



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 10:10 AM UTC

PDB ID : 5FI2 / pdb_00005fi2
Title : Crystal structure of human GAC in complex with inhibitor UPGL_00009: 2-phenyl- {N}-[5-[[{(3 {R})-1-[5-(2-phenylethanoylamino)-1,3,4-thiadiazol- 2-yl]pyrrolidin-3-yl]amino]-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

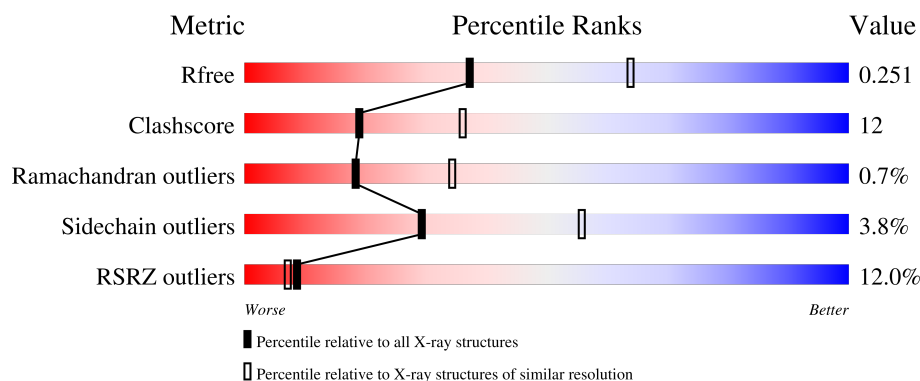
1 Overall quality at a glance

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% 17% • 24%
1	B	539	9% 57% 17% •• 24%
1	C	539	10% 60% 14% • 24%
1	D	539	9% 56% 19% • 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13548 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:

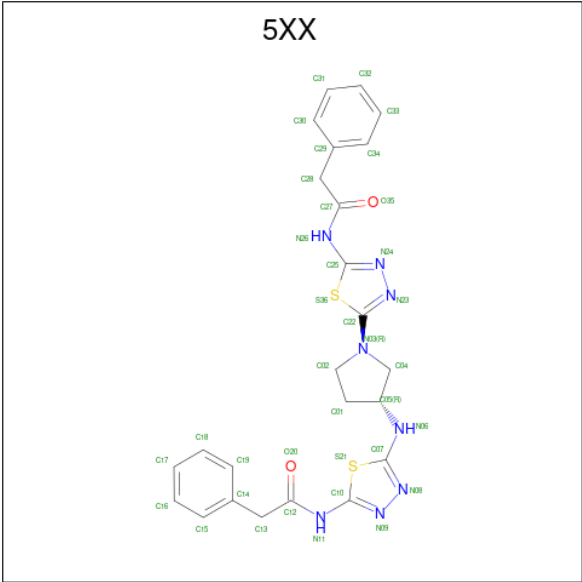
Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MET	-	initiating methionine	UNP O94925
A	60	ARG	-	expression tag	UNP O94925
A	61	GLY	-	expression tag	UNP O94925
A	62	SER	-	expression tag	UNP O94925
A	63	HIS	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	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 {R})-1-[5-(2-phenylethanoylamino)-1,3,4-thiadiazol-2-yl]pyrrolidin-3-yl]amino]-1,3,4-thiadiazol-2-yl]ethanamide (CCD ID: 5XX) (formula: C₂₄H₂₄N₈O₂S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			36	24	8	2	2		
2	D	1	Total	C	N	O	S	0	0
			36	24	8	2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	180	Total	O	0	0
			180	180		
3	B	167	Total	O	0	0
			167	167		
3	C	177	Total	O	0	0
			177	177		
3	D	176	Total	O	0	0
			176	176		

TRP
LYS
LYS
VAL
SER
PRO
GLU
SER
ASN
GLU
ASP
ILE
SER
THR
VAL
VAL
TYR
ARG
MET
GLU
SER
LEU
GLY
GLU
LYS
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	98.05Å 138.62Å 176.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.83 – 2.50 44.83 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.83-2.50) 99.9 (44.83-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.225 , 0.265 (Not available) , 0.251	Depositor DCC
R_{free} test set	2000 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.7	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	0.94	EDS
Total number of atoms	13548	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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 59.57 % 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 1.7307e-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: 5XX

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	0.69	0/3266	0.90	5/4408 (0.1%)
1	B	0.69	0/3266	0.91	8/4408 (0.2%)
1	C	0.67	0/3266	0.91	6/4408 (0.1%)
1	D	0.70	0/3266	0.93	10/4408 (0.2%)
All	All	0.69	0/13064	0.91	29/17632 (0.2%)

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	D	0	2
All	All	0	3

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	313	SER	N-CA-C	-8.92	101.55	111.28
1	B	251	GLN	CA-CB-CG	7.44	128.97	114.10
1	A	220	ILE	CA-C-N	6.91	126.16	118.97
1	A	220	ILE	C-N-CA	6.91	126.16	118.97
1	D	317	PHE	N-CA-C	6.32	124.27	110.80
1	C	316	ARG	N-CA-C	-6.29	106.19	114.31
1	D	220	ILE	CA-C-N	6.25	125.74	119.24
1	D	220	ILE	C-N-CA	6.25	125.74	119.24
1	C	465	TYR	CB-CA-C	-6.25	109.38	116.63
1	B	220	ILE	CA-C-N	6.22	125.44	118.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	ILE	C-N-CA	6.22	125.44	118.97
1	A	502	PRO	N-CA-C	5.94	117.94	110.70
1	A	465	TYR	CB-CA-C	-5.91	109.77	116.63
1	C	502	PRO	N-CA-C	5.83	117.82	110.70
1	D	465	TYR	CB-CA-C	-5.79	109.92	116.63
1	D	502	PRO	N-CA-C	5.70	117.66	110.70
1	B	536	ALA	CB-CA-C	-5.62	110.08	116.54
1	D	189	SER	N-CA-C	-5.62	105.53	112.38
1	C	439	CYS	CA-C-N	5.58	124.93	118.85
1	C	439	CYS	C-N-CA	5.58	124.93	118.85
1	B	317	PHE	CA-C-N	-5.50	113.95	123.25
1	B	317	PHE	C-N-CA	-5.50	113.95	123.25
1	B	502	PRO	N-CA-C	5.48	117.39	110.70
1	D	536	ALA	CB-CA-C	-5.35	110.42	116.63
1	C	247	ASP	N-CA-C	-5.35	105.49	112.23
1	B	379	SER	N-CA-C	5.34	117.54	111.02
1	A	193	MET	CB-CG-SD	5.26	128.49	112.70
1	D	502	PRO	CA-C-N	-5.17	114.47	119.90
1	D	502	PRO	C-N-CA	-5.17	114.47	119.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	250	PRO	Peptide
1	D	316	ARG	Peptide
1	D	317	PHE	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	85	0
1	B	3194	0	3167	79	0
1	C	3194	0	3167	60	0
1	D	3194	0	3167	94	0
2	A	36	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	36	0	0	0	1
3	A	180	0	0	18	1
3	B	167	0	0	19	4
3	C	177	0	0	6	0
3	D	176	0	0	13	2
All	All	13548	0	12668	300	4

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 12.

All (300) 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:530:ASP:O	3:A:701:HOH:O	1.84	0.95
1:C:318:ASN:O	3:C:602:HOH:O	1.87	0.93
1:B:364:MET:SD	3:B:748:HOH:O	2.27	0.92
1:B:271:ARG:O	3:B:601:HOH:O	1.86	0.92
1:B:252:LEU:HD21	3:B:754:HOH:O	1.71	0.91
1:C:249:ILE:HD11	1:C:252:LEU:HG	1.51	0.90
1:A:528:ASN:ND2	1:D:528:ASN:OD1	2.06	0.88
1:B:251:GLN:HE21	1:B:375:ALA:HB1	1.38	0.87
1:A:364:MET:SD	3:A:847:HOH:O	2.34	0.85
1:C:512:LYS:NZ	3:C:601:HOH:O	1.85	0.84
1:D:239:LYS:NZ	3:D:702:HOH:O	2.10	0.82
1:B:433:LEU:O	3:B:602:HOH:O	1.97	0.81
1:A:433:LEU:O	3:A:702:HOH:O	1.98	0.80
1:A:154:PRO:HD2	1:A:157:LYS:HD2	1.62	0.80
1:D:234:TYR:CD2	1:D:274:THR:HG23	2.15	0.80
1:C:167:LEU:O	3:C:603:HOH:O	1.97	0.79
1:A:316:ARG:HH22	1:A:319:LYS:HD2	1.47	0.79
1:A:164:SER:HB2	1:A:224:MET:HE1	1.65	0.78
1:B:313:SER:O	1:C:316:ARG:NH2	2.16	0.78
1:A:234:TYR:CD2	1:A:274:THR:HG23	2.19	0.78
1:A:247:ASP:CA	1:A:252:LEU:HD11	2.08	0.76
1:A:152:LYS:HE3	1:A:193:MET:HE2	1.68	0.76
1:B:249:ILE:HD13	1:B:379:SER:OG	1.84	0.75
1:D:179:ASP:OD1	1:D:182:ARG:NH2	2.20	0.74
1:B:530:ASP:O	3:B:604:HOH:O	2.06	0.72
1:A:334:ASN:OD1	3:A:703:HOH:O	2.07	0.72
1:A:424:GLU:OE1	3:A:704:HOH:O	2.08	0.71
1:D:142:LEU:O	1:D:145:THR:OG1	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ASN:OD1	3:A:705:HOH:O	2.08	0.71
1:D:221:PRO:O	3:D:701:HOH:O	2.08	0.71
1:D:187:THR:HG23	1:D:188:THR:HG23	1.70	0.70
1:A:247:ASP:HA	1:A:252:LEU:HD11	1.74	0.70
1:A:244:LYS:NZ	3:A:713:HOH:O	2.25	0.69
1:A:315:LEU:C	1:A:318:ASN:HD21	2.00	0.69
1:B:146:ILE:O	1:B:157:LYS:NZ	2.22	0.68
1:D:285:SER:OG	1:D:288:LYS:NZ	2.26	0.68
1:C:144:TYR:OH	1:C:196:LYS:NZ	2.24	0.68
1:B:234:TYR:CD2	1:B:274:THR:HG23	2.28	0.68
1:D:144:TYR:OH	1:D:196:LYS:NZ	2.22	0.68
1:B:526:PHE:O	3:B:605:HOH:O	2.11	0.68
1:D:313:SER:C	1:D:317:PHE:CZ	2.72	0.67
1:C:314:GLY:C	1:C:316:ARG:H	2.00	0.67
1:C:234:TYR:CD2	1:C:274:THR:HG23	2.29	0.67
1:A:374:ASN:OD1	3:A:707:HOH:O	2.11	0.67
1:B:252:LEU:CG	3:B:754:HOH:O	2.40	0.67
1:D:197:ASP:O	3:D:704:HOH:O	2.12	0.67
1:D:519:ASP:OD2	3:D:703:HOH:O	2.12	0.67
1:A:530:ASP:O	3:A:708:HOH:O	2.11	0.67
1:B:252:LEU:CD2	3:B:754:HOH:O	2.34	0.66
1:A:246:ALA:CB	1:A:252:LEU:HD13	2.21	0.65
1:C:150:GLN:OE1	1:C:151:GLU:N	2.30	0.65
1:B:321:PHE:O	3:B:607:HOH:O	2.14	0.65
1:B:318:ASN:HD21	1:B:333:VAL:HG11	1.61	0.64
1:B:316:ARG:HD3	1:B:466:ASP:OD1	1.97	0.64
1:C:233:LEU:HD22	1:C:519:ASP:HB3	1.79	0.64
1:D:164:SER:O	3:D:705:HOH:O	2.14	0.64
1:A:246:ALA:HB3	1:A:252:LEU:HD13	1.78	0.64
1:D:301:THR:OG1	1:D:454:ASN:ND2	2.29	0.63
1:D:148:GLU:OE2	1:D:157:LYS:NZ	2.21	0.63
1:D:444:GLU:HB2	3:D:708:HOH:O	1.96	0.63
1:D:154:PRO:HD2	1:D:157:LYS:HD3	1.79	0.63
1:B:507:MET:O	3:B:608:HOH:O	2.16	0.63
1:D:497:MET:HE1	1:D:516:PHE:CE1	2.34	0.63
1:B:487:ILE:HD12	1:B:513:GLY:HA3	1.82	0.62
1:D:316:ARG:O	1:D:318:ASN:N	2.32	0.61
1:A:215:ARG:NH1	3:A:718:HOH:O	2.33	0.61
1:C:306:ARG:HH12	1:D:257:PRO:HB2	1.67	0.60
1:B:315:LEU:O	1:B:316:ARG:HB2	2.00	0.60
1:D:155:VAL:HG21	1:D:185:LEU:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:497:MET:HE1	1:C:516:PHE:CE1	2.36	0.60
1:D:302:GLU:OE2	1:D:306:ARG:NH2	2.35	0.59
1:A:317:PHE:CE2	1:D:317:PHE:HB3	2.37	0.59
1:B:233:LEU:HD22	1:B:519:ASP:HB3	1.82	0.59
1:D:234:TYR:CD2	1:D:274:THR:CG2	2.85	0.59
1:B:314:GLY:O	1:B:316:ARG:N	2.35	0.58
1:D:450:GLU:OE1	3:D:706:HOH:O	2.16	0.58
1:B:374:ASN:OD1	3:B:609:HOH:O	2.17	0.58
1:D:316:ARG:HB2	1:D:317:PHE:CD2	2.37	0.58
1:B:528:ASN:OD1	1:C:528:ASN:OD1	2.21	0.57
1:D:222:ASP:O	3:D:707:HOH:O	2.17	0.57
1:A:247:ASP:HA	1:A:252:LEU:CD1	2.33	0.57
1:B:470:GLN:NE2	3:B:617:HOH:O	2.33	0.56
1:C:250:PRO:HD2	1:C:379:SER:HB2	1.87	0.56
1:A:472:ALA:HA	3:A:762:HOH:O	2.04	0.56
1:C:248:TYR:OH	1:C:380:GLU:OE2	2.15	0.56
1:A:233:LEU:HD22	1:A:519:ASP:HB3	1.88	0.55
1:C:497:MET:HE1	1:C:516:PHE:HE1	1.71	0.55
1:B:316:ARG:HD3	1:B:466:ASP:CG	2.31	0.55
1:B:466:ASP:OD1	1:B:466:ASP:N	2.39	0.55
1:D:184:THR:O	1:D:187:THR:HG22	2.06	0.55
1:A:251:GLN:O	1:A:254:LYS:HE2	2.07	0.55
1:D:314:GLY:CA	1:D:317:PHE:HZ	2.19	0.55
1:A:533:ARG:NH1	3:A:725:HOH:O	2.40	0.55
1:B:137:SER:OG	1:B:140:ASP:OD2	2.24	0.54
1:D:445:ARG:NH2	3:D:714:HOH:O	2.39	0.54
1:B:244:LYS:NZ	3:B:628:HOH:O	2.40	0.54
1:D:431:ALA:HB1	1:D:440:PRO:HG2	1.90	0.54
1:A:146:ILE:O	1:A:157:LYS:NZ	2.32	0.54
1:D:331:PRO:HD2	1:D:458:LEU:HD13	1.90	0.54
1:A:316:ARG:NH2	1:A:319:LYS:HD2	2.20	0.53
1:D:314:GLY:C	1:D:317:PHE:HZ	2.16	0.53
1:B:497:MET:HE1	1:B:516:PHE:CE1	2.44	0.53
1:D:139:GLU:OE1	1:D:139:GLU:N	2.35	0.53
1:A:317:PHE:CE2	1:D:317:PHE:HD2	2.26	0.53
1:B:251:GLN:NE2	1:B:375:ALA:HB1	2.17	0.53
1:A:152:LYS:HG3	1:A:193:MET:CB	2.39	0.53
1:A:252:LEU:C	1:A:252:LEU:HD12	2.34	0.53
1:B:252:LEU:HG	3:B:754:HOH:O	2.08	0.52
1:A:234:TYR:CD2	1:A:274:THR:CG2	2.91	0.52
1:B:194:LEU:HA	1:B:198:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ILE:HD12	1:C:252:LEU:H	1.74	0.52
1:A:138:LEU:O	1:A:142:LEU:HG	2.10	0.52
1:D:233:LEU:HD22	1:D:519:ASP:HB3	1.91	0.52
1:D:313:SER:HB3	1:D:317:PHE:CE1	2.44	0.52
1:A:386:ARG:NH2	3:A:728:HOH:O	2.42	0.52
1:A:142:LEU:O	1:A:146:ILE:HD12	2.10	0.52
1:B:466:ASP:HB2	1:B:507:MET:SD	2.50	0.51
1:B:478:PRO:HD2	1:B:490:VAL:O	2.09	0.51
1:D:445:ARG:NE	3:D:714:HOH:O	2.41	0.51
1:A:152:LYS:HG3	1:A:193:MET:HB3	1.92	0.51
1:B:466:ASP:CG	3:B:608:HOH:O	2.53	0.51
1:A:317:PHE:HE2	1:D:317:PHE:HB3	1.76	0.51
1:C:194:LEU:HD23	1:C:198:LEU:HG	1.93	0.51
1:A:223:PHE:O	1:A:227:THR:HG23	2.11	0.51
1:A:150:GLN:OE1	1:A:150:GLN:N	2.44	0.51
1:A:359:GLN:OE1	3:A:710:HOH:O	2.19	0.51
1:B:140:ASP:OD1	1:B:196:LYS:HE2	2.11	0.51
1:C:216:ARG:HG2	1:C:216:ARG:HH11	1.76	0.51
1:D:317:PHE:CD1	1:D:317:PHE:C	2.89	0.50
1:C:382:GLU:O	3:C:604:HOH:O	2.18	0.50
1:D:313:SER:O	1:D:317:PHE:CZ	2.65	0.50
1:D:144:TYR:HA	1:D:147:ALA:HB3	1.94	0.50
1:B:318:ASN:ND2	1:B:333:VAL:HG11	2.26	0.50
1:A:252:LEU:HD12	1:A:253:ALA:N	2.27	0.49
1:A:323:ASN:HA	1:D:316:ARG:HH21	1.77	0.49
1:B:249:ILE:O	1:B:251:GLN:N	2.45	0.49
1:D:249:ILE:HB	1:D:379:SER:HB3	1.94	0.49
1:C:184:THR:O	1:C:187:THR:OG1	2.30	0.49
1:A:331:PRO:HD2	1:A:458:LEU:HD13	1.93	0.49
1:C:306:ARG:NH1	1:D:257:PRO:HB2	2.27	0.49
1:B:434:ALA:HB2	1:B:490:VAL:HG13	1.94	0.49
1:C:188:THR:HG22	1:C:190:ASP:H	1.77	0.49
3:A:859:HOH:O	1:D:492:PRO:HB3	2.13	0.49
1:B:252:LEU:HD11	3:B:754:HOH:O	2.12	0.49
1:A:147:ALA:C	1:A:149:GLY:H	2.21	0.49
1:C:435:ASN:HA	3:C:628:HOH:O	2.12	0.49
1:A:171:ASP:OD1	1:A:173:ARG:HD3	2.13	0.48
1:D:231:ASP:O	1:D:235:GLU:HG2	2.13	0.48
1:A:348:VAL:HG23	1:A:353:LYS:HG3	1.96	0.48
1:C:257:PRO:HB3	1:C:503:PRO:HG3	1.95	0.48
1:B:223:PHE:O	1:B:227:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ILE:HD12	1:C:251:GLN:H	1.77	0.48
1:A:188:THR:O	1:A:188:THR:OG1	2.18	0.48
1:A:529:TYR:CZ	1:D:478:PRO:HG3	2.49	0.48
1:C:173:ARG:HD2	1:C:441:ILE:C	2.38	0.48
1:A:317:PHE:HE2	1:D:317:PHE:HD2	1.62	0.48
1:A:487:ILE:HD12	1:A:513:GLY:HA3	1.96	0.48
1:C:190:ASP:O	1:C:192:VAL:HG12	2.14	0.48
1:D:472:ALA:HA	3:D:752:HOH:O	2.13	0.48
1:D:497:MET:HE1	1:D:516:PHE:HE1	1.77	0.48
1:A:317:PHE:HE2	1:D:317:PHE:CD2	2.31	0.48
1:B:147:ALA:C	1:B:149:GLY:H	2.21	0.48
1:A:497:MET:HE1	1:A:516:PHE:CE1	2.50	0.47
1:C:378:GLN:O	1:C:381:ARG:HG2	2.13	0.47
1:B:364:MET:HE2	1:B:447:LEU:HD11	1.96	0.47
1:D:262:VAL:HG13	1:D:497:MET:HE3	1.96	0.47
1:B:169:THR:OG1	1:B:178:MET:SD	2.72	0.47
1:D:388:PHE:HA	1:D:410:LEU:HD11	1.95	0.47
1:B:139:GLU:HG3	1:B:207:ILE:HD13	1.96	0.47
1:B:191:GLY:HA3	1:B:192:VAL:HA	1.66	0.47
1:B:342:SER:HA	1:B:409:ILE:HD12	1.95	0.47
1:A:315:LEU:C	1:A:318:ASN:ND2	2.72	0.47
1:D:161:ALA:HB1	1:D:214:PHE:HE1	1.80	0.47
1:D:173:ARG:HD2	1:D:441:ILE:C	2.38	0.47
1:D:487:ILE:HD12	1:D:513:GLY:HA3	1.96	0.47
1:B:161:ALA:HB1	1:B:214:PHE:HE1	1.78	0.47
1:B:317:PHE:HZ	1:C:317:PHE:CD2	2.33	0.47
1:A:216:ARG:HD3	1:A:544:GLU:OE2	2.16	0.46
1:D:142:LEU:O	1:D:146:ILE:HD12	2.15	0.46
1:B:217:LYS:HB3	1:B:217:LYS:HE3	1.58	0.46
1:C:333:VAL:HG23	1:C:336:GLY:H	1.80	0.46
1:D:188:THR:HB	1:D:190:ASP:HB2	1.97	0.46
1:D:378:GLN:O	1:D:381:ARG:HG2	2.14	0.46
1:C:143:PHE:CG	1:C:196:LYS:HG3	2.50	0.46
1:B:478:PRO:HG3	1:C:529:TYR:CE1	2.51	0.46
1:A:435:ASN:HA	3:A:730:HOH:O	2.16	0.46
1:C:314:GLY:C	1:C:316:ARG:N	2.70	0.46
1:D:313:SER:O	1:D:317:PHE:CE2	2.69	0.46
1:A:191:GLY:HA3	1:A:192:VAL:HA	1.55	0.46
1:C:452:VAL:O	1:C:456:LEU:HG	2.15	0.46
1:A:315:LEU:O	1:A:315:LEU:HD23	2.16	0.45
1:C:288:LYS:HE3	1:C:337:ALA:CB	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:SER:HB3	1:D:259:LEU:HG	1.98	0.45
1:A:139:GLU:HG3	1:A:207:ILE:HD13	1.97	0.45
1:D:194:LEU:HD23	1:D:198:LEU:HG	1.98	0.45
1:D:345:LYS:HE2	1:D:356:TYR:CE1	2.52	0.45
1:C:216:ARG:HG2	1:C:216:ARG:NH1	2.31	0.45
1:B:243:GLY:HA3	1:B:511:VAL:HG21	1.98	0.45
1:B:533:ARG:NH1	3:B:612:HOH:O	2.24	0.45
1:A:329:HIS:ND1	1:A:329:HIS:N	2.65	0.45
1:B:257:PRO:HB3	1:B:503:PRO:HG3	1.98	0.45
1:B:383:SER:O	1:B:383:SER:OG	2.26	0.45
1:C:401:PRO:O	1:C:404:THR:OG1	2.28	0.45
1:A:357:VAL:O	1:A:361:LEU:HG	2.17	0.45
2:A:601:5XX:C28	1:D:316:ARG:HH22	2.30	0.44
1:B:345:LYS:HD2	1:B:345:LYS:HA	1.87	0.44
1:B:171:ASP:OD1	1:B:173:ARG:HD3	2.17	0.44
1:B:255:PHE:CE1	1:B:500:TRP:HZ2	2.35	0.44
1:D:313:SER:CB	1:D:317:PHE:CE1	3.01	0.44
1:A:262:VAL:HG13	1:A:497:MET:HE3	2.00	0.44
1:C:148:GLU:C	1:C:150:GLN:H	2.26	0.44
1:A:317:PHE:CZ	1:D:317:PHE:HB3	2.53	0.44
1:D:374:ASN:O	1:D:378:GLN:HG2	2.17	0.44
1:D:421:VAL:HG21	1:D:426:ALA:HB2	2.00	0.44
1:A:140:ASP:O	1:A:143:PHE:HB3	2.18	0.44
1:A:203:VAL:HG23	1:A:207:ILE:HD13	1.99	0.44
1:C:140:ASP:OD1	1:C:196:LYS:HG2	2.18	0.44
1:C:152:LYS:HE2	1:C:193:MET:HB2	2.00	0.44
1:A:313:SER:CB	1:A:329:HIS:CD2	3.01	0.43
1:A:447:LEU:O	3:A:711:HOH:O	2.21	0.43
1:B:528:ASN:ND2	1:C:529:TYR:OH	2.51	0.43
1:C:191:GLY:HA3	1:C:192:VAL:HA	1.60	0.43
1:D:191:GLY:HA3	1:D:192:VAL:HA	1.52	0.43
1:D:345:LYS:HB3	1:D:353:LYS:HG2	2.00	0.43
1:A:173:ARG:HD2	1:A:441:ILE:C	2.43	0.43
1:B:262:VAL:HG13	1:B:497:MET:HE3	2.00	0.43
1:B:331:PRO:HD2	1:B:458:LEU:HD13	2.00	0.43
1:B:182:ARG:O	3:B:610:HOH:O	2.21	0.43
1:C:161:ALA:HB1	1:C:214:PHE:HE1	1.84	0.43
1:C:302:GLU:CD	1:C:302:GLU:H	2.25	0.43
1:D:234:TYR:CE2	1:D:274:THR:HG23	2.52	0.43
1:C:317:PHE:CD2	1:C:320:LEU:HD12	2.54	0.43
1:D:188:THR:C	1:D:190:ASP:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:246:ALA:HB2	1:C:483:VAL:HG22	2.01	0.43
1:B:409:ILE:HD13	1:B:409:ILE:HA	1.91	0.43
1:B:431:ALA:HB1	1:B:440:PRO:HG2	2.00	0.43
1:D:264:VAL:HG22	1:D:497:MET:HG2	2.01	0.43
1:D:524:CYS:HA	1:D:539:LEU:O	2.19	0.43
1:C:262:VAL:HG13	1:C:497:MET:HE3	2.01	0.43
1:D:233:LEU:CD2	1:D:519:ASP:HB3	2.49	0.43
1:B:251:GLN:HG3	1:B:254:LYS:NZ	2.33	0.43
1:A:315:LEU:O	1:A:318:ASN:ND2	2.50	0.43
1:A:317:PHE:HD1	1:A:320:LEU:HD12	1.83	0.43
1:C:487:ILE:HD12	1:C:513:GLY:HA3	1.99	0.43
1:D:383:SER:O	1:D:383:SER:OG	2.36	0.43
1:B:159:ILE:O	1:B:163:LYS:HG3	2.18	0.43
1:A:146:ILE:HD12	1:A:146:ILE:H	1.84	0.42
1:B:252:LEU:CD1	3:B:754:HOH:O	2.67	0.42
1:D:139:GLU:HG2	1:D:200:LYS:HG3	2.01	0.42
1:C:194:LEU:HA	1:C:198:LEU:HD23	2.01	0.42
1:A:320:LEU:HD13	2:A:601:5XX:C29	2.50	0.42
1:B:345:LYS:HB3	1:B:353:LYS:HG2	2.01	0.42
1:C:168:ARG:NE	3:C:613:HOH:O	2.32	0.42
1:A:313:SER:HA	1:A:329:HIS:HD2	1.85	0.42
1:B:458:LEU:HD23	1:B:458:LEU:HA	1.82	0.42
1:D:171:ASP:OD1	1:D:173:ARG:HD3	2.18	0.42
1:B:401:PRO:O	1:B:404:THR:OG1	2.34	0.42
1:D:234:TYR:CG	1:D:274:THR:CG2	3.02	0.42
1:D:353:LYS:HB3	1:D:412:PHE:CZ	2.55	0.42
1:B:260:TRP:CE3	1:B:501:SER:HB2	2.54	0.42
1:C:234:TYR:CD2	1:C:274:THR:CG2	3.01	0.42
1:A:180:MET:HG2	1:A:202:CYS:HA	2.01	0.42
1:C:264:VAL:HG22	1:C:497:MET:HG2	2.02	0.42
1:D:280:PRO:HA	1:D:421:VAL:O	2.19	0.42
1:A:431:ALA:HB1	1:A:440:PRO:HG2	2.02	0.41
1:A:445:ARG:HD3	3:A:706:HOH:O	2.18	0.41
1:B:138:LEU:HD23	1:B:138:LEU:HA	1.88	0.41
1:D:215:ARG:HD2	3:D:772:HOH:O	2.18	0.41
1:A:319:LYS:HZ2	2:A:601:5XX:C12	2.33	0.41
1:D:147:ALA:O	1:D:150:GLN:HG2	2.20	0.41
1:C:247:ASP:OD1	1:C:248:TYR:N	2.53	0.41
1:C:302:GLU:O	1:C:306:ARG:HG3	2.21	0.41
1:A:529:TYR:CE1	1:D:478:PRO:HG3	2.55	0.41
1:B:316:ARG:NE	1:B:466:ASP:HB3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLU:HB3	1:A:545:GLY:H	1.61	0.41
1:A:260:TRP:CE3	1:A:501:SER:HB2	2.56	0.41
1:A:360:PHE:CE1	1:A:446:VAL:HG12	2.54	0.41
1:A:527:HIS:CG	1:D:453:ARG:HD2	2.56	0.41
1:D:479:ALA:HB2	1:D:489:LEU:HD12	2.01	0.41
1:A:161:ALA:HB1	1:A:214:PHE:HE1	1.86	0.41
1:B:138:LEU:O	1:B:142:LEU:HG	2.21	0.41
1:B:248:TYR:C	1:B:249:ILE:HG13	2.45	0.41
1:C:363:LYS:HD3	1:C:444:GLU:OE2	2.20	0.41
1:D:277:THR:O	1:D:422:THR:HB	2.20	0.41
1:B:152:LYS:HB3	1:B:193:MET:HB3	2.03	0.41
1:D:248:TYR:CD2	1:D:249:ILE:HG23	2.56	0.41
1:D:439:CYS:HA	1:D:440:PRO:HD3	1.89	0.41
1:B:277:THR:HA	1:B:423:CYS:HB2	2.03	0.41
1:A:356:TYR:O	1:A:359:GLN:HG2	2.21	0.40
1:B:439:CYS:HA	1:B:440:PRO:HD3	1.88	0.40
1:C:138:LEU:HD12	1:C:138:LEU:H	1.84	0.40
1:D:314:GLY:HA2	3:D:864:HOH:O	2.20	0.40
1:A:479:ALA:HB2	1:A:489:LEU:HD12	2.01	0.40
1:B:299:LEU:HD13	1:B:303:TYR:CE2	2.57	0.40
1:C:227:THR:HB	1:C:272:HIS:CE1	2.56	0.40
1:D:196:LYS:HE2	1:D:196:LYS:HB2	1.82	0.40
1:C:223:PHE:O	1:C:227:THR:HG23	2.21	0.40
1:C:182:ARG:O	1:C:186:GLN:HG2	2.22	0.40
1:D:182:ARG:O	1:D:186:GLN:HG2	2.21	0.40
1:D:314:GLY:N	1:D:317:PHE:HZ	2.20	0.40

All (4) 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)
3:A:854:HOH:O	3:B:744:HOH:O[1_455]	1.84	0.36
3:B:738:HOH:O	3:D:849:HOH:O[3_847]	2.01	0.19
2:D:601:5XX:S36	3:B:603:HOH:O[4_497]	2.11	0.09
3:B:681:HOH:O	3:D:735:HOH:O[3_847]	2.12	0.08

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%)	388 (95%)	20 (5%)	0	100	100
1	B	408/539 (76%)	388 (95%)	13 (3%)	7 (2%)	7	13
1	C	408/539 (76%)	387 (95%)	19 (5%)	2 (0%)	24	43
1	D	408/539 (76%)	389 (95%)	17 (4%)	2 (0%)	24	43
All	All	1632/2156 (76%)	1552 (95%)	69 (4%)	11 (1%)	18	34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	315	LEU
1	B	316	ARG
1	C	248	TYR
1	D	316	ARG
1	D	317	PHE
1	B	190	ASP
1	B	250	PRO
1	B	246	ALA
1	B	249	ILE
1	B	191	GLY
1	C	544	GLU

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%)	338 (96%)	15 (4%)	26	52
1	B	353/462 (76%)	338 (96%)	15 (4%)	26	52
1	C	353/462 (76%)	340 (96%)	13 (4%)	30	57
1	D	353/462 (76%)	343 (97%)	10 (3%)	38	66
All	All	1412/1848 (76%)	1359 (96%)	53 (4%)	29	56

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	LYS
1	A	173	ARG
1	A	190	ASP
1	A	193	MET
1	A	224	MET
1	A	240	GLN
1	A	241	SER
1	A	287	VAL
1	A	319	LYS
1	A	329	HIS
1	A	345	LYS
1	A	359	GLN
1	A	528	ASN
1	A	539	LEU
1	A	543	ARG
1	B	142	LEU
1	B	173	ARG
1	B	200	LYS
1	B	240	GLN
1	B	249	ILE
1	B	251	GLN
1	B	316	ARG
1	B	318	ASN
1	B	319	LYS
1	B	379	SER
1	B	383	SER
1	B	466	ASP
1	B	506	LYS
1	B	539	LEU
1	B	544	GLU
1	C	148	GLU
1	C	151	GLU
1	C	155	VAL

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Mol	Chain	Res	Type
1	C	183	LEU
1	C	185	LEU
1	C	187	THR
1	C	196	LYS
1	C	240	GLN
1	C	249	ILE
1	C	258	ASP
1	C	302	GLU
1	C	528	ASN
1	C	544	GLU
1	D	173	ARG
1	D	196	LYS
1	D	205	SER
1	D	240	GLN
1	D	315	LEU
1	D	319	LYS
1	D	324	GLU
1	D	345	LYS
1	D	387	ASN
1	D	528	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	240	GLN
1	A	329	HIS
1	A	470	GLN
1	A	528	ASN
1	B	156	HIS
1	B	251	GLN
1	B	318	ASN
1	B	346	GLN
1	B	415	GLN
1	B	528	ASN
1	C	229	HIS
1	C	367	ASN
1	C	534	HIS
1	D	334	ASN
1	D	350	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 oligosaccharides 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	5XX	D	601	-	40,40,40	3.13	12 (30%)	48,54,54	4.09	21 (43%)
2	5XX	A	601	-	40,40,40	3.06	13 (32%)	48,54,54	3.44	20 (41%)

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	5XX	D	601	-	-	11/24/33/33	0/5/5/5
2	5XX	A	601	-	-	6/24/33/33	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	5XX	C01-C05	-9.58	1.27	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	5XX	C01-C05	-9.50	1.27	1.52
2	D	601	5XX	C04-N03	-8.11	1.31	1.46
2	D	601	5XX	C07-N06	8.02	1.46	1.34
2	A	601	5XX	C04-N03	-8.01	1.31	1.46
2	A	601	5XX	C07-N06	6.88	1.45	1.34
2	D	601	5XX	C04-C05	6.09	1.63	1.53
2	A	601	5XX	C04-C05	5.71	1.63	1.53
2	A	601	5XX	C10-N11	5.03	1.45	1.38
2	D	601	5XX	C10-N11	4.76	1.45	1.38
2	D	601	5XX	C22-N03	4.49	1.44	1.34
2	A	601	5XX	C12-N11	4.14	1.44	1.37
2	A	601	5XX	C22-N03	3.88	1.43	1.34
2	D	601	5XX	C12-N11	3.86	1.44	1.37
2	A	601	5XX	C25-N26	3.71	1.43	1.38
2	D	601	5XX	C02-N03	3.64	1.54	1.47
2	D	601	5XX	C27-N26	3.54	1.43	1.37
2	D	601	5XX	C25-N26	3.37	1.43	1.38
2	A	601	5XX	C02-N03	3.36	1.54	1.47
2	A	601	5XX	C27-N26	3.18	1.43	1.37
2	A	601	5XX	C10-N09	2.84	1.35	1.31
2	D	601	5XX	C10-N09	2.69	1.35	1.31
2	D	601	5XX	C07-N08	2.47	1.34	1.31
2	A	601	5XX	C07-N08	2.29	1.34	1.31
2	A	601	5XX	C25-N24	2.23	1.34	1.31

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	5XX	S21-C07-N08	-9.59	103.81	114.52
2	D	601	5XX	S36-C25-N24	-9.01	104.46	114.52
2	A	601	5XX	S21-C10-N09	-8.78	104.72	114.52
2	A	601	5XX	S21-C07-N08	-8.70	104.81	114.52
2	D	601	5XX	N11-C10-N09	8.69	128.57	120.81
2	D	601	5XX	N26-C25-N24	8.39	128.31	120.81
2	D	601	5XX	S21-C10-N09	-8.35	105.20	114.52
2	A	601	5XX	S36-C25-N24	-7.58	106.05	114.52
2	D	601	5XX	C02-N03-C04	-7.15	104.03	112.38
2	D	601	5XX	C28-C27-N26	6.81	122.70	114.40
2	D	601	5XX	C13-C12-N11	6.16	121.92	114.40
2	D	601	5XX	S36-C22-N23	-6.13	103.84	114.44
2	A	601	5XX	C02-N03-C04	-6.09	105.26	112.38
2	A	601	5XX	N26-C25-N24	5.96	126.14	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	5XX	S36-C22-N03	5.89	128.19	120.31
2	A	601	5XX	N03-C22-N23	5.77	128.06	116.91
2	D	601	5XX	N03-C22-N23	5.71	127.94	116.91
2	A	601	5XX	N11-C10-N09	5.53	125.75	120.81
2	D	601	5XX	C22-N23-N24	5.34	117.61	107.08
2	D	601	5XX	C27-N26-C25	-5.28	114.66	123.69
2	A	601	5XX	C13-C12-N11	5.20	120.74	114.40
2	D	601	5XX	C07-N08-N09	5.15	118.58	112.02
2	A	601	5XX	S36-C22-N23	-4.52	106.63	114.44
2	A	601	5XX	C22-N23-N24	4.44	115.84	107.08
2	A	601	5XX	S21-C10-N11	4.33	129.52	123.72
2	A	601	5XX	C07-N08-N09	4.06	117.18	112.02
2	D	601	5XX	C25-N24-N23	3.93	117.02	112.02
2	A	601	5XX	C05-N06-C07	-3.86	117.71	124.48
2	A	601	5XX	C10-N09-N08	3.83	116.89	112.02
2	A	601	5XX	S36-C22-N03	3.74	125.31	120.31
2	A	601	5XX	C25-N24-N23	3.48	116.44	112.02
2	A	601	5XX	C27-N26-C25	-3.08	118.42	123.69
2	D	601	5XX	C04-N03-C22	3.08	129.21	123.83
2	A	601	5XX	S36-C25-N26	3.05	127.81	123.72
2	A	601	5XX	C29-C28-C27	2.97	121.19	112.33
2	D	601	5XX	C05-N06-C07	2.90	129.58	124.48
2	D	601	5XX	C10-N09-N08	2.83	115.62	112.02
2	A	601	5XX	C01-C05-N06	-2.76	106.34	111.98
2	D	601	5XX	C12-N11-C10	-2.69	119.08	123.69
2	D	601	5XX	S36-C25-N26	2.61	127.21	123.72
2	D	601	5XX	C01-C02-N03	2.40	106.02	102.93

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	5XX	N24-C25-N26-C27
2	A	601	5XX	S36-C25-N26-C27
2	A	601	5XX	C28-C27-N26-C25
2	A	601	5XX	O35-C27-N26-C25
2	D	601	5XX	N09-C10-N11-C12
2	D	601	5XX	S21-C10-N11-C12
2	D	601	5XX	N23-C22-N03-C02
2	D	601	5XX	N23-C22-N03-C04
2	D	601	5XX	S36-C22-N03-C02
2	D	601	5XX	S36-C22-N03-C04

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Mol	Chain	Res	Type	Atoms
2	D	601	5XX	C01-C05-N06-C07
2	D	601	5XX	S21-C07-N06-C05
2	D	601	5XX	N24-C25-N26-C27
2	D	601	5XX	S36-C25-N26-C27
2	D	601	5XX	N08-C07-N06-C05
2	A	601	5XX	N09-C10-N11-C12
2	A	601	5XX	S21-C10-N11-C12

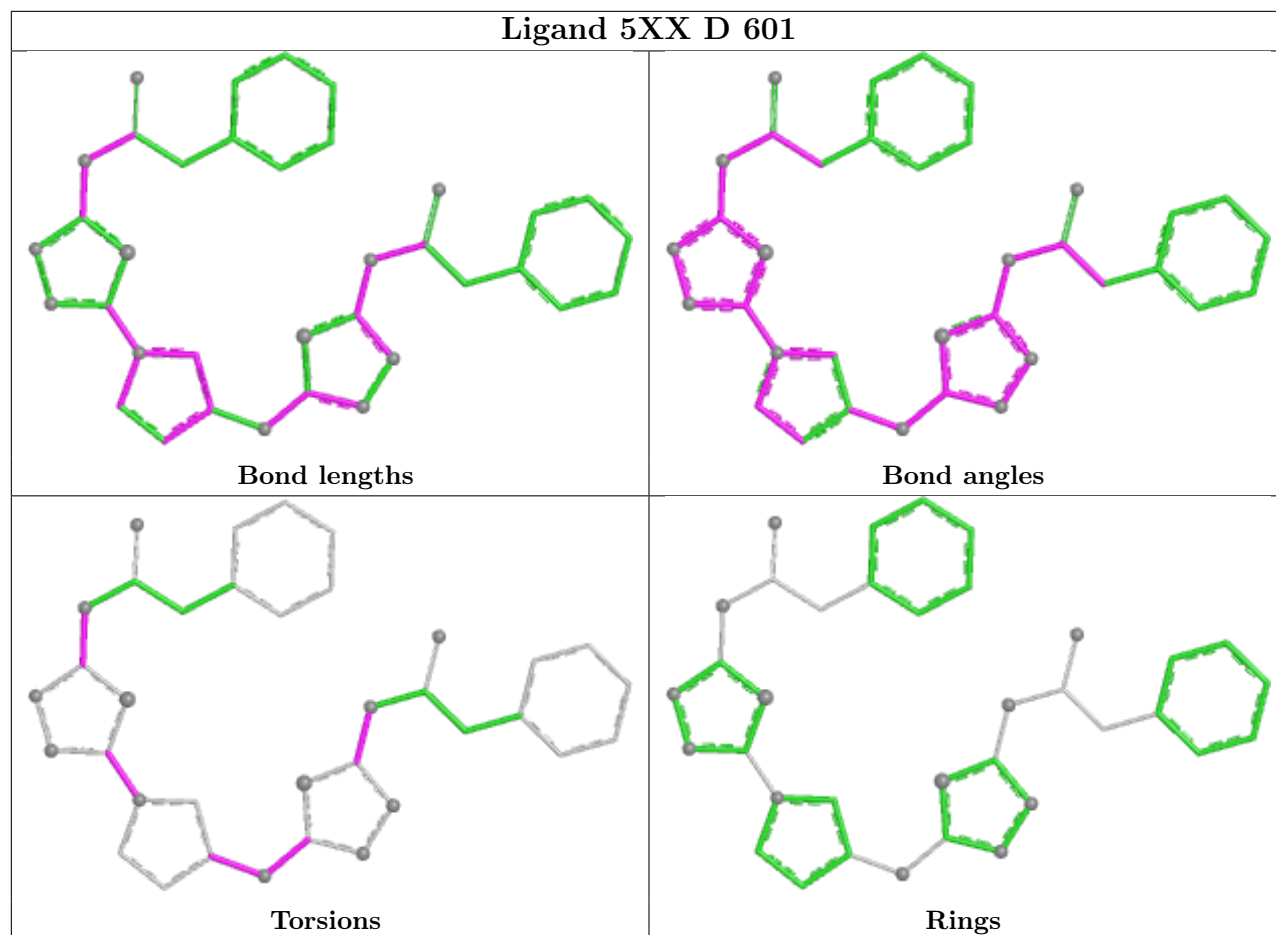
There are no ring outliers.

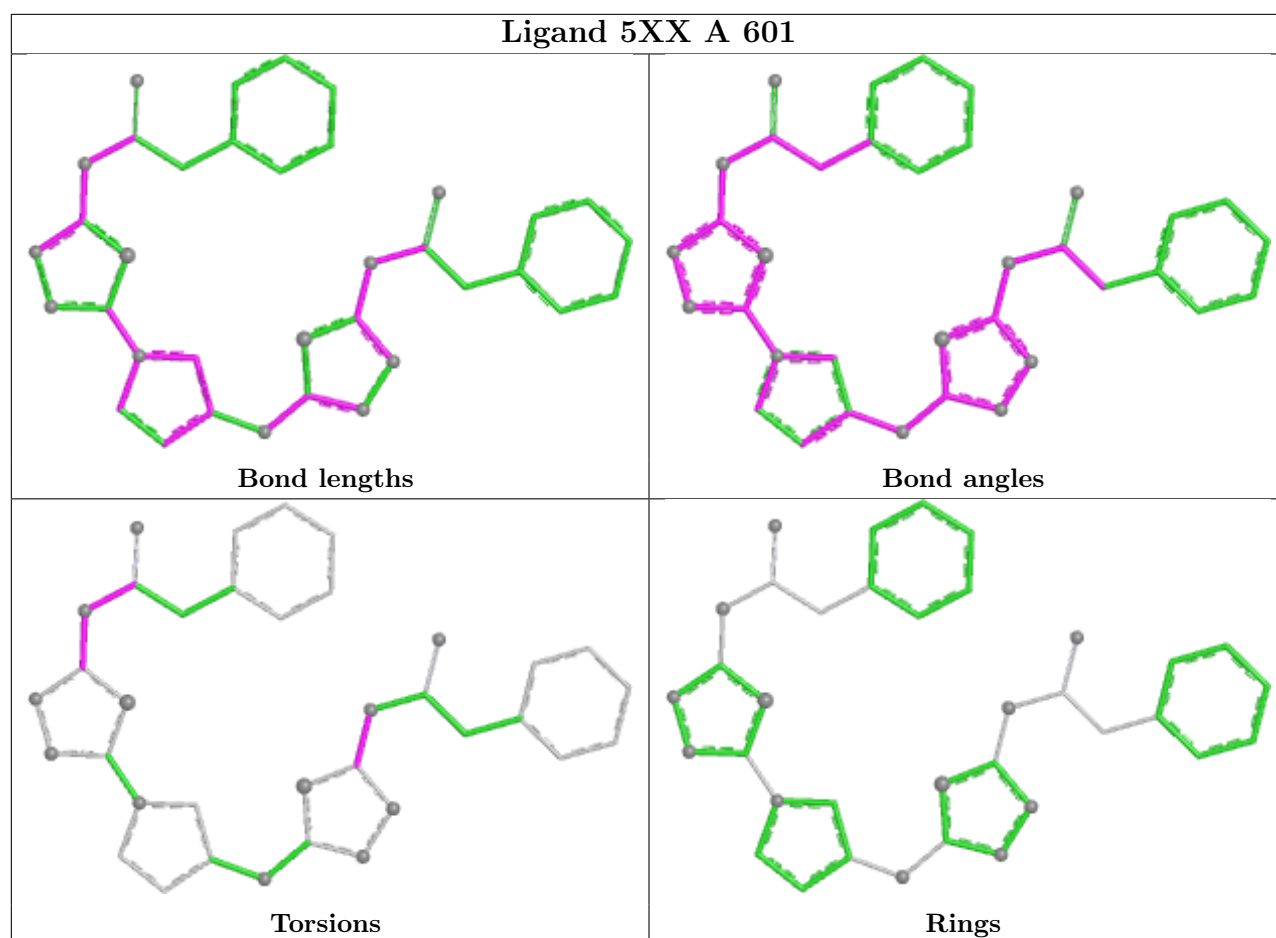
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	5XX	0	1
2	A	601	5XX	3	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.

Ligand 5XX D 601





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%)	0.83	45 (10%) 10 8	12, 22, 62, 80	0
1	B	410/539 (76%)	0.96	51 (12%) 8 6	11, 22, 66, 91	0
1	C	410/539 (76%)	0.87	52 (12%) 8 6	10, 22, 68, 99	0
1	D	410/539 (76%)	0.82	48 (11%) 9 7	11, 22, 65, 98	0
All	All	1640/2156 (76%)	0.87	196 (11%) 9 7	10, 22, 66, 99	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	315	LEU	15.8
1	B	250	PRO	10.6
1	A	317	PHE	9.5
1	B	317	PHE	9.2
1	B	318	ASN	9.0
1	B	249	ILE	8.9
1	B	248	TYR	8.3
1	B	252	LEU	8.0
1	B	255	PHE	7.9
1	D	188	THR	7.6
1	C	248	TYR	7.3
1	C	317	PHE	7.2
1	A	137	SER	6.8
1	D	314	GLY	6.8
1	D	545	GLY	6.8
1	B	314	GLY	6.7
1	C	316	ARG	6.7
1	D	187	THR	6.5
1	A	252	LEU	6.4
1	B	316	ARG	5.9
1	B	192	VAL	5.9

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Mol	Chain	Res	Type	RSRZ
1	C	250	PRO	5.8
1	A	192	VAL	5.7
1	D	316	ARG	5.6
1	D	190	ASP	5.6
1	D	189	SER	5.6
1	A	136	PRO	5.6
1	C	315	LEU	5.5
1	C	252	LEU	5.4
1	B	190	ASP	5.3
1	C	251	GLN	5.3
1	B	251	GLN	5.2
1	C	255	PHE	5.1
1	B	253	ALA	5.1
1	C	187	THR	5.1
1	A	318	ASN	5.1
1	B	466	ASP	5.0
1	D	317	PHE	5.0
1	A	315	LEU	5.0
1	D	315	LEU	5.0
1	A	316	ARG	4.9
1	B	247	ASP	4.9
1	C	149	GLY	4.8
1	C	256	SER	4.8
1	C	545	GLY	4.7
1	D	136	PRO	4.7
1	C	246	ALA	4.5
1	A	143	PHE	4.5
1	B	545	GLY	4.5
1	A	141	LEU	4.4
1	C	247	ASP	4.4
1	A	193	MET	4.4
1	C	254	LYS	4.3
1	A	140	ASP	4.3
1	A	545	GLY	4.3
1	C	144	TYR	4.3
1	A	190	ASP	4.2
1	A	152	LYS	4.2
1	B	256	SER	4.1
1	A	188	THR	4.1
1	C	197	ASP	4.0
1	D	144	TYR	4.0
1	A	314	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	189	SER	3.9
1	A	267	VAL	3.9
1	C	249	ILE	3.9
1	C	188	THR	3.9
1	D	191	GLY	3.8
1	B	136	PRO	3.8
1	C	136	PRO	3.8
1	A	319	LYS	3.7
1	D	147	ALA	3.7
1	D	152	LYS	3.7
1	D	319	LYS	3.7
1	A	138	LEU	3.7
1	D	192	VAL	3.6
1	D	140	ASP	3.6
1	B	254	LYS	3.5
1	B	246	ALA	3.5
1	C	138	LEU	3.5
1	C	192	VAL	3.5
1	A	146	ILE	3.5
1	D	318	ASN	3.5
1	A	154	PRO	3.3
1	D	254	LYS	3.3
1	D	197	ASP	3.3
1	C	147	ALA	3.3
1	A	144	TYR	3.3
1	C	318	ASN	3.3
1	B	191	GLY	3.3
1	A	251	GLN	3.2
1	D	149	GLY	3.2
1	D	212	GLN	3.2
1	A	142	LEU	3.2
1	D	313	SER	3.2
1	A	201	LYS	3.2
1	A	189	SER	3.1
1	A	150	GLN	3.1
1	C	319	LYS	3.1
1	C	190	ASP	3.1
1	C	191	GLY	3.0
1	C	146	ILE	3.0
1	C	150	GLN	3.0
1	B	143	PHE	3.0
1	C	382	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	207	ILE	3.0
1	B	267	VAL	3.0
1	D	145	THR	3.0
1	A	199	PHE	3.0
1	A	191	GLY	2.9
1	B	144	TYR	2.9
1	C	183	LEU	2.9
1	C	151	GLU	2.8
1	D	250	PRO	2.8
1	D	185	LEU	2.8
1	B	193	MET	2.8
1	D	199	PHE	2.8
1	A	149	GLY	2.8
1	B	137	SER	2.8
1	B	206	ASN	2.8
1	D	539	LEU	2.8
1	D	153	ILE	2.7
1	B	465	TYR	2.7
1	D	155	VAL	2.7
1	D	186	GLN	2.7
1	D	267	VAL	2.7
1	B	151	GLU	2.7
1	D	150	GLN	2.7
1	B	313	SER	2.7
1	D	138	LEU	2.7
1	A	203	VAL	2.7
1	C	544	GLU	2.7
1	D	382	GLU	2.7
1	C	229	HIS	2.7
1	A	153	ILE	2.6
1	A	543	ARG	2.6
1	C	148	GLU	2.6
1	B	189	SER	2.6
1	B	146	ILE	2.6
1	B	142	LEU	2.6
1	B	138	LEU	2.6
1	C	253	ALA	2.6
1	B	379	SER	2.5
1	D	146	ILE	2.5
1	B	229	HIS	2.5
1	B	347	GLY	2.5
1	C	347	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	383	SER	2.5
1	D	543	ARG	2.5
1	D	137	SER	2.5
1	D	251	GLN	2.4
1	C	350	ASN	2.4
1	B	382	GLU	2.4
1	A	196	LYS	2.4
1	D	544	GLU	2.4
1	A	197	ASP	2.4
1	A	382	GLU	2.4
1	C	257	PRO	2.3
1	B	244	LYS	2.3
1	C	137	SER	2.3
1	B	188	THR	2.3
1	A	320	LEU	2.3
1	B	141	LEU	2.3
1	B	169	THR	2.3
1	C	186	GLN	2.3
1	C	313	SER	2.3
1	B	319	LYS	2.3
1	C	267	VAL	2.3
1	B	153	ILE	2.2
1	C	379	SER	2.2
1	D	302	GLU	2.2
1	B	145	THR	2.2
1	C	314	GLY	2.2
1	D	141	LEU	2.2
1	D	198	LEU	2.2
1	C	155	VAL	2.2
1	A	313	SER	2.2
1	C	153	ILE	2.2
1	A	250	PRO	2.2
1	C	196	LYS	2.2
1	B	237	ALA	2.1
1	C	245	VAL	2.1
1	A	206	ASN	2.1
1	D	387	ASN	2.1
1	D	252	LEU	2.1
1	A	246	ALA	2.1
1	B	147	ALA	2.1
1	D	476	GLY	2.1
1	B	216	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	151	GLU	2.0
1	D	193	MET	2.0
1	C	543	ARG	2.0
1	A	198	LEU	2.0
1	A	416	LEU	2.0
1	C	322	LEU	2.0
1	B	257	PRO	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](#)

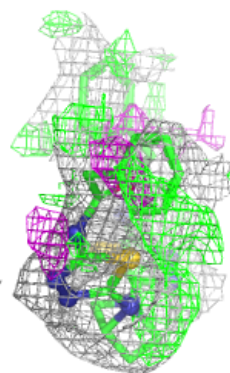
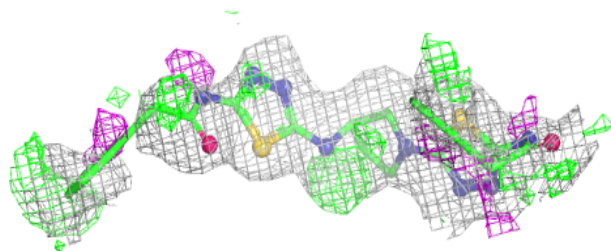
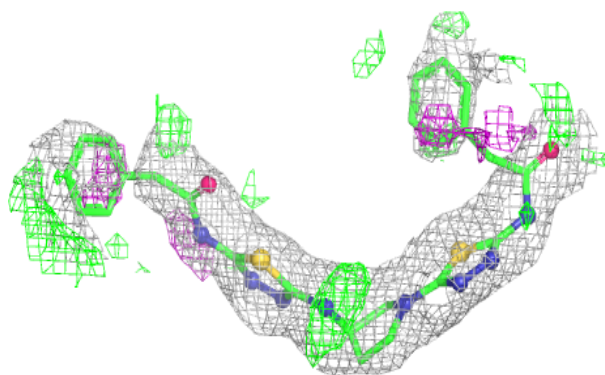
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	5XX	A	601	36/36	0.72	0.23	34,49,73,75	0
2	5XX	D	601	36/36	0.80	0.19	36,46,60,69	0

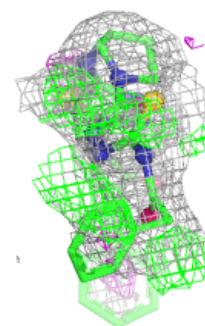
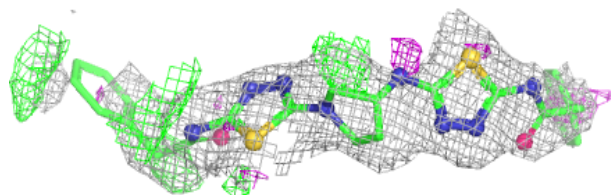
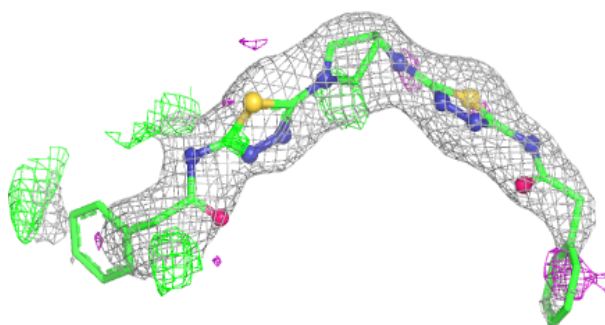
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5XX 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 5XX 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.