
2	B	601	Q9M	O12-C10	-4.81	1.35	1.46
2	D	601	Q9M	C16-N17	4.48	1.44	1.38
2	B	601	Q9M	C18-N17	4.38	1.45	1.37
2	B	601	Q9M	O12-C13	4.33	1.41	1.35
2	D	601	Q9M	O12-C10	-4.16	1.36	1.46
2	D	601	Q9M	C09-C10	-3.75	1.46	1.53
2	B	601	Q9M	C02-N03	3.75	1.44	1.37
2	D	601	Q9M	C07-N08	3.66	1.42	1.34
2	B	601	Q9M	C13-N14	3.51	1.33	1.29
2	D	601	Q9M	C09-N08	3.49	1.50	1.47
2	B	601	Q9M	C09-C10	-3.14	1.47	1.53
2	B	601	Q9M	O29-C02	-2.88	1.17	1.23
2	D	601	Q9M	O29-C02	-2.85	1.17	1.23
2	D	601	Q9M	C11-N08	2.83	1.49	1.47
2	B	601	Q9M	O26-C18	-2.48	1.18	1.23
2	B	601	Q9M	C11-N08	2.41	1.49	1.47

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	Q9M	C10-O12-C13	-21.46	103.61	117.71
2	B	601	Q9M	C10-O12-C13	-16.88	106.61	117.71
2	D	601	Q9M	S27-C16-N15	-16.01	96.64	114.52
2	D	601	Q9M	S28-C07-N08	12.07	136.46	120.31
2	D	601	Q9M	C16-N15-N14	11.10	126.14	112.02
2	D	601	Q9M	C19-C18-N17	10.43	127.12	114.40
2	D	601	Q9M	N17-C16-N15	10.20	129.92	120.81
2	B	601	Q9M	C13-N14-N15	10.10	117.48	105.84
2	B	601	Q9M	S27-C13-N14	-9.29	104.95	117.59
2	D	601	Q9M	S27-C13-N14	-9.13	105.17	117.59
2	B	601	Q9M	S28-C07-N08	8.83	132.13	120.31
2	B	601	Q9M	N17-C16-N15	8.67	128.56	120.81
2	B	601	Q9M	C01-C02-N03	8.58	124.87	114.40
2	D	601	Q9M	C01-C02-N03	8.51	124.78	114.40
2	D	601	Q9M	S28-C04-N05	-8.06	105.52	114.52
2	B	601	Q9M	S28-C04-N05	-7.37	106.29	114.52
2	D	601	Q9M	C10-C09-N08	-7.34	80.68	87.96
2	D	601	Q9M	S27-C16-N17	7.22	133.39	123.72
2	B	601	Q9M	S27-C16-N15	-7.12	106.57	114.52
2	D	601	Q9M	O12-C13-S27	6.94	131.12	116.13
2	D	601	Q9M	C16-S27-C13	6.32	99.68	86.65
2	B	601	Q9M	C19-C18-N17	6.30	122.08	114.40
2	B	601	Q9M	C10-C09-N08	-6.26	81.75	87.96
2	D	601	Q9M	C13-N14-N15	5.66	112.36	105.84
2	B	601	Q9M	O12-C13-S27	5.65	128.33	116.13
2	D	601	Q9M	C10-C11-N08	-5.53	82.48	87.96
2	D	601	Q9M	C07-N06-N05	5.18	117.30	107.08
2	D	601	Q9M	C09-N08-C07	5.16	145.09	129.57
2	D	601	Q9M	C18-N17-C16	-4.97	115.19	123.69
2	D	601	Q9M	S28-C07-N06	-4.93	105.92	114.44
2	B	601	Q9M	C02-N03-C04	-4.72	115.61	123.69
2	D	601	Q9M	S28-C04-N03	4.71	130.02	123.72
2	D	601	Q9M	O26-C18-C19	-4.57	112.09	121.99
2	B	601	Q9M	C18-N17-C16	-4.51	115.97	123.69
2	B	601	Q9M	N03-C04-N05	4.50	124.84	120.81
2	D	601	Q9M	C02-N03-C04	-4.46	116.06	123.69
2	B	601	Q9M	C16-S27-C13	4.44	95.81	86.65
2	B	601	Q9M	C04-N05-N06	4.43	117.65	112.02
2	B	601	Q9M	C10-C11-N08	-4.35	83.64	87.96
2	B	601	Q9M	C09-N08-C07	4.34	142.62	129.57
2	D	601	Q9M	N03-C04-N05	4.07	124.45	120.81
2	D	601	Q9M	C30-C01-C02	-3.95	100.54	112.33
2	B	601	Q9M	S28-C04-N03	3.73	128.72	123.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	Q9M	C11-N08-C07	-3.72	118.38	129.57
2	D	601	Q9M	C04-N05-N06	3.48	116.45	112.02
2	B	601	Q9M	O29-C02-C01	-3.17	115.12	121.99
2	D	601	Q9M	O29-C02-C01	-3.17	115.12	121.99
2	B	601	Q9M	C07-N06-N05	2.94	112.88	107.08
2	B	601	Q9M	C30-C01-C02	-2.59	104.60	112.33
2	B	601	Q9M	C11-N08-C07	-2.58	121.83	129.57
2	B	601	Q9M	C16-N15-N14	2.48	115.18	112.02
2	B	601	Q9M	S28-C07-N06	-2.47	110.16	114.44

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	Q9M	N05-C04-N03-C02
2	B	601	Q9M	S28-C04-N03-C02
2	B	601	Q9M	N15-C16-N17-C18
2	B	601	Q9M	S27-C16-N17-C18
2	D	601	Q9M	N05-C04-N03-C02
2	D	601	Q9M	S28-C04-N03-C02
2	B	601	Q9M	C09-C10-O12-C13
2	B	601	Q9M	C11-C10-O12-C13
2	D	601	Q9M	S27-C16-N17-C18
2	B	601	Q9M	O26-C18-C19-C20
2	B	601	Q9M	N17-C18-C19-C20

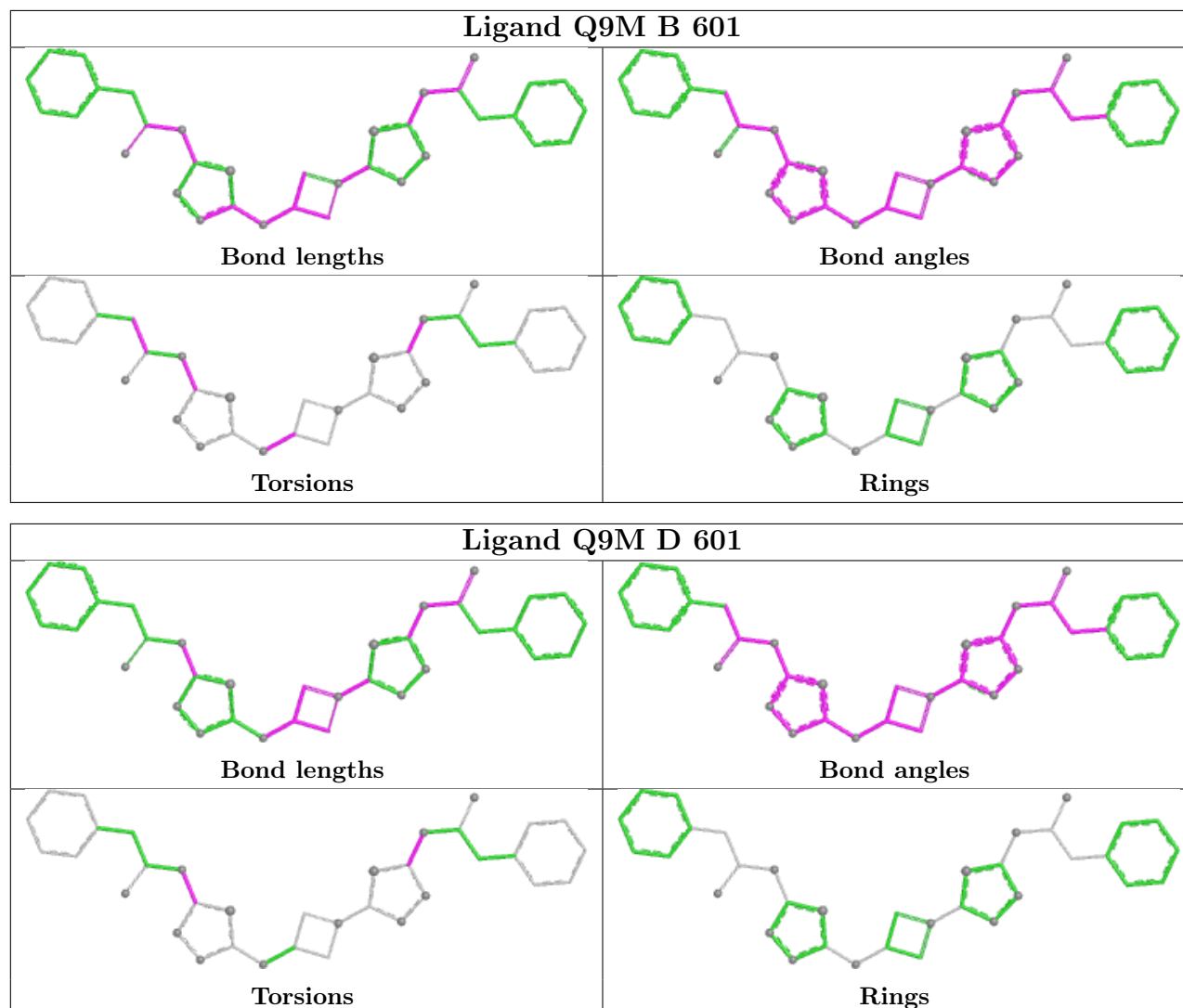
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	Q9M	2	0
2	D	601	Q9M	1	1

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	402/527 (76%)	0.50	42 (10%)	11	10	16, 27, 75, 174	0
1	B	409/527 (77%)	0.43	41 (10%)	12	10	16, 27, 72, 160	0
1	C	410/527 (77%)	0.49	43 (10%)	11	10	17, 27, 83, 132	0
1	D	409/527 (77%)	0.36	33 (8%)	18	15	17, 27, 71, 121	0
All	All	1630/2108 (77%)	0.45	159 (9%)	13	11	16, 27, 76, 174	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	189	THR	13.7
1	A	189	THR	9.7
1	D	316	LEU	8.2
1	C	316	LEU	7.9
1	D	318	PHE	7.0
1	A	137	PRO	6.9
1	A	188	THR	6.8
1	B	193	VAL	6.6
1	A	257	SER	6.5
1	B	137	PRO	6.4
1	C	258	PRO	6.4
1	C	189	THR	6.2
1	A	318	PHE	6.0
1	C	253	LEU	5.8
1	B	150	GLY	5.7
1	B	190	SER	5.7
1	C	317	ARG	5.7
1	B	318	PHE	5.6
1	A	190	SER	5.6
1	C	254	ALA	5.5
1	C	249	TYR	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	546	GLY	5.4
1	A	258	PRO	5.2
1	A	148	ALA	5.2
1	A	317	ARG	5.1
1	C	318	PHE	5.1
1	D	191	ASP	5.0
1	A	249	TYR	5.0
1	D	137	PRO	5.0
1	A	145	TYR	4.8
1	C	257	SER	4.7
1	C	538	LYS	4.7
1	A	150	GLY	4.7
1	C	137	PRO	4.6
1	A	225	MET	4.5
1	B	188	THR	4.5
1	B	145	TYR	4.4
1	C	250	ILE	4.4
1	A	186	LEU	4.4
1	C	193	VAL	4.4
1	B	191	ASP	4.1
1	A	192	GLY	4.1
1	C	319	ASN	4.1
1	C	198	ASP	4.1
1	D	190	SER	4.0
1	D	193	VAL	4.0
1	A	316	LEU	4.0
1	B	317	ARG	3.9
1	D	383	GLU	3.8
1	D	142	LEU	3.7
1	D	151	GLN	3.7
1	A	248	ASP	3.7
1	B	192	GLY	3.7
1	B	186	LEU	3.7
1	C	256	PHE	3.6
1	B	316	LEU	3.6
1	A	191	ASP	3.5
1	A	319	ASN	3.5
1	C	190	SER	3.5
1	B	252	GLN	3.5
1	C	145	TYR	3.4
1	B	251	PRO	3.4
1	B	143	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	193	VAL	3.4
1	A	185	THR	3.3
1	C	151	GLN	3.3
1	C	152	GLU	3.3
1	C	150	GLY	3.3
1	D	144	PHE	3.3
1	A	184	LEU	3.3
1	B	152	GLU	3.2
1	D	195	LEU	3.2
1	C	138	SER	3.2
1	B	148	ALA	3.1
1	D	317	ARG	3.1
1	C	252	GLN	3.1
1	C	191	ASP	3.1
1	D	319	ASN	3.1
1	D	189	THR	3.1
1	C	248	ASP	3.1
1	C	251	PRO	3.0
1	A	195	LEU	3.0
1	A	320	LYS	3.0
1	B	138	SER	3.0
1	D	149	GLU	3.0
1	C	149	GLU	2.9
1	B	153	LYS	2.9
1	A	383	GLU	2.9
1	C	186	LEU	2.9
1	C	192	GLY	2.9
1	D	150	GLY	2.9
1	B	217	ARG	2.9
1	A	187	GLN	2.9
1	A	147	ILE	2.8
1	B	185	THR	2.8
1	B	194	MET	2.8
1	A	507	LYS	2.8
1	C	320	LYS	2.8
1	B	142	LEU	2.8
1	A	149	GLU	2.8
1	C	213	GLN	2.8
1	D	145	TYR	2.8
1	A	151	GLN	2.7
1	B	319	ASN	2.7
1	B	255	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	139	LEU	2.6
1	D	353	GLU	2.6
1	D	194	MET	2.6
1	B	156	VAL	2.6
1	B	249	TYR	2.6
1	B	149	GLU	2.5
1	D	360	GLN	2.5
1	C	188	THR	2.5
1	A	348	GLY	2.5
1	D	192	GLY	2.5
1	B	165	SER	2.5
1	B	200	PHE	2.5
1	B	146	THR	2.5
1	C	325	GLU	2.4
1	A	138	SER	2.4
1	D	138	SER	2.4
1	B	141	ASP	2.4
1	B	250	ILE	2.4
1	D	186	LEU	2.4
1	A	156	VAL	2.4
1	C	255	LYS	2.4
1	A	544	ARG	2.4
1	D	152	GLU	2.4
1	D	141	ASP	2.3
1	A	202	LYS	2.3
1	A	545	GLU	2.3
1	D	147	ILE	2.3
1	D	154	ILE	2.3
1	A	205	GLN	2.3
1	C	194	MET	2.2
1	B	197	LYS	2.2
1	C	143	LEU	2.2
1	D	143	LEU	2.2
1	B	242	SER	2.2
1	B	544	ARG	2.2
1	A	247	ALA	2.1
1	C	148	ALA	2.1
1	D	185	THR	2.1
1	B	545	GLU	2.1
1	C	153	LYS	2.1
1	D	225	MET	2.1
1	A	537	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	139	LEU	2.1
1	A	141	ASP	2.1
1	C	139	LEU	2.1
1	D	217	ARG	2.1
1	B	151	GLN	2.1
1	C	144	PHE	2.1
1	C	242	SER	2.1
1	B	383	GLU	2.0
1	D	200	PHE	2.0
1	A	153	LYS	2.0
1	B	147	ILE	2.0
1	C	259	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

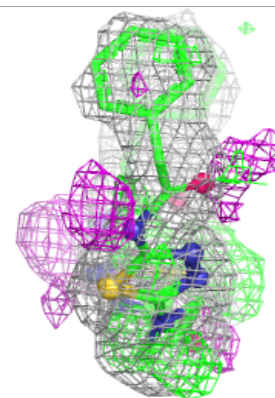
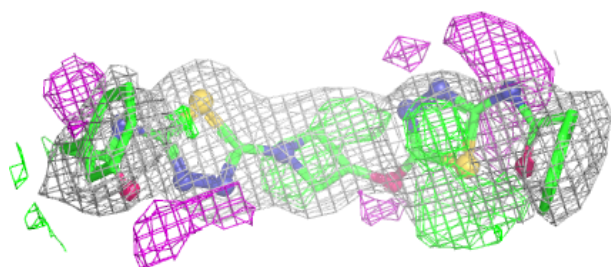
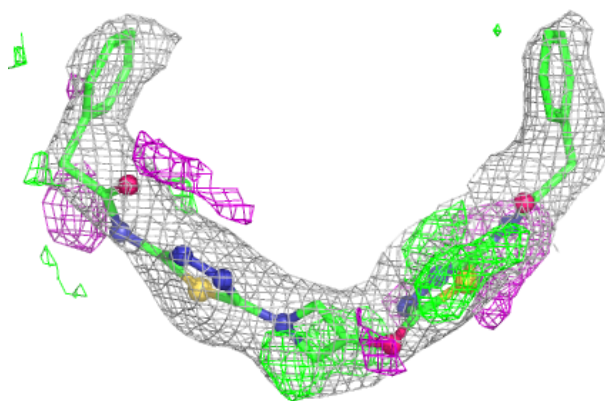
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	Q9M	D	601	35/35	0.79	0.21	35,62,72,74	0
2	Q9M	B	601	35/35	0.87	0.18	32,59,68,70	0

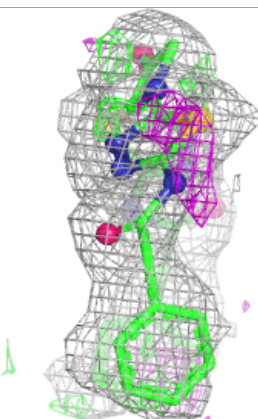
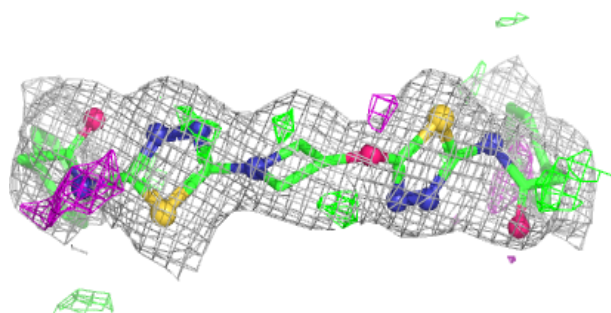
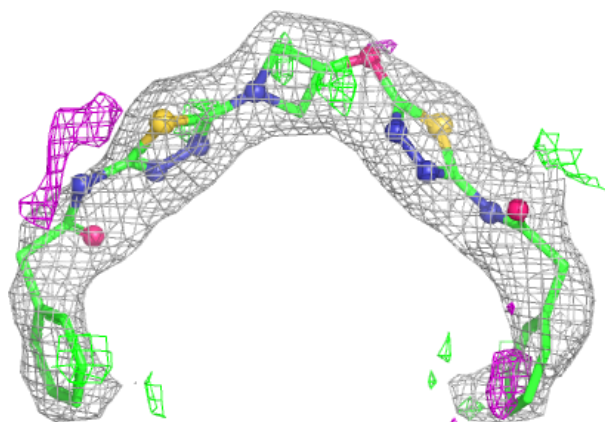
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around Q9M 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)

**Electron density around Q9M 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.