



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:07 PM UTC

PDB ID : 5FI7 / pdb_00005fi7
Title : Crystal structure of human GAC in complex with inhibitor UPGL_00015: 2-phenyl- {N}-[5-[(3 {S})-3-[[5-(2-phenylethanoylamino)-1,3,4-thiadiazol-2-yl]oxy]pyrrolidin-1-yl]-1,3,4-thiadiazol-2-yl]ethanamide
Authors : Huang, Q.; Cerione, R.
Deposited on : 2015-12-22
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

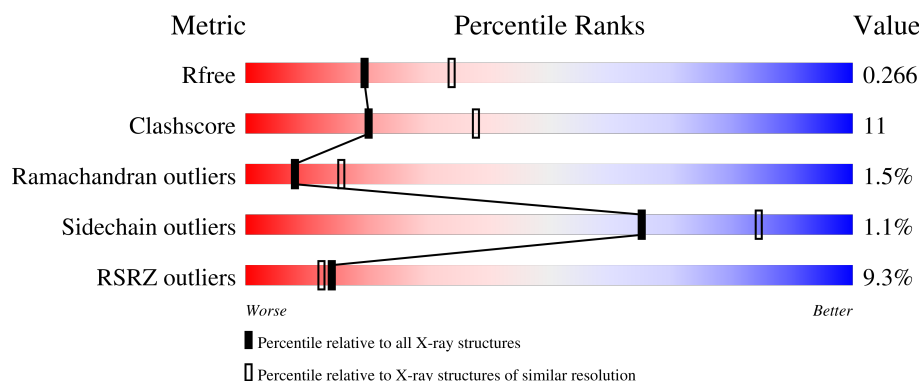
1 Overall quality at a glance

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	539	 8% 58% 16% 24%
1	B	539	 6% 60% 15% 24%
1	C	539	 8% 58% 16% 24%
1	D	539	 6% 60% 15% 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13050 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	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	B	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	C	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			
1	D	410	Total	C	N	O	S	1	0	0
			3194	2036	540	590	28			

There are 48 discrepancies between the modelled and reference sequences:

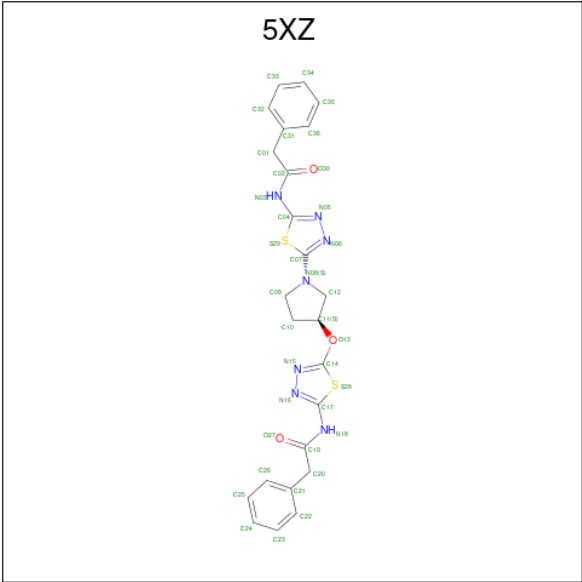
Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MET	-	initiating methionine	UNP O94925
A	60	ARG	-	expression tag	UNP O94925
A	61	GLY	-	expression tag	UNP O94925
A	62	SER	-	expression tag	UNP O94925
A	63	HIS	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	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	GLY	-	expression tag	UNP O94925
A	70	SER	-	expression tag	UNP O94925
B	59	MET	-	initiating methionine	UNP O94925
B	60	ARG	-	expression tag	UNP O94925
B	61	GLY	-	expression tag	UNP O94925
B	62	SER	-	expression tag	UNP O94925
B	63	HIS	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	68	HIS	-	expression tag	UNP O94925
B	69	GLY	-	expression tag	UNP O94925
B	70	SER	-	expression tag	UNP O94925
C	59	MET	-	initiating methionine	UNP O94925
C	60	ARG	-	expression tag	UNP O94925
C	61	GLY	-	expression tag	UNP O94925
C	62	SER	-	expression tag	UNP O94925
C	63	HIS	-	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	GLY	-	expression tag	UNP O94925
C	70	SER	-	expression tag	UNP O94925
D	59	MET	-	initiating methionine	UNP O94925
D	60	ARG	-	expression tag	UNP O94925
D	61	GLY	-	expression tag	UNP O94925
D	62	SER	-	expression tag	UNP O94925
D	63	HIS	-	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	GLY	-	expression tag	UNP O94925
D	70	SER	-	expression tag	UNP O94925

- Molecule 2 is 2-phenyl- {N}-[5-[(3 {S})-3-[[5-(2-phenylethanoylamino)-1,3,4-thiadiazol-2-yl]oxy]pyrrolidin-1-yl]-1,3,4-thiadiazol-2-yl]ethanamide (CCD ID: 5XZ) (formula: C₂₄H₂₃N₇O₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			36	24	7	3	2		
2	C	1	Total	C	N	O	S	0	0
			36	24	7	3	2		

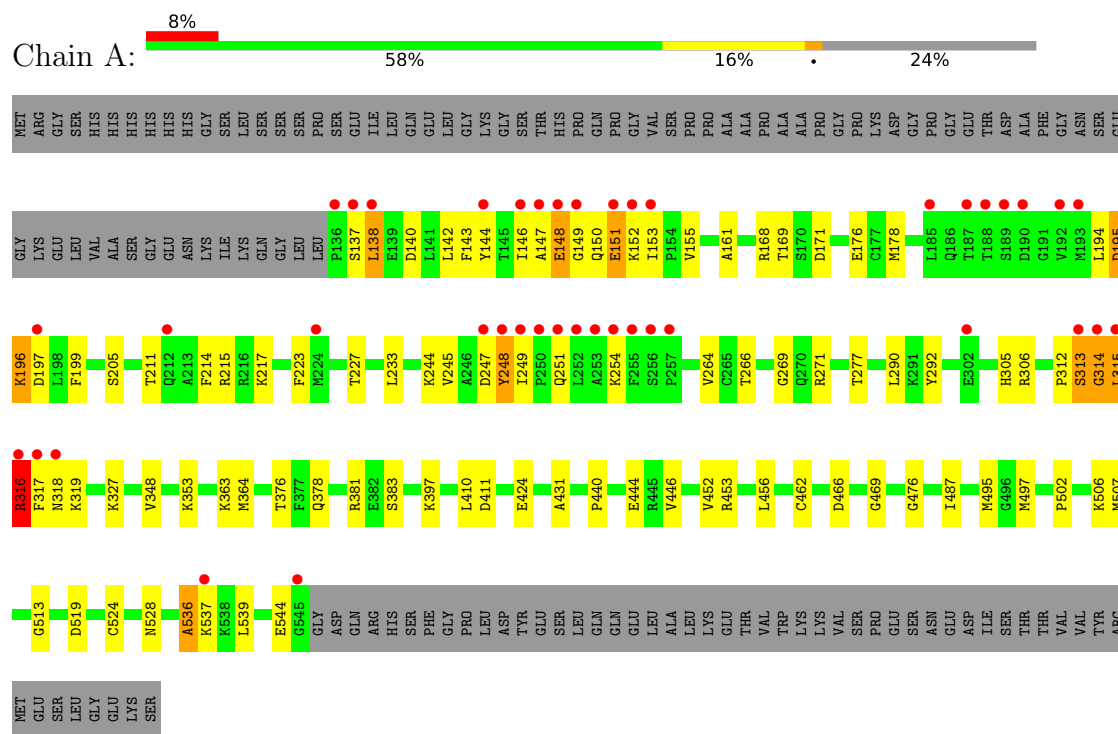
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	51	Total	O	0	0
			51	51		
3	B	53	Total	O	0	0
			53	53		
3	C	48	Total	O	0	0
			48	48		
3	D	50	Total	O	0	0
			50	50		

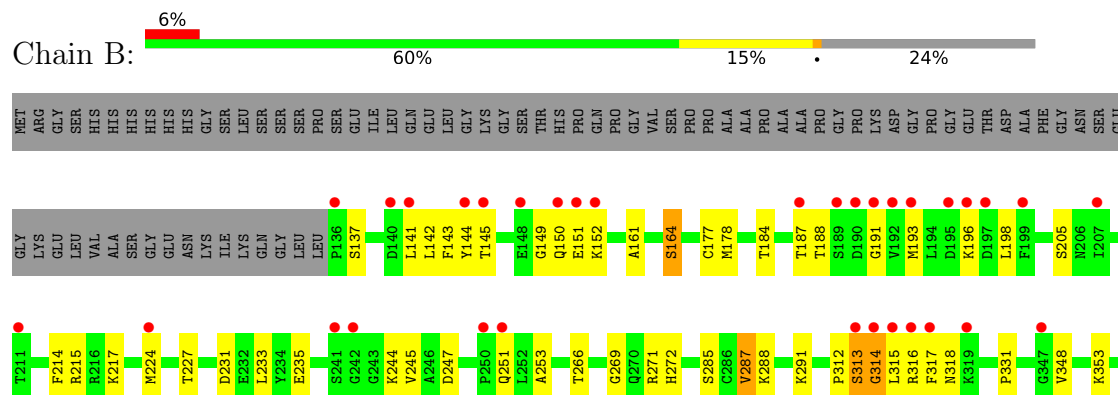
3 Residue-property plots

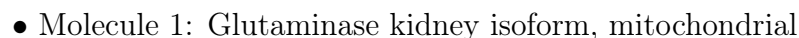
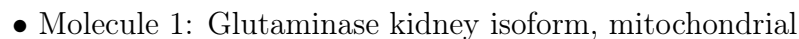
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	99.17Å 138.83Å 176.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.90 – 2.50 44.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.90-2.50) 87.5 (44.90-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.218 , 0.267 0.218 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (1.86%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.892	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13050	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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 57.70 % 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 2.2787e-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: 5XZ

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	0.36	0/3266	0.62	3/4408 (0.1%)
1	B	0.38	0/3266	0.59	0/4408
1	C	0.44	0/3266	0.62	0/4408
1	D	0.37	0/3266	0.59	0/4408
All	All	0.39	0/13064	0.61	3/17632 (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	B	0	1
1	C	0	2
1	D	0	1
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	ALA	CB-CA-C	-6.76	108.79	116.63
1	A	316	ARG	CA-C-N	5.86	131.98	121.66
1	A	316	ARG	C-N-CA	5.86	131.98	121.66

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	314	GLY	Peptide
1	C	252	LEU	Peptide
1	C	315	LEU	Peptide
1	D	312	PRO	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	3194	0	3167	83	0
1	B	3194	0	3167	63	0
1	C	3194	0	3167	89	0
1	D	3194	0	3167	74	0
2	A	36	0	0	2	0
2	C	36	0	0	1	0
3	A	51	0	0	2	0
3	B	53	0	0	1	0
3	C	48	0	0	2	0
3	D	50	0	0	1	0
All	All	13050	0	12668	288	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 11.

All (288) 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:140:ASP:OD2	1:C:196:LYS:NZ	1.86	1.08
1:D:146:ILE:O	1:D:157:LYS:NZ	2.01	0.93
1:B:489:LEU:HD23	1:B:497:MET:HE2	1.50	0.91
1:C:345:LYS:HE3	1:C:356:TYR:CE2	2.06	0.90
1:B:489:LEU:HD23	1:B:497:MET:CE	2.03	0.88
1:C:137:SER:OG	1:C:140:ASP:OD1	1.94	0.84
1:A:148:GLU:HG3	1:A:150:GLN:HG2	1.58	0.83
1:D:313:SER:HA	1:D:316:ARG:CZ	2.08	0.83
1:C:316:ARG:HD2	1:C:317:PHE:CE2	2.12	0.83
1:B:362:ASN:ND2	3:B:602:HOH:O	2.13	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:GLU:OE1	1:D:139:GLU:N	2.13	0.81
1:B:316:ARG:HH21	1:B:317:PHE:HE1	1.28	0.80
1:A:142:LEU:HD22	1:A:199:PHE:HZ	1.49	0.78
1:D:140:ASP:OD2	1:D:196:LYS:NZ	2.15	0.77
1:C:312:PRO:HA	1:C:462:CYS:SG	2.25	0.77
1:C:297:ASN:HD22	1:C:448:SER:H	1.33	0.76
1:C:508:GLY:O	3:C:701:HOH:O	2.02	0.76
1:D:195:ASP:OD1	1:D:198:LEU:N	2.17	0.76
1:A:315:LEU:HD11	1:A:466:ASP:O	1.86	0.76
1:C:215:ARG:HE	1:C:215:ARG:HA	1.50	0.75
1:C:345:LYS:HE3	1:C:356:TYR:CD2	2.22	0.74
1:B:187:THR:HG23	1:B:188:THR:HG23	1.70	0.74
1:A:233:LEU:HD22	1:A:519:ASP:HB3	1.71	0.73
1:B:493:ASN:HD21	1:D:532:LEU:H	1.37	0.73
1:B:251:GLN:OE1	1:B:251:GLN:N	2.19	0.70
1:B:493:ASN:ND2	1:D:532:LEU:H	1.88	0.70
1:D:207:ILE:O	1:D:211:THR:HG23	1.92	0.70
1:C:184:THR:HA	1:C:187:THR:HB	1.74	0.69
1:C:316:ARG:CZ	1:C:317:PHE:CD2	2.76	0.69
1:A:148:GLU:CG	1:A:150:GLN:HG2	2.23	0.69
1:B:313:SER:OG	1:B:314:GLY:N	2.26	0.68
1:B:528:ASN:OD1	1:D:528:ASN:ND2	2.27	0.68
1:C:146:ILE:O	1:C:157:LYS:NZ	2.23	0.68
1:C:316:ARG:NH1	1:C:317:PHE:CE2	2.62	0.67
1:A:142:LEU:HD23	1:A:146:ILE:HD13	1.76	0.67
1:C:313:SER:HA	1:C:316:ARG:CZ	2.25	0.67
1:A:397:LYS:NZ	3:A:702:HOH:O	2.29	0.66
1:B:233:LEU:HD22	1:B:519:ASP:HB3	1.77	0.66
1:A:316:ARG:HA	1:A:316:ARG:NE	2.12	0.65
1:C:255:PHE:HD1	1:C:259:LEU:HD13	1.61	0.65
1:C:306:ARG:NH2	1:D:258:ASP:OD1	2.30	0.65
1:A:537:LYS:H	1:A:537:LYS:HD3	1.62	0.65
1:C:345:LYS:CE	1:C:356:TYR:CE2	2.80	0.64
1:C:323:ASN:HB3	1:C:329:HIS:HD2	1.62	0.64
1:C:302:GLU:OE2	1:D:241:SER:HB3	1.98	0.63
1:A:152:LYS:HG2	1:A:195:ASP:HA	1.81	0.63
1:C:306:ARG:HH12	1:D:257:PRO:HB2	1.63	0.63
1:D:215:ARG:HE	1:D:215:ARG:HA	1.64	0.63
1:C:381:ARG:NH2	1:C:411:ASP:OD2	2.31	0.62
1:C:316:ARG:HG2	1:C:317:PHE:H	1.64	0.62
1:D:181:LEU:O	1:D:185:LEU:HD12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HD22	1:A:199:PHE:CZ	2.33	0.62
1:A:290:LEU:HB3	1:A:364:MET:HE1	1.81	0.62
1:C:521:VAL:O	1:C:538:LYS:NZ	2.27	0.62
1:A:161:ALA:HB1	1:A:214:PHE:HE1	1.65	0.61
1:C:491:VAL:HG21	1:C:495:MET:HE3	1.82	0.61
1:D:317:PHE:O	1:D:319:LYS:N	2.33	0.61
1:B:251:GLN:HE21	1:B:375:ALA:C	2.08	0.61
1:B:251:GLN:NE2	1:B:379:SER:OG	2.25	0.61
1:D:348:VAL:HG23	1:D:353:LYS:HG3	1.81	0.61
1:A:317:PHE:CE1	1:C:316:ARG:HG3	2.36	0.61
1:C:316:ARG:CG	1:C:317:PHE:H	2.13	0.61
1:A:194:LEU:O	1:A:196:LYS:N	2.32	0.61
1:A:315:LEU:C	1:A:317:PHE:H	2.08	0.60
1:C:323:ASN:HB3	1:C:329:HIS:CD2	2.36	0.60
1:D:139:GLU:HB2	1:D:200:LYS:HD2	1.84	0.60
1:C:144:TYR:O	1:C:148:GLU:HG3	2.02	0.60
1:A:137:SER:OG	1:A:138:LEU:N	2.35	0.60
1:A:469:GLY:HA3	1:C:311:GLU:HG2	1.83	0.60
1:A:142:LEU:HD12	1:A:211:THR:HG23	1.84	0.59
1:B:287:VAL:HG13	1:B:291:LYS:HD3	1.85	0.59
1:C:142:LEU:HD22	1:C:199:PHE:HZ	1.67	0.59
1:D:248:TYR:CD1	1:D:249:ILE:HG12	2.37	0.59
1:B:497:MET:HE1	1:B:516:PHE:HE1	1.68	0.59
1:D:152:LYS:HB3	1:D:193:MET:HB3	1.83	0.59
1:A:244:LYS:HE2	1:A:245:VAL:O	2.02	0.59
1:D:466:ASP:HB2	1:D:507:MET:HE2	1.84	0.59
1:A:195:ASP:O	1:A:197:ASP:N	2.36	0.59
1:A:169:THR:HB	1:A:178:MET:HE2	1.84	0.58
1:B:152:LYS:HG3	1:B:193:MET:SD	2.43	0.58
1:D:313:SER:HA	1:D:316:ARG:NH1	2.19	0.58
1:C:312:PRO:HB3	1:C:461:SER:HB2	1.86	0.58
1:D:316:ARG:HH22	1:D:329:HIS:CG	2.20	0.58
1:B:489:LEU:HD23	1:B:497:MET:HE3	1.85	0.57
1:B:143:PHE:CE2	1:B:196:LYS:HG2	2.39	0.57
1:C:161:ALA:HB1	1:C:214:PHE:HE1	1.68	0.57
1:C:313:SER:HA	1:C:316:ARG:NH1	2.19	0.57
1:D:331:PRO:HD2	1:D:458:LEU:HD13	1.87	0.57
1:B:142:LEU:O	1:B:145:THR:OG1	2.18	0.57
1:C:313:SER:OG	1:C:314:GLY:N	2.29	0.57
1:B:251:GLN:HE22	1:B:379:SER:CB	2.17	0.57
1:B:285:SER:OG	1:B:288:LYS:NZ	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLN:NE2	1:B:152:LYS:HD3	2.20	0.56
1:B:316:ARG:NH2	1:D:316:ARG:HH11	2.05	0.55
1:C:181:LEU:HD23	1:C:202:CYS:SG	2.46	0.55
1:A:290:LEU:HD22	1:A:364:MET:CE	2.37	0.55
1:D:313:SER:O	1:D:316:ARG:HB2	2.07	0.55
1:C:181:LEU:O	1:C:185:LEU:HD12	2.07	0.54
1:C:316:ARG:HD2	1:C:317:PHE:CZ	2.41	0.54
1:D:487:ILE:HD12	1:D:513:GLY:HA3	1.88	0.54
1:A:364:MET:HG3	1:A:446:VAL:HG11	1.89	0.54
1:A:316:ARG:HH21	1:A:318:ASN:CG	2.15	0.54
1:D:316:ARG:HG2	1:D:317:PHE:CD2	2.43	0.54
1:B:524:CYS:HA	1:B:539:LEU:O	2.06	0.54
1:A:223:PHE:O	1:A:227:THR:HG23	2.08	0.54
1:C:357:VAL:O	1:C:361:LEU:HG	2.08	0.54
1:C:487:ILE:HD12	1:C:513:GLY:HA3	1.90	0.54
1:A:147:ALA:C	1:A:149:GLY:H	2.16	0.53
1:C:151:GLU:CD	1:C:152:LYS:H	2.17	0.53
1:B:247:ASP:HA	1:B:253:ALA:HB2	1.90	0.53
1:D:313:SER:O	1:D:316:ARG:HD3	2.09	0.53
1:D:142:LEU:CD2	1:D:211:THR:HG22	2.39	0.53
1:A:319:LYS:HE3	2:A:601:5XZ:C24	2.38	0.53
1:B:453:ARG:HD3	1:D:527:HIS:CD2	2.42	0.53
1:A:144:TYR:OH	1:A:196:LYS:NZ	2.25	0.53
1:B:184:THR:O	1:B:187:THR:HG22	2.09	0.53
1:A:528:ASN:ND2	1:C:528:ASN:OD1	2.40	0.52
1:D:233:LEU:HD22	1:D:519:ASP:HB3	1.91	0.52
1:A:316:ARG:NH2	1:A:318:ASN:OD1	2.40	0.52
1:C:297:ASN:ND2	1:C:448:SER:H	2.03	0.52
1:A:528:ASN:HD21	1:C:528:ASN:CG	2.17	0.52
1:B:184:THR:HG21	1:B:198:LEU:HD21	1.92	0.52
1:A:266:THR:HA	1:A:495:MET:HA	1.91	0.51
1:A:251:GLN:HG2	1:A:254:LYS:NZ	2.25	0.51
1:B:312:PRO:HA	1:B:462:CYS:SG	2.51	0.51
1:A:150:GLN:HG3	1:A:151:GLU:N	2.25	0.51
1:A:245:VAL:HG22	1:A:502:PRO:HB2	1.93	0.51
1:A:363:LYS:NZ	3:A:706:HOH:O	2.37	0.51
1:A:292:TYR:OH	1:A:305:HIS:NE2	2.33	0.51
1:C:191:GLY:HA3	1:C:193:MET:H	1.75	0.50
1:A:251:GLN:O	1:A:254:LYS:HG2	2.11	0.50
1:C:342:SER:HA	1:C:409:ILE:HD12	1.94	0.50
1:D:138:LEU:HD23	1:D:141:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:ALA:HB1	1:C:440:PRO:HG2	1.93	0.50
1:B:151:GLU:OE1	1:B:196:LYS:NZ	2.33	0.50
1:B:231:ASP:O	1:B:235:GLU:HG2	2.11	0.50
1:D:476:GLY:O	1:D:528:ASN:HB2	2.10	0.50
1:C:247:ASP:HA	1:C:253:ALA:HB2	1.94	0.50
1:D:161:ALA:HB1	1:D:214:PHE:HE1	1.76	0.49
1:A:315:LEU:C	1:A:317:PHE:N	2.67	0.49
1:D:248:TYR:O	1:D:249:ILE:HD13	2.13	0.49
1:D:251:GLN:H	1:D:251:GLN:NE2	2.10	0.49
1:C:465:TYR:HE1	3:C:701:HOH:O	1.94	0.49
1:B:527:HIS:CD2	1:D:453:ARG:HD2	2.48	0.49
1:B:164:SER:HA	1:B:224:MET:HE3	1.93	0.49
1:C:255:PHE:HD1	1:C:259:LEU:CD1	2.25	0.48
1:C:316:ARG:NH1	1:C:317:PHE:CD2	2.81	0.48
1:C:301:THR:OG1	1:C:454:ASN:OD1	2.29	0.48
1:A:452:VAL:O	1:A:456:LEU:HG	2.12	0.48
1:C:244:LYS:O	1:C:244:LYS:HG2	2.12	0.48
1:A:316:ARG:HH22	1:A:319:LYS:NZ	2.11	0.48
1:B:528:ASN:CG	1:D:528:ASN:HD21	2.20	0.48
1:A:247:ASP:O	1:A:249:ILE:N	2.46	0.48
1:C:252:LEU:HD23	1:C:252:LEU:O	2.13	0.48
1:B:431:ALA:HB1	1:B:440:PRO:HG3	1.95	0.48
1:B:478:PRO:HG3	1:D:529:TYR:CE1	2.50	0.47
1:A:151:GLU:O	1:A:152:LYS:HG3	2.14	0.47
1:A:248:TYR:CD1	1:A:249:ILE:HG23	2.49	0.47
1:A:150:GLN:CG	1:A:151:GLU:H	2.27	0.47
1:B:315:LEU:O	1:B:318:ASN:ND2	2.46	0.47
1:D:317:PHE:O	1:D:319:LYS:HG3	2.14	0.47
1:B:161:ALA:HB1	1:B:214:PHE:HE1	1.79	0.47
1:C:266:THR:HA	1:C:495:MET:HA	1.96	0.47
1:A:524:CYS:HA	1:A:539:LEU:O	2.14	0.47
1:B:478:PRO:HD2	1:B:490:VAL:O	2.14	0.47
1:B:489:LEU:CD2	1:B:497:MET:HE2	2.34	0.47
1:A:363:LYS:HD3	1:A:444:GLU:OE2	2.14	0.47
1:B:361:LEU:HD22	1:B:429:MET:CE	2.45	0.47
1:C:187:THR:HG22	1:C:188:THR:HG23	1.97	0.47
1:D:223:PHE:O	1:D:227:THR:HG23	2.15	0.47
1:A:269:GLY:O	1:A:271:ARG:HG2	2.15	0.46
1:C:255:PHE:CD1	1:C:259:LEU:HD13	2.47	0.46
1:C:476:GLY:O	1:C:528:ASN:HB2	2.15	0.46
1:A:306:ARG:O	1:A:327:LYS:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:CYS:SG	1:B:178:MET:HE2	2.55	0.46
1:A:150:GLN:HG3	1:A:151:GLU:H	1.79	0.46
1:C:299:LEU:HD13	1:C:303:TYR:CE2	2.50	0.46
1:B:317:PHE:N	1:B:317:PHE:CD1	2.83	0.46
1:C:146:ILE:HD12	1:C:146:ILE:H	1.80	0.46
1:C:251:GLN:HA	1:C:251:GLN:NE2	2.30	0.46
1:A:348:VAL:O	1:A:353:LYS:HE3	2.16	0.46
1:A:453:ARG:HD3	1:C:527:HIS:CD2	2.51	0.46
1:A:476:GLY:O	1:A:528:ASN:HB2	2.16	0.46
1:C:316:ARG:NE	1:C:317:PHE:CD2	2.84	0.46
1:D:318:ASN:N	1:D:318:ASN:OD1	2.48	0.46
1:A:148:GLU:H	1:A:148:GLU:HG2	1.59	0.46
1:A:378:GLN:NE2	1:A:381:ARG:HD3	2.31	0.46
1:B:313:SER:HG	1:B:314:GLY:N	2.14	0.46
1:C:152:LYS:HB3	1:C:193:MET:HB3	1.98	0.46
1:C:392:TYR:CE2	1:C:406:MET:HE1	2.51	0.46
1:D:219:VAL:N	1:D:268:ASP:OD2	2.48	0.46
1:B:244:LYS:HE3	1:B:245:VAL:O	2.17	0.45
1:A:151:GLU:HB2	1:A:152:LYS:H	1.52	0.45
1:D:138:LEU:O	1:D:142:LEU:HD23	2.16	0.45
1:C:479:ALA:HB2	1:C:489:LEU:HD12	1.99	0.45
1:A:152:LYS:HE2	1:A:195:ASP:OD2	2.17	0.45
1:C:215:ARG:HA	1:C:215:ARG:NE	2.24	0.45
1:D:195:ASP:OD1	1:D:197:ASP:N	2.50	0.45
1:A:140:ASP:HA	1:A:143:PHE:HB3	1.99	0.45
1:C:302:GLU:OE2	1:D:241:SER:CB	2.64	0.45
1:D:241:SER:HB2	1:D:242:GLY:H	1.56	0.45
1:D:260:TRP:CE3	1:D:501:SER:HB2	2.52	0.45
1:C:151:GLU:OE1	1:C:152:LYS:N	2.50	0.45
1:D:262:VAL:HG13	1:D:497:MET:CE	2.46	0.45
1:D:438:PHE:CE2	1:D:445:ARG:HB2	2.52	0.45
1:A:316:ARG:HH21	1:A:318:ASN:ND2	2.15	0.44
1:B:529:TYR:OH	1:D:478:PRO:HD3	2.17	0.44
1:C:314:GLY:O	1:C:316:ARG:HB3	2.17	0.44
1:B:266:THR:HA	1:B:495:MET:HA	1.99	0.44
1:C:316:ARG:NH1	1:C:317:PHE:HE2	2.12	0.44
1:C:191:GLY:HA3	1:C:193:MET:N	2.33	0.44
1:C:316:ARG:HD2	1:C:317:PHE:CD2	2.50	0.44
1:A:244:LYS:HE3	1:A:247:ASP:OD2	2.17	0.44
1:D:364:MET:HG3	1:D:446:VAL:HG11	1.99	0.44
1:A:431:ALA:HB1	1:A:440:PRO:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:GLY:O	1:B:528:ASN:HB2	2.18	0.44
1:D:313:SER:OG	1:D:316:ARG:NH2	2.51	0.44
1:B:398:LYS:HA	1:B:398:LYS:HD3	1.81	0.44
1:B:537:LYS:HE2	1:B:537:LYS:HA	1.98	0.44
1:C:256:SER:O	1:C:259:LEU:HD12	2.18	0.44
1:D:141:LEU:HD23	1:D:142:LEU:HD22	1.99	0.44
1:B:144:TYR:CE1	1:B:149:GLY:HA2	2.52	0.44
1:C:140:ASP:OD2	1:C:196:LYS:HG3	2.18	0.44
1:C:320:LEU:HD22	2:C:601:5XZ:C07	2.48	0.44
1:A:316:ARG:HH22	1:A:319:LYS:CE	2.31	0.43
1:B:193:MET:HB2	1:B:193:MET:HE3	1.58	0.43
1:D:191:GLY:HA3	1:D:192:VAL:HA	1.61	0.43
1:D:339:VAL:HG23	1:D:394:LEU:HD13	2.00	0.43
1:D:364:MET:HE2	1:D:447:LEU:HD21	2.01	0.43
1:A:150:GLN:NE2	1:A:151:GLU:OE2	2.52	0.43
1:A:312:PRO:HA	1:A:462:CYS:SG	2.59	0.43
1:D:142:LEU:HG	1:D:211:THR:HG22	2.00	0.43
1:D:155:VAL:HG23	1:D:192:VAL:O	2.19	0.43
1:D:317:PHE:CE1	1:D:320:LEU:HB2	2.52	0.43
1:B:227:THR:HB	1:B:272:HIS:CE1	2.54	0.43
1:C:302:GLU:O	1:C:306:ARG:HG3	2.19	0.43
1:A:251:GLN:HG2	1:A:254:LYS:HZ2	1.84	0.43
1:A:316:ARG:HH22	1:A:319:LYS:HE2	1.83	0.43
1:B:141:LEU:HD23	1:B:141:LEU:HA	1.78	0.43
1:B:529:TYR:CE1	1:D:478:PRO:HG3	2.54	0.43
1:A:319:LYS:HE3	2:A:601:5XZ:C25	2.49	0.43
1:B:331:PRO:HD2	1:B:458:LEU:HD13	2.01	0.43
1:A:264:VAL:HG22	1:A:497:MET:HE3	2.01	0.42
1:B:348:VAL:HG23	1:B:353:LYS:HG3	2.00	0.42
1:B:506:LYS:HD3	1:B:506:LYS:N	2.33	0.42
1:A:251:GLN:CD	1:A:376:THR:OG1	2.63	0.42
1:B:489:LEU:CD2	1:B:497:MET:CE	2.88	0.42
1:D:141:LEU:CD2	1:D:142:LEU:HD22	2.49	0.42
1:C:226:PHE:CZ	1:C:230:ILE:HD11	2.54	0.42
1:A:168:ARG:O	1:A:171:ASP:HB2	2.20	0.42
1:A:487:ILE:HD12	1:A:513:GLY:HA3	2.02	0.42
1:C:180:MET:HG2	1:C:202:CYS:HA	2.01	0.42
1:D:359:GLN:HG3	1:D:363:LYS:NZ	2.34	0.42
1:B:215:ARG:O	1:B:217:LYS:NZ	2.49	0.42
1:C:223:PHE:O	1:C:227:THR:HG23	2.20	0.42
1:C:252:LEU:C	1:C:254:LYS:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:ILE:HA	1:D:409:ILE:HD13	1.84	0.41
1:A:506:LYS:HA	1:A:506:LYS:HD2	1.87	0.41
1:C:162:LEU:HD21	1:C:174:LEU:HD13	2.01	0.41
1:C:313:SER:HG	1:C:314:GLY:H	1.62	0.41
1:D:445:ARG:NH1	3:D:609:HOH:O	2.47	0.41
1:A:277:THR:O	1:A:424:GLU:HG3	2.21	0.41
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.92	0.41
1:A:536:ALA:HB2	1:C:449:PRO:HG2	2.02	0.41
1:C:401:PRO:O	1:C:404:THR:OG1	2.35	0.41
1:B:269:GLY:O	1:B:271:ARG:HG2	2.20	0.41
1:B:356:TYR:HA	1:B:359:GLN:HE21	1.86	0.41
1:D:189:SER:HB2	1:D:190:ASP:H	1.62	0.41
1:A:215:ARG:HB3	1:A:217:LYS:NZ	2.36	0.41
1:C:497:MET:HE1	1:C:516:PHE:CE1	2.55	0.41
1:D:208:VAL:O	1:D:211:THR:OG1	2.39	0.41
1:D:317:PHE:C	1:D:319:LYS:H	2.28	0.41
1:D:410:LEU:HD23	1:D:410:LEU:HA	1.88	0.41
1:D:431:ALA:HB1	1:D:440:PRO:HG3	2.01	0.41
1:B:386:ARG:O	1:B:390:ILE:HG13	2.21	0.41
1:D:155:VAL:H	1:D:192:VAL:HG23	1.86	0.41
1:A:215:ARG:HA	1:A:215:ARG:HD3	1.78	0.40
1:A:317:PHE:CD1	1:C:316:ARG:HG3	2.56	0.40
1:C:140:ASP:CG	1:C:196:LYS:HZ2	2.03	0.40
1:D:180:MET:HG2	1:D:202:CYS:HA	2.02	0.40
1:A:378:GLN:O	1:A:381:ARG:HG2	2.21	0.40
1:D:312:PRO:HA	1:D:462:CYS:SG	2.62	0.40
1:A:143:PHE:CE1	1:A:196:LYS:HA	2.57	0.40
1:D:248:TYR:CE1	1:D:249:ILE:HG12	2.57	0.40
1:A:176:GLU:H	1:A:176:GLU:CD	2.29	0.40
1:A:313:SER:OG	1:A:314:GLY:N	2.54	0.40
1:C:292:TYR:OH	1:C:305:HIS:NE2	2.38	0.40
1:C:434:ALA:HB2	1:C:490:VAL:HG13	2.03	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	408/539 (76%)	379 (93%)	17 (4%)	12 (3%)	3	5
1	B	408/539 (76%)	388 (95%)	18 (4%)	2 (0%)	24	43
1	C	408/539 (76%)	379 (93%)	22 (5%)	7 (2%)	7	13
1	D	408/539 (76%)	386 (95%)	19 (5%)	3 (1%)	18	34
All	All	1632/2156 (76%)	1532 (94%)	76 (5%)	24 (2%)	8	16

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	GLU
1	A	248	TYR
1	A	313	SER
1	A	316	ARG
1	A	544	GLU
1	C	148	GLU
1	C	313	SER
1	D	189	SER
1	D	318	ASN
1	A	195	ASP
1	A	196	LYS
1	A	315	LEU
1	B	313	SER
1	C	190	ASP
1	C	251	GLN
1	A	148	GLU
1	C	152	LYS
1	C	316	ARG
1	D	316	ARG
1	A	153	ILE
1	A	138	LEU
1	C	248	TYR
1	A	314	GLY
1	B	191	GLY

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	353/462 (76%)	348 (99%)	5 (1%)	59	81
1	B	353/462 (76%)	349 (99%)	4 (1%)	65	84
1	C	353/462 (76%)	350 (99%)	3 (1%)	73	88
1	D	353/462 (76%)	349 (99%)	4 (1%)	65	84
All	All	1412/1848 (76%)	1396 (99%)	16 (1%)	65	84

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	VAL
1	A	205	SER
1	A	383	SER
1	A	411	ASP
1	A	507	MET
1	B	137	SER
1	B	164	SER
1	B	205	SER
1	B	287	VAL
1	C	359	GLN
1	C	411	ASP
1	C	462	CYS
1	D	137	SER
1	D	189	SER
1	D	241	SER
1	D	360	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	GLN
1	A	350	ASN
1	A	515	HIS

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Mol	Chain	Res	Type
1	B	150	GLN
1	B	270	GLN
1	B	359	GLN
1	B	415	GLN
1	B	493	ASN
1	B	534	HIS
1	C	186	GLN
1	C	297	ASN
1	C	329	HIS
1	C	470	GLN
1	D	186	GLN
1	D	251	GLN
1	D	334	ASN
1	D	346	GLN
1	D	367	ASN
1	D	374	ASN
1	D	415	GLN
1	D	454	ASN

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	5XZ	C	601	-	40,40,40	3.37	14 (35%)	50,54,54	4.81	26 (52%)
2	5XZ	A	601	-	40,40,40	3.40	14 (35%)	50,54,54	3.72	20 (40%)

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	5XZ	C	601	-	-	10/22/33/33	0/5/5/5
2	5XZ	A	601	-	-	10/22/33/33	0/5/5/5

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	5XZ	C12-C11	-14.26	1.30	1.52
2	C	601	5XZ	C12-C11	-14.14	1.30	1.52
2	C	601	5XZ	C12-N08	8.42	1.62	1.46
2	A	601	5XZ	C12-N08	8.34	1.62	1.46
2	A	601	5XZ	C09-N08	-8.00	1.30	1.47
2	C	601	5XZ	C09-N08	-7.68	1.31	1.47
2	A	601	5XZ	C14-N15	4.44	1.34	1.29
2	C	601	5XZ	C14-N15	4.32	1.34	1.29
2	A	601	5XZ	O13-C14	4.27	1.41	1.35
2	C	601	5XZ	O13-C14	4.13	1.41	1.35
2	C	601	5XZ	C07-N08	3.79	1.43	1.34
2	A	601	5XZ	C07-N08	3.55	1.42	1.34
2	C	601	5XZ	C17-N18	3.49	1.43	1.38
2	A	601	5XZ	C04-N03	3.40	1.43	1.38
2	C	601	5XZ	C19-N18	3.31	1.43	1.37
2	A	601	5XZ	C02-N03	3.11	1.42	1.37
2	A	601	5XZ	C19-N18	3.08	1.42	1.37
2	C	601	5XZ	C02-N03	3.08	1.42	1.37
2	C	601	5XZ	C04-N03	3.07	1.42	1.38
2	A	601	5XZ	C17-N18	2.92	1.42	1.38
2	A	601	5XZ	C04-N05	2.69	1.35	1.31
2	C	601	5XZ	C17-N16	2.56	1.35	1.31
2	A	601	5XZ	N16-N15	-2.48	1.34	1.39
2	C	601	5XZ	N06-N05	-2.30	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	5XZ	C04-N05	2.29	1.34	1.31
2	C	601	5XZ	N16-N15	-2.23	1.34	1.39
2	A	601	5XZ	C17-N16	2.21	1.34	1.31
2	A	601	5XZ	N06-N05	-2.06	1.35	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	5XZ	C11-O13-C14	-17.87	105.97	117.71
2	C	601	5XZ	C20-C19-N18	10.53	127.24	114.40
2	A	601	5XZ	C11-O13-C14	-9.81	111.27	117.71
2	A	601	5XZ	C14-N15-N16	9.07	116.29	105.84
2	C	601	5XZ	C14-N15-N16	9.04	116.26	105.84
2	C	601	5XZ	S28-C17-N16	-8.69	104.82	114.52
2	C	601	5XZ	S28-C14-N15	-8.65	105.83	117.59
2	A	601	5XZ	S28-C14-N15	-8.39	106.17	117.59
2	C	601	5XZ	C19-N18-C17	-7.99	110.03	123.69
2	A	601	5XZ	S29-C04-N05	-7.81	105.81	114.52
2	A	601	5XZ	S28-C17-N16	-7.72	105.90	114.52
2	C	601	5XZ	S29-C04-N05	-7.36	106.31	114.52
2	A	601	5XZ	N03-C04-N05	7.34	127.37	120.81
2	C	601	5XZ	S29-C07-N08	6.66	129.22	120.31
2	C	601	5XZ	O13-C14-S28	5.92	128.91	116.13
2	A	601	5XZ	N08-C07-N06	5.62	127.78	116.91
2	C	601	5XZ	N18-C17-N16	5.35	125.59	120.81
2	A	601	5XZ	O13-C14-S28	5.22	127.40	116.13
2	C	601	5XZ	C07-N06-N05	5.17	117.28	107.08
2	C	601	5XZ	S29-C07-N06	-5.13	105.56	114.44
2	C	601	5XZ	C09-N08-C12	-5.13	106.38	112.38
2	A	601	5XZ	S29-C07-N06	-5.01	105.77	114.44
2	A	601	5XZ	C07-N06-N05	4.88	116.71	107.08
2	C	601	5XZ	N03-C04-N05	4.78	125.08	120.81
2	A	601	5XZ	C09-N08-C12	-4.66	106.94	112.38
2	A	601	5XZ	S28-C17-N18	4.60	129.88	123.72
2	A	601	5XZ	S29-C07-N08	4.59	126.45	120.31
2	C	601	5XZ	C01-C02-N03	4.40	119.76	114.40
2	C	601	5XZ	C17-S28-C14	4.37	95.66	86.65
2	C	601	5XZ	S28-C17-N18	4.34	129.53	123.72
2	C	601	5XZ	N08-C07-N06	4.30	125.22	116.91
2	C	601	5XZ	C17-N16-N15	4.25	117.43	112.02
2	A	601	5XZ	C17-S28-C14	3.95	94.79	86.65
2	C	601	5XZ	C10-C09-N08	3.89	107.94	102.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	5XZ	C17-N16-N15	3.79	116.84	112.02
2	A	601	5XZ	N18-C17-N16	3.79	124.20	120.81
2	C	601	5XZ	S29-C04-N03	3.64	128.59	123.72
2	A	601	5XZ	C01-C02-N03	3.52	118.70	114.40
2	A	601	5XZ	C04-N05-N06	3.24	116.14	112.02
2	A	601	5XZ	C20-C19-N18	3.19	118.29	114.40
2	C	601	5XZ	C04-N05-N06	2.96	115.78	112.02
2	C	601	5XZ	O27-C19-N18	-2.88	116.98	122.44
2	C	601	5XZ	O27-C19-C20	-2.87	115.78	121.99
2	A	601	5XZ	S29-C04-N03	2.32	126.82	123.72
2	C	601	5XZ	C21-C20-C19	-2.27	105.55	112.33
2	C	601	5XZ	O13-C11-C12	2.25	113.58	108.30

There are no chirality outliers.

All (20) torsion outliers are listed below:

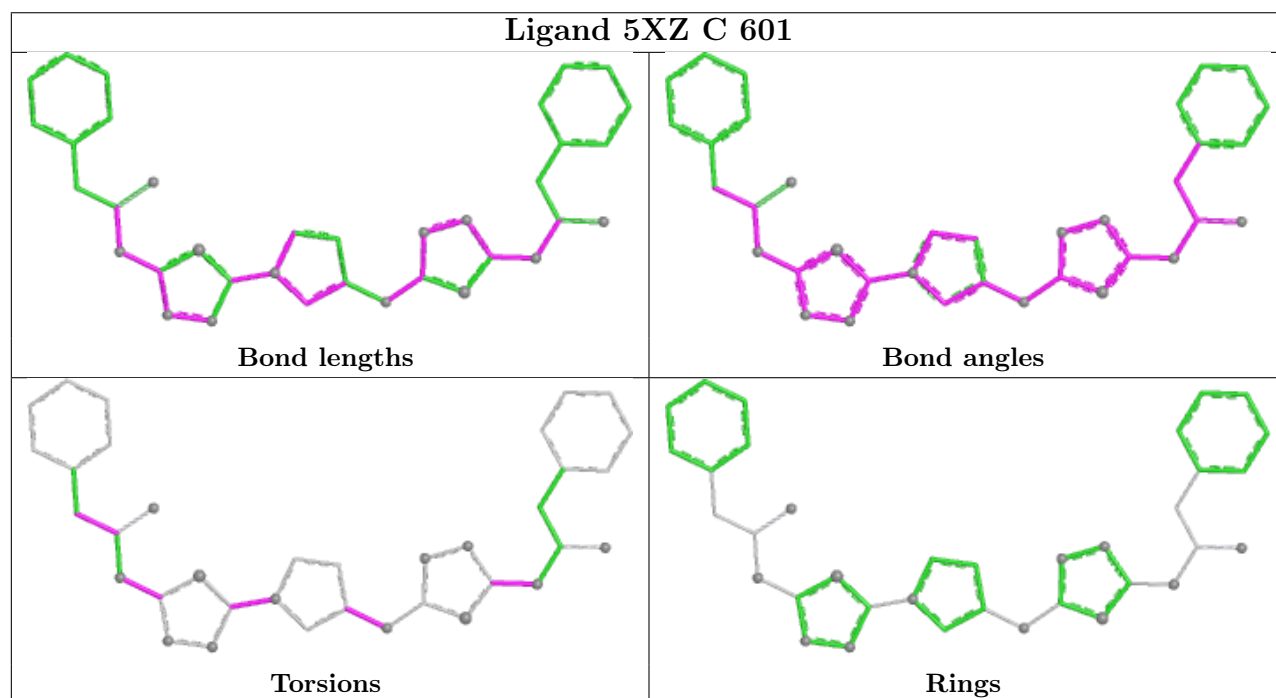
Mol	Chain	Res	Type	Atoms
2	A	601	5XZ	N16-C17-N18-C19
2	A	601	5XZ	S28-C17-N18-C19
2	A	601	5XZ	S29-C04-N03-C02
2	A	601	5XZ	N06-C07-N08-C09
2	A	601	5XZ	N06-C07-N08-C12
2	A	601	5XZ	S29-C07-N08-C09
2	A	601	5XZ	S29-C07-N08-C12
2	C	601	5XZ	N16-C17-N18-C19
2	C	601	5XZ	S28-C17-N18-C19
2	C	601	5XZ	N05-C04-N03-C02
2	C	601	5XZ	S29-C04-N03-C02
2	C	601	5XZ	S29-C07-N08-C12
2	C	601	5XZ	C12-C11-O13-C14
2	A	601	5XZ	N05-C04-N03-C02
2	C	601	5XZ	N06-C07-N08-C12
2	A	601	5XZ	O27-C19-C20-C21
2	C	601	5XZ	C10-C11-O13-C14
2	A	601	5XZ	N18-C19-C20-C21
2	C	601	5XZ	C31-C01-C02-N03
2	C	601	5XZ	C31-C01-C02-O30

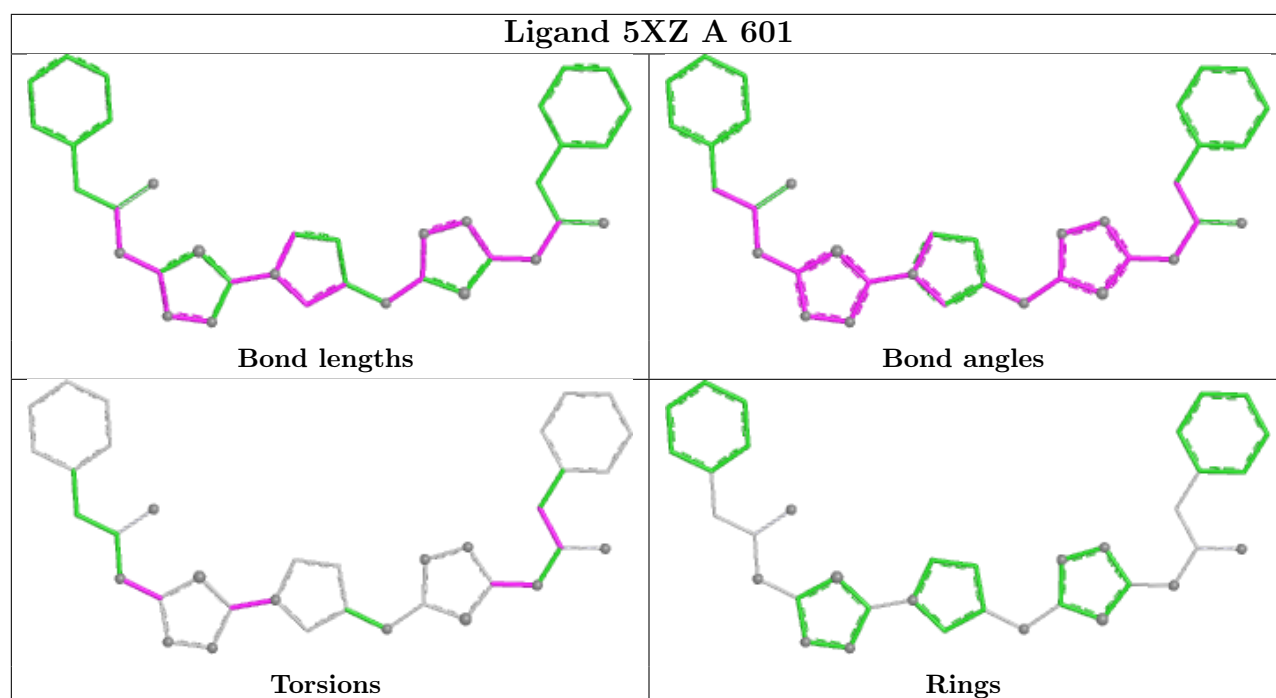
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	5XZ	1	0
2	A	601	5XZ	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	410/539 (76%)	0.66	41 (10%)	12 10	23, 38, 95, 170	0
1	B	410/539 (76%)	0.53	34 (8%)	17 15	20, 38, 87, 155	0
1	C	410/539 (76%)	0.65	44 (10%)	11 9	22, 38, 88, 165	0
1	D	410/539 (76%)	0.50	34 (8%)	17 15	20, 36, 79, 141	0
All	All	1640/2156 (76%)	0.59	153 (9%)	14 12	20, 38, 89, 170	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	314	GLY	9.8
1	C	313	SER	9.5
1	C	252	LEU	9.5
1	B	144	TYR	7.6
1	C	317	PHE	7.5
1	A	317	PHE	7.3
1	D	315	LEU	7.3
1	C	315	LEU	6.8
1	D	313	SER	6.8
1	D	317	PHE	6.4
1	A	251	GLN	6.3
1	A	318	ASN	6.3
1	C	314	GLY	6.2
1	C	255	PHE	6.1
1	A	189	SER	6.1
1	C	248	TYR	6.0
1	A	187	THR	5.9
1	B	317	PHE	5.9
1	B	187	THR	5.8
1	B	316	ARG	5.7
1	A	314	GLY	5.6

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Mol	Chain	Res	Type	RSRZ
1	B	545	GLY	5.6
1	A	313	SER	5.6
1	A	315	LEU	5.6
1	D	318	ASN	5.4
1	B	314	GLY	5.1
1	A	188	THR	4.9
1	D	136	PRO	4.8
1	A	545	GLY	4.7
1	D	316	ARG	4.7
1	B	313	SER	4.5
1	C	192	VAL	4.5
1	A	192	VAL	4.5
1	C	249	ILE	4.3
1	D	142	LEU	4.3
1	C	190	ASP	4.3
1	B	315	LEU	4.3
1	D	144	TYR	4.2
1	A	190	ASP	4.2
1	B	136	PRO	4.1
1	B	192	VAL	4.1
1	B	145	THR	4.1
1	D	143	PHE	4.1
1	B	141	LEU	4.0
1	D	192	VAL	4.0
1	A	144	TYR	4.0
1	C	185	LEU	4.0
1	B	152	LYS	4.0
1	D	545	GLY	4.0
1	A	136	PRO	4.0
1	C	545	GLY	4.0
1	C	144	TYR	3.9
1	A	247	ASP	3.9
1	D	191	GLY	3.8
1	A	316	ARG	3.7
1	A	152	LYS	3.7
1	C	189	SER	3.6
1	C	247	ASP	3.6
1	A	252	LEU	3.6
1	C	191	GLY	3.5
1	C	250	PRO	3.4
1	B	148	GLU	3.4
1	A	248	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	250	PRO	3.3
1	D	267	VAL	3.3
1	A	137	SER	3.3
1	D	189	SER	3.3
1	C	136	PRO	3.2
1	A	255	PHE	3.2
1	C	379	SER	3.2
1	D	137	SER	3.2
1	B	190	ASP	3.2
1	A	148	GLU	3.1
1	C	318	ASN	3.1
1	A	149	GLY	3.1
1	C	141	LEU	3.0
1	A	138	LEU	3.0
1	B	189	SER	3.0
1	A	146	ILE	2.9
1	C	138	LEU	2.9
1	C	151	GLU	2.9
1	D	138	LEU	2.8
1	C	143	PHE	2.8
1	B	193	MET	2.8
1	C	254	LYS	2.8
1	C	316	ARG	2.8
1	D	188	THR	2.7
1	A	193	MET	2.7
1	B	191	GLY	2.6
1	B	211	THR	2.6
1	C	253	ALA	2.6
1	A	197	ASP	2.6
1	B	197	ASP	2.6
1	A	302	GLU	2.6
1	B	151	GLU	2.6
1	B	207	ILE	2.6
1	D	190	ASP	2.5
1	D	141	LEU	2.5
1	D	151	GLU	2.5
1	A	253	ALA	2.5
1	A	257	PRO	2.5
1	B	347	GLY	2.5
1	D	146	ILE	2.5
1	C	187	THR	2.5
1	D	544	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	249	ILE	2.4
1	B	196	LYS	2.4
1	A	185	LEU	2.4
1	C	312	PRO	2.4
1	A	537	LYS	2.4
1	C	188	THR	2.4
1	B	140	ASP	2.4
1	C	251	GLN	2.4
1	A	147	ALA	2.4
1	B	319	LYS	2.4
1	A	256	SER	2.4
1	C	193	MET	2.3
1	C	197	ASP	2.3
1	C	201	LYS	2.3
1	D	543	ARG	2.3
1	C	256	SER	2.3
1	D	241	SER	2.3
1	C	142	LEU	2.3
1	D	153	ILE	2.3
1	B	251	GLN	2.3
1	D	185	LEU	2.3
1	D	224	MET	2.3
1	C	257	PRO	2.2
1	A	254	LYS	2.2
1	C	382	GLU	2.2
1	B	199	PHE	2.2
1	A	212	GLN	2.2
1	D	193	MET	2.2
1	B	242	GLY	2.2
1	C	149	GLY	2.2
1	B	224	MET	2.1
1	A	153	ILE	2.1
1	C	146	ILE	2.1
1	A	151	GLU	2.1
1	D	382	GLU	2.1
1	B	250	PRO	2.1
1	C	244	LYS	2.1
1	D	150	GLN	2.1
1	B	195	ASP	2.1
1	B	150	GLN	2.1
1	D	445	ARG	2.1
1	C	137	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	152	LYS	2.0
1	D	207	ILE	2.0
1	C	465	TYR	2.0
1	A	224	MET	2.0
1	B	241	SER	2.0
1	C	150	GLN	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](#)

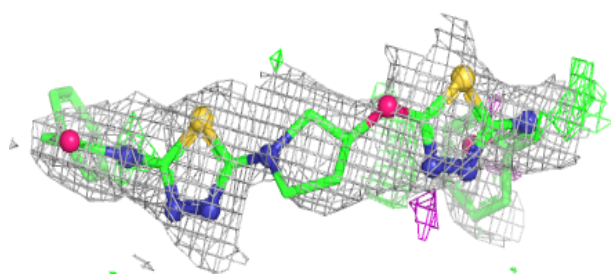
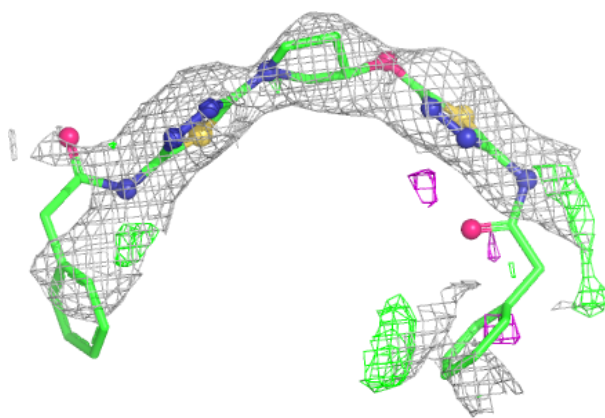
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	5XZ	C	601	36/36	0.66	0.28	93,105,114,121	0
2	5XZ	A	601	36/36	0.71	0.25	82,97,117,119	0

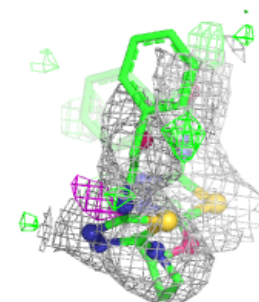
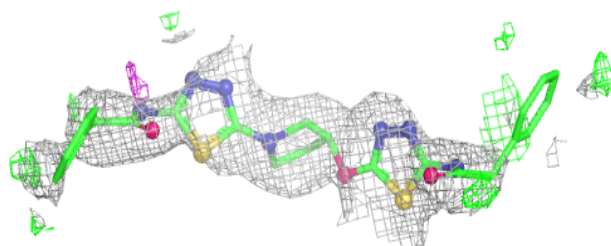
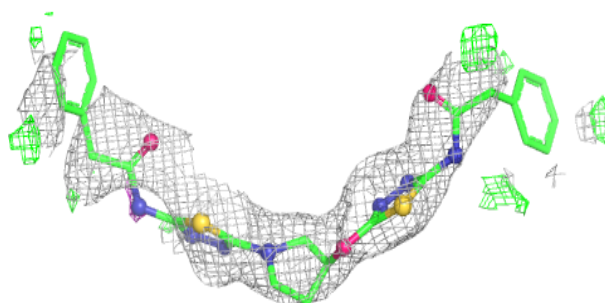
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5XZ 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)

**Electron density around 5XZ A 601:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.