



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:14 AM UTC

PDB ID : 5HGQ / pdb_00005hgq
Title : Loa loa Lysyl-tRNA synthetase in complex with Cladosporin.
Authors : Sharma, A.; Sharma, M.; Yogavel, M.; Sharma, A.
Deposited on : 2016-01-08
Resolution : 3.28 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

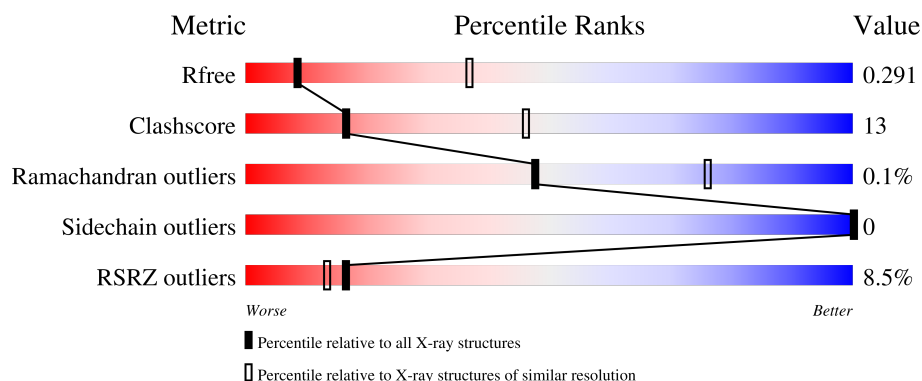
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.28 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	524	6% 64% 25% 11%
1	B	524	9% 66% 26% 8%
1	C	524	7% 66% 24% 10%
1	D	524	8% 63% 26% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14637 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.

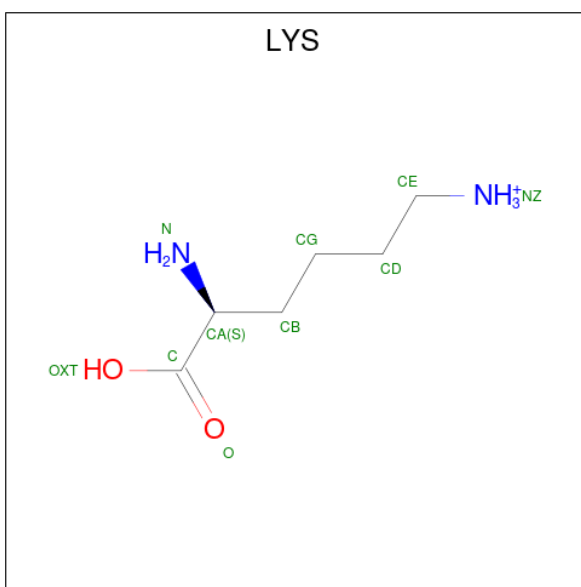
- Molecule 1 is a protein called Lysine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	0	0
			3584	2315	610	641	18			
1	D	470	Total	C	N	O	S	0	0	0
			3634	2344	620	654	16			
1	B	482	Total	C	N	O	S	0	0	0
			3668	2367	635	647	19			
1	C	473	Total	C	N	O	S	0	0	0
			3614	2335	616	644	19			

There are 8 discrepancies between the modelled and reference sequences:

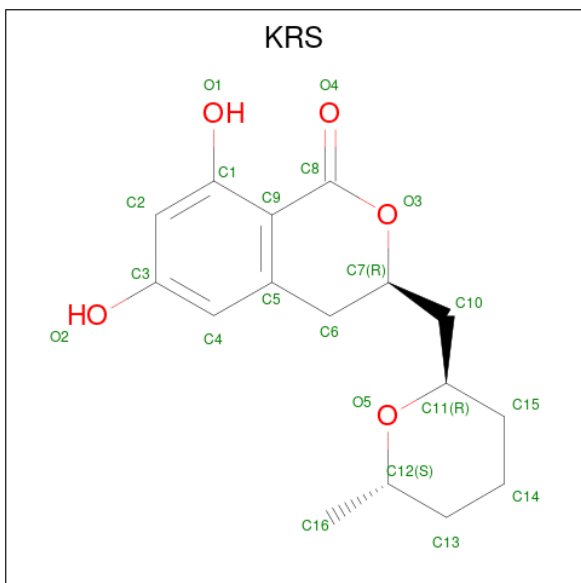
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP E1FQP0
A	0	ALA	-	cloning artifact	UNP E1FQP0
D	-1	MET	-	cloning artifact	UNP E1FQP0
D	0	ALA	-	cloning artifact	UNP E1FQP0
B	-1	MET	-	cloning artifact	UNP E1FQP0
B	0	ALA	-	cloning artifact	UNP E1FQP0
C	-1	MET	-	cloning artifact	UNP E1FQP0
C	0	ALA	-	cloning artifact	UNP E1FQP0

- Molecule 2 is LYSINE (CCD ID: LYS) (formula: $C_6H_{15}N_2O_2$).



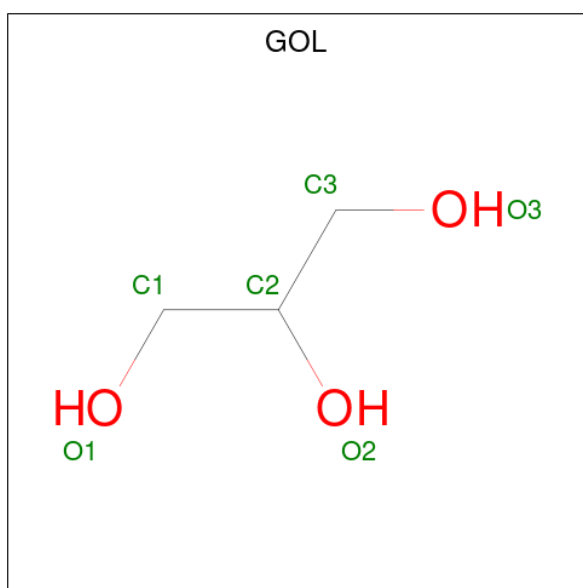
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	D	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		
2	C	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is cladosporin (CCD ID: KRS) (formula: C₁₆H₂₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	D	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		

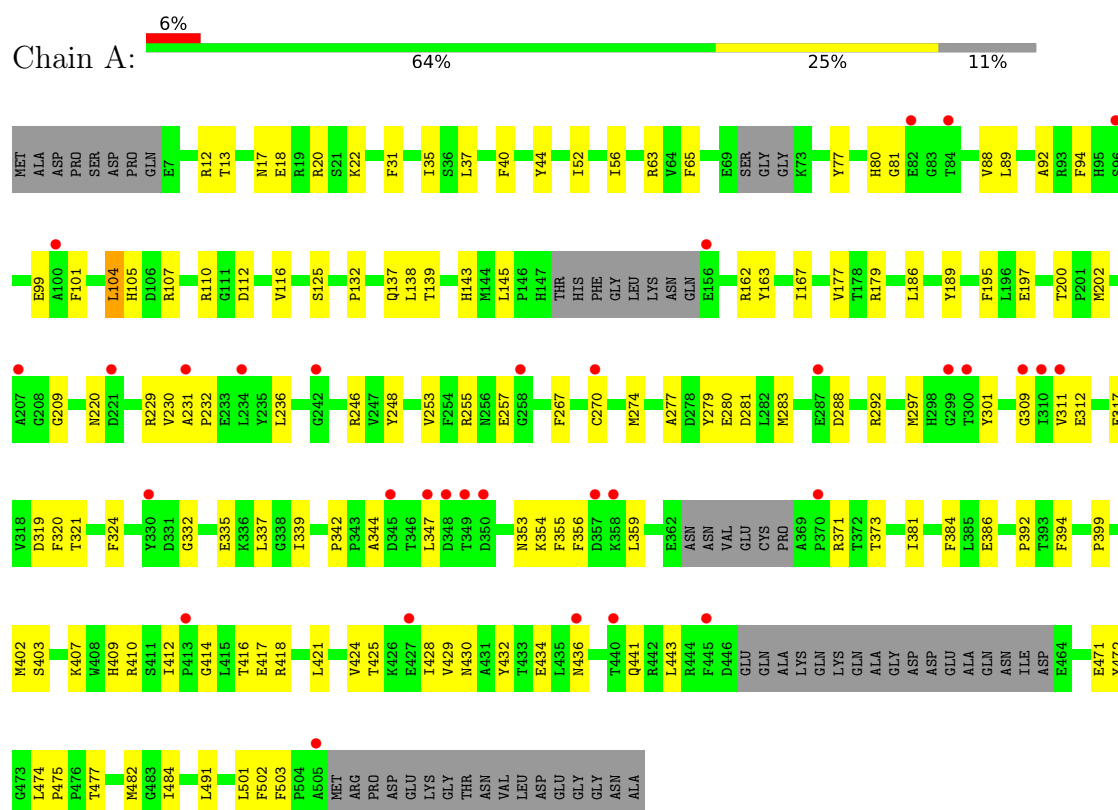
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	O	0	0
			2	2		
5	D	1	Total	O	0	0
			1	1		
5	B	3	Total	O	0	0
			3	3		
5	C	1	Total	O	0	0
			1	1		

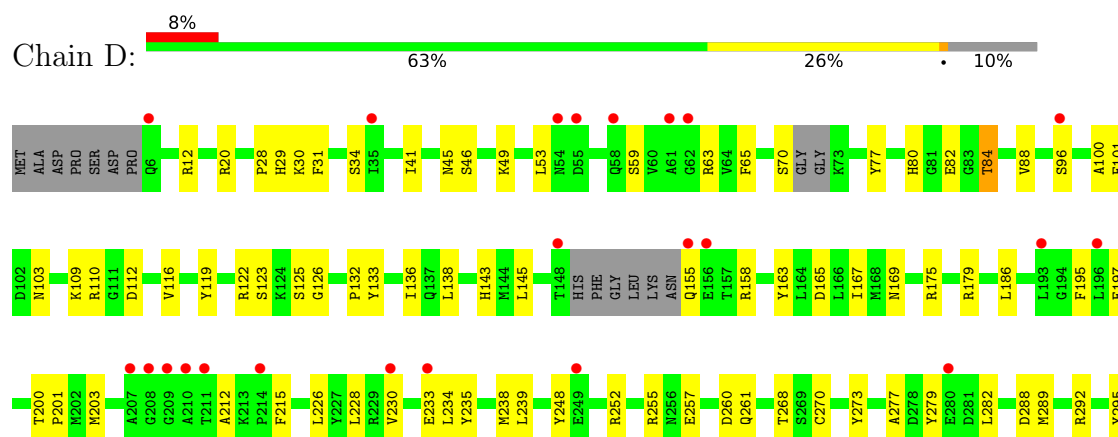
3 Residue-property plots

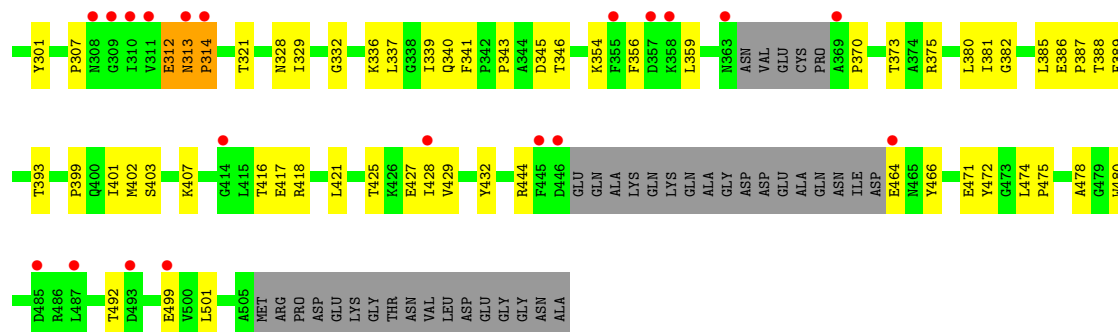
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

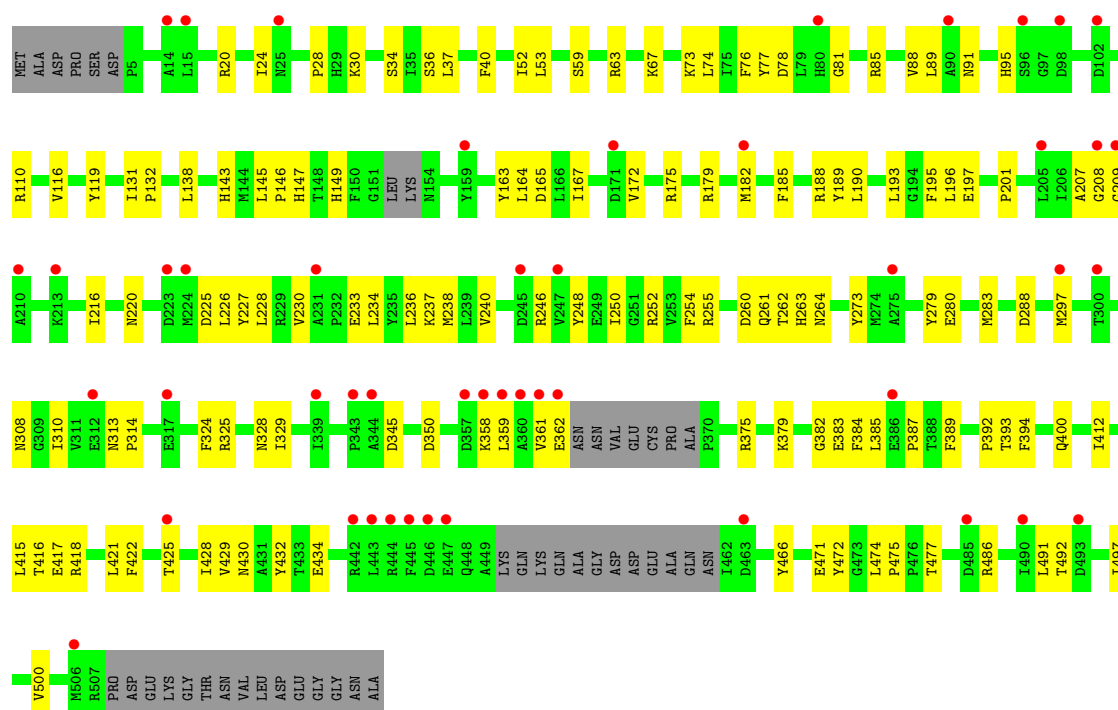


• Molecule 1: Lysine-tRNA ligase

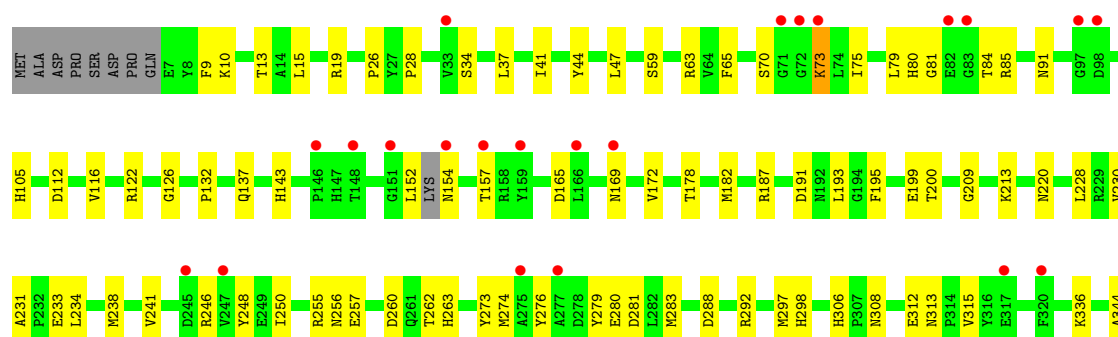


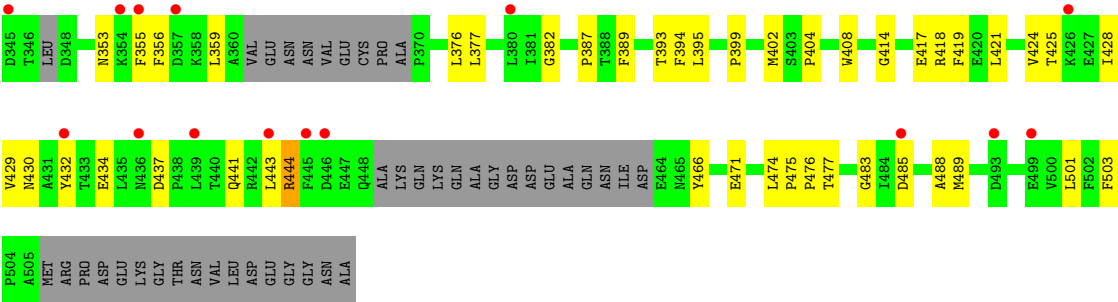


• Molecule 1: Lysine-tRNA ligase



• Molecule 1: Lysine-tRNA ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	120.17Å 147.35Å 160.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.75 – 3.28 43.75 – 3.28	Depositor EDS
% Data completeness (in resolution range)	90.8 (43.75-3.28) 82.3 (43.75-3.28)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.23 (at 3.25Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.254 , 0.292 0.254 , 0.291	Depositor DCC
R_{free} test set	2000 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.911	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	14637	wwPDB-VP
Average B, all atoms (Å ²)	42.0	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 26.53 % 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 2.5923e-03. 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: GOL, KRS

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	0.27	0/3674	0.59	4/4999 (0.1%)
1	B	0.26	0/3759	0.60	4/5105 (0.1%)
1	C	0.26	0/3706	0.63	6/5027 (0.1%)
1	D	0.29	0/3722	0.65	5/5059 (0.1%)
All	All	0.27	0/14861	0.62	19/20190 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	THR	N-CA-C	-17.75	94.39	114.62
1	C	73	LYS	N-CA-C	9.38	121.50	111.28
1	A	309	GLY	N-CA-C	9.27	123.70	112.49
1	B	220	ASN	N-CA-C	8.36	120.39	111.28
1	C	220	ASN	N-CA-C	7.29	119.23	111.28
1	D	84	THR	N-CA-C	7.24	119.31	110.41
1	D	313	ASN	N-CA-C	6.97	123.06	113.16
1	C	443	LEU	N-CA-C	-5.93	98.71	108.49
1	B	384	PHE	N-CA-C	5.88	120.50	112.68
1	C	313	ASN	N-CA-C	5.88	121.51	113.16
1	D	312	GLU	N-CA-C	5.81	118.71	109.65
1	D	101	PHE	N-CA-C	-5.74	105.02	111.28
1	C	444	ARG	N-CA-C	5.68	118.16	108.90
1	A	220	ASN	N-CA-C	5.52	117.30	111.28
1	B	383	GLU	N-CA-C	5.48	117.33	111.36
1	A	347	LEU	N-CA-C	5.46	117.58	110.43
1	D	82	GLU	CB-CA-C	-5.31	108.88	115.89
1	A	104	LEU	N-CA-C	5.30	117.14	111.36
1	B	359	LEU	N-CA-C	-5.06	105.76	112.24

There are no chirality outliers.

There are no planarity outliers.

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	3584	0	3353	94	0
1	B	3668	0	3416	94	1
1	C	3614	0	3338	96	2
1	D	3634	0	3446	106	1
2	A	10	0	12	0	0
2	B	10	0	12	1	0
2	C	10	0	12	2	0
2	D	10	0	12	0	0
3	A	21	0	19	1	0
3	B	21	0	19	4	0
3	C	21	0	19	5	0
3	D	21	0	19	1	0
4	D	6	0	8	0	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	14637	0	13685	365	2

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 13.

All (365) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ASN:CB	1:B:313:ASN:CB	2.00	1.39
1:C:404:PRO:HB3	1:C:444:ARG:HH21	1.26	0.98
1:A:63:ARG:NH2	1:B:472:TYR:O	2.01	0.93
1:A:65:PHE:CB	1:A:80:HIS:CD2	2.55	0.90
1:A:65:PHE:CB	1:A:80:HIS:NE2	2.35	0.89
1:D:252:ARG:NH1	1:C:200:THR:O	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:VAL:HG12	1:A:312:GLU:H	1.40	0.85
1:D:354:LYS:HG3	1:D:373:THR:HG23	1.61	0.83
1:A:421:LEU:HB3	1:A:429:VAL:HG22	1.58	0.83
1:A:407:LYS:HE2	1:A:436:ASN:HB2	1.61	0.82
1:C:116:VAL:HG13	1:C:132:PRO:HB3	1.61	0.82
1:C:187:ARG:O	1:C:191:ASP:HB2	1.81	0.80
1:B:182:MET:HB2	1:B:297:MET:HE1	1.64	0.80
1:C:404:PRO:HB3	1:C:444:ARG:NH2	1.96	0.79
1:A:104:LEU:HD12	1:A:104:LEU:O	1.83	0.79
1:B:77:TYR:HB2	1:B:88:VAL:HG22	1.68	0.75
1:D:230:VAL:HG23	1:D:255:ARG:HG2	1.68	0.74
1:B:116:VAL:HG13	1:B:132:PRO:HB3	1.69	0.74
1:C:421:LEU:HB3	1:C:429:VAL:HB	1.69	0.74
1:B:313:ASN:CB	1:B:314:PRO:HD2	2.18	0.73
1:A:162:ARG:NE	1:A:502:PHE:O	2.21	0.73
1:C:112:ASP:OD2	1:C:137:GLN:NE2	2.21	0.73
1:D:122:ARG:NH1	1:D:126:GLY:O	2.23	0.72
1:D:12:ARG:HH12	1:D:109:LYS:HB2	1.53	0.72
1:D:100:ALA:HB3	1:D:103:ASN:HB2	1.72	0.71
1:D:337:LEU:HD22	1:D:359:LEU:CD1	2.20	0.71
1:D:370:PRO:O	1:D:375:ARG:NH1	2.23	0.71
1:C:306:HIS:CD2	1:C:315:VAL:HG22	2.25	0.71
1:C:122:ARG:NH1	1:C:126:GLY:O	2.24	0.71
1:D:428:ILE:HG13	1:D:429:VAL:HG23	1.73	0.70
1:B:216:ILE:HD11	1:B:225:ASP:HB2	1.72	0.70
1:B:165:ASP:OD2	1:B:172:VAL:HG21	1.92	0.70
1:A:116:VAL:HG13	1:A:132:PRO:HB3	1.73	0.70
1:D:346:THR:HG21	1:D:401:ILE:HD13	1.74	0.70
1:D:116:VAL:HG13	1:D:132:PRO:HB3	1.73	0.69
1:B:428:ILE:HG13	1:B:429:VAL:HG23	1.73	0.69
1:B:260:ASP:OD1	1:B:261:GLN:N	2.26	0.68
1:B:52:ILE:HD12	1:B:131:ILE:HD12	1.74	0.68
1:A:281:ASP:OD2	1:B:30:LYS:NZ	2.26	0.68
1:D:407:LYS:NZ	1:C:28:PRO:O	2.26	0.68
1:D:418:ARG:HA	1:D:432:TYR:HB3	1.76	0.68
1:A:418:ARG:HA	1:A:432:TYR:HB3	1.74	0.68
1:B:313:ASN:CB	1:B:314:PRO:CD	2.72	0.68
1:B:262:THR:O	1:B:486:ARG:NH2	2.25	0.67
1:D:301:TYR:HD2	1:D:321:THR:HG22	1.57	0.67
1:D:474:LEU:HD12	1:D:475:PRO:HD2	1.75	0.67
1:A:52:ILE:HD11	1:A:94:PHE:HE2	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:LEU:HD12	1:A:475:PRO:HD2	1.76	0.67
1:B:345:ASP:CB	1:B:350:ASP:OD2	2.43	0.67
1:C:428:ILE:HG13	1:C:429:VAL:HG23	1.76	0.67
1:C:474:LEU:HD12	1:C:475:PRO:HD2	1.76	0.67
1:D:233:GLU:HG3	1:D:273:TYR:OH	1.95	0.66
1:D:295:TYR:HB2	1:D:301:TYR:CE1	2.30	0.66
1:B:358:LYS:O	1:B:361:VAL:HG22	1.94	0.66
1:A:354:LYS:HG3	1:A:373:THR:HG23	1.78	0.66
1:B:362:GLU:CB	1:B:379:LYS:HZ1	2.09	0.65
1:C:273:TYR:OH	2:C:601:LYS:NZ	2.29	0.65
1:D:12:ARG:NH1	1:D:109:LYS:HB2	2.11	0.65
1:B:474:LEU:HD12	1:B:475:PRO:HD2	1.78	0.65
1:A:280:GLU:HG2	1:A:283:MET:HE2	1.78	0.65
1:D:260:ASP:OD1	1:D:261:GLN:N	2.28	0.64
1:A:471:GLU:OE1	1:B:143:HIS:NE2	2.29	0.64
1:A:441:GLN:OE1	1:A:441:GLN:HA	1.98	0.64
1:D:203:MET:HE2	1:D:226:LEU:HD12	1.80	0.64
1:C:34:SER:HB3	1:C:59:SER:H	1.61	0.63
1:A:143:HIS:NE2	1:B:471:GLU:OE2	2.31	0.63
1:A:200:THR:O	1:B:252:ARG:NH2	2.31	0.63
1:D:175:ARG:HH11	1:D:492:THR:HB	1.64	0.63
1:A:92:ALA:HB2	1:A:101:PHE:CD2	2.34	0.63
1:A:101:PHE:CE1	1:A:105:HIS:CD2	2.86	0.63
1:D:100:ALA:HB3	1:D:103:ASN:CB	2.29	0.62
1:D:12:ARG:HH22	1:D:109:LYS:H	1.47	0.62
1:D:288:ASP:OD1	1:D:292:ARG:NE	2.32	0.62
1:D:212:ALA:HB1	1:D:257:GLU:OE2	1.99	0.62
1:A:35:ILE:HD11	1:A:40:PHE:HD2	1.63	0.62
1:D:295:TYR:HB2	1:D:301:TYR:HE1	1.64	0.62
1:A:77:TYR:HB2	1:A:88:VAL:HB	1.81	0.62
1:B:78:ASP:OD1	1:B:85:ARG:NH1	2.31	0.62
1:A:101:PHE:CD1	1:A:105:HIS:CD2	2.87	0.62
1:D:228:LEU:HD21	1:C:228:LEU:HD11	1.81	0.61
1:D:472:TYR:O	1:C:63:ARG:NH2	2.33	0.61
1:A:472:TYR:O	1:B:63:ARG:NH2	2.34	0.61
1:D:30:LYS:NZ	1:C:281:ASP:OD2	2.34	0.61
1:A:428:ILE:HG13	1:A:429:VAL:HG13	1.81	0.61
1:C:10:LYS:O	1:C:13:THR:CG2	2.49	0.60
1:A:288:ASP:OD1	1:A:292:ARG:NE	2.34	0.60
1:D:31:PHE:HB2	1:D:138:LEU:HD21	1.82	0.60
1:D:20:ARG:NH2	1:C:437:ASP:OD2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:158:ARG:NH2	1:D:499:GLU:OE1	2.34	0.60
1:D:403:SER:HB2	1:D:416:THR:HG21	1.83	0.60
1:C:9:PHE:O	1:C:13:THR:HG22	2.01	0.60
1:D:385:LEU:O	1:D:388:THR:HG22	2.02	0.59
1:B:421:LEU:HB3	1:B:429:VAL:HB	1.84	0.59
1:C:308:ASN:O	1:C:312:GLU:HB2	2.03	0.59
1:D:155:GLN:O	1:D:158:ARG:HG2	2.03	0.59
1:D:382:GLY:HA2	1:D:386:GLU:HB2	1.84	0.59
1:C:344:ALA:HB1	1:C:414:GLY:HA3	1.84	0.58
1:B:233:GLU:HG3	1:B:273:TYR:OH	2.02	0.58
1:A:37:LEU:HD22	1:A:81:GLY:HA3	1.84	0.58
1:D:12:ARG:NH2	1:D:112:ASP:OD2	2.37	0.58
1:C:355:PHE:HD1	1:C:355:PHE:O	1.87	0.58
1:B:375:ARG:O	1:B:379:LYS:HG2	2.03	0.58
1:C:297:MET:HG3	1:C:298:HIS:ND1	2.19	0.58
1:B:230:VAL:HG23	1:B:255:ARG:HG2	1.84	0.58
1:B:264:ASN:H	3:B:602:KRS:H3	1.69	0.58
1:D:252:ARG:HG3	1:D:268:THR:HG22	1.85	0.58
1:C:404:PRO:HD3	1:C:444:ARG:HH22	1.69	0.57
1:D:197:GLU:HB2	1:D:248:TYR:CZ	2.40	0.57
1:B:475:PRO:O	1:B:477:THR:OG1	2.22	0.57
1:C:152:LEU:CB	1:C:154:ASN:N	2.68	0.56
1:A:13:THR:O	1:A:17:ASN:ND2	2.28	0.56
1:A:195:PHE:HB3	1:A:248:TYR:HD2	1.70	0.56
1:D:59:SER:HA	1:D:116:VAL:O	2.06	0.56
1:C:10:LYS:C	1:C:13:THR:HG22	2.31	0.56
1:D:346:THR:HG21	1:D:401:ILE:HG21	1.87	0.56
1:D:421:LEU:HB3	1:D:429:VAL:HB	1.88	0.56
1:C:404:PRO:CB	1:C:444:ARG:NH2	2.67	0.56
1:C:434:GLU:HB2	1:C:477:THR:HG23	1.87	0.55
1:A:99:GLU:OE2	1:A:107:ARG:NH2	2.38	0.55
1:D:49:LYS:O	1:D:123:SER:O	2.24	0.55
1:C:10:LYS:O	1:C:13:THR:HG22	2.07	0.54
1:C:257:GLU:OE1	3:C:602:KRS:O2	2.21	0.54
1:A:335:GLU:OE1	1:D:125:SER:OG	2.22	0.54
1:C:356:PHE:CE1	1:C:359:LEU:HG	2.43	0.54
1:A:429:VAL:HG12	1:A:482:MET:HB2	1.89	0.54
1:B:325:ARG:HG3	1:B:393:THR:HG23	1.89	0.54
1:C:356:PHE:CD1	1:C:356:PHE:C	2.86	0.54
1:D:195:PHE:HB3	1:D:248:TYR:HD2	1.71	0.54
1:B:362:GLU:CB	1:B:379:LYS:NZ	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:GLU:N	1:A:317:GLU:OE1	2.41	0.53
1:A:311:VAL:HG12	1:A:312:GLU:N	2.16	0.53
1:C:279:TYR:CD1	1:C:417:GLU:HB3	2.43	0.53
1:D:158:ARG:NH1	1:D:165:ASP:OD2	2.42	0.53
1:D:282:LEU:HD13	1:D:480:TRP:HB2	1.91	0.53
1:D:28:PRO:HD2	1:D:138:LEU:O	2.08	0.53
1:B:28:PRO:HD2	1:B:138:LEU:O	2.09	0.53
1:A:12:ARG:NH2	1:A:107:ARG:O	2.38	0.53
1:B:430:ASN:HB2	3:B:602:KRS:H17	1.91	0.53
1:B:179:ARG:NH1	1:B:500:VAL:O	2.42	0.52
1:D:234:LEU:O	1:D:238:MET:HG3	2.10	0.52
1:A:197:GLU:HB2	1:A:248:TYR:CZ	2.44	0.52
1:D:464:GLU:HG3	1:D:466:TYR:H	1.75	0.52
1:B:20:ARG:HA	1:B:24:ILE:O	2.10	0.52
1:C:75:ILE:HD12	1:C:105:HIS:CD2	2.45	0.52
1:C:262:THR:HG22	1:C:489:MET:HE1	1.91	0.52
1:A:317:GLU:O	1:A:317:GLU:HG2	2.09	0.52
1:D:235:TYR:O	1:D:239:LEU:HD12	2.10	0.52
1:D:399:PRO:HD2	1:D:402:MET:SD	2.51	0.51
1:A:104:LEU:HD12	1:A:104:LEU:C	2.34	0.51
1:A:179:ARG:HH12	1:A:501:LEU:HD23	1.75	0.51
1:C:165:ASP:OD1	1:C:169:ASN:ND2	2.44	0.51
1:C:288:ASP:O	1:C:292:ARG:HG3	2.10	0.51
1:C:394:PHE:CE1	1:C:421:LEU:HD12	2.46	0.51
1:C:418:ARG:HD2	1:C:432:TYR:HE1	1.75	0.51
1:D:346:THR:HG23	1:D:373:THR:HG21	1.93	0.51
1:D:332:GLY:O	1:D:336:LYS:HB2	2.11	0.51
1:D:387:PRO:HA	1:D:425:THR:HG23	1.93	0.51
1:A:101:PHE:CE1	1:A:105:HIS:NE2	2.79	0.50
1:A:186:LEU:HD21	1:A:270:CYS:SG	2.51	0.50
1:B:67:LYS:NZ	1:B:77:TYR:OH	2.44	0.50
1:A:230:VAL:HG23	1:A:255:ARG:HG2	1.93	0.50
1:D:100:ALA:CB	1:D:103:ASN:OD1	2.59	0.50
1:D:471:GLU:OE1	1:C:143:HIS:NE2	2.44	0.50
1:B:77:TYR:HB2	1:B:88:VAL:CG2	2.39	0.50
1:A:335:GLU:HG3	1:D:123:SER:OG	2.11	0.50
1:A:434:GLU:HB2	1:A:477:THR:HG23	1.93	0.50
1:D:337:LEU:HD22	1:D:359:LEU:HD11	1.93	0.50
1:B:34:SER:CB	1:B:59:SER:H	2.24	0.50
1:C:418:ARG:HD2	1:C:432:TYR:CE1	2.47	0.50
1:D:201:PRO:HD3	1:C:503:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:MET:HE2	1:B:491:LEU:HD12	1.92	0.50
1:A:18:GLU:O	1:A:22:LYS:HG3	2.12	0.49
1:A:399:PRO:HD2	1:A:402:MET:SD	2.52	0.49
1:B:248:TYR:CE1	1:B:250:ILE:HG13	2.47	0.49
1:B:382:GLY:O	1:B:387:PRO:HD3	2.12	0.49
1:C:209:GLY:HA3	1:C:231:ALA:HB3	1.94	0.49
1:C:355:PHE:HA	1:C:376:LEU:HD13	1.94	0.49
1:A:110:ARG:NH2	1:A:145:LEU:O	2.46	0.49
1:C:430:ASN:O	2:C:601:LYS:HD2	2.12	0.49
1:A:163:TYR:O	1:A:167:ILE:HG13	2.13	0.49
1:C:276:TYR:N	1:C:476:PRO:O	2.42	0.49
1:A:403:SER:HB2	1:A:416:THR:HG21	1.94	0.49
1:A:52:ILE:HD11	1:A:94:PHE:CE2	2.46	0.49
1:D:77:TYR:HB2	1:D:88:VAL:HB	1.94	0.49
1:C:230:VAL:HG23	1:C:255:ARG:HG2	1.95	0.49
1:B:34:SER:N	1:B:59:SER:O	2.46	0.48
1:D:215:PHE:HB2	1:D:228:LEU:HB2	1.95	0.48
1:B:179:ARG:O	1:B:182:MET:HB3	2.14	0.48
1:C:234:LEU:O	1:C:238:MET:HG3	2.13	0.48
1:A:257:GLU:OE1	3:A:602:KRS:O2	2.13	0.48
1:C:387:PRO:HA	1:C:425:THR:OG1	2.13	0.48
1:C:441:GLN:OE1	1:C:441:GLN:HA	2.13	0.48
1:D:63:ARG:NH2	1:C:241:VAL:O	2.46	0.48
1:D:427:GLU:HG2	3:D:603:KRS:H19	1.95	0.48
1:B:418:ARG:HA	1:B:432:TYR:HB3	1.96	0.48
1:A:381:ILE:HG22	1:A:386:GLU:HG3	1.96	0.48
1:D:100:ALA:HB3	1:D:103:ASN:CG	2.39	0.48
1:D:289:MET:HE1	1:D:480:TRP:CZ2	2.48	0.48
1:D:444:ARG:HD3	1:D:444:ARG:HA	1.52	0.48
1:A:359:LEU:HD12	1:A:384:PHE:CZ	2.48	0.48
1:A:31:PHE:HB2	1:A:138:LEU:HD21	1.95	0.48
1:B:236:LEU:O	1:B:240:VAL:HG23	2.14	0.48
1:A:332:GLY:HA2	1:D:125:SER:HB3	1.96	0.48
1:B:280:GLU:HA	1:B:283:MET:HE2	1.95	0.48
1:B:400:GLN:HG3	1:B:416:THR:HG22	1.96	0.47
1:C:193:LEU:N	1:C:193:LEU:HD12	2.28	0.47
1:C:10:LYS:O	1:C:13:THR:HG23	2.14	0.47
1:C:399:PRO:HD2	1:C:402:MET:SD	2.54	0.47
1:A:209:GLY:HA3	1:A:231:ALA:HB3	1.95	0.47
1:A:409:HIS:HB3	1:A:412:ILE:O	2.13	0.47
1:B:37:LEU:HD22	1:B:81:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:GLU:HB2	3:C:602:KRS:O2	2.15	0.47
1:A:177:VAL:HA	1:B:196:LEU:HD11	1.95	0.47
1:D:238:MET:HE2	1:D:466:TYR:HD1	1.79	0.47
1:B:228:LEU:HD23	1:B:254:PHE:CD2	2.49	0.47
1:A:410:ARG:NH2	1:A:417:GLU:OE2	2.47	0.47
1:A:202:MET:HA	1:A:229:ARG:HB3	1.97	0.47
1:C:195:PHE:CD1	1:C:246:ARG:HB3	2.50	0.47
1:D:53:LEU:O	1:D:119:TYR:HB3	2.15	0.46
1:B:328:ASN:OD1	1:B:329:ILE:N	2.48	0.46
1:C:483:GLY:N	3:C:602:KRS:H17	2.30	0.46
1:A:279:TYR:CD1	1:A:417:GLU:HB3	2.50	0.46
1:A:344:ALA:HB3	1:A:414:GLY:HA3	1.97	0.46
1:A:424:VAL:O	1:A:425:THR:HG22	2.16	0.46
1:B:110:ARG:NH2	1:B:145:LEU:O	2.48	0.46
1:C:10:LYS:CA	1:C:13:THR:HG22	2.46	0.46
1:C:280:GLU:HA	1:C:283:MET:HE2	1.97	0.46
1:C:424:VAL:O	1:C:425:THR:HG22	2.16	0.46
1:A:443:LEU:HD12	1:A:443:LEU:N	2.30	0.46
1:C:353:ASN:C	1:C:353:ASN:ND2	2.73	0.46
1:A:274:MET:HE2	1:A:277:ALA:HB2	1.98	0.46
1:A:418:ARG:HH21	1:A:430:ASN:HD21	1.63	0.46
1:D:307:PRO:HD2	1:D:314:PRO:O	2.16	0.46
1:C:404:PRO:CG	1:C:444:ARG:NH2	2.78	0.46
1:A:125:SER:OG	1:D:332:GLY:HA2	2.16	0.46
1:B:261:GLN:O	1:B:497:ILE:N	2.42	0.46
1:B:53:LEU:O	1:B:119:TYR:HB3	2.16	0.46
1:D:356:PHE:HD2	1:D:380:LEU:HD11	1.80	0.45
1:B:233:GLU:OE1	1:B:432:TYR:OH	2.28	0.45
1:C:44:TYR:HB3	1:C:47:LEU:HD22	1.98	0.45
1:B:237:LYS:NZ	1:B:434:GLU:OE1	2.47	0.45
1:B:260:ASP:HB3	1:B:263:HIS:HB2	1.98	0.45
1:A:44:TYR:OH	1:A:56:ILE:HG21	2.16	0.45
1:D:31:PHE:CD2	1:D:136:ILE:HD11	2.51	0.45
1:D:186:LEU:HD21	1:D:270:CYS:SG	2.56	0.45
1:D:41:ILE:HD11	1:D:84:THR:HG21	1.98	0.45
1:A:22:LYS:HE3	1:A:22:LYS:HB3	1.79	0.45
1:C:485:ASP:OD2	1:C:501:LEU:HD21	2.17	0.45
1:B:172:VAL:O	1:B:175:ARG:HB3	2.16	0.45
1:B:193:LEU:O	1:B:246:ARG:NH1	2.50	0.45
1:C:37:LEU:HD12	1:C:81:GLY:HA3	1.99	0.45
1:C:428:ILE:C	3:C:602:KRS:H18	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:PHE:CD1	1:B:246:ARG:HB3	2.52	0.45
1:A:317:GLU:O	1:A:317:GLU:CG	2.64	0.45
1:A:354:LYS:HA	1:A:354:LYS:HD3	1.69	0.45
1:C:19:ARG:HH12	1:C:26:PRO:HA	1.82	0.45
1:B:234:LEU:O	1:B:238:MET:HG3	2.18	0.44
1:C:248:TYR:CE1	1:C:250:ILE:HG13	2.52	0.44
1:C:356:PHE:CD1	1:C:356:PHE:O	2.70	0.44
1:A:503:PHE:HB2	1:B:201:PRO:CG	2.47	0.44
1:C:187:ARG:HG2	1:C:248:TYR:OH	2.16	0.44
1:A:324:PHE:HB3	1:A:392:PRO:O	2.17	0.44
1:B:190:LEU:HD13	1:B:248:TYR:CE1	2.52	0.44
1:C:260:ASP:HB2	1:C:263:HIS:HB2	2.00	0.44
1:C:394:PHE:HE1	1:C:421:LEU:HD12	1.82	0.44
1:D:228:LEU:HD23	1:D:228:LEU:HA	1.83	0.44
1:A:195:PHE:CZ	1:A:274:MET:HG3	2.53	0.44
1:D:163:TYR:O	1:D:167:ILE:HG13	2.18	0.44
1:C:246:ARG:HG2	1:C:274:MET:HG3	1.99	0.44
1:C:389:PHE:CE1	1:C:393:THR:HG21	2.52	0.44
1:C:483:GLY:H	3:C:602:KRS:H17	1.82	0.44
1:B:73:LYS:HE2	1:B:91:ASN:OD1	2.18	0.44
1:B:208:GLY:HA2	1:B:209:GLY:HA2	1.71	0.44
1:C:41:ILE:HD12	1:C:84:THR:HG21	2.00	0.44
1:A:301:TYR:O	1:A:320:PHE:HB2	2.18	0.43
1:B:110:ARG:NH2	1:B:146:PRO:O	2.44	0.43
1:A:189:TYR:OH	1:A:288:ASP:OD2	2.33	0.43
1:D:165:ASP:OD1	1:D:169:ASN:ND2	2.51	0.43
1:D:337:LEU:HD11	1:D:380:LEU:HD13	2.00	0.43
1:B:345:ASP:CB	1:B:350:ASP:CG	2.91	0.43
1:B:264:ASN:N	3:B:602:KRS:H3	2.33	0.43
1:C:73:LYS:HE2	1:C:91:ASN:OD1	2.18	0.43
1:A:319:ASP:CG	1:A:321:THR:HG1	2.25	0.43
1:A:342:PRO:HD3	1:A:353:ASN:HD22	1.83	0.43
1:A:482:MET:HE3	1:A:484:ILE:HD13	2.01	0.43
1:B:207:ALA:HB2	1:B:227:TYR:CB	2.49	0.43
2:B:601:LYS:HB3	3:B:602:KRS:H16	2.00	0.43
1:D:31:PHE:HD2	1:D:136:ILE:HD11	1.83	0.43
1:D:279:TYR:CD1	1:D:417:GLU:HB3	2.54	0.43
1:D:329:ILE:HG23	1:D:381:ILE:HD11	2.01	0.43
1:B:279:TYR:CD1	1:B:417:GLU:HB3	2.53	0.43
1:C:79:LEU:O	1:C:85:ARG:HA	2.19	0.43
1:C:353:ASN:ND2	1:C:353:ASN:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:PRO:HA	1:B:422:PHE:O	2.19	0.43
1:D:65:PHE:HB2	1:D:80:HIS:CD2	2.53	0.43
1:D:399:PRO:HB2	1:D:401:ILE:HG12	2.01	0.43
1:B:89:LEU:O	1:B:132:PRO:HD2	2.19	0.43
1:D:328:ASN:OD1	1:D:329:ILE:N	2.52	0.42
1:D:339:ILE:HG12	1:D:340:GLN:N	2.34	0.42
1:D:339:ILE:HG12	1:D:340:GLN:H	1.83	0.42
1:B:207:ALA:HB2	1:B:227:TYR:HB3	2.00	0.42
1:A:195:PHE:HB3	1:A:248:TYR:CD2	2.52	0.42
1:A:112:ASP:OD2	1:A:137:GLN:NE2	2.52	0.42
1:A:253:VAL:HG12	1:A:267:PHE:O	2.19	0.42
1:A:339:ILE:HG21	1:A:356:PHE:HZ	1.85	0.42
1:D:179:ARG:HH12	1:D:501:LEU:HD23	1.84	0.42
1:C:15:LEU:HD23	1:C:15:LEU:HA	1.79	0.42
1:C:233:GLU:HG3	1:C:273:TYR:OH	2.19	0.42
1:C:169:ASN:O	1:C:172:VAL:HG22	2.20	0.42
1:B:185:PHE:HA	1:B:188:ARG:HG2	2.01	0.42
1:C:213:LYS:HE2	1:C:256:ASN:O	2.20	0.42
1:A:337:LEU:O	1:D:70:SER:OG	2.26	0.42
1:D:329:ILE:HD12	1:D:381:ILE:CD1	2.50	0.42
1:D:343:PRO:O	1:D:345:ASP:N	2.52	0.42
1:B:394:PHE:CE1	1:B:421:LEU:HD12	2.55	0.42
1:A:195:PHE:CD2	1:A:246:ARG:HB3	2.55	0.42
1:B:189:TYR:OH	1:B:288:ASP:OD2	2.37	0.42
1:B:238:MET:HE2	1:B:466:TYR:HA	2.02	0.42
1:C:59:SER:HA	1:C:116:VAL:O	2.19	0.42
1:A:394:PHE:CD1	1:A:421:LEU:HD13	2.54	0.41
1:D:389:PHE:CE1	1:D:393:THR:HG21	2.55	0.41
1:B:164:LEU:HD12	1:B:164:LEU:HA	1.83	0.41
1:D:34:SER:CB	1:D:59:SER:H	2.33	0.41
1:B:216:ILE:HD12	1:B:226:LEU:O	2.20	0.41
1:C:389:PHE:CD1	1:C:393:THR:HG21	2.55	0.41
1:A:355:PHE:HE1	1:A:371:ARG:HD3	1.85	0.41
1:B:74:LEU:HD23	1:B:76:PHE:CZ	2.55	0.41
1:C:395:LEU:O	1:C:419:PHE:HA	2.20	0.41
1:A:139:THR:HG21	1:B:474:LEU:H	1.84	0.41
1:D:277:ALA:O	1:D:478:ALA:HB2	2.21	0.41
1:D:337:LEU:HD12	1:D:341:PHE:CZ	2.56	0.41
1:D:418:ARG:CA	1:D:432:TYR:HB3	2.47	0.41
1:C:377:LEU:HD13	1:C:399:PRO:HG2	2.03	0.41
1:B:175:ARG:HG3	1:B:492:THR:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:THR:HB	1:D:201:PRO:HD2	2.03	0.41
1:B:324:PHE:HB2	1:B:394:PHE:CE2	2.55	0.41
1:B:400:GLN:HG3	1:B:416:THR:CG2	2.51	0.41
1:C:178:THR:O	1:C:182:MET:N	2.50	0.41
1:A:17:ASN:O	1:A:20:ARG:HB3	2.20	0.41
1:A:337:LEU:HD21	1:A:384:PHE:CD2	2.56	0.41
1:D:268:THR:HG21	1:C:199:GLU:OE2	2.21	0.41
1:B:147:HIS:C	1:B:149:HIS:H	2.29	0.41
1:B:412:ILE:HG21	1:B:415:LEU:HD13	2.03	0.41
1:D:45:ASN:OD1	1:D:46:SER:N	2.54	0.41
1:D:143:HIS:NE2	1:C:471:GLU:OE1	2.54	0.41
1:D:312:GLU:HB3	1:D:313:ASN:H	1.74	0.41
1:B:36:SER:O	1:B:40:PHE:N	2.49	0.41
1:B:163:TYR:O	1:B:167:ILE:HG13	2.21	0.41
1:C:65:PHE:HB2	1:C:80:HIS:CD2	2.56	0.41
1:C:382:GLY:O	1:C:387:PRO:HD3	2.20	0.41
1:B:193:LEU:HD23	1:B:193:LEU:HA	1.91	0.41
1:A:232:PRO:O	1:A:236:LEU:HG	2.22	0.40
1:D:29:HIS:HE1	1:C:408:TRP:O	2.04	0.40
1:D:96:SER:CB	1:D:133:TYR:HB2	2.51	0.40
1:B:197:GLU:HA	1:B:248:TYR:O	2.21	0.40
1:B:389:PHE:O	1:B:425:THR:N	2.51	0.40
1:A:89:LEU:O	1:A:132:PRO:HD2	2.21	0.40
1:A:297:MET:SD	1:A:491:LEU:HD13	2.61	0.40
1:B:110:ARG:HH22	1:B:146:PRO:C	2.28	0.40
1:C:238:MET:HE2	1:C:466:TYR:HD1	1.84	0.40
1:B:59:SER:HA	1:B:116:VAL:O	2.21	0.40
1:D:356:PHE:CD2	1:D:380:LEU:HD11	2.56	0.40
1:C:182:MET:HE1	1:C:488:ALA:HB2	2.04	0.40
1:D:110:ARG:NH1	1:D:145:LEU:HB2	2.36	0.40
1:B:385:LEU:HD23	1:B:385:LEU:HA	1.85	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:SER:CB	1:C:70:SER:OG[2_455]	1.98	0.22
1:B:95:HIS:O	1:C:336:LYS:NZ[2_455]	2.18	0.02

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	455/524 (87%)	441 (97%)	14 (3%)	0	100	100
1	B	474/524 (90%)	453 (96%)	20 (4%)	1 (0%)	43	71
1	C	463/524 (88%)	442 (96%)	21 (4%)	0	100	100
1	D	460/524 (88%)	438 (95%)	21 (5%)	1 (0%)	43	71
All	All	1852/2096 (88%)	1774 (96%)	76 (4%)	2 (0%)	48	76

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	314	PRO
1	B	310	ILE

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	346/459 (75%)	346 (100%)	0	100	100
1	B	345/459 (75%)	345 (100%)	0	100	100
1	C	340/459 (74%)	340 (100%)	0	100	100
1	D	363/459 (79%)	363 (100%)	0	100	100
All	All	1394/1836 (76%)	1394 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	218	HIS
1	A	430	ASN
1	D	95	HIS
1	D	137	GLN
1	D	220	ASN
1	B	117	ASN
1	B	263	HIS
1	C	80	HIS
1	C	174	ASN
1	C	353	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](#)

9 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	$\# Z > 2$
3	KRS	C	602	-	23,23,23	1.69	6 (26%)	33,33,33	1.69	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	D	601	-	5,5,5	0.38	0	5,5,5	0.37	0
2	LYS	C	601	-	8,9,9	0.84	1 (12%)	7,10,10	0.97	1 (14%)
3	KRS	A	602	-	23,23,23	1.72	6 (26%)	33,33,33	1.49	6 (18%)
2	LYS	A	601	-	8,9,9	0.83	1 (12%)	7,10,10	1.10	1 (14%)
3	KRS	B	602	-	23,23,23	1.73	6 (26%)	33,33,33	1.47	6 (18%)
2	LYS	B	601	-	8,9,9	0.85	1 (12%)	7,10,10	1.04	1 (14%)
2	LYS	D	602	-	8,9,9	0.84	1 (12%)	7,10,10	1.07	1 (14%)
3	KRS	D	603	-	23,23,23	1.75	7 (30%)	33,33,33	1.45	7 (21%)

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
3	KRS	C	602	-	-	4/4/26/26	0/3/3/3
4	GOL	D	601	-	-	2/4/4/4	-
2	LYS	C	601	-	-	4/9/9/9	-
3	KRS	A	602	-	-	0/4/26/26	0/3/3/3
2	LYS	A	601	-	-	4/9/9/9	-
3	KRS	B	602	-	-	0/4/26/26	0/3/3/3
2	LYS	B	601	-	-	2/9/9/9	-
2	LYS	D	602	-	-	2/9/9/9	-
3	KRS	D	603	-	-	0/4/26/26	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	KRS	C6-C5	4.03	1.59	1.51
3	D	603	KRS	C6-C5	4.02	1.59	1.51
3	B	602	KRS	C6-C5	3.96	1.59	1.51
3	C	602	KRS	C6-C5	3.84	1.58	1.51
3	B	602	KRS	C14-C15	-3.73	1.43	1.53
3	A	602	KRS	C14-C15	-3.72	1.43	1.53
3	D	603	KRS	C14-C15	-3.71	1.43	1.53
3	C	602	KRS	C14-C15	-3.67	1.44	1.53
3	B	602	KRS	O2-C3	3.30	1.44	1.37
3	D	603	KRS	O2-C3	3.24	1.44	1.37
3	A	602	KRS	O2-C3	3.20	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	KRS	O2-C3	3.10	1.43	1.37
3	B	602	KRS	O3-C7	-2.81	1.40	1.46
3	A	602	KRS	O3-C7	-2.81	1.40	1.46
3	D	603	KRS	O3-C7	-2.80	1.40	1.46
3	C	602	KRS	O3-C7	-2.76	1.40	1.46
3	D	603	KRS	C14-C13	-2.75	1.46	1.53
3	C	602	KRS	C14-C13	-2.69	1.46	1.53
3	B	602	KRS	C14-C13	-2.67	1.46	1.53
3	A	602	KRS	C14-C13	-2.65	1.46	1.53
3	B	602	KRS	O3-C8	2.26	1.38	1.34
2	C	601	LYS	OXT-C	-2.26	1.23	1.30
2	D	602	LYS	OXT-C	-2.25	1.23	1.30
2	B	601	LYS	OXT-C	-2.24	1.23	1.30
2	A	601	LYS	OXT-C	-2.23	1.23	1.30
3	C	602	KRS	O3-C8	2.18	1.38	1.34
3	D	603	KRS	O3-C8	2.17	1.38	1.34
3	A	602	KRS	O3-C8	2.05	1.38	1.34
3	D	603	KRS	C4-C3	2.02	1.42	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	KRS	C11-C10-C7	-4.16	108.14	114.43
3	C	602	KRS	C11-C10-C7	-3.77	108.73	114.43
3	B	602	KRS	O5-C12-C13	3.50	112.56	109.91
3	C	602	KRS	C10-C7-C6	-3.38	107.09	113.44
3	D	603	KRS	O5-C11-C15	3.27	113.35	109.91
3	C	602	KRS	C14-C13-C12	3.26	113.22	111.00
3	D	603	KRS	O3-C8-O4	3.24	121.08	117.53
3	C	602	KRS	O3-C8-O4	3.22	121.06	117.53
3	A	602	KRS	O3-C8-O4	3.13	120.96	117.53
3	B	602	KRS	O3-C8-O4	3.05	120.88	117.53
3	D	603	KRS	C11-C10-C7	-2.83	110.16	114.43
3	C	602	KRS	O5-C12-C13	2.80	112.03	109.91
3	A	602	KRS	O5-C11-C15	2.80	112.85	109.91
3	A	602	KRS	O5-C12-C13	2.72	111.97	109.91
2	A	601	LYS	OXT-C-O	-2.72	117.91	124.08
3	D	603	KRS	O5-C12-C13	2.72	111.97	109.91
3	B	602	KRS	C10-C7-C6	-2.70	108.36	113.44
3	B	602	KRS	C11-C10-C7	-2.70	110.36	114.43
3	B	602	KRS	O5-C11-C15	2.69	112.74	109.91
3	C	602	KRS	O5-C11-C15	2.67	112.72	109.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	LYS	OXT-C-O	-2.65	118.08	124.08
2	D	602	LYS	OXT-C-O	-2.62	118.14	124.08
3	C	602	KRS	C10-C11-C15	-2.57	108.02	113.75
3	B	602	KRS	C10-C11-C15	-2.56	108.04	113.75
3	A	602	KRS	C10-C11-C15	-2.48	108.22	113.75
2	C	601	LYS	OXT-C-O	-2.45	118.53	124.08
3	C	602	KRS	O3-C7-C6	2.43	113.16	110.16
3	D	603	KRS	C10-C7-C6	-2.38	108.95	113.44
3	A	602	KRS	C10-C7-C6	-2.23	109.24	113.44
3	D	603	KRS	C10-C11-C15	-2.23	108.79	113.75
3	D	603	KRS	O3-C7-C10	2.04	109.32	106.10

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	LYS	O-C-CA-N
2	D	602	LYS	C-CA-CB-CG
2	B	601	LYS	O-C-CA-N
3	C	602	KRS	C11-C10-C7-O3
3	C	602	KRS	C11-C10-C7-C6
4	D	601	GOL	C1-C2-C3-O3
2	B	601	LYS	OXT-C-CA-N
2	A	601	LYS	OXT-C-CA-N
3	C	602	KRS	C7-C10-C11-O5
2	C	601	LYS	OXT-C-CA-N
2	C	601	LYS	CG-CD-CE-NZ
4	D	601	GOL	O2-C2-C3-O3
2	D	602	LYS	OXT-C-CA-N
3	C	602	KRS	C7-C10-C11-C15
2	C	601	LYS	O-C-CA-N
2	A	601	LYS	OXT-C-CA-CB
2	A	601	LYS	O-C-CA-CB
2	C	601	LYS	CA-CB-CG-CD

There are no ring outliers.

6 monomers are involved in 13 short contacts:

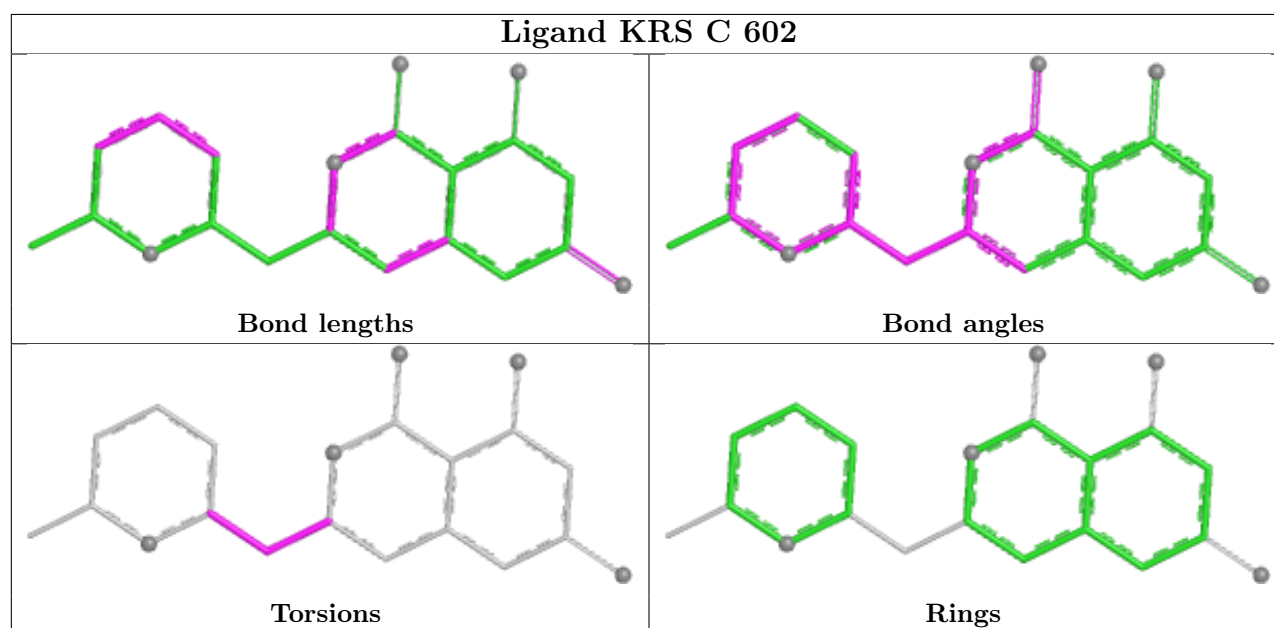
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	KRS	5	0
2	C	601	LYS	2	0

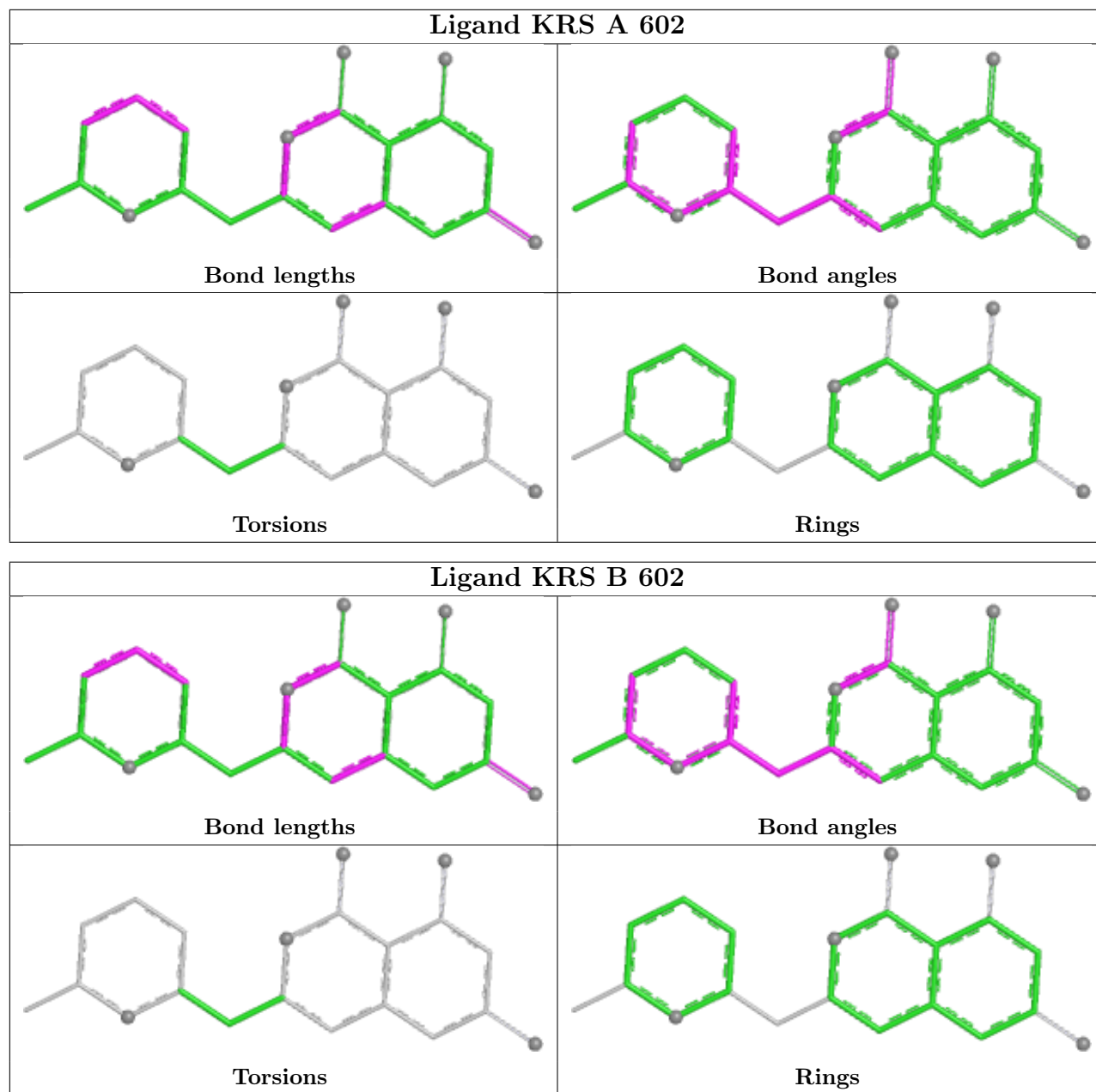
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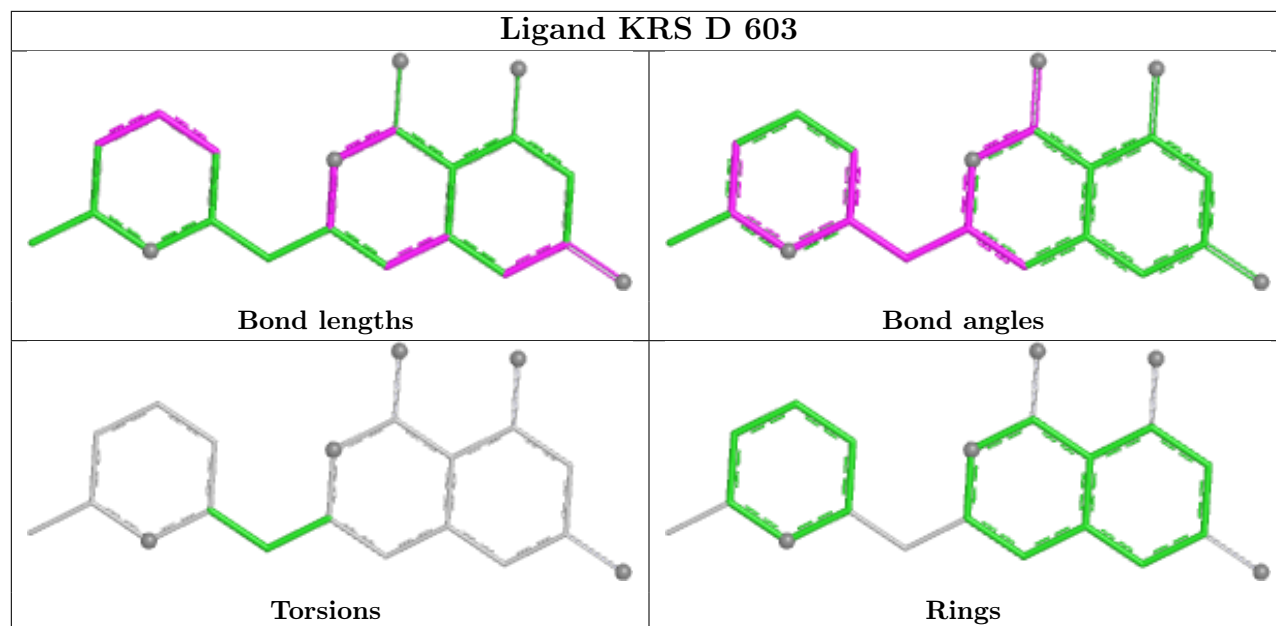
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	KRS	1	0
3	B	602	KRS	4	0
2	B	601	LYS	1	0
3	D	603	KRS	1	0

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	465/524 (88%)	0.72	33 (7%)	22	16	22, 39, 71, 100	0
1	B	482/524 (91%)	0.88	48 (9%)	12	10	23, 43, 74, 103	0
1	C	473/524 (90%)	0.80	37 (7%)	19	15	27, 39, 68, 86	0
1	D	470/524 (89%)	0.87	43 (9%)	15	12	25, 38, 70, 97	0
All	All	1890/2096 (90%)	0.82	161 (8%)	16	13	22, 40, 71, 103	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	209	GLY	8.3
1	D	211	THR	6.0
1	D	208	GLY	5.4
1	B	25	ASN	5.4
1	D	210	ALA	4.9
1	D	207	ALA	4.3
1	A	358	LYS	4.2
1	B	359	LEU	4.1
1	D	309	GLY	4.1
1	C	98	ASP	4.0
1	B	358	LYS	4.0
1	B	506	MET	3.8
1	C	154	ASN	3.7
1	C	436	ASN	3.7
1	B	490	ILE	3.7
1	A	310	ILE	3.7
1	A	350	ASP	3.7
1	D	363	ASN	3.6
1	B	361	VAL	3.5
1	D	358	LYS	3.5
1	B	297	MET	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	447	GLU	3.4
1	B	300	THR	3.3
1	D	308	ASN	3.3
1	A	207	ALA	3.3
1	A	348	ASP	3.3
1	B	446	ASP	3.2
1	C	247	VAL	3.2
1	D	493	ASP	3.2
1	B	209	GLY	3.1
1	C	82	GLU	3.1
1	B	443	LEU	3.1
1	A	309	GLY	3.1
1	D	445	PHE	3.1
1	B	208	GLY	3.0
1	D	310	ILE	3.0
1	D	313	ASN	3.0
1	A	231	ALA	2.9
1	A	347	LEU	2.9
1	A	100	ALA	2.9
1	D	311	VAL	2.9
1	C	151	GLY	2.9
1	A	505	ALA	2.9
1	B	344	ALA	2.9
1	C	148	THR	2.9
1	C	317	GLU	2.9
1	D	62	GLY	2.9
1	B	357	ASP	2.8
1	C	345	ASP	2.8
1	B	445	PHE	2.8
1	D	233	GLU	2.8
1	B	210	ALA	2.8
1	D	214	PRO	2.8
1	A	427	GLU	2.7
1	C	73	LYS	2.7
1	B	223	ASP	2.7
1	A	300	THR	2.7
1	D	357	ASP	2.7
1	C	245	ASP	2.7
1	B	339	ILE	2.6
1	D	249	GLU	2.6
1	B	247	VAL	2.6
1	B	171	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	35	ILE	2.6
1	D	148	THR	2.6
1	B	205	LEU	2.6
1	B	98	ASP	2.6
1	D	414	GLY	2.6
1	D	96	SER	2.5
1	D	6	GLN	2.5
1	D	155	GLN	2.5
1	B	312	GLU	2.5
1	B	317	GLU	2.5
1	A	370	PRO	2.5
1	B	343	PRO	2.5
1	A	299	GLY	2.5
1	B	159	TYR	2.5
1	B	386	GLU	2.5
1	A	345	ASP	2.5
1	A	436	ASN	2.5
1	C	357	ASP	2.5
1	A	330	TYR	2.5
1	C	439	LEU	2.5
1	A	357	ASP	2.5
1	D	54	ASN	2.5
1	B	231	ALA	2.4
1	B	360	ALA	2.4
1	B	96	SER	2.4
1	C	380	LEU	2.4
1	B	362	GLU	2.4
1	D	446	ASP	2.4
1	C	354	LYS	2.4
1	B	485	ASP	2.4
1	C	97	GLY	2.4
1	C	445	PHE	2.4
1	C	443	LEU	2.4
1	C	169	ASN	2.4
1	A	82	GLU	2.4
1	A	287	GLU	2.3
1	A	258	GLY	2.3
1	B	425	THR	2.3
1	B	493	ASP	2.3
1	D	280	GLU	2.3
1	D	314	PRO	2.3
1	C	71	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	440	THR	2.3
1	C	146	PRO	2.3
1	C	72	GLY	2.3
1	D	196	LEU	2.3
1	A	445	PHE	2.3
1	C	159	TYR	2.3
1	A	234	LEU	2.2
1	B	245	ASP	2.2
1	B	224	MET	2.2
1	D	428	ILE	2.2
1	C	432	TYR	2.2
1	D	464	GLU	2.2
1	D	487	LEU	2.2
1	C	83	GLY	2.2
1	A	221	ASP	2.2
1	C	426	LYS	2.2
1	C	446	ASP	2.2
1	C	485	ASP	2.2
1	B	90	ALA	2.2
1	C	499	GLU	2.2
1	B	80	HIS	2.2
1	A	84	THR	2.1
1	A	96	SER	2.1
1	B	213	LYS	2.1
1	B	275	ALA	2.1
1	A	413	PRO	2.1
1	C	355	PHE	2.1
1	D	55	ASP	2.1
1	B	102	ASP	2.1
1	A	349	THR	2.1
1	B	15	LEU	2.1
1	B	182	MET	2.1
1	A	242	GLY	2.1
1	D	485	ASP	2.1
1	B	463	ASP	2.1
1	C	166	LEU	2.1
1	B	442	ARG	2.1
1	D	58	GLN	2.1
1	D	499	GLU	2.1
1	D	355	PHE	2.1
1	A	311	VAL	2.1
1	C	33	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	320	PHE	2.1
1	D	61	ALA	2.1
1	B	14	ALA	2.1
1	C	277	ALA	2.1
1	A	156	GLU	2.1
1	D	156	GLU	2.1
1	D	230	VAL	2.0
1	A	270	CYS	2.0
1	C	275	ALA	2.0
1	D	193	LEU	2.0
1	B	444	ARG	2.0
1	D	369	ALA	2.0
1	C	157	THR	2.0
1	C	493	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](#)

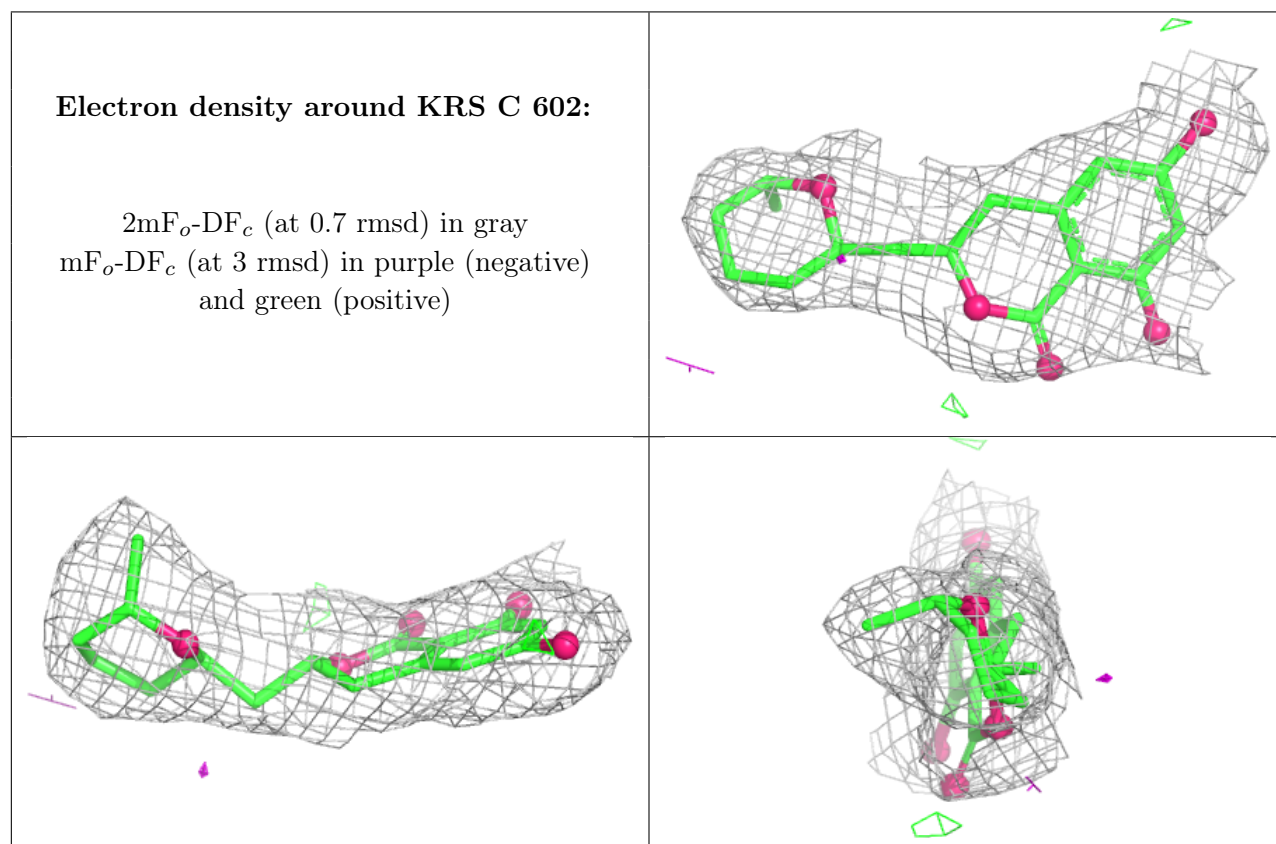
There are no oligosaccharides in this entry.

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.

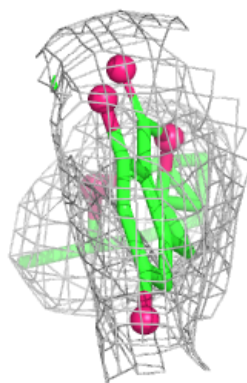
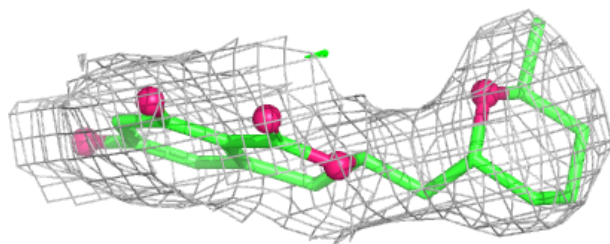
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LYS	C	601	10/10	0.81	0.23	44,53,60,62	0
2	LYS	D	602	10/10	0.82	0.21	30,51,66,72	0
3	KRS	C	602	21/21	0.85	0.16	19,30,41,43	0
2	LYS	A	601	10/10	0.87	0.14	25,30,46,48	0
2	LYS	B	601	10/10	0.88	0.18	34,37,44,44	0
4	GOL	D	601	6/6	0.89	0.10	38,40,41,46	0
3	KRS	A	602	21/21	0.92	0.12	10,19,37,44	0
3	KRS	D	603	21/21	0.92	0.11	11,22,29,33	0
3	KRS	B	602	21/21	0.93	0.10	23,29,34,43	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.

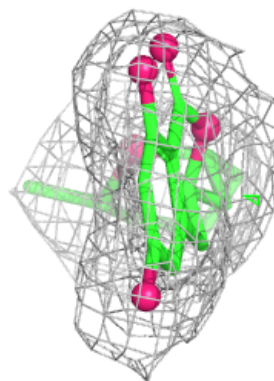
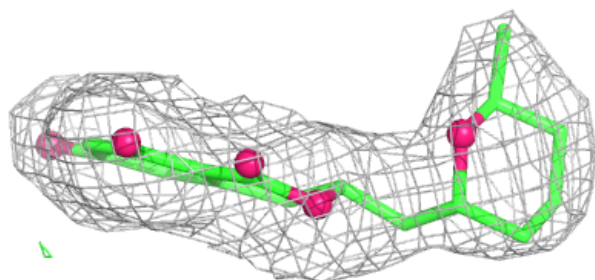
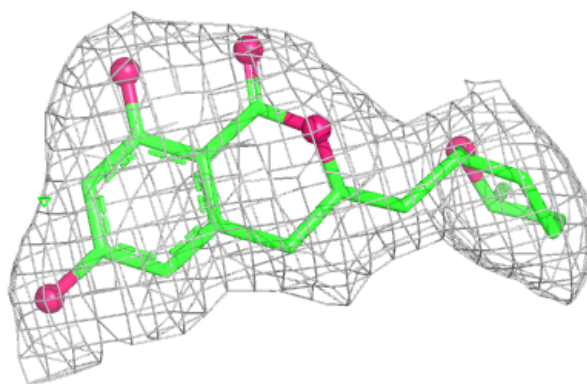


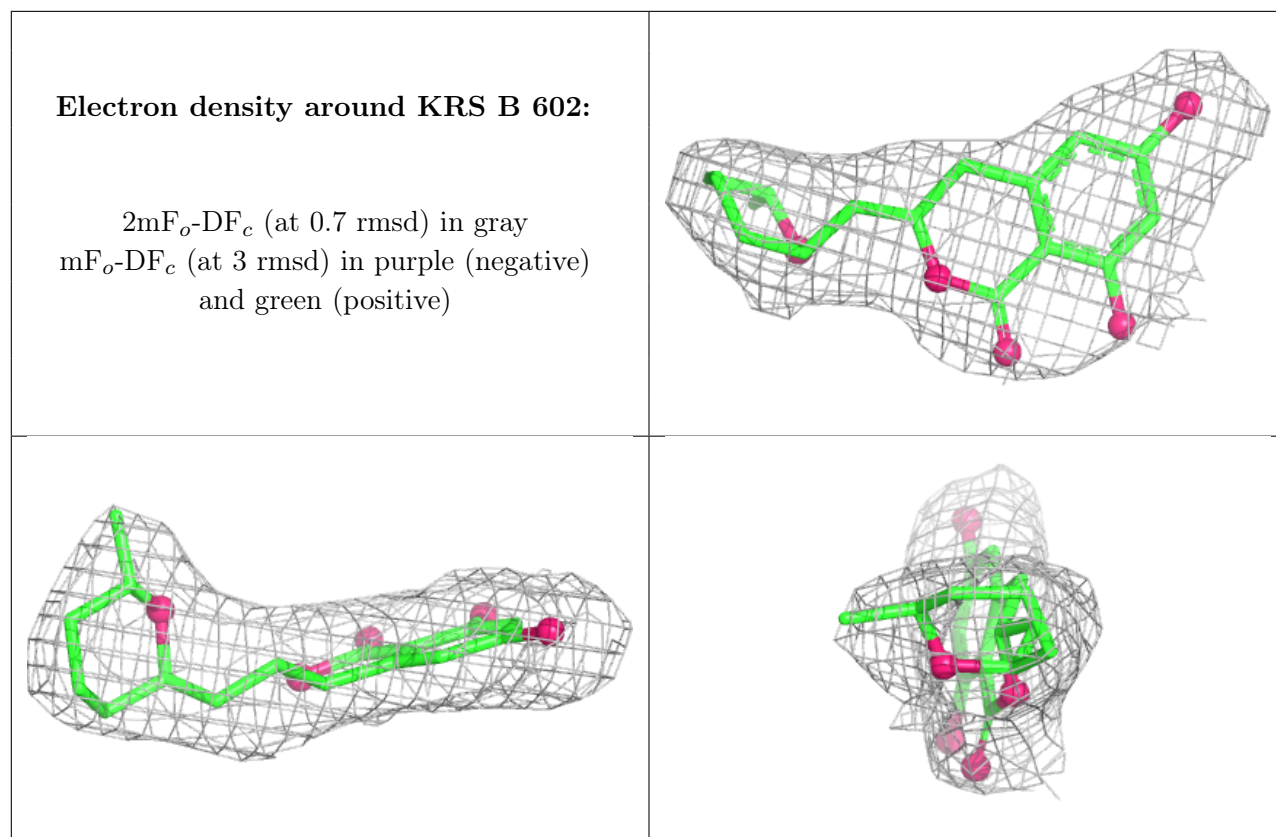
Electron density around KRS A 602:

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

**Electron density around KRS D 603:**

$2mF_o-DF_c$ (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.