



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:58 PM UTC

PDB ID : 5FI6 / pdb_00005fi6
Title : Crystal structure of human GAC in complex with inhibitor UPGL_00011: 2-phenyl- {N}-[5-[[[(3 {S})-1-[5-(2-phenylethanoylamino)-1,3,4-thiadiazol-2-yl]p-yrrolidin-3-yl]amino]-1,3,4-thiadiazol-2-yl]ethanamide
Authors : Huang, Q.; Cerione, R.
Deposited on : 2015-12-22
Resolution : 2.52 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

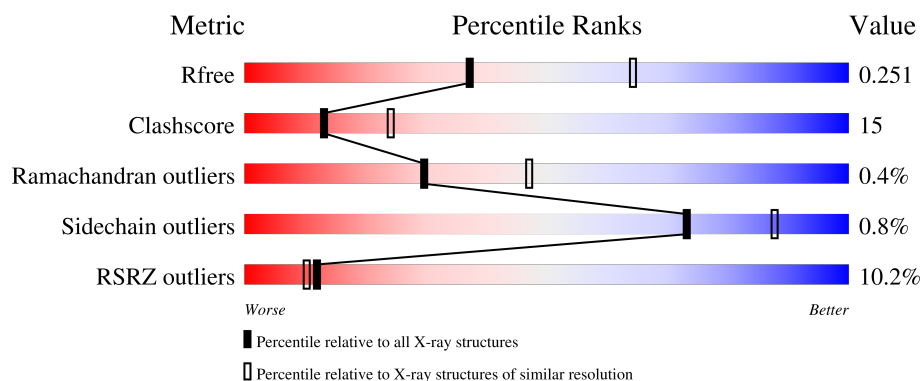
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.52 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	6% 55% 19% • 24%
1	B	539	8% 53% 23% 24%
1	C	539	8% 57% 19% 24%
1	D	539	10% 56% 19% • 24%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13115 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:

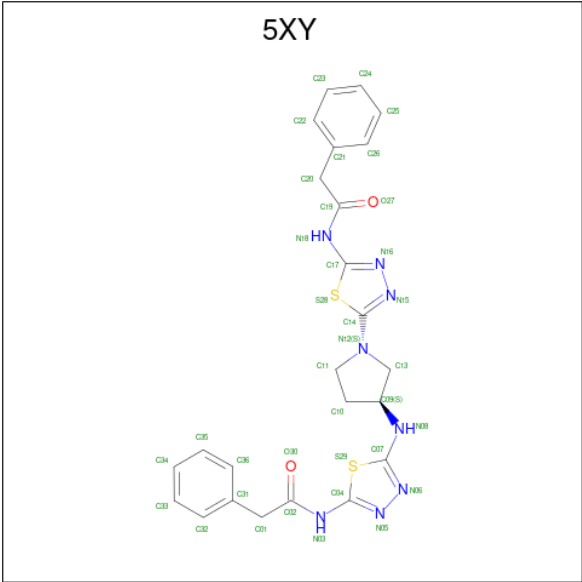
Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MET	-	initiating methionine	UNP O94925
A	60	ARG	-	expression tag	UNP O94925
A	61	GLY	-	expression tag	UNP O94925
A	62	SER	-	expression tag	UNP O94925
A	63	HIS	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag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

Continued on next page...

Continued from previous page...

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})-1-[5-(2-phenylethanoylamino)-1,3,4-thiadiazol-2-yl]pyrrolidin-3-yl]amino]-1,3,4-thiadiazol-2-yl]ethanamide (CCD ID: 5XY) (formula: C₂₄H₂₄N₈O₂S₂).



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

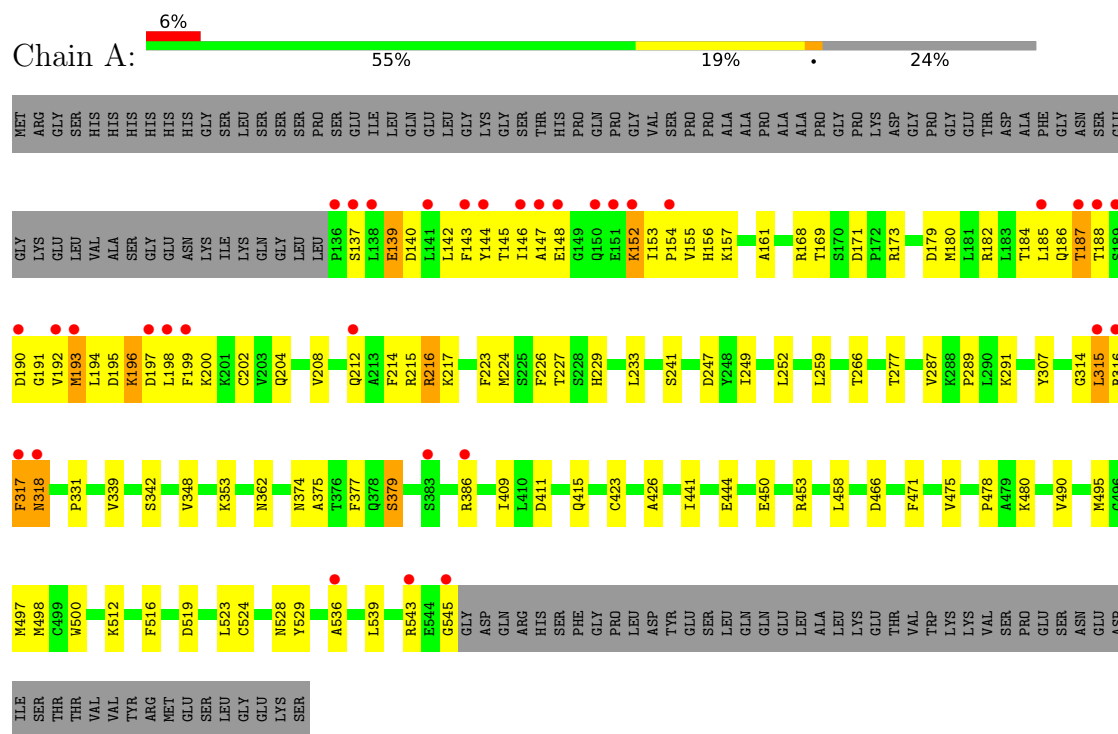
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total	O	0	0
			75	75		
3	B	56	Total	O	0	0
			56	56		
3	C	77	Total	O	0	0
			77	77		
3	D	59	Total	O	0	0
			59	59		

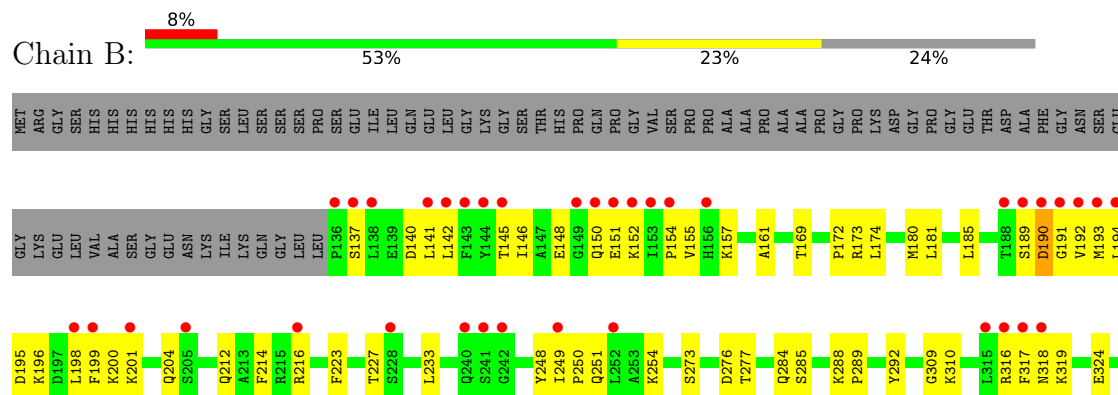
3 Residue-property plots [i](#)

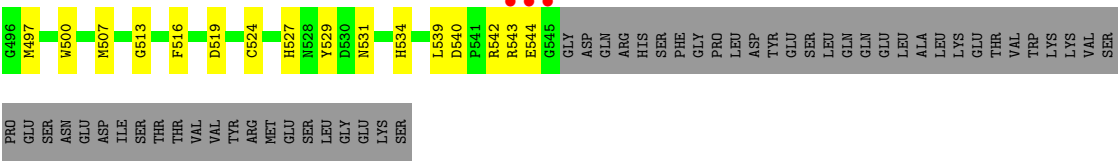
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutaminase kidney isoform, mitochondrial



- Molecule 1: Glutaminase kidney isoform, mitochondrial





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

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.69Å 139.03Å 176.78Å 90.00° 95.56° 90.00°	Depositor
Resolution (Å)	47.30 – 2.52 47.30 – 2.52	Depositor EDS
% Data completeness (in resolution range)	97.3 (47.30-2.52) 97.6 (47.30-2.52)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.209 , 0.253 0.211 , 0.251	Depositor DCC
R_{free} test set	1996 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å ²)	41.9	Xtriage
Anisotropy	0.733	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13115	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5XY

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	0.46	2/3266 (0.1%)	0.67	3/4408 (0.1%)
1	B	0.44	1/3266 (0.0%)	0.61	0/4408
1	C	0.41	0/3266	0.60	0/4408
1	D	0.51	4/3266 (0.1%)	0.62	0/4408
All	All	0.45	7/13064 (0.1%)	0.62	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	A	0	1
1	C	0	2
1	D	0	1
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	316	ARG	NE-CZ	-10.25	1.21	1.33
1	D	316	ARG	CZ-NH1	-7.86	1.21	1.32
1	D	316	ARG	CZ-NH2	-7.35	1.23	1.33
1	D	316	ARG	CD-NE	-6.66	1.36	1.46
1	B	196	LYS	CD-CE	-6.55	1.32	1.52
1	A	386	ARG	NE-CZ	6.01	1.39	1.33
1	A	196	LYS	CD-CE	-6.00	1.34	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	MET	CB-CG-SD	7.45	135.05	112.70
1	A	152	LYS	CB-CG-CD	-5.95	97.61	111.30
1	A	193	MET	CG-SD-CE	5.33	112.63	100.90

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	317	PHE	Peptide
1	C	315	LEU	Peptide
1	C	316	ARG	Peptide
1	D	140	ASP	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	3194	0	3167	109	0
1	B	3194	0	3167	97	0
1	C	3194	0	3167	88	0
1	D	3194	0	3167	103	0
2	A	36	0	0	2	0
2	C	36	0	0	2	0
3	A	75	0	0	9	0
3	B	56	0	0	5	0
3	C	77	0	0	5	0
3	D	59	0	0	4	0
All	All	13115	0	12668	380	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (380) 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:152:LYS:NZ	1:A:193:MET:HB3	1.52	1.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:249:ILE:CG2	1:C:252:LEU:HD12	1.71	1.19
1:A:152:LYS:HZ1	1:A:193:MET:CG	1.60	1.14
1:A:152:LYS:NZ	1:A:193:MET:CB	2.14	1.10
1:D:195:ASP:H	1:D:198:LEU:HD21	1.16	1.09
1:C:249:ILE:HG22	1:C:252:LEU:HD12	1.36	1.03
1:C:249:ILE:HD11	1:C:379:SER:HB2	1.38	1.01
1:C:249:ILE:HD11	1:C:379:SER:CB	1.92	1.00
1:A:152:LYS:HZ1	1:A:193:MET:CB	1.73	0.97
1:B:544:GLU:O	3:B:601:HOH:O	1.82	0.96
1:A:152:LYS:CE	1:A:193:MET:HB3	1.97	0.94
1:D:195:ASP:H	1:D:198:LEU:CD2	1.82	0.92
1:C:249:ILE:HG21	1:C:252:LEU:HD12	1.52	0.90
1:D:152:LYS:HZ3	1:D:193:MET:C	1.82	0.88
1:A:152:LYS:HZ3	1:A:193:MET:HB3	1.39	0.87
1:B:185:LEU:HD22	1:B:192:VAL:HG11	1.57	0.87
1:D:233:LEU:HD22	1:D:519:ASP:HB3	1.57	0.86
1:B:444:GLU:OE1	3:B:602:HOH:O	1.91	0.86
1:C:180:MET:HE2	1:C:201:LYS:HE2	1.58	0.85
1:B:152:LYS:HE2	1:B:193:MET:SD	2.16	0.85
1:A:152:LYS:NZ	1:A:193:MET:CG	2.40	0.84
1:B:276:ASP:O	3:B:603:HOH:O	1.95	0.84
1:A:152:LYS:HZ3	1:A:193:MET:CB	1.91	0.83
1:B:470:GLN:HG2	3:D:608:HOH:O	1.78	0.83
1:D:386:ARG:NH2	1:D:387:ASN:OD1	2.11	0.82
1:A:185:LEU:HD23	1:A:192:VAL:HG23	1.65	0.79
1:A:362:ASN:OD1	3:A:701:HOH:O	2.00	0.78
1:D:195:ASP:N	1:D:198:LEU:HD21	1.95	0.78
1:A:197:ASP:OD2	3:A:702:HOH:O	2.01	0.77
1:A:497:MET:HE1	1:A:516:PHE:HE1	1.50	0.77
1:D:143:PHE:CE2	1:D:153:ILE:HG13	2.20	0.76
1:B:146:ILE:O	1:B:157:LYS:NZ	2.20	0.75
1:C:249:ILE:CD1	1:C:379:SER:HB2	2.16	0.75
1:B:216:ARG:NH2	1:B:544:GLU:OE2	2.18	0.75
1:D:497:MET:HE1	1:D:516:PHE:HE1	1.50	0.75
1:A:233:LEU:HD22	1:A:519:ASP:HB3	1.69	0.74
1:C:351:ALA:O	3:C:701:HOH:O	2.05	0.74
1:A:450:GLU:OE1	3:A:703:HOH:O	2.05	0.73
1:C:140:ASP:HA	1:C:196:LYS:HZ1	1.54	0.72
1:A:497:MET:HE1	1:A:516:PHE:CE1	2.26	0.71
1:A:249:ILE:HD11	1:A:379:SER:OG	1.91	0.70
1:A:444:GLU:OE1	3:A:704:HOH:O	2.07	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:497:MET:HE1	1:D:516:PHE:CE1	2.26	0.70
1:C:139:GLU:HG3	1:C:200:LYS:HD2	1.74	0.69
1:D:186:GLN:O	3:D:602:HOH:O	2.10	0.69
1:C:140:ASP:HA	1:C:196:LYS:NZ	2.07	0.69
1:D:179:ASP:OD1	1:D:182:ARG:NH1	2.20	0.68
1:B:233:LEU:HD22	1:B:519:ASP:HB3	1.75	0.68
1:A:226:PHE:CE2	1:A:495:MET:HE1	2.29	0.68
1:A:185:LEU:CD2	1:A:192:VAL:HG23	2.24	0.68
1:B:324:GLU:OE2	1:D:316:ARG:HB2	1.93	0.67
1:C:249:ILE:HG23	1:C:251:GLN:H	1.60	0.67
1:C:161:ALA:HB1	1:C:214:PHE:HE1	1.61	0.66
1:B:368:GLU:OE1	3:B:604:HOH:O	2.13	0.66
1:D:143:PHE:O	1:D:153:ILE:HD11	1.96	0.65
1:D:540:ASP:O	1:D:543:ARG:HG3	1.96	0.65
1:A:152:LYS:HD2	1:A:153:ILE:N	2.12	0.65
1:A:188:THR:HG23	1:A:190:ASP:OD1	1.97	0.64
1:D:152:LYS:NZ	1:D:193:MET:C	2.54	0.64
1:B:161:ALA:HB1	1:B:214:PHE:HE1	1.63	0.64
1:D:164:SER:HA	1:D:224:MET:HE3	1.79	0.64
1:B:317:PHE:HE2	1:D:317:PHE:CD1	2.15	0.64
1:A:466:ASP:O	3:A:705:HOH:O	2.15	0.64
1:D:143:PHE:HB2	1:D:199:PHE:CD2	2.33	0.63
1:A:152:LYS:HB2	1:A:194:LEU:O	1.99	0.62
1:A:179:ASP:OD1	1:A:182:ARG:NH1	2.32	0.62
1:A:185:LEU:HD23	1:A:192:VAL:CG2	2.28	0.62
1:A:184:THR:O	1:A:187:THR:OG1	2.18	0.62
1:C:171:ASP:OD1	1:C:173:ARG:HD3	2.00	0.62
1:D:143:PHE:CD2	1:D:153:ILE:HD12	2.34	0.62
1:A:142:LEU:HD22	1:A:199:PHE:HZ	1.65	0.61
1:A:543:ARG:NH1	1:A:545:GLY:O	2.32	0.61
1:C:182:ARG:NH1	3:C:705:HOH:O	2.31	0.61
1:B:154:PRO:HG3	1:B:193:MET:HE2	1.81	0.61
1:C:345:LYS:HB3	1:C:353:LYS:HG2	1.83	0.61
1:D:249:ILE:HB	1:D:252:LEU:HD12	1.83	0.60
1:B:479:ALA:HB2	1:B:489:LEU:HD12	1.84	0.60
1:B:316:ARG:HH22	1:B:319:LYS:HD3	1.67	0.60
1:A:314:GLY:O	1:A:316:ARG:N	2.33	0.60
1:B:378:GLN:O	1:B:381:ARG:HG2	2.01	0.60
1:A:140:ASP:OD1	1:A:196:LYS:HE3	2.00	0.60
1:C:181:LEU:O	1:C:185:LEU:HG	2.02	0.60
1:C:277:THR:O	1:C:424:GLU:HG3	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:SER:OG	1:B:140:ASP:OD2	2.20	0.59
1:B:181:LEU:O	1:B:185:LEU:HG	2.01	0.59
1:C:497:MET:HE1	1:C:516:PHE:CE1	2.37	0.59
1:D:152:LYS:HZ3	1:D:193:MET:HB2	1.67	0.59
1:B:374:ASN:N	3:B:606:HOH:O	2.35	0.59
1:C:137:SER:O	1:C:140:ASP:HB2	2.01	0.59
1:A:249:ILE:HG22	1:A:252:LEU:HB2	1.85	0.59
1:B:195:ASP:OD2	1:B:198:LEU:N	2.28	0.59
1:D:542:ARG:NH1	3:D:601:HOH:O	2.03	0.58
1:B:251:GLN:OE1	1:B:376:THR:HA	2.04	0.58
1:B:317:PHE:HE2	1:D:317:PHE:CG	2.21	0.58
1:C:168:ARG:NH2	1:C:424:GLU:OE2	2.30	0.58
1:D:377:PHE:CE1	1:D:415:GLN:HG3	2.37	0.58
1:C:155:VAL:HG21	1:C:185:LEU:HD21	1.85	0.58
1:A:226:PHE:HE2	1:A:495:MET:HE1	1.68	0.58
1:A:316:ARG:HH22	2:A:601:5XY:C35	2.17	0.58
1:C:320:LEU:HD23	2:C:601:5XY:C17	2.32	0.58
1:D:387:ASN:HD22	1:D:414:PHE:HE1	1.52	0.58
1:B:141:LEU:O	1:B:145:THR:HG23	2.04	0.58
1:C:271:ARG:NH2	3:C:706:HOH:O	2.32	0.58
1:B:277:THR:HA	1:B:423:CYS:HB2	1.86	0.58
1:B:360:PHE:CE1	1:B:447:LEU:HD21	2.39	0.57
1:C:194:LEU:HD23	1:C:198:LEU:HD23	1.85	0.57
1:C:249:ILE:CG2	1:C:252:LEU:H	2.17	0.57
1:D:361:LEU:HD23	1:D:364:MET:HE3	1.86	0.57
1:D:188:THR:HG22	1:D:192:VAL:HG12	1.85	0.57
1:A:374:ASN:OD1	3:A:706:HOH:O	2.17	0.57
1:B:198:LEU:HD12	1:B:201:LYS:HD3	1.85	0.57
1:A:137:SER:OG	1:A:140:ASP:OD2	2.18	0.57
1:C:146:ILE:O	1:C:157:LYS:NZ	2.37	0.57
1:B:316:ARG:C	1:B:317:PHE:HD1	2.12	0.56
1:D:143:PHE:CD2	1:D:153:ILE:CD1	2.88	0.56
1:D:178:MET:O	1:D:182:ARG:HG3	2.04	0.56
1:D:140:ASP:OD1	1:D:143:PHE:HD1	1.88	0.56
1:A:215:ARG:O	1:A:216:ARG:HB2	2.05	0.56
1:A:528:ASN:HD21	1:C:528:ASN:ND2	2.04	0.56
1:A:144:TYR:HA	1:A:147:ALA:HB3	1.86	0.56
1:C:223:PHE:O	1:C:227:THR:HG23	2.06	0.56
1:B:273:SER:HB3	1:B:277:THR:HG21	1.87	0.56
1:D:140:ASP:OD2	1:D:144:TYR:N	2.39	0.56
1:B:527:HIS:CD2	1:D:453:ARG:HD2	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:ALA:HB1	1:C:440:PRO:HG2	1.88	0.56
1:D:147:ALA:HB1	1:D:150:GLN:O	2.05	0.56
1:D:161:ALA:HB1	1:D:214:PHE:HE1	1.70	0.56
1:C:249:ILE:HG21	1:C:252:LEU:CD1	2.32	0.55
1:C:249:ILE:HD11	1:C:379:SER:C	2.32	0.55
1:A:536:ALA:HB2	1:C:449:PRO:HG2	1.87	0.55
1:D:184:THR:O	1:D:187:THR:HG22	2.07	0.55
1:A:152:LYS:HD2	1:A:152:LYS:C	2.32	0.55
1:D:142:LEU:O	1:D:145:THR:HB	2.07	0.55
1:D:143:PHE:HB2	1:D:199:PHE:CE2	2.42	0.55
1:B:318:ASN:ND2	1:B:466:ASP:OD1	2.39	0.55
1:B:536:ALA:HB2	1:D:449:PRO:HG2	1.87	0.55
1:C:249:ILE:HG22	1:C:252:LEU:CD1	2.24	0.54
1:D:194:LEU:HD23	1:D:198:LEU:HG	1.89	0.54
1:A:478:PRO:HD2	1:A:490:VAL:O	2.07	0.54
1:D:140:ASP:CG	1:D:143:PHE:HB3	2.32	0.54
1:A:249:ILE:CD1	1:A:379:SER:OG	2.55	0.54
1:A:148:GLU:CD	1:A:157:LYS:HZ1	2.15	0.54
1:C:478:PRO:HD2	1:C:490:VAL:O	2.08	0.54
1:D:348:VAL:O	1:D:353:LYS:HE3	2.07	0.54
1:A:152:LYS:HZ3	1:A:193:MET:CA	2.20	0.54
1:A:266:THR:HA	1:A:495:MET:HA	1.89	0.54
1:A:152:LYS:CE	1:A:193:MET:HE2	2.39	0.53
1:A:154:PRO:HB2	1:A:156:HIS:CD2	2.43	0.53
1:B:248:TYR:OH	1:B:380:GLU:OE2	2.23	0.53
1:C:318:ASN:OD1	1:C:318:ASN:N	2.40	0.53
1:A:194:LEU:HD23	1:A:198:LEU:HG	1.90	0.53
1:A:524:CYS:HA	1:A:539:LEU:O	2.09	0.53
1:D:146:ILE:O	1:D:157:LYS:NZ	2.42	0.53
1:D:249:ILE:HD12	1:D:379:SER:HB3	1.90	0.53
1:B:155:VAL:HG21	1:B:185:LEU:HD21	1.88	0.53
1:B:331:PRO:HD2	1:B:458:LEU:HD13	1.90	0.53
1:A:289:PRO:HD3	1:A:480:LYS:HG2	1.90	0.53
1:D:249:ILE:HD12	1:D:379:SER:CB	2.39	0.53
1:A:377:PHE:CE1	1:A:415:GLN:HG3	2.44	0.53
1:D:152:LYS:NZ	1:D:193:MET:HB2	2.23	0.53
1:D:195:ASP:OD1	1:D:198:LEU:HD22	2.09	0.53
1:A:152:LYS:CD	1:A:193:MET:HB3	2.39	0.52
1:B:150:GLN:HG3	1:B:151:GLU:H	1.74	0.52
1:B:431:ALA:HB1	1:B:440:PRO:HG2	1.91	0.52
1:B:173:ARG:O	1:B:174:LEU:HD23	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:LEU:HD22	1:D:199:PHE:HA	1.90	0.52
1:A:453:ARG:HD2	1:C:527:HIS:CG	2.45	0.52
1:C:444:GLU:OE1	3:C:702:HOH:O	2.19	0.52
1:D:211:THR:O	1:D:215:ARG:HB2	2.10	0.52
1:D:266:THR:HA	1:D:495:MET:HA	1.92	0.52
1:B:194:LEU:HD23	1:B:198:LEU:HG	1.92	0.52
1:B:250:PRO:O	1:B:254:LYS:HD3	2.10	0.51
1:C:249:ILE:CD1	1:C:379:SER:CB	2.77	0.51
1:B:527:HIS:CG	1:D:453:ARG:HD2	2.45	0.51
1:D:142:LEU:HA	1:D:215:ARG:HH12	1.75	0.51
1:A:171:ASP:OD1	1:A:173:ARG:HD3	2.10	0.51
1:A:529:TYR:CE1	1:C:478:PRO:HG3	2.46	0.51
1:B:140:ASP:OD2	1:B:140:ASP:N	2.41	0.51
1:D:140:ASP:HA	1:D:143:PHE:H	1.75	0.51
1:A:314:GLY:C	1:A:316:ARG:H	2.19	0.51
1:B:373:SER:OG	1:B:376:THR:HG23	2.11	0.51
1:D:195:ASP:OD1	1:D:198:LEU:CD2	2.59	0.51
1:C:315:LEU:HD23	1:C:315:LEU:O	2.10	0.50
1:B:190:ASP:OD2	1:B:190:ASP:N	2.41	0.50
1:D:198:LEU:HD23	1:D:199:PHE:N	2.26	0.50
1:A:249:ILE:CG1	1:A:379:SER:OG	2.59	0.50
1:A:316:ARG:HG3	1:C:324:GLU:CD	2.37	0.50
1:B:361:LEU:HD23	1:B:364:MET:HE3	1.93	0.50
1:A:229:HIS:ND1	1:A:523:LEU:HD21	2.27	0.50
1:D:348:VAL:HG12	1:D:352:GLU:HB2	1.93	0.50
1:B:453:ARG:HD2	1:D:527:HIS:CG	2.47	0.50
1:B:497:MET:HE1	1:B:516:PHE:CE1	2.47	0.50
1:B:521:VAL:O	1:B:538:LYS:NZ	2.25	0.50
1:C:294:ILE:HG12	1:C:360:PHE:HD2	1.77	0.50
1:D:144:TYR:HA	1:D:147:ALA:HB3	1.94	0.50
1:D:288:LYS:HE3	1:D:337:ALA:HB2	1.94	0.50
1:A:142:LEU:HD23	1:A:146:ILE:HG13	1.95	0.49
1:C:152:LYS:CB	1:C:193:MET:HE2	2.42	0.49
1:D:144:TYR:OH	1:D:196:LYS:HD3	2.12	0.49
1:D:277:THR:HA	1:D:423:CYS:HB2	1.93	0.49
1:B:200:LYS:HE2	1:B:204:GLN:HB2	1.93	0.49
1:B:145:THR:O	1:B:148:GLU:HG3	2.13	0.49
1:D:198:LEU:HD23	1:D:199:PHE:H	1.78	0.49
1:A:342:SER:HA	1:A:409:ILE:HD12	1.95	0.49
1:D:345:LYS:HB3	1:D:353:LYS:HG2	1.95	0.49
1:A:528:ASN:HD21	1:C:528:ASN:CG	2.20	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:GLN:NE2	1:B:152:LYS:NZ	2.60	0.49
1:D:251:GLN:HA	1:D:254:LYS:HE3	1.93	0.49
1:B:142:LEU:HD23	1:B:199:PHE:HZ	1.78	0.48
1:C:287:VAL:O	1:C:291:LYS:HG2	2.13	0.48
1:D:531:ASN:HB3	1:D:534:HIS:O	2.12	0.48
1:A:377:PHE:HZ	1:A:411:ASP:OD1	1.97	0.48
1:A:426:ALA:HB3	1:A:498:MET:HG2	1.96	0.48
1:C:349:ASN:OD1	1:C:352:GLU:HG3	2.14	0.48
1:D:151:GLU:OE1	1:D:151:GLU:HA	2.14	0.48
2:A:601:5XY:O27	1:B:319:LYS:HE3	2.14	0.48
1:D:259:LEU:HD13	1:D:500:TRP:CH2	2.49	0.48
1:A:453:ARG:HD2	1:C:527:HIS:CD2	2.49	0.48
1:B:309:GLY:O	1:B:330:ASN:HA	2.13	0.48
1:D:223:PHE:O	1:D:227:THR:HG23	2.14	0.48
1:B:353:LYS:HB3	1:B:412:PHE:CE2	2.49	0.48
1:B:189:SER:O	1:B:191:GLY:N	2.46	0.47
1:B:478:PRO:HG3	1:D:529:TYR:CE1	2.48	0.47
1:C:277:THR:HA	1:C:423:CYS:HB2	1.96	0.47
1:D:188:THR:CG2	1:D:192:VAL:HG12	2.44	0.47
1:A:316:ARG:HD3	2:C:601:5XY:C24	2.44	0.47
1:D:466:ASP:CB	1:D:507:MET:HE2	2.44	0.47
1:B:316:ARG:NH2	1:B:319:LYS:HD3	2.29	0.47
1:B:359:GLN:O	1:B:363:LYS:HG3	2.15	0.47
1:A:143:PHE:HZ	1:A:152:LYS:HA	1.79	0.47
1:A:215:ARG:HB3	1:A:217:LYS:HE3	1.96	0.47
1:C:259:LEU:HD13	1:C:500:TRP:CH2	2.50	0.47
1:B:223:PHE:O	1:B:227:THR:HG23	2.14	0.47
1:B:310:LYS:HD2	1:D:473:PHE:CD2	2.50	0.47
1:A:331:PRO:CD	1:A:458:LEU:HD13	2.45	0.47
1:D:259:LEU:HD13	1:D:500:TRP:HH2	1.80	0.47
1:B:152:LYS:HG2	1:B:193:MET:HG2	1.96	0.46
1:B:317:PHE:N	1:B:317:PHE:CD1	2.83	0.46
1:C:358:MET:HE3	1:C:358:MET:HB3	1.79	0.46
1:D:145:THR:OG1	1:D:215:ARG:NH2	2.49	0.46
1:C:292:TYR:OH	1:C:454:ASN:HB3	2.15	0.46
1:D:248:TYR:CE2	1:D:249:ILE:HG12	2.49	0.46
1:B:363:LYS:HD3	1:B:444:GLU:OE2	2.14	0.46
1:D:152:LYS:HZ3	1:D:193:MET:CB	2.28	0.46
1:A:161:ALA:HB1	1:A:214:PHE:HE1	1.79	0.46
1:C:431:ALA:CB	1:C:440:PRO:HG2	2.45	0.46
1:D:208:VAL:O	1:D:212:GLN:HG3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:GLN:OE1	1:D:417:CYS:HB3	2.15	0.46
1:C:137:SER:O	1:C:141:LEU:HG	2.15	0.46
1:A:152:LYS:NZ	1:A:193:MET:CE	2.79	0.46
1:A:223:PHE:O	1:A:227:THR:HG23	2.16	0.46
1:A:512:LYS:HG3	3:A:744:HOH:O	2.16	0.46
1:B:142:LEU:HD23	1:B:199:PHE:CZ	2.50	0.46
1:D:143:PHE:O	1:D:147:ALA:N	2.49	0.46
1:A:152:LYS:HD3	1:A:193:MET:HB3	1.98	0.46
1:B:284:GLN:HG3	1:B:483:VAL:HG12	1.98	0.46
1:C:194:LEU:HA	1:C:198:LEU:HD23	1.98	0.46
1:C:249:ILE:HD11	1:C:379:SER:HB3	1.90	0.46
1:A:224:MET:HA	1:A:224:MET:HE2	1.98	0.45
1:A:277:THR:HA	1:A:423:CYS:HB2	1.97	0.45
1:C:260:TRP:HE3	1:C:500:TRP:O	1.99	0.45
1:C:479:ALA:HB2	1:C:489:LEU:HD12	1.98	0.45
1:D:195:ASP:O	1:D:197:ASP:N	2.49	0.45
1:D:316:ARG:NH1	1:D:319:LYS:HE3	2.30	0.45
1:A:339:VAL:O	1:A:342:SER:OG	2.31	0.45
1:B:342:SER:HA	1:B:409:ILE:HD12	1.99	0.45
1:B:373:SER:HB2	1:B:420:GLU:OE2	2.17	0.45
1:C:152:LYS:HB2	1:C:193:MET:HE2	1.98	0.45
1:A:249:ILE:HG13	1:A:379:SER:OG	2.15	0.45
1:B:317:PHE:HD1	1:B:317:PHE:N	2.15	0.45
1:C:491:VAL:HG21	1:C:495:MET:HE2	1.99	0.45
1:A:348:VAL:O	1:A:353:LYS:HE3	2.16	0.45
1:B:212:GLN:H	1:B:212:GLN:HG3	1.55	0.45
1:C:309:GLY:O	1:C:330:ASN:HA	2.17	0.45
1:A:471:PHE:CE1	1:A:475:VAL:HG21	2.52	0.45
1:D:457:SER:O	1:D:460:HIS:HB3	2.16	0.45
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.64	0.45
1:A:173:ARG:HD2	1:A:441:ILE:C	2.42	0.44
1:A:208:VAL:O	1:A:212:GLN:HG3	2.17	0.44
1:D:148:GLU:O	1:D:150:GLN:N	2.46	0.44
1:B:285:SER:HB3	1:B:288:LYS:HD2	2.00	0.44
1:C:361:LEU:HD23	1:C:364:MET:HE3	1.99	0.44
1:A:155:VAL:HG22	1:A:194:LEU:HD11	1.99	0.44
1:D:175:LYS:O	1:D:179:ASP:N	2.46	0.44
1:C:410:LEU:HD23	1:C:410:LEU:HA	1.85	0.44
1:A:140:ASP:HB3	1:A:196:LYS:NZ	2.32	0.44
1:B:249:ILE:HD11	1:B:379:SER:HB3	1.98	0.44
1:A:180:MET:HG2	1:A:202:CYS:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLY:HA3	1:A:192:VAL:HA	1.76	0.44
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.84	0.44
1:D:524:CYS:HA	1:D:539:LEU:O	2.17	0.44
1:A:287:VAL:O	1:A:291:LYS:HG2	2.18	0.44
1:B:461:SER:O	1:B:468:SER:HB3	2.18	0.44
1:C:396:GLU:O	1:C:398:LYS:HE2	2.18	0.44
1:B:360:PHE:CE1	1:B:447:LEU:CD2	3.00	0.43
1:A:375:ALA:O	1:A:379:SER:HB3	2.18	0.43
1:B:152:LYS:HG2	1:B:193:MET:CG	2.49	0.43
1:B:316:ARG:HA	1:B:316:ARG:HD2	1.42	0.43
1:C:249:ILE:CG1	1:C:379:SER:HB2	2.48	0.43
1:A:307:TYR:HB3	1:A:339:VAL:HG11	2.00	0.43
1:C:296:VAL:HG11	1:C:454:ASN:HD22	1.84	0.43
1:B:250:PRO:HG2	1:B:251:GLN:NE2	2.33	0.43
1:C:191:GLY:HA3	1:C:192:VAL:HA	1.77	0.43
1:D:288:LYS:HE3	1:D:337:ALA:CB	2.49	0.43
1:B:505:ASP:HB3	1:B:511:VAL:HG22	2.01	0.43
1:D:288:LYS:HA	1:D:291:LYS:HE2	2.01	0.43
1:D:450:GLU:OE1	3:D:603:HOH:O	2.19	0.43
1:B:369:TYR:CZ	1:B:371:GLY:HA3	2.54	0.43
1:B:529:TYR:CE1	1:D:478:PRO:HG3	2.53	0.43
1:A:148:GLU:OE2	1:A:157:LYS:NZ	2.52	0.42
1:D:355:ASP:O	1:D:359:GLN:HG3	2.19	0.42
1:D:466:ASP:HB3	1:D:507:MET:HE2	2.00	0.42
1:B:292:TYR:HA	1:B:340:VAL:HG11	2.01	0.42
1:C:262:VAL:HG13	1:C:497:MET:HE3	2.00	0.42
1:A:247:ASP:C	1:A:249:ILE:H	2.26	0.42
1:B:339:VAL:HG23	1:B:394:LEU:HD13	2.00	0.42
1:B:348:VAL:O	1:B:353:LYS:HE3	2.19	0.42
1:C:228:SER:O	1:C:232:GLU:HG3	2.18	0.42
1:D:334:ASN:ND2	1:D:386:ARG:NH2	2.67	0.42
1:C:173:ARG:HD2	1:C:441:ILE:C	2.43	0.42
1:C:369:TYR:CZ	1:C:371:GLY:HA3	2.54	0.42
1:D:250:PRO:O	1:D:254:LYS:HG3	2.20	0.42
1:D:318:ASN:OD1	1:D:318:ASN:N	2.29	0.42
1:A:140:ASP:HB3	1:A:196:LYS:HZ2	1.83	0.42
1:A:217:LYS:HA	1:A:217:LYS:HD3	1.91	0.42
1:A:182:ARG:O	1:A:186:GLN:HG2	2.20	0.42
1:C:136:PRO:HB2	1:C:141:LEU:HD21	2.01	0.42
1:B:180:MET:HE2	1:B:180:MET:HB2	1.92	0.42
1:B:471:PHE:CZ	1:B:475:VAL:HG11	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:289:PRO:HD3	1:D:480:LYS:HG2	2.02	0.42
1:D:487:ILE:HD12	1:D:513:GLY:HA3	2.02	0.42
1:A:168:ARG:HD2	3:A:713:HOH:O	2.19	0.42
1:A:195:ASP:OD2	3:A:707:HOH:O	2.21	0.42
1:A:318:ASN:ND2	1:A:466:ASP:OD2	2.52	0.42
1:B:478:PRO:HD2	1:B:490:VAL:O	2.20	0.42
1:D:478:PRO:HD2	1:D:490:VAL:O	2.19	0.42
1:A:200:LYS:O	1:A:204:GLN:HB3	2.20	0.42
1:A:259:LEU:HD13	1:A:500:TRP:CH2	2.54	0.41
1:B:150:GLN:HG3	1:B:151:GLU:N	2.35	0.41
1:B:150:GLN:HG2	1:B:152:LYS:HD3	2.01	0.41
1:B:421:VAL:HG21	1:B:426:ALA:HB2	2.00	0.41
1:C:363:LYS:HG2	3:C:728:HOH:O	2.19	0.41
1:C:366:GLY:HA3	1:C:441:ILE:HD11	2.02	0.41
1:B:476:GLY:O	1:B:528:ASN:HB2	2.20	0.41
1:D:249:ILE:HG22	1:D:252:LEU:H	1.85	0.41
1:A:142:LEU:HD22	1:A:199:PHE:CZ	2.51	0.41
1:A:316:ARG:O	1:A:317:PHE:HD1	2.03	0.41
1:C:234:TYR:CE1	1:C:260:TRP:CD1	3.08	0.41
1:A:289:PRO:CD	1:A:480:LYS:HG2	2.50	0.41
1:C:249:ILE:HG13	1:C:250:PRO:HD2	2.02	0.41
1:D:215:ARG:HB3	1:D:217:LYS:HE2	2.02	0.41
1:B:141:LEU:HD12	1:B:141:LEU:HA	1.89	0.41
1:B:172:PRO:C	1:B:174:LEU:H	2.28	0.41
1:C:247:ASP:HA	1:C:253:ALA:HB2	2.03	0.41
1:D:198:LEU:HA	1:D:201:LYS:HB2	2.03	0.41
1:A:217:LYS:HE2	1:A:217:LYS:N	2.36	0.41
1:C:219:VAL:HG21	1:C:494:VAL:HA	2.01	0.41
1:C:273:SER:HB3	1:C:277:THR:HG21	2.03	0.41
1:C:363:LYS:HD3	1:C:444:GLU:OE2	2.19	0.41
1:A:318:ASN:HD21	1:A:466:ASP:CG	2.29	0.41
1:B:422:THR:H	1:B:425:SER:HG	1.67	0.41
1:B:386:ARG:O	1:B:389:ALA:HB3	2.20	0.41
1:C:263:SER:OG	1:C:424:GLU:HG2	2.21	0.41
1:C:438:PHE:CE2	1:C:445:ARG:HB2	2.56	0.41
1:C:199:PHE:O	1:C:203:VAL:HG22	2.21	0.40
1:C:296:VAL:HG11	1:C:454:ASN:ND2	2.36	0.40
1:C:477:LEU:HD21	1:C:526:PHE:O	2.22	0.40
1:D:315:LEU:HD12	1:D:315:LEU:HA	1.89	0.40
1:A:247:ASP:C	1:A:249:ILE:N	2.79	0.40
1:B:495:MET:HE3	1:B:497:MET:SD	2.61	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:MET:HA	1:C:224:MET:HE2	2.04	0.40
1:C:249:ILE:HG23	1:C:252:LEU:H	1.86	0.40
1:A:139:GLU:H	1:A:139:GLU:HG2	1.12	0.40
1:A:249:ILE:HD11	1:A:379:SER:C	2.46	0.40
1:B:288:LYS:N	1:B:289:PRO:HD2	2.36	0.40
1:B:477:LEU:HD23	1:B:477:LEU:HA	1.89	0.40
1:C:139:GLU:HG3	1:C:200:LYS:CD	2.47	0.40
1:D:198:LEU:HD23	1:D:198:LEU:N	2.35	0.40
1:D:215:ARG:HB3	1:D:217:LYS:CE	2.51	0.40
1:D:219:VAL:HG13	1:D:220:ILE:HG13	2.02	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%)	390 (96%)	14 (3%)	4 (1%)	12	23
1	B	408/539 (76%)	385 (94%)	22 (5%)	1 (0%)	43	62
1	C	408/539 (76%)	390 (96%)	18 (4%)	0	100	100
1	D	408/539 (76%)	385 (94%)	22 (5%)	1 (0%)	43	62
All	All	1632/2156 (76%)	1550 (95%)	76 (5%)	6 (0%)	30	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	THR
1	A	318	ASN
1	B	190	ASP
1	A	315	LEU
1	D	196	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	216	ARG

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	80
1	B	353/462 (76%)	352 (100%)	1 (0%)	86	94
1	C	353/462 (76%)	351 (99%)	2 (1%)	78	90
1	D	353/462 (76%)	349 (99%)	4 (1%)	65	83
All	All	1412/1848 (76%)	1400 (99%)	12 (1%)	73	88

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	GLU
1	A	145	THR
1	A	169	THR
1	A	241	SER
1	A	379	SER
1	B	169	THR
1	C	169	THR
1	C	318	ASN
1	D	198	LEU
1	D	316	ARG
1	D	318	ASN
1	D	544	GLU

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	186	GLN
1	A	240	GLN
1	A	346	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	359	GLN
1	A	470	GLN
1	A	528	ASN
1	B	150	GLN
1	B	186	GLN
1	B	240	GLN
1	B	435	ASN
1	C	186	GLN
1	C	362	ASN
1	C	435	ASN
1	C	454	ASN
1	D	367	ASN
1	D	528	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	5XY	A	601	-	40,40,40	2.93	15 (37%)	48,54,54	3.80	17 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	5XY	C	601	-	40,40,40	3.03	14 (35%)	48,54,54	3.58	19 (39%)

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	5XY	A	601	-	-	9/24/33/33	0/5/5/5
2	5XY	C	601	-	-	12/24/33/33	0/5/5/5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	5XY	C13-C09	-10.75	1.34	1.53
2	A	601	5XY	C13-C09	-10.35	1.35	1.53
2	C	601	5XY	C13-N12	8.33	1.62	1.46
2	A	601	5XY	C13-N12	8.07	1.62	1.46
2	A	601	5XY	C11-N12	-7.48	1.31	1.47
2	C	601	5XY	C11-N12	-7.27	1.32	1.47
2	A	601	5XY	C07-N08	5.08	1.42	1.34
2	C	601	5XY	C07-N08	4.82	1.42	1.34
2	C	601	5XY	C04-N03	3.94	1.44	1.38
2	C	601	5XY	C02-N03	3.53	1.43	1.37
2	C	601	5XY	C14-N12	3.46	1.42	1.34
2	A	601	5XY	C14-N12	3.40	1.42	1.34
2	C	601	5XY	C17-N18	3.12	1.42	1.38
2	A	601	5XY	C19-N18	2.97	1.42	1.37
2	C	601	5XY	C04-N05	2.97	1.35	1.31
2	A	601	5XY	C17-N18	2.90	1.42	1.38
2	C	601	5XY	C17-N16	2.89	1.35	1.31
2	A	601	5XY	C17-N16	2.88	1.35	1.31
2	A	601	5XY	C04-N03	2.86	1.42	1.38
2	A	601	5XY	C02-N03	2.79	1.42	1.37
2	C	601	5XY	C19-N18	2.72	1.42	1.37
2	C	601	5XY	C10-C11	2.69	1.57	1.52
2	A	601	5XY	C10-C11	2.64	1.57	1.52
2	C	601	5XY	C14-N15	2.34	1.35	1.31
2	A	601	5XY	C04-N05	2.32	1.34	1.31
2	A	601	5XY	N16-N15	-2.25	1.34	1.39
2	A	601	5XY	C07-N06	2.23	1.34	1.31
2	A	601	5XY	N06-N05	-2.15	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	5XY	C07-N06	2.07	1.34	1.31

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	5XY	N03-C04-N05	9.93	129.68	120.81
2	A	601	5XY	C11-N12-C13	-9.90	100.82	112.38
2	C	601	5XY	N03-C04-N05	9.24	129.06	120.81
2	C	601	5XY	S29-C04-N05	-8.55	104.97	114.52
2	A	601	5XY	S29-C07-N06	-8.50	105.03	114.52
2	A	601	5XY	S29-C04-N05	-8.07	105.50	114.52
2	A	601	5XY	N18-C17-N16	8.06	128.01	120.81
2	A	601	5XY	S28-C17-N16	-7.98	105.61	114.52
2	C	601	5XY	S29-C07-N06	-7.66	105.97	114.52
2	C	601	5XY	S28-C17-N16	-7.55	106.09	114.52
2	C	601	5XY	N18-C17-N16	7.44	127.46	120.81
2	A	601	5XY	S28-C14-N12	5.95	128.27	120.31
2	C	601	5XY	N12-C14-N15	5.37	127.29	116.91
2	C	601	5XY	C01-C02-N03	5.21	120.76	114.40
2	C	601	5XY	C20-C19-N18	5.16	120.69	114.40
2	C	601	5XY	S28-C14-N15	-5.06	105.69	114.44
2	C	601	5XY	C14-N15-N16	5.03	117.00	107.08
2	C	601	5XY	S28-C14-N12	4.99	126.98	120.31
2	C	601	5XY	C11-N12-C13	-4.91	106.64	112.38
2	A	601	5XY	C09-C13-N12	4.84	108.83	103.55
2	A	601	5XY	C20-C19-N18	4.80	120.25	114.40
2	A	601	5XY	C14-N15-N16	4.79	116.54	107.08
2	A	601	5XY	S28-C14-N15	-4.79	106.15	114.44
2	A	601	5XY	N12-C14-N15	4.45	125.52	116.91
2	C	601	5XY	C09-C13-N12	4.32	108.25	103.55
2	C	601	5XY	C04-N05-N06	4.29	117.47	112.02
2	A	601	5XY	C07-N06-N05	4.03	117.14	112.02
2	A	601	5XY	C17-N16-N15	3.70	116.73	112.02
2	A	601	5XY	C04-N05-N06	3.29	116.21	112.02
2	A	601	5XY	C11-N12-C14	3.14	129.33	123.83
2	C	601	5XY	C07-N06-N05	3.13	116.00	112.02
2	A	601	5XY	C01-C02-N03	3.01	118.07	114.40
2	C	601	5XY	C11-N12-C14	2.92	128.94	123.83
2	C	601	5XY	C17-N16-N15	2.89	115.69	112.02
2	C	601	5XY	O30-C02-C01	-2.07	117.50	121.99
2	C	601	5XY	S28-C17-N18	2.03	126.44	123.72

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	5XY	N15-C14-N12-C13
2	A	601	5XY	S28-C14-N12-C13
2	A	601	5XY	N15-C14-N12-C11
2	A	601	5XY	S28-C14-N12-C11
2	A	601	5XY	N16-C17-N18-C19
2	A	601	5XY	S28-C17-N18-C19
2	A	601	5XY	N05-C04-N03-C02
2	A	601	5XY	S29-C04-N03-C02
2	A	601	5XY	C13-C09-N08-C07
2	C	601	5XY	N15-C14-N12-C13
2	C	601	5XY	S28-C14-N12-C13
2	C	601	5XY	N15-C14-N12-C11
2	C	601	5XY	S28-C14-N12-C11
2	C	601	5XY	N16-C17-N18-C19
2	C	601	5XY	S28-C17-N18-C19
2	C	601	5XY	N05-C04-N03-C02
2	C	601	5XY	S29-C04-N03-C02
2	C	601	5XY	S29-C07-N08-C09
2	C	601	5XY	N06-C07-N08-C09
2	C	601	5XY	O27-C19-C20-C21
2	C	601	5XY	N18-C19-C20-C21

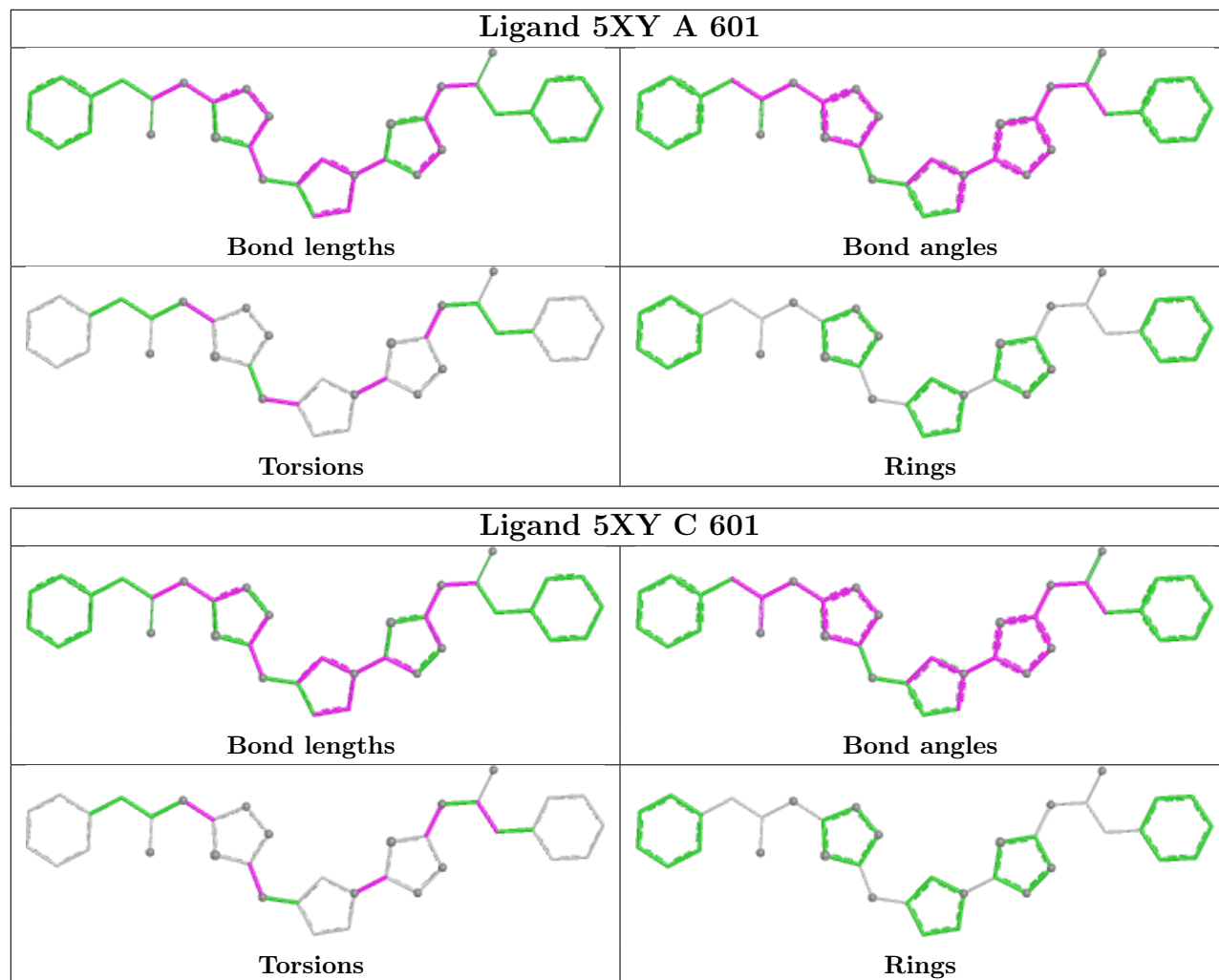
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	5XY	2	0
2	C	601	5XY	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%)	0.62	33 (8%)	18 16	30, 44, 79, 114	0
1	B	410/539 (76%)	0.74	42 (10%)	12 10	33, 48, 80, 98	0
1	C	410/539 (76%)	0.72	41 (10%)	12 11	31, 44, 80, 95	0
1	D	410/539 (76%)	0.80	52 (12%)	8 6	34, 47, 87, 111	0
All	All	1640/2156 (76%)	0.72	168 (10%)	12 10	30, 46, 81, 114	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	317	PHE	9.0
1	A	188	THR	8.1
1	D	140	ASP	6.7
1	A	136	PRO	6.4
1	D	188	THR	6.1
1	C	317	PHE	5.6
1	C	136	PRO	5.5
1	A	317	PHE	5.4
1	D	315	LEU	5.3
1	B	317	PHE	5.1
1	D	545	GLY	4.9
1	B	138	LEU	4.6
1	B	136	PRO	4.6
1	D	193	MET	4.6
1	A	152	LYS	4.6
1	A	545	GLY	4.4
1	D	249	ILE	4.3
1	D	141	LEU	4.3
1	D	144	TYR	4.3
1	D	136	PRO	4.2
1	C	138	LEU	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	138	LEU	4.2
1	D	155	VAL	4.1
1	D	151	GLU	4.1
1	B	143	PHE	4.0
1	B	316	ARG	3.9
1	D	152	LYS	3.9
1	A	148	GLU	3.9
1	D	251	GLN	3.8
1	D	318	ASN	3.8
1	C	149	GLY	3.7
1	C	360	PHE	3.6
1	B	188	THR	3.6
1	C	192	VAL	3.6
1	C	315	LEU	3.6
1	B	318	ASN	3.6
1	D	248	TYR	3.6
1	D	189	SER	3.6
1	B	545	GLY	3.5
1	C	545	GLY	3.5
1	A	190	ASP	3.5
1	D	148	GLU	3.5
1	A	189	SER	3.5
1	A	318	ASN	3.4
1	C	188	THR	3.4
1	A	185	LEU	3.4
1	B	360	PHE	3.4
1	B	190	ASP	3.4
1	D	192	VAL	3.3
1	D	250	PRO	3.3
1	D	252	LEU	3.3
1	C	190	ASP	3.2
1	A	199	PHE	3.2
1	A	383	SER	3.2
1	B	141	LEU	3.2
1	D	194	LEU	3.1
1	C	155	VAL	3.1
1	C	249	ILE	3.1
1	C	143	PHE	3.1
1	A	193	MET	3.1
1	B	198	LEU	3.1
1	B	144	TYR	3.1
1	B	192	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	196	LYS	3.0
1	B	252	LEU	3.0
1	A	144	TYR	3.0
1	D	142	LEU	3.0
1	B	153	ILE	2.9
1	A	147	ALA	2.9
1	A	138	LEU	2.9
1	D	153	ILE	2.9
1	C	142	LEU	2.9
1	C	144	TYR	2.9
1	B	205	SER	2.9
1	A	141	LEU	2.8
1	B	539	LEU	2.8
1	D	150	GLN	2.8
1	B	199	PHE	2.8
1	D	199	PHE	2.8
1	B	154	PRO	2.8
1	C	252	LEU	2.8
1	D	185	LEU	2.8
1	C	199	PHE	2.8
1	D	187	THR	2.7
1	B	152	LYS	2.7
1	A	137	SER	2.7
1	D	198	LEU	2.7
1	A	187	THR	2.7
1	A	151	GLU	2.7
1	B	142	LEU	2.7
1	D	224	MET	2.7
1	C	161	ALA	2.7
1	D	190	ASP	2.7
1	B	149	GLY	2.7
1	B	137	SER	2.7
1	B	145	THR	2.7
1	D	139	GLU	2.7
1	D	156	HIS	2.6
1	B	193	MET	2.6
1	A	315	LEU	2.6
1	D	137	SER	2.6
1	D	197	ASP	2.6
1	A	198	LEU	2.6
1	B	376	THR	2.6
1	A	543	ARG	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	150	GLN	2.6
1	C	251	GLN	2.6
1	B	194	LEU	2.5
1	A	192	VAL	2.5
1	D	316	ARG	2.5
1	D	386	ARG	2.5
1	B	189	SER	2.5
1	A	212	GLN	2.5
1	B	156	HIS	2.5
1	C	156	HIS	2.5
1	C	189	SER	2.5
1	B	151	GLU	2.4
1	C	191	GLY	2.4
1	D	164	SER	2.4
1	D	543	ARG	2.4
1	D	145	THR	2.4
1	D	184	THR	2.4
1	D	254	LYS	2.4
1	C	198	LEU	2.4
1	D	255	PHE	2.4
1	C	137	SER	2.3
1	C	316	ARG	2.3
1	C	141	LEU	2.3
1	B	201	LYS	2.3
1	A	154	PRO	2.3
1	C	205	SER	2.3
1	D	205	SER	2.3
1	C	544	GLU	2.3
1	A	386	ARG	2.3
1	D	257	PRO	2.3
1	A	146	ILE	2.3
1	B	315	LEU	2.2
1	D	383	SER	2.2
1	C	150	GLN	2.2
1	D	149	GLY	2.2
1	C	543	ARG	2.2
1	C	152	LYS	2.2
1	C	465	TYR	2.2
1	D	212	GLN	2.2
1	B	191	GLY	2.2
1	A	316	ARG	2.2
1	A	536	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	207	ILE	2.2
1	B	242	GLY	2.1
1	D	146	ILE	2.1
1	B	216	ARG	2.1
1	B	241	SER	2.1
1	C	386	ARG	2.1
1	C	166	GLY	2.1
1	A	143	PHE	2.1
1	C	194	LEU	2.1
1	D	544	GLU	2.1
1	B	228	SER	2.1
1	C	193	MET	2.1
1	A	150	GLN	2.1
1	B	240	GLN	2.1
1	C	318	ASN	2.1
1	B	249	ILE	2.1
1	C	197	ASP	2.1
1	B	383	SER	2.1
1	C	255	PHE	2.0
1	C	200	LYS	2.0
1	A	197	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](#)

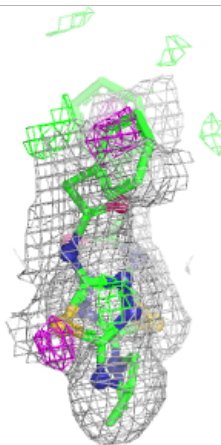
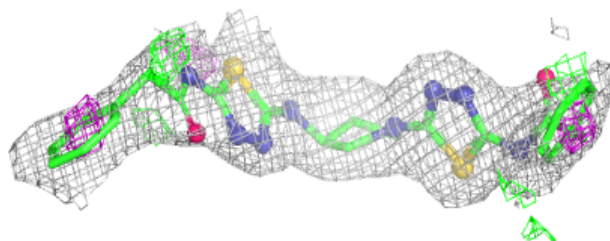
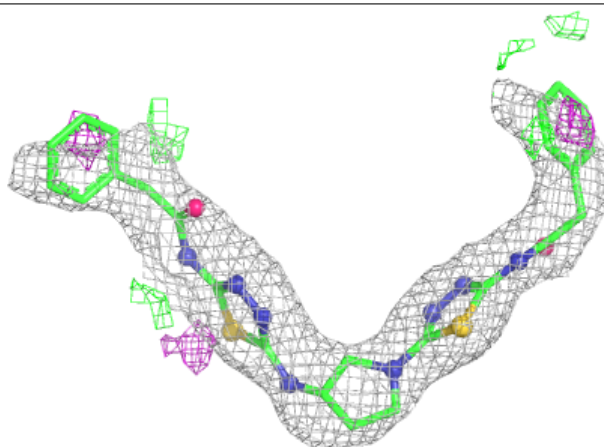
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

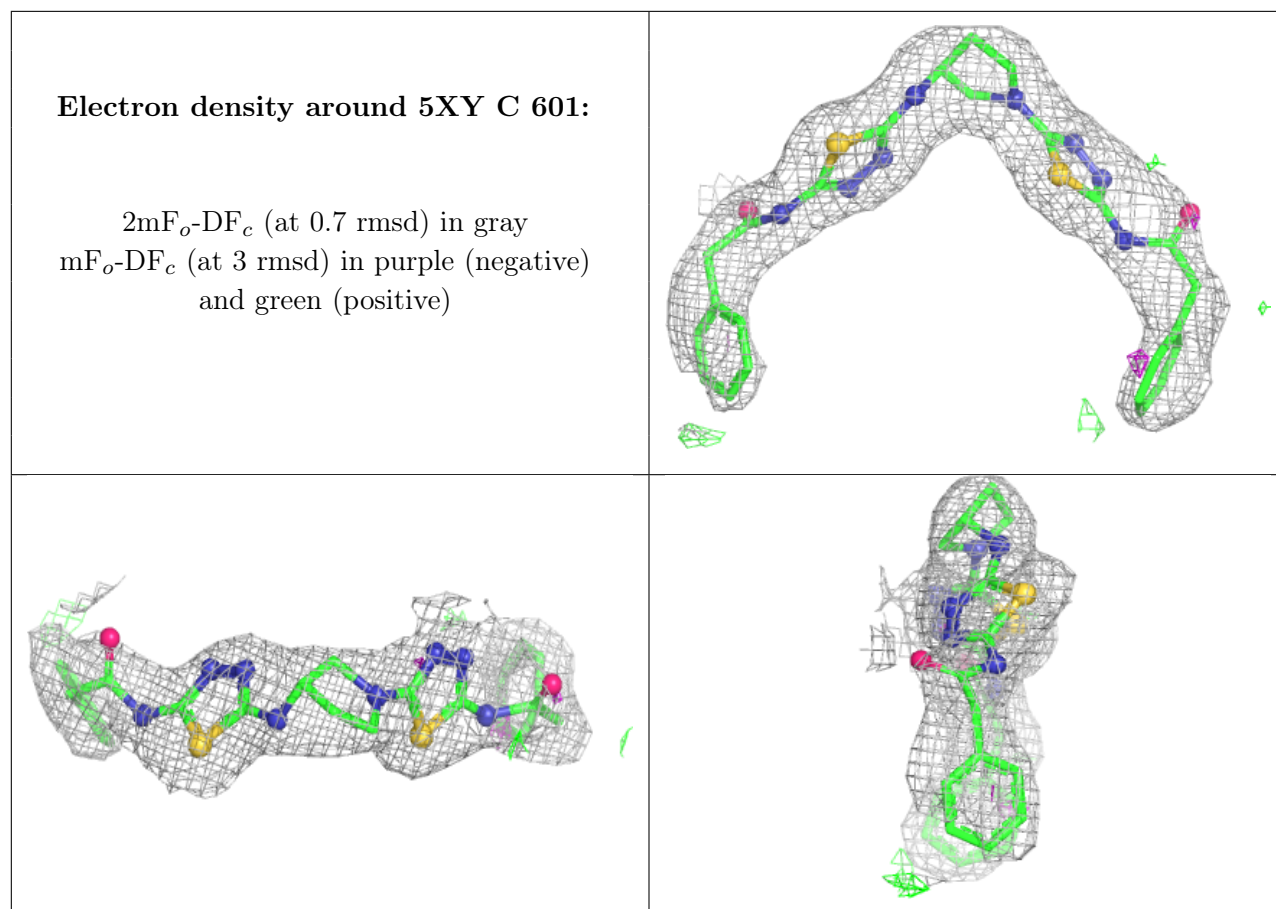
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	5XY	A	601	36/36	0.86	0.17	48,65,82,85	0
2	5XY	C	601	36/36	0.88	0.16	52,67,83,84	0

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 5XY 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.