Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 10:35 AM EDT

PDB ID	:	4YCW
Title	:	Crystal structure of cladosporin in complex with plasmodium like human lysyl-tRNA synthetase mutant
Authors	:	Fang, P.; Wang, J.; Guo, M.
Deposited on	:	2015-02-20
Resolution	:	2.90 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.90 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.

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
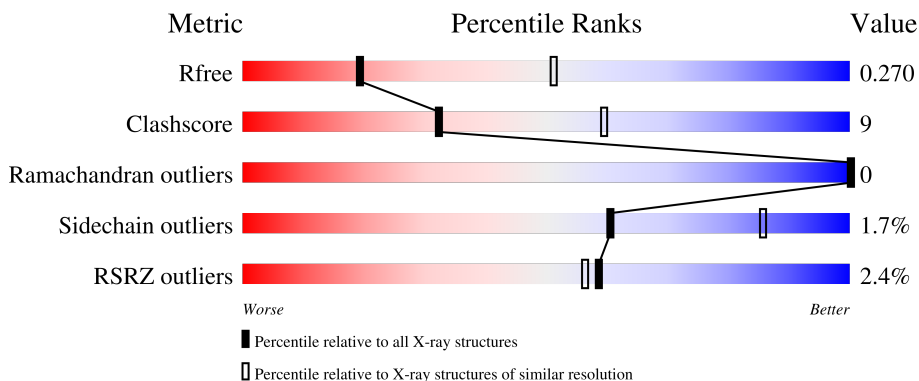
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 <=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	513	85% 12% ·
1	B	513	% 81% 16% ·
1	E	513	4% 75% 21% · ·
1	F	513	4% 74% 21% · ·
2	C	42	17% 5% 79%

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Mol	Chain	Length	Quality of chain
2	D	42	17% 5% 79%
2	G	42	2% 21% 79%
2	H	42	12% 10% 79%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 16000 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	501	Total	C	N	O	S	0	0	0
			3998	2563	669	738	28			
1	B	501	Total	C	N	O	S	0	0	0
			3976	2547	673	728	28			
1	E	499	Total	C	N	O	S	0	0	0
			3776	2400	655	696	25			
1	F	498	Total	C	N	O	S	0	0	0
			3811	2429	650	705	27			

There are 16 discrepancies between the modelled and reference sequences:

| Chain	Residue	Modelled	Actual	Comment	Reference
A	69	MET	-	initiating methionine	UNP Q15046
A	300	THR	PRO	conflict	UNP Q15046
A	321	VAL	GLN	conflict	UNP Q15046
A	337	SER	THR	conflict	UNP Q15046
B	69	MET	-	initiating methionine	UNP Q15046
B	300	THR	PRO	conflict	UNP Q15046
B	321	VAL	GLN	conflict	UNP Q15046
B	337	SER	THR	conflict	UNP Q15046
E	69	MET	-	initiating methionine	UNP Q15046
E	300	THR	PRO	conflict	UNP Q15046
E	321	VAL	GLN	conflict	UNP Q15046
E	337	SER	THR	conflict	UNP Q15046
F	69	MET	-	initiating methionine	UNP Q15046
F	300	THR	PRO	conflict	UNP Q15046
F	321	VAL	GLN	conflict	UNP Q15046
F	337	SER	THR	conflict	UNP Q15046

- Molecule 2 is a protein called Aminoacyl tRNA synthase complex-interacting multifunctional protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	S	0	0	0
			78	53	12	12	1			
2	D	9	Total	C	N	O	S	0	0	0
			78	53	12	12	1			
2	G	9	Total	C	N	O	S	0	0	0
			78	53	12	12	1			
2	H	9	Total	C	N	O	S	0	0	0
			76	51	12	12	1			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	37	HIS	-	expression tag	UNP Q13155
C	38	HIS	-	expression tag	UNP Q13155
C	39	HIS	-	expression tag	UNP Q13155
C	40	HIS	-	expression tag	UNP Q13155
C	41	HIS	-	expression tag	UNP Q13155
C	42	HIS	-	expression tag	UNP Q13155
D	37	HIS	-	expression tag	UNP Q13155
D	38	HIS	-	expression tag	UNP Q13155
D	39	HIS	-	expression tag	UNP Q13155
D	40	HIS	-	expression tag	UNP Q13155
D	41	HIS	-	expression tag	UNP Q13155
D	42	HIS	-	expression tag	UNP Q13155
G	37	HIS	-	expression tag	UNP Q13155
G	38	HIS	-	expression tag	UNP Q13155
G	39	HIS	-	expression tag	UNP Q13155
G	40	HIS	-	expression tag	UNP Q13155
G	41	HIS	-	expression tag	UNP Q13155
G	42	HIS	-	expression tag	UNP Q13155
H	37	HIS	-	expression tag	UNP Q13155
H	38	HIS	-	expression tag	UNP Q13155
H	39	HIS	-	expression tag	UNP Q13155
H	40	HIS	-	expression tag	UNP Q13155
H	41	HIS	-	expression tag	UNP Q13155
H	42	HIS	-	expression tag	UNP Q13155

- Molecule 3 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).
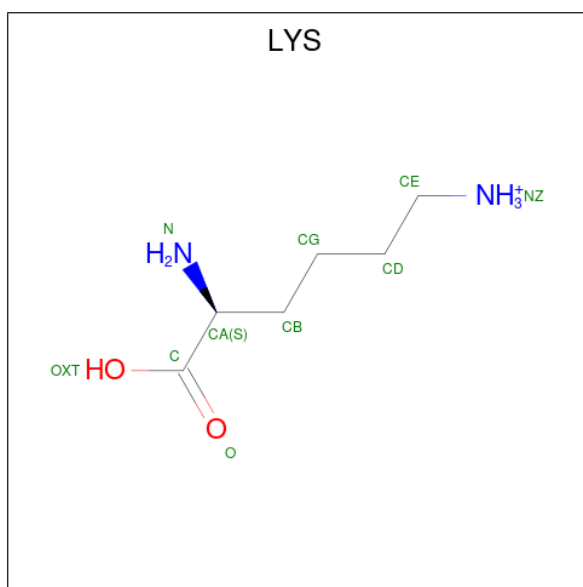
LYS

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 9	C 6	N 2	O 1	0	0
3	B	1	Total 9	C 6	N 2	O 1	0	0
3	E	1	Total 9	C 6	N 2	O 1	0	0
3	F	1	Total 9	C 6	N 2	O 1	0	0

- Molecule 4 is cladosporin (three-letter code: KRS) (formula: $C_{16}H_{20}O_5$).

KRS
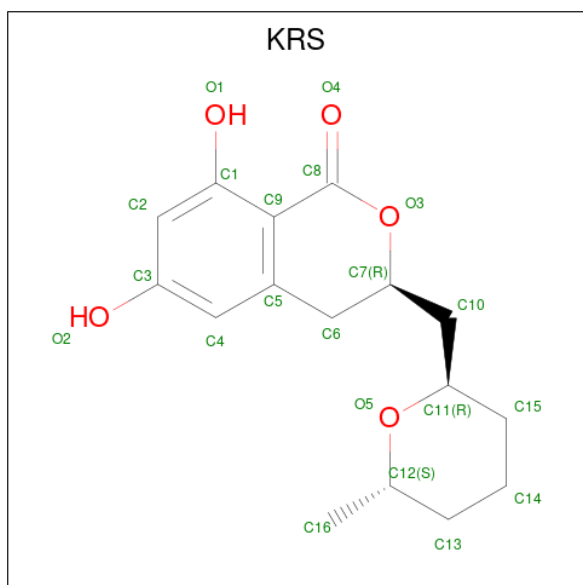
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 21	C 16	O 5	0	0
4	B	1	Total 21	C 16	O 5	0	0
4	E	1	Total 21	C 16	O 5	0	0
4	F	1	Total 21	C 16	O 5	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0
5	B	3	Total 3	O 3	0	0
5	E	2	Total 2	O 2	0	0
5	F	1	Total 1	O 1	0	0

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 geomet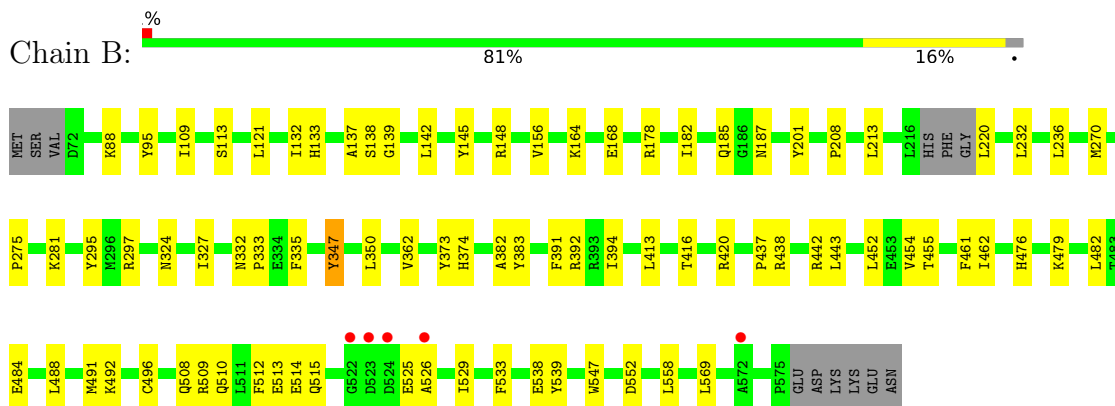ric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
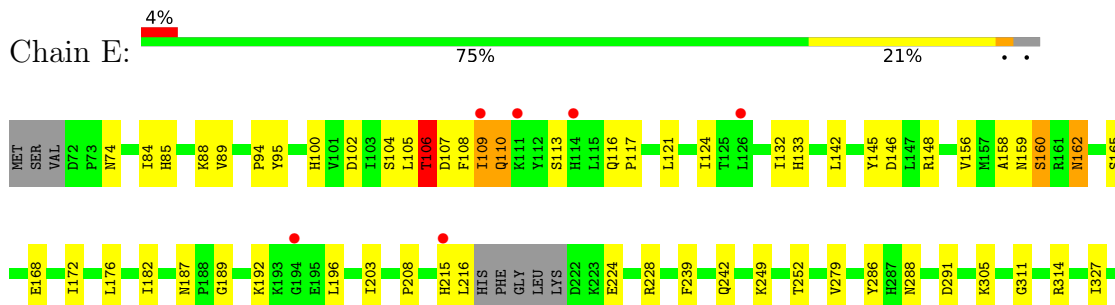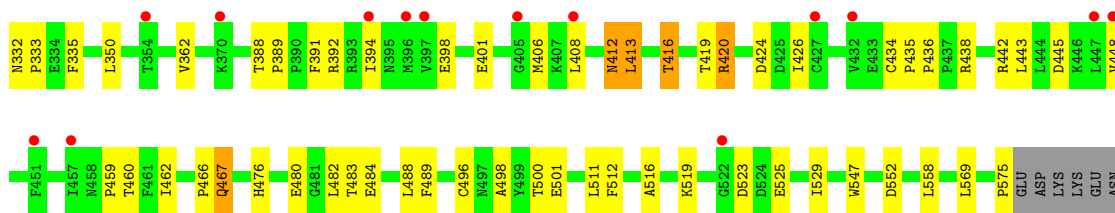
• Molecule 1: Lysine–tRNA ligase

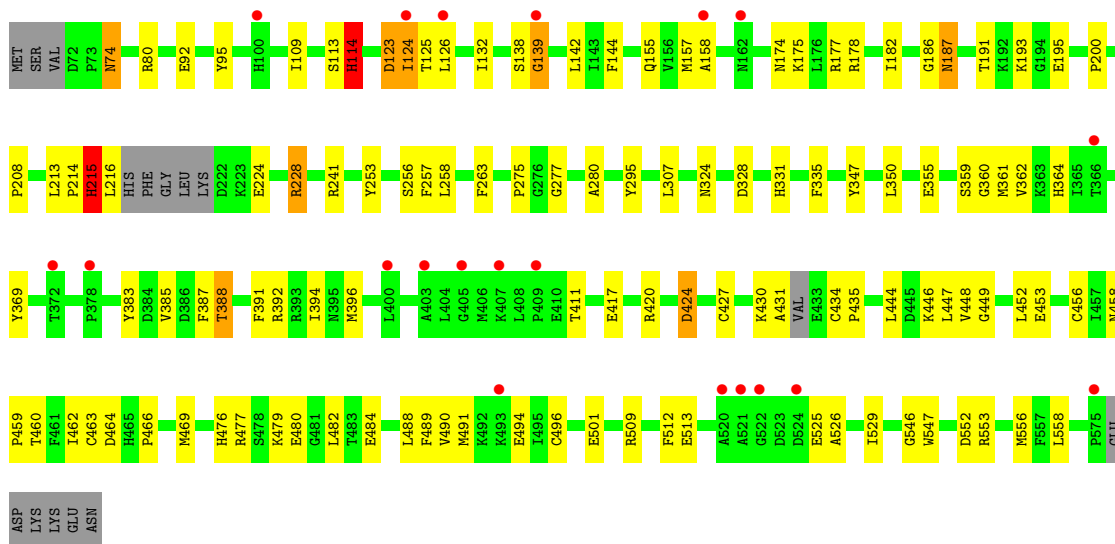Chain A:

• Molecule 1: Lysine–tRNA ligase

Chain B:

• Molecule 1: Lysine–tRNA ligase

Chain E:

N332 P333 E334 F335 L350 T354 V362 K370 T388 P389 P390 F391 R392 R393 I394 N395 M396 V397 E398 E401 G405 M406 K407 L408 N412 L413 T416 T419 R420 D424 D425 I426 C427 V432 E433 C434 P435 P436 P437 R438 R442 L443 L444 D445 K446 L447 V448

F451 I457 N458 P459 T460 F461 I462 P466 Q467 H476 E480 G481 L482 T483 E484 L488 F489 C496 N497 A498 Y499 T500 E501 L511 F512 A516 K519 G522 D523 D524 E525 I529 W547 D552 L558 L569 P575 GLU ASP LYS LYS GLU ASN

• Molecule 1: Lysine–tRNA ligase

Chain F:

MET SER VAL D72 P73 N74 R80 E92 Y95 H100 I109 S113 H114 D123 I124 T125 L126 I132 S138 G139 L142 F143 F144 Q155 V156 M157 A158 N162 N174 K175 L176 R177 R178 I182 G186 N187 T191 K192 K193 G194 E195 P200

P208 L213 P214 H215 I216 HIS PHE GLY LEU LYS D222 K223 E224 R228 R241 Y253 S256 F257 L258 F263 P275 G276 G277 A280 Y295 L307 N324 D328 H331 F335 Y347 L350 E355 S359 G360 V362 K363 H364 T365 T366

Y369 T372 P378 Y383 D384 V385 D386 F387 T388 F391 R392 R393 I394 N395 M396 L400 A403 L404 G405 M406 K407 L408 P409 E410 T411 E417 R420 D424 C427 K430 A431 VAL E433 E434 P435 L444 D445 K446 L447 V448 G449 L452 E453 C456 I457 N458

P459 T460 F461 I462 C463 D464 H465 P466 M469 H476 R477 S478 K479 E480 G481 L482 T483 E484 L488 F489 V490 M491 K492 K493 E494 I495 C496 E501 R509 F512 E513 A520 A521 G522 D523 D524 E525 A526 I529 G546 W547 D552 R553 M556 F557 L558 P575 GLU

ASP LYS LYS GLU ASN

• Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2

Chain C:

MET P2 K7 P8 Y9 H10 GLY GLY GLY ALA PRO LEU ARG VAL GLU LEU PRO THR CYS MET TYR ARG LEU PRO ASN VAL HIS GLY ARG SER TYR GLY HIS HIS HIS HIS HIS HIS

• Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2

Chain D:

MET P2 K7 P8 Y9 H10 GLY GLY GLY ALA PRO LEU ARG VAL GLU LEU PRO THR CYS MET TYR ARG LEU PRO ASN VAL HIS GLY ARG SER TYR GLY HIS HIS HIS HIS HIS HIS

• Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2

Chain G:

MET P2 K7 H10 GLY GLY GLY ALA PRO LEU ARG VAL GLU LEU PRO THR CYS MET TYR ARG LEU PRO ASN VAL HIS GLY ARG SER TYR GLY HIS HIS HIS HIS HIS HIS

• Molecule 2: Aminoacyl tRNA synthase complex-interacting multifunctional protein 2

Chain H:

12% 10% 79%

MET P2 M3 Y4 Q5 P8 Y9 H10 GLY GLY GLY ALA PRO LEU ARG VAL GLU LEU PRO THR CYS MET TYR ARG LEU PRO ASN VAL HIS GLY ARG SER TYR GLY HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	51.28Å 75.56Å 162.99Å 90.80° 99.09° 109.83°	Depositor
Resolution (Å)	35.45 – 2.90 35.45 – 2.89	Depositor EDS
% Data completeness (in resolution range)	88.7 (35.45-2.90) 88.8 (35.45-2.89)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.90Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.268 0.226 , 0.270	Depositor DCC
R_{free} test set	2297 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	49.6	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 19.7	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.448 for h,-h-k,-h-l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	16000	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.24	0/4091	0.43	0/5538
1	B	0.23	0/4068	0.44	0/5509
1	E	0.33	0/3859	0.57	2/5251 (0.0%)
1	F	0.36	0/3902	0.59	4/5304 (0.1%)
2	C	0.20	0/82	0.34	0/111
2	D	0.20	0/82	0.36	0/111
2	G	0.28	0/82	0.33	0/111
2	H	0.27	0/80	0.53	0/108
All	All	0.30	0/16246	0.51	6/22043 (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	E	0	2
1	F	0	2
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	467	GLN	CA-CB-CG	5.84	126.26	113.40
1	F	215	HIS	CB-CA-C	5.64	121.69	110.40
1	E	108	PHE	N-CA-C	-5.41	96.40	111.00
1	F	228	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	F	114	HIS	N-CA-C	5.21	125.07	111.00
1	F	139	GLY	N-CA-C	-5.01	100.56	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	106	THR	Peptide
1	E	162	ASN	Peptide
1	F	526	ALA	Peptide
1	F	74	ASN	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	3998	0	3916	40	0
1	B	3976	0	3896	52	0
1	E	3776	0	3549	96	1
1	F	3811	0	3537	90	0
2	C	78	0	69	1	0
2	D	78	0	69	1	0
2	G	78	0	69	0	0
2	H	76	0	62	2	0
3	A	9	0	12	0	0
3	B	9	0	12	0	0
3	E	9	0	12	1	0
3	F	9	0	12	2	0
4	A	21	0	18	0	0
4	B	21	0	18	1	0
4	E	21	0	18	4	0
4	F	21	0	18	0	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	E	2	0	0	0	0
5	F	1	0	0	0	0
All	All	16000	0	15287	274	1

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 9.

All (274) 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:F:224:GLU:HG2	1:F:228:ARG:HH22	1.16	1.10
1:E:420:ARG:HG3	1:E:420:ARG:HH11	1.27	1.00
1:E:413:LEU:O	1:E:416:THR:OG1	1.85	0.93
1:A:228:ARG:NH1	1:A:574:LYS:O	2.00	0.93
1:F:191:THR:HG22	1:F:195:GLU:H	1.34	0.90
1:F:174:ASN:O	1:F:177:ARG:NH1	2.10	0.84
1:F:224:GLU:HG2	1:F:228:ARG:NH2	1.96	0.81
1:B:392:ARG:HH12	1:B:455:THR:HG22	1.45	0.78
1:F:435:PRO:HD2	1:F:446:LYS:NZ	1.98	0.77
1:E:335:PHE:HE2	4:E:602:KRS:H14	1.50	0.77
1:F:253:TYR:CE1	1:F:257:PHE:HB2	2.20	0.76
1:F:434:CYS:HA	1:F:446:LYS:HZ3	1.51	0.75
1:E:159:ASN:OD1	1:E:160:SER:N	2.21	0.73
1:E:488:LEU:HB3	1:E:496:CYS:HB2	1.68	0.73
1:F:420:ARG:NH2	1:F:420:ARG:HG2	2.03	0.73
1:F:420:ARG:HG2	1:F:420:ARG:HH21	1.54	0.72
1:E:445:ASP:HA	1:E:448:VAL:HG12	1.71	0.72
1:F:435:PRO:HD2	1:F:446:LYS:HZ3	1.54	0.72
1:B:488:LEU:HB3	1:B:496:CYS:HB2	1.71	0.71
1:A:488:LEU:HB3	1:A:496:CYS:HB2	1.72	0.71
1:F:355:GLU:HG2	1:F:391:PHE:HD2	1.55	0.71
1:E:107:ASP:HA	1:E:109:ILE:HG23	1.72	0.71
1:E:104:SER:O	1:E:106:THR:OG1	2.10	0.69
1:F:124:ILE:O	1:F:187:ASN:ND2	2.24	0.69
1:F:464:ASP:HB3	1:F:482:LEU:HD13	1.73	0.69
1:F:488:LEU:HB3	1:F:496:CYS:HB2	1.73	0.69
1:F:494:GLU:O	1:F:553:ARG:NH1	2.26	0.69
1:E:412:ASN:HB3	1:E:413:LEU:CD2	2.22	0.68
1:F:411:THR:OG1	1:F:480:GLU:O	2.10	0.68
1:E:420:ARG:HG3	1:E:420:ARG:NH1	1.96	0.68
1:F:215:HIS:ND1	1:F:216:LEU:N	2.41	0.68
1:F:448:VAL:HG23	1:F:452:LEU:HD12	1.75	0.68
1:A:104:SER:OG	1:A:107:ASP:OD1	2.10	0.67
1:F:392:ARG:HB3	1:F:460:THR:HG22	1.74	0.67
1:E:107:ASP:HB3	1:E:110:GLN:H	1.60	0.67
1:F:449:GLY:HA2	1:F:453:GLU:OE2	1.95	0.66
1:F:109:ILE:O	1:F:113:SER:HB2	1.95	0.66
1:B:437:PRO:O	1:B:442:ARG:NH2	2.29	0.65
1:F:253:TYR:O	1:F:256:SER:N	2.30	0.65
1:F:125:THR:HA	1:F:187:ASN:ND2	2.12	0.65
1:F:253:TYR:CZ	1:F:257:PHE:HB2	2.32	0.65
1:F:92:GLU:OE2	1:F:175:LYS:NZ	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:328:ASP:OD2	1:F:331:HIS:ND1	2.30	0.65
1:F:191:THR:HG23	1:F:193:LYS:H	1.62	0.65
1:F:494:GLU:HB3	1:F:553:ARG:HH12	1.63	0.64
1:A:350:LEU:HD13	1:A:547:TRP:HB2	1.79	0.64
1:A:424:ASP:OD2	1:A:438:ARG:NH2	2.30	0.64
1:A:394:ILE:HD11	1:A:462:ILE:HG12	1.80	0.63
1:F:350:LEU:HD13	1:F:547:TRP:HB2	1.79	0.63
1:F:215:HIS:O	1:F:216:LEU:HG	1.99	0.62
1:F:144:PHE:CE1	1:F:157:MET:HG3	2.35	0.62
1:F:434:CYS:HA	1:F:446:LYS:NZ	2.14	0.62
1:E:142:LEU:HD12	1:E:158:ALA:O	2.00	0.61
1:F:509:ARG:O	1:F:513:GLU:HG2	2.01	0.61
1:E:288:ASN:HD22	1:F:324:ASN:ND2	1.99	0.60
1:E:84:ILE:HG23	1:E:88:LYS:NZ	2.16	0.60
1:B:515:GLN:HG2	1:B:526:ALA:HB1	1.83	0.60
1:E:311:GLY:O	1:F:241:ARG:NH2	2.34	0.60
1:B:392:ARG:HH12	1:B:455:THR:CG2	2.15	0.60
1:F:420:ARG:HH21	1:F:420:ARG:CG	2.15	0.59
1:E:165:SER:HB2	1:E:168:GLU:HG3	1.85	0.59
1:E:332:ASN:O	4:E:602:KRS:H3	2.03	0.59
1:A:202:GLU:OE2	1:E:412:ASN:OD1	2.20	0.59
1:B:508:GLN:HE21	1:B:533:PHE:HE2	1.51	0.58
1:E:416:THR:HB	1:E:419:THR:H	1.68	0.57
2:H:8:PRO:HB3	2:H:10:HIS:CE1	2.39	0.57
1:A:409:PRO:HG2	1:A:419:THR:HG23	1.86	0.57
1:E:107:ASP:HB3	1:E:110:GLN:HG2	1.86	0.57
1:B:178:ARG:NH1	1:B:213:LEU:HB2	2.19	0.57
1:E:394:ILE:HG23	1:E:462:ILE:HA	1.87	0.57
1:A:327:ILE:HG12	1:A:333:PRO:HD3	1.87	0.57
1:B:327:ILE:HG12	1:B:333:PRO:HD3	1.87	0.56
1:E:392:ARG:HB3	1:E:460:THR:HG22	1.87	0.56
1:F:280:ALA:O	1:F:525:GLU:HG3	2.05	0.56
3:E:601:LYS:O	4:E:602:KRS:H16	2.05	0.56
1:E:88:LYS:HZ1	1:E:94:PRO:HB2	1.70	0.56
1:E:406:MET:CE	1:E:426:ILE:HD11	2.35	0.56
1:F:258:LEU:HB3	1:F:263:PHE:HB2	1.87	0.56
1:A:178:ARG:NH1	1:A:213:LEU:HB3	2.21	0.56
1:B:362:VAL:HG22	1:B:558:LEU:HD21	1.87	0.56
1:E:350:LEU:HD13	1:E:547:TRP:HB2	1.87	0.56
1:B:513:GLU:HA	1:B:529:ILE:HD11	1.86	0.56
1:E:420:ARG:HH11	1:E:420:ARG:CG	2.09	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:394:ILE:HG22	1:F:462:ILE:HA	1.87	0.55
1:B:383:TYR:HB2	1:B:491:MET:HE1	1.89	0.55
1:E:467:GLN:NE2	1:E:511:LEU:HD11	2.20	0.55
1:F:123:ASP:OD1	1:F:124:ILE:N	2.40	0.55
1:A:383:TYR:HB2	1:A:491:MET:HE1	1.87	0.55
1:F:361:MET:HA	1:F:364:HIS:H	1.72	0.55
1:A:86:GLN:OE1	1:A:90:ASN:ND2	2.40	0.55
1:A:504:ASP:OD1	1:B:88:LYS:NZ	2.36	0.54
1:B:270:MET:HA	1:B:297:ARG:HD3	1.89	0.54
1:B:164:LYS:HG2	1:B:201:TYR:CZ	2.43	0.54
1:A:145:TYR:HB2	1:A:156:VAL:HB	1.90	0.54
1:A:362:VAL:HG22	1:A:558:LEU:HD21	1.89	0.54
1:B:509:ARG:NH2	1:B:538:GLU:OE2	2.41	0.54
1:E:335:PHE:CE2	4:E:602:KRS:H14	2.38	0.54
1:F:459:PRO:HA	1:F:489:PHE:O	2.07	0.54
1:F:178:ARG:NH1	1:F:213:LEU:HB3	2.24	0.53
1:B:350:LEU:HD13	1:B:547:TRP:HB2	1.88	0.53
1:B:373:TYR:HB3	1:B:491:MET:HE2	1.90	0.53
1:B:479:LYS:HD3	1:B:482:LEU:HD12	1.89	0.53
1:E:466:PRO:HA	1:E:482:LEU:HA	1.90	0.53
1:E:88:LYS:HZ2	1:E:94:PRO:HD2	1.74	0.53
1:E:107:ASP:HB3	1:E:110:GLN:CG	2.39	0.53
1:E:512:PHE:HB3	1:E:529:ILE:HG12	1.91	0.52
1:E:162:ASN:N	1:E:162:ASN:OD1	2.42	0.52
1:E:459:PRO:HA	1:E:489:PHE:O	2.10	0.52
1:A:423:LEU:HD12	1:A:440:THR:HG23	1.92	0.52
1:E:401:GLU:HB3	1:E:406:MET:O	2.08	0.52
1:B:512:PHE:HB3	1:B:529:ILE:HG12	1.91	0.52
1:A:335:PHE:HB2	1:A:552:ASP:OD2	2.10	0.51
1:F:459:PRO:HB3	1:F:490:VAL:HG22	1.92	0.51
1:E:88:LYS:HZ2	1:E:94:PRO:CG	2.24	0.51
1:B:121:LEU:O	1:B:187:ASN:HB3	2.10	0.51
1:E:413:LEU:CD2	1:E:413:LEU:N	2.73	0.51
1:F:191:THR:HG23	1:F:193:LYS:N	2.26	0.51
1:A:104:SER:HB2	1:A:150:GLU:OE2	2.11	0.51
1:E:132:ILE:HD11	1:E:182:ILE:HD13	1.91	0.51
1:E:239:PHE:O	1:E:242:GLN:HB2	2.11	0.51
1:A:146:ASP:OD1	1:A:153:LYS:NZ	2.32	0.51
1:F:494:GLU:HB3	1:F:553:ARG:NH1	2.26	0.51
1:E:362:VAL:HG22	1:E:558:LEU:HD21	1.93	0.50
1:A:121:LEU:O	1:A:187:ASN:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:424:ASP:OD2	1:A:438:ARG:HD3	2.11	0.50
1:F:253:TYR:CE1	1:F:361:MET:SD	3.04	0.50
1:A:274:ILE:HD12	1:A:275:PRO:HD2	1.93	0.50
1:B:145:TYR:HB2	1:B:156:VAL:HB	1.92	0.50
1:E:88:LYS:HZ2	1:E:94:PRO:HG2	1.76	0.50
1:F:224:GLU:CG	1:F:228:ARG:HH22	2.05	0.50
1:F:430:LYS:O	1:F:431:ALA:HB2	2.11	0.50
1:E:391:PHE:CD2	1:E:459:PRO:HB2	2.46	0.50
1:F:335:PHE:HB2	1:F:552:ASP:OD2	2.11	0.50
1:F:157:MET:O	1:F:200:PRO:HD2	2.12	0.50
1:E:476:HIS:HA	1:E:484:GLU:HG3	1.94	0.50
1:F:512:PHE:HB3	1:F:529:ILE:HG12	1.94	0.49
1:A:394:ILE:HB	1:A:399:GLU:OE1	2.12	0.49
1:A:539:TYR:CE1	1:B:232:LEU:HD21	2.48	0.49
1:E:467:GLN:OE1	1:E:483:THR:CG2	2.61	0.49
1:B:510:GLN:O	1:B:514:GLU:HG3	2.11	0.49
1:E:239:PHE:HA	1:E:242:GLN:HB2	1.95	0.49
1:E:406:MET:HE2	1:E:426:ILE:HD11	1.94	0.49
1:E:133:HIS:HD2	1:E:133:HIS:O	1.95	0.49
1:B:335:PHE:HB2	1:B:552:ASP:OD2	2.12	0.49
1:B:347:TYR:CD2	1:B:484:GLU:HB3	2.48	0.49
1:A:95:TYR:CE1	1:A:208:PRO:HD2	2.48	0.48
1:A:416:THR:HG22	1:A:418:GLU:H	1.78	0.48
1:E:215:HIS:ND1	1:E:216:LEU:HG	2.28	0.48
1:E:412:ASN:HB3	1:E:413:LEU:HD22	1.92	0.48
1:E:133:HIS:O	1:E:133:HIS:CD2	2.66	0.48
1:E:189:GLY:O	1:E:196:LEU:HD12	2.13	0.48
1:B:452:LEU:O	1:B:455:THR:HB	2.13	0.48
1:E:412:ASN:CB	1:E:413:LEU:CD2	2.91	0.48
1:E:109:ILE:HA	1:E:196:LEU:HD23	1.96	0.48
1:A:347:TYR:CD2	1:A:484:GLU:HB3	2.49	0.48
1:E:412:ASN:CB	1:E:413:LEU:HD23	2.43	0.48
1:B:220:LEU:HD22	1:B:236:LEU:HD12	1.95	0.47
1:E:85:HIS:O	1:E:89:VAL:HG23	2.14	0.47
1:E:314:ARG:NH2	2:H:4:TYR:O	2.35	0.47
1:E:406:MET:SD	1:E:426:ILE:HD12	2.54	0.47
1:B:413:LEU:O	1:B:416:THR:HG22	2.14	0.47
1:E:249:LYS:HA	1:E:252:THR:OG1	2.15	0.47
1:F:396:MET:SD	1:F:469:MET:HE1	2.54	0.47
1:F:424:ASP:O	1:F:427:CYS:HB2	2.14	0.47
1:B:332:ASN:O	4:B:602:KRS:H3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:100:HIS:NE2	1:E:102:ASP:OD1	2.47	0.47
1:F:359:SER:OG	1:F:360:GLY:N	2.47	0.47
1:E:84:ILE:HG23	1:E:88:LYS:HZ3	1.80	0.47
1:F:132:ILE:HD11	1:F:182:ILE:HD13	1.97	0.46
1:B:525:GLU:HG2	1:B:526:ALA:N	2.31	0.46
1:B:95:TYR:CE1	1:B:208:PRO:HD2	2.51	0.46
1:B:138:SER:HB2	1:B:142:LEU:HB3	1.96	0.46
1:E:228:ARG:NH1	1:E:575:PRO:HA	2.30	0.46
1:E:305:LYS:HD3	1:E:501:GLU:HB3	1.96	0.46
1:E:435:PRO:O	1:E:442:ARG:NH1	2.48	0.46
1:F:124:ILE:HD12	1:F:126:LEU:HD13	1.97	0.46
1:A:232:LEU:HD21	1:B:539:TYR:CE2	2.51	0.46
1:E:286:TYR:OH	1:E:291:ASP:OD1	2.34	0.46
1:A:510:GLN:O	1:A:514:GLU:HG3	2.16	0.46
1:F:347:TYR:OH	1:F:463:CYS:HB3	2.15	0.46
1:E:391:PHE:CE2	1:E:459:PRO:HB2	2.51	0.46
1:F:501:GLU:OE2	3:F:601:LYS:NZ	2.34	0.46
1:B:515:GLN:HG2	1:B:526:ALA:CB	2.45	0.45
1:F:138:SER:OG	1:F:142:LEU:O	2.25	0.45
1:A:307:LEU:HD11	1:B:569:LEU:HD13	1.98	0.45
1:B:374:HIS:NE2	1:B:382:ALA:HB2	2.32	0.45
1:E:106:THR:HB	1:E:107:ASP:C	2.36	0.45
1:E:516:ALA:HB2	1:E:529:ILE:HG13	1.98	0.45
1:F:142:LEU:HD12	1:F:158:ALA:O	2.16	0.45
1:F:385:VAL:HG23	1:F:458:ASN:HA	1.98	0.45
1:F:391:PHE:CE1	1:F:459:PRO:HG2	2.51	0.45
1:E:109:ILE:HA	1:E:196:LEU:CD2	2.46	0.45
1:F:275:PRO:HD3	1:F:295:TYR:CD1	2.51	0.45
1:F:435:PRO:HD2	1:F:446:LYS:HZ1	1.78	0.45
1:A:95:TYR:HE1	1:A:207:SER:HG	1.62	0.45
1:F:95:TYR:CE1	1:F:208:PRO:HD2	2.52	0.45
1:A:281:LYS:HB2	1:A:324:ASN:O	2.17	0.45
1:F:124:ILE:C	1:F:187:ASN:HD21	2.20	0.45
1:A:501:GLU:OE2	1:A:546:GLY:HA3	2.17	0.45
1:F:213:LEU:HA	1:F:214:PRO:HD3	1.76	0.45
1:F:434:CYS:HA	1:F:435:PRO:HD2	1.86	0.45
1:A:132:ILE:HD11	1:A:182:ILE:HD13	1.98	0.45
1:A:383:TYR:HB2	1:A:491:MET:CE	2.47	0.44
1:E:95:TYR:CE2	1:E:208:PRO:HD2	2.52	0.44
1:F:355:GLU:HG2	1:F:391:PHE:CD2	2.45	0.44
1:E:117:PRO:HB3	1:E:192:LYS:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:406:MET:CE	1:E:426:ILE:CD1	2.94	0.44
1:E:569:LEU:HD13	1:F:307:LEU:HD11	2.00	0.44
1:F:138:SER:OG	1:F:139:GLY:N	2.50	0.44
1:F:369:TYR:CG	1:F:388:THR:HG23	2.52	0.44
1:A:270:MET:HA	1:A:297:ARG:HD3	2.00	0.44
1:B:454:VAL:HA	1:B:492:LYS:HG2	2.00	0.44
2:D:7:LYS:HA	2:D:8:PRO:HD3	1.90	0.44
1:E:84:ILE:HG23	1:E:88:LYS:HZ1	1.82	0.44
2:C:7:LYS:HA	2:C:8:PRO:HD3	1.91	0.43
1:E:124:ILE:O	1:E:187:ASN:OD1	2.35	0.43
1:E:480:GLU:C	1:E:482:LEU:H	2.22	0.43
1:B:275:PRO:HD3	1:B:295:TYR:CD1	2.53	0.43
1:E:133:HIS:CG	1:E:148:ARG:HH21	2.36	0.43
1:F:501:GLU:OE2	1:F:546:GLY:HA3	2.18	0.43
1:B:438:ARG:HG2	1:B:443:LEU:HD21	2.00	0.43
1:E:88:LYS:NZ	1:E:94:PRO:HB2	2.33	0.43
1:E:438:ARG:CB	1:E:443:LEU:HD11	2.49	0.43
1:E:88:LYS:HZ2	1:E:94:PRO:CD	2.31	0.43
1:F:277:GLY:O	3:F:601:LYS:N	2.51	0.43
1:A:373:TYR:HB3	1:A:491:MET:HE2	2.00	0.42
1:B:133:HIS:CG	1:B:148:ARG:HD2	2.53	0.42
1:E:498:ALA:HB2	1:E:547:TRP:CD1	2.54	0.42
1:B:132:ILE:HD11	1:B:182:ILE:HD13	2.00	0.42
1:B:281:LYS:HB2	1:B:324:ASN:O	2.19	0.42
1:B:392:ARG:NH1	1:B:455:THR:HG22	2.24	0.42
1:F:476:HIS:HA	1:F:484:GLU:CG	2.49	0.42
1:E:133:HIS:CD2	1:E:133:HIS:C	2.93	0.42
1:E:401:GLU:OE2	1:E:408:LEU:HB2	2.19	0.42
1:F:552:ASP:O	1:F:556:MET:HG3	2.19	0.42
1:F:362:VAL:HG21	1:F:387:PHE:CD2	2.54	0.42
1:F:383:TYR:HB2	1:F:491:MET:HE2	2.02	0.42
1:E:388:THR:HA	1:E:389:PRO:HD2	1.90	0.42
1:A:414:PHE:HA	1:A:419:THR:HG21	2.01	0.42
1:B:137:ALA:HB1	1:B:139:GLY:HA2	2.01	0.42
1:F:114:HIS:ND1	1:F:114:HIS:C	2.73	0.42
1:E:327:ILE:HG12	1:E:333:PRO:HD3	2.02	0.42
1:B:476:HIS:HB3	1:B:479:LYS:O	2.20	0.42
1:B:383:TYR:HB2	1:B:491:MET:CE	2.50	0.41
1:E:145:TYR:HB2	1:E:156:VAL:HB	2.01	0.41
1:E:279:VAL:HG13	1:E:525:GLU:O	2.20	0.41
1:F:186:GLY:HA3	1:F:200:PRO:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:GLN:HA	1:E:113:SER:OG	2.20	0.41
1:F:477:ARG:HG2	1:F:484:GLU:OE2	2.20	0.41
1:B:394:ILE:HD11	1:B:462:ILE:HG12	2.00	0.41
1:E:172:ILE:O	1:E:176:LEU:HG	2.20	0.41
1:B:164:LYS:HE2	1:B:164:LYS:HB3	1.73	0.41
1:E:434:CYS:HA	1:E:435:PRO:HD2	1.90	0.41
1:F:80:ARG:NH1	1:F:177:ARG:HB2	2.34	0.41
1:B:185:GLN:O	1:B:201:TYR:N	2.47	0.41
1:E:146:ASP:OD2	1:E:148:ARG:NH1	2.52	0.41
1:E:224:GLU:O	1:E:228:ARG:HG3	2.21	0.41
1:A:411:THR:HA	1:A:414:PHE:CD1	2.56	0.41
1:E:435:PRO:HA	1:E:436:PRO:HD3	1.79	0.41
1:E:172:ILE:HG12	1:E:203:ILE:HB	2.02	0.41
1:F:394:ILE:O	1:F:463:CYS:N	2.53	0.41
1:F:466:PRO:HA	1:F:482:LEU:HA	2.03	0.41
1:E:88:LYS:NZ	1:E:94:PRO:HG2	2.36	0.40
1:E:335:PHE:HB2	1:E:552:ASP:OD2	2.21	0.40
1:E:519:LYS:HA	1:E:523:ASP:O	2.21	0.40
1:F:453:GLU:HA	1:F:456:CYS:SG	2.61	0.40
1:A:275:PRO:HD3	1:A:295:TYR:CD1	2.56	0.40
1:B:164:LYS:HB3	1:B:168:GLU:OE2	2.21	0.40
1:F:476:HIS:HA	1:F:484:GLU:HG2	2.02	0.40
1:F:476:HIS:HB3	1:F:479:LYS:O	2.20	0.40
1:B:109:ILE:O	1:B:113:SER:OG	2.33	0.40
1:B:391:PHE:HB2	1:B:461:PHE:CE2	2.57	0.40
1:F:558:LEU:HD23	1:F:558:LEU:HA	1.89	0.40
1:F:444:LEU:HA	1:F:447:LEU:HB2	2.04	0.40

All (1) 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:E:74:ASN:ND2	1:E:116:GLN:OE1[1_455]	2.17	0.03

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	497/513 (97%)	486 (98%)	11 (2%)	0	100	100
1	B	497/513 (97%)	489 (98%)	8 (2%)	0	100	100
1	E	495/513 (96%)	477 (96%)	18 (4%)	0	100	100
1	F	492/513 (96%)	476 (97%)	16 (3%)	0	100	100
2	C	7/42 (17%)	7 (100%)	0	0	100	100
2	D	7/42 (17%)	7 (100%)	0	0	100	100
2	G	7/42 (17%)	7 (100%)	0	0	100	100
2	H	7/42 (17%)	7 (100%)	0	0	100	100
All	All	2009/2220 (90%)	1956 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/455 (94%)	425 (100%)	2 (0%)	88	96
1	B	423/455 (93%)	421 (100%)	2 (0%)	88	96
1	E	376/455 (83%)	363 (96%)	13 (4%)	36	70
1	F	379/455 (83%)	369 (97%)	10 (3%)	46	77
2	C	8/36 (22%)	8 (100%)	0	100	100
2	D	8/36 (22%)	8 (100%)	0	100	100
2	G	8/36 (22%)	8 (100%)	0	100	100
2	H	7/36 (19%)	6 (86%)	1 (14%)	3	10
All	All	1636/1964 (83%)	1608 (98%)	28 (2%)	60	86

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	215	HIS
1	A	399	GLU
1	B	347	TYR
1	B	420	ARG
1	E	105	LEU
1	E	106	THR
1	E	109	ILE
1	E	110	GLN
1	E	121	LEU
1	E	160	SER
1	E	398	GLU
1	E	412	ASN
1	E	413	LEU
1	E	416	THR
1	E	420	ARG
1	E	424	ASP
1	E	500	THR
1	F	74	ASN
1	F	114	HIS
1	F	123	ASP
1	F	124	ILE
1	F	155	GLN
1	F	187	ASN
1	F	215	HIS
1	F	388	THR
1	F	417	GLU
1	F	424	ASP
2	H	5	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	HIS
1	B	287	HIS
1	E	110	GLN
1	E	133	HIS
1	E	288	ASN
1	E	412	ASN
1	F	155	GLN
1	F	187	ASN
2	H	10	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	LYS	B	601	-	7,8,9	0.46	0	3,8,10	0.50	0
3	LYS	E	601	-	7,8,9	0.46	0	3,8,10	0.46	0
4	KRS	B	602	-	23,23,23	1.66	3 (13%)	33,33,33	2.50	10 (30%)
4	KRS	F	602	-	23,23,23	1.92	3 (13%)	33,33,33	1.44	7 (21%)
3	LYS	F	601	-	7,8,9	0.45	0	3,8,10	0.46	0
4	KRS	E	602	-	23,23,23	1.97	3 (13%)	33,33,33	1.38	7 (21%)
3	LYS	A	601	-	7,8,9	0.45	0	3,8,10	0.48	0
4	KRS	A	602	-	23,23,23	1.93	3 (13%)	33,33,33	1.43	6 (18%)

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	LYS	B	601	-	-	0/6/7/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LYS	E	601	-	-	0/6/7/9	-
4	KRS	B	602	-	-	0/4/26/26	0/3/3/3
4	KRS	F	602	-	-	0/4/26/26	0/3/3/3
3	LYS	F	601	-	-	0/6/7/9	-
4	KRS	E	602	-	-	0/4/26/26	0/3/3/3
3	LYS	A	601	-	-	0/6/7/9	-
4	KRS	A	602	-	-	0/4/26/26	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	602	KRS	O3-C8	7.12	1.46	1.35
4	A	602	KRS	O3-C8	6.99	1.46	1.35
4	F	602	KRS	O3-C8	6.88	1.45	1.35
4	B	602	KRS	O3-C8	5.08	1.43	1.35
4	F	602	KRS	C9-C1	4.45	1.48	1.41
4	E	602	KRS	C9-C1	4.44	1.48	1.41
4	A	602	KRS	C9-C1	4.35	1.48	1.41
4	E	602	KRS	C9-C5	3.37	1.48	1.41
4	A	602	KRS	C9-C5	3.29	1.48	1.41
4	F	602	KRS	C9-C5	3.28	1.48	1.41
4	B	602	KRS	O5-C12	-2.92	1.39	1.44
4	B	602	KRS	O3-C7	-2.53	1.40	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	602	KRS	O5-C12-C13	-9.05	103.60	109.96
4	B	602	KRS	C14-C13-C12	-5.95	106.93	111.04
4	B	602	KRS	C11-C10-C7	-3.94	108.31	114.39
4	A	602	KRS	C7-O3-C8	-3.86	112.74	118.69
4	F	602	KRS	C7-O3-C8	-3.71	112.97	118.69
4	E	602	KRS	C7-O3-C8	-3.60	113.14	118.69
4	B	602	KRS	O3-C8-O4	3.40	121.39	117.60
4	B	602	KRS	O1-C1-C9	-3.28	115.00	121.14
4	E	602	KRS	C1-C9-C8	3.18	123.55	119.81
4	B	602	KRS	C4-C5-C9	-2.77	116.15	119.47
4	F	602	KRS	C1-C9-C8	2.71	123.00	119.81
4	A	602	KRS	C1-C9-C8	2.70	122.99	119.81
4	B	602	KRS	O3-C7-C10	-2.69	101.89	106.17
4	F	602	KRS	C14-C13-C12	-2.63	109.22	111.04
4	B	602	KRS	C1-C9-C5	2.62	121.44	118.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	602	KRS	C11-C10-C7	-2.59	110.39	114.39
4	F	602	KRS	C11-C10-C7	-2.54	110.48	114.39
4	B	602	KRS	O1-C1-C2	2.45	126.03	119.46
4	A	602	KRS	C14-C13-C12	-2.32	109.44	111.04
4	B	602	KRS	C2-C3-C4	2.31	123.62	120.43
4	E	602	KRS	C2-C1-C9	-2.28	118.29	120.93
4	F	602	KRS	C2-C1-C9	-2.26	118.31	120.93
4	E	602	KRS	C11-C10-C7	-2.23	110.95	114.39
4	A	602	KRS	C2-C1-C9	-2.20	118.38	120.93
4	F	602	KRS	C10-C7-C6	-2.19	109.33	113.44
4	E	602	KRS	O3-C8-O4	2.12	119.96	117.60
4	E	602	KRS	C10-C7-C6	-2.11	109.47	113.44
4	E	602	KRS	O3-C7-C10	2.09	109.50	106.17
4	F	602	KRS	C1-C2-C3	2.01	121.52	119.70
4	A	602	KRS	O3-C8-O4	2.01	119.84	117.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	LYS	1	0
4	B	602	KRS	1	0
3	F	601	LYS	2	0
4	E	602	KRS	4	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 then 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 KRS B 602

Bond lengths

Bond angles

Torsions

Rings

Ligand KRS F 602

Bond lengths

Bond angles

Torsions

Rings

Ligand KRS E 602

Bond lengths

Bond angles

Torsions

Rings

Ligand KRS A 602

Bond lengths

Bond angles

Torsions

Rings
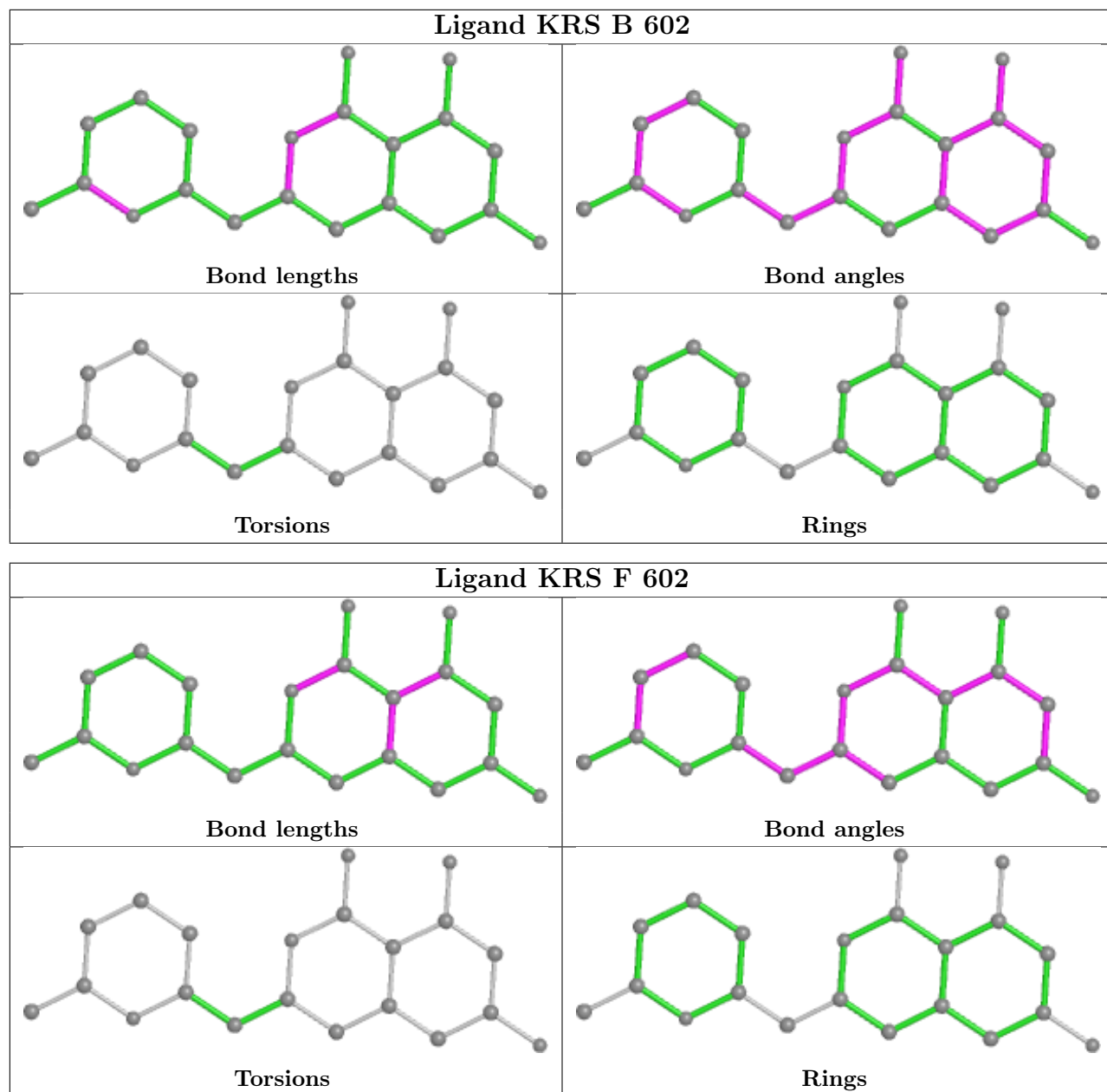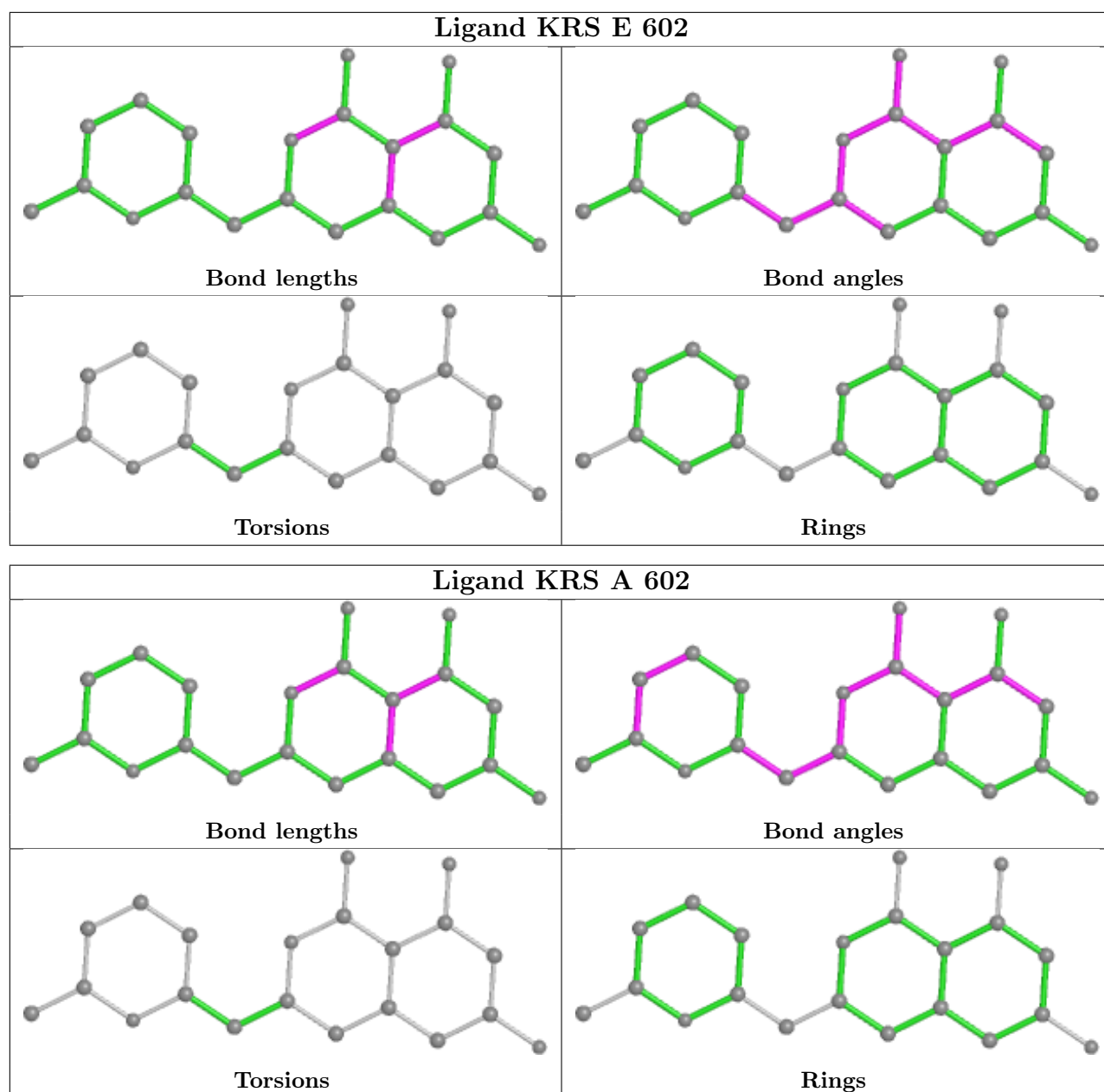
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	501/513 (97%)	-0.40	2 (0%)	92	93	27, 46, 80, 202	2 (0%)
1	B	501/513 (97%)	-0.35	5 (0%)	82	82	25, 47, 83, 174	1 (0%)
1	E	499/513 (97%)	0.11	20 (4%)	38	33	34, 72, 128, 198	1 (0%)
1	F	498/513 (97%)	0.13	20 (4%)	38	33	38, 72, 126, 160	4 (0%)
2	C	9/42 (21%)	-0.01	0	100	100	30, 49, 58, 81	0
2	D	9/42 (21%)	-0.51	0	100	100	34, 47, 62, 68	0
2	G	9/42 (21%)	0.41	1 (11%)	5	4	62, 90, 104, 108	0
2	H	9/42 (21%)	0.25	0	100	100	63, 82, 90, 106	0
All	All	2035/2220 (91%)	-0.13	48 (2%)	59	56	25, 57, 117, 202	8 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	194	GLY	10.1
1	F	575	PRO	6.0
1	B	523	ASP	5.7
1	F	405	GLY	5.7
1	E	405	GLY	5.5
1	E	397	VAL	5.2
1	F	400	LEU	5.0
1	E	109	ILE	5.0
1	F	139	GLY	4.0
1	E	114	HIS	4.0
1	F	522	GLY	3.6
1	B	526	ALA	3.3
1	F	126	LEU	3.3
1	B	522	GLY	3.3
1	E	522	GLY	3.3
1	F	520	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	394	ILE	3.1
1	B	524	ASP	3.0
1	F	403	ALA	3.0
1	B	572	ALA	2.9
1	E	447	LEU	2.9
1	F	521	ALA	2.9
1	E	396	MET	2.8
1	E	370	LYS	2.7
1	E	408	LEU	2.7
1	E	126	LEU	2.7
1	E	427	CYS	2.7
1	F	378	PRO	2.6
1	A	528	PHE	2.6
1	F	124	ILE	2.6
1	F	493	LYS	2.5
1	E	457	ILE	2.4
1	F	158	ALA	2.4
1	F	409	PRO	2.3
1	F	407	LYS	2.3
1	F	372	THR	2.2
1	A	520	ALA	2.2
1	E	451	PHE	2.2
1	E	448	VAL	2.2
1	E	111	LYS	2.1
1	F	524	ASP	2.1
1	F	100	HIS	2.1
1	E	354	THR	2.1
1	F	366	THR	2.1
1	E	215	HIS	2.1
1	E	432	VAL	2.1
2	G	7	LYS	2.1
1	F	162	ASN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å^2)	Q<0.9
3	LYS	A	601	9/10	0.91	0.16	28,29,34,37	0
3	LYS	E	601	9/10	0.92	0.15	30,36,38,43	0
3	LYS	B	601	9/10	0.93	0.16	26,31,39,40	0
4	KRS	E	602	21/21	0.93	0.18	44,54,62,66	0
4	KRS	B	602	21/21	0.95	0.13	28,40,47,49	0
3	LYS	F	601	9/10	0.95	0.17	36,44,57,58	0
4	KRS	F	602	21/21	0.95	0.21	36,47,56,61	0
4	KRS	A	602	21/21	0.97	0.16	26,33,45,51	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 E 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
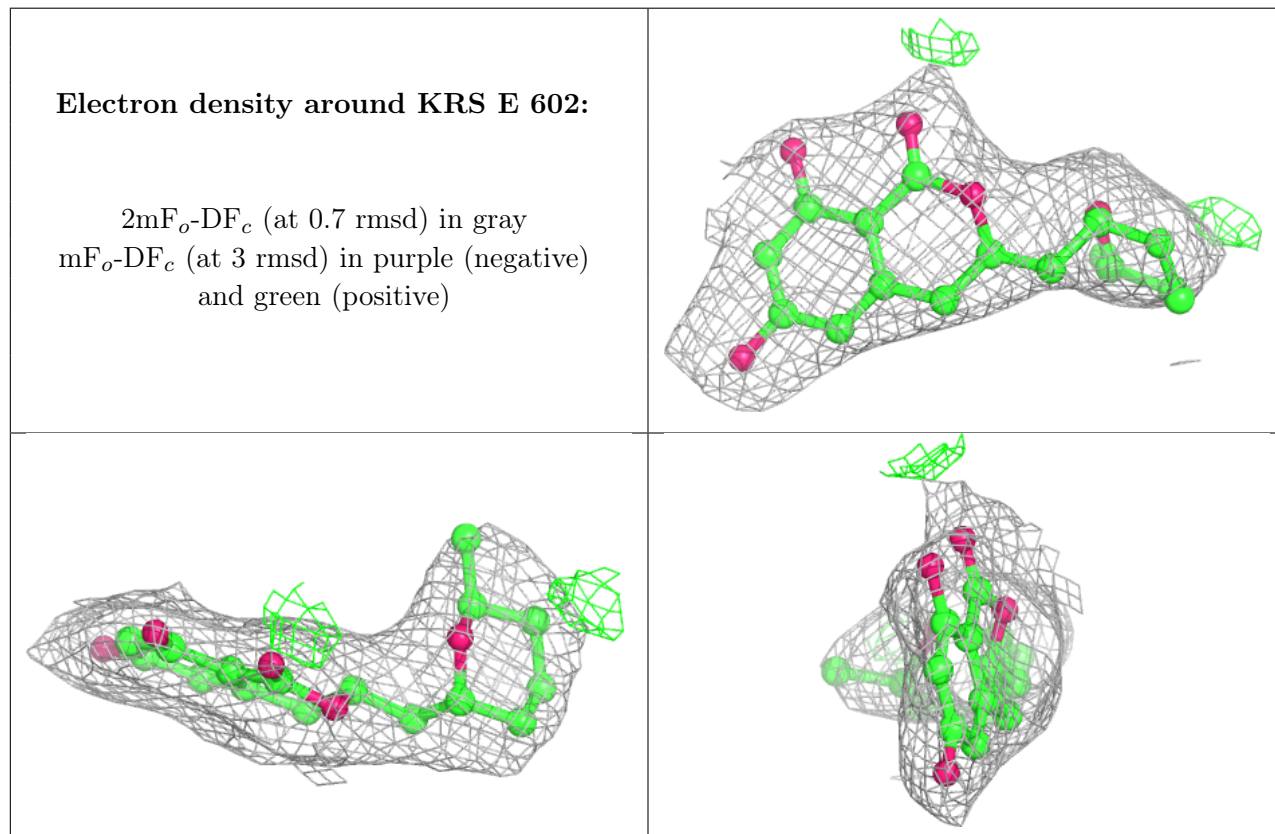
Electron density around KRS B 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
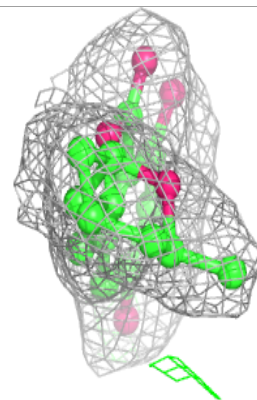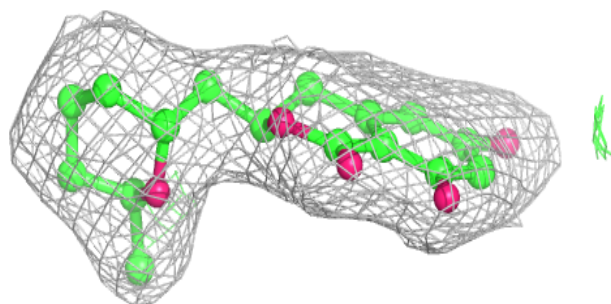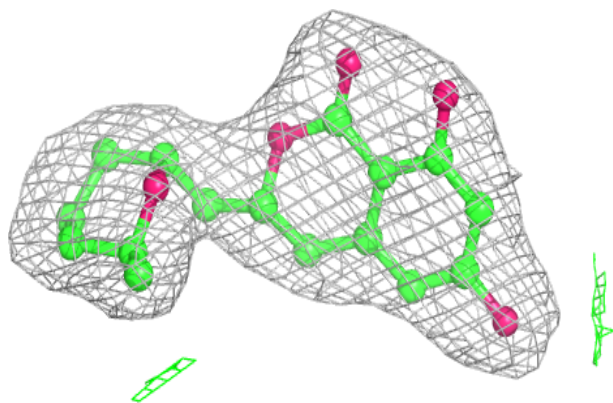
Electron density around KRS F 602:

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

Electron density around KRS A 602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
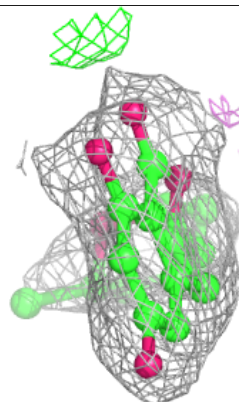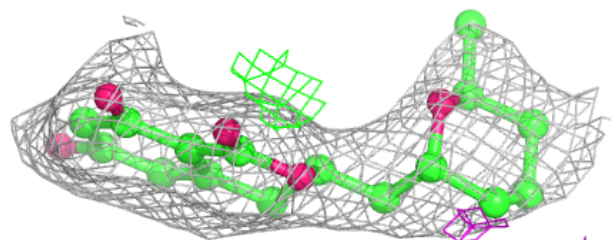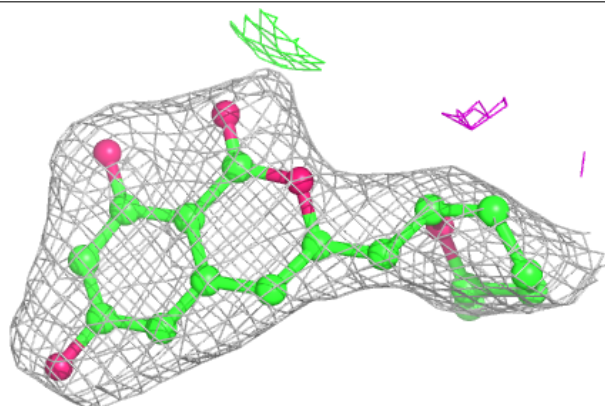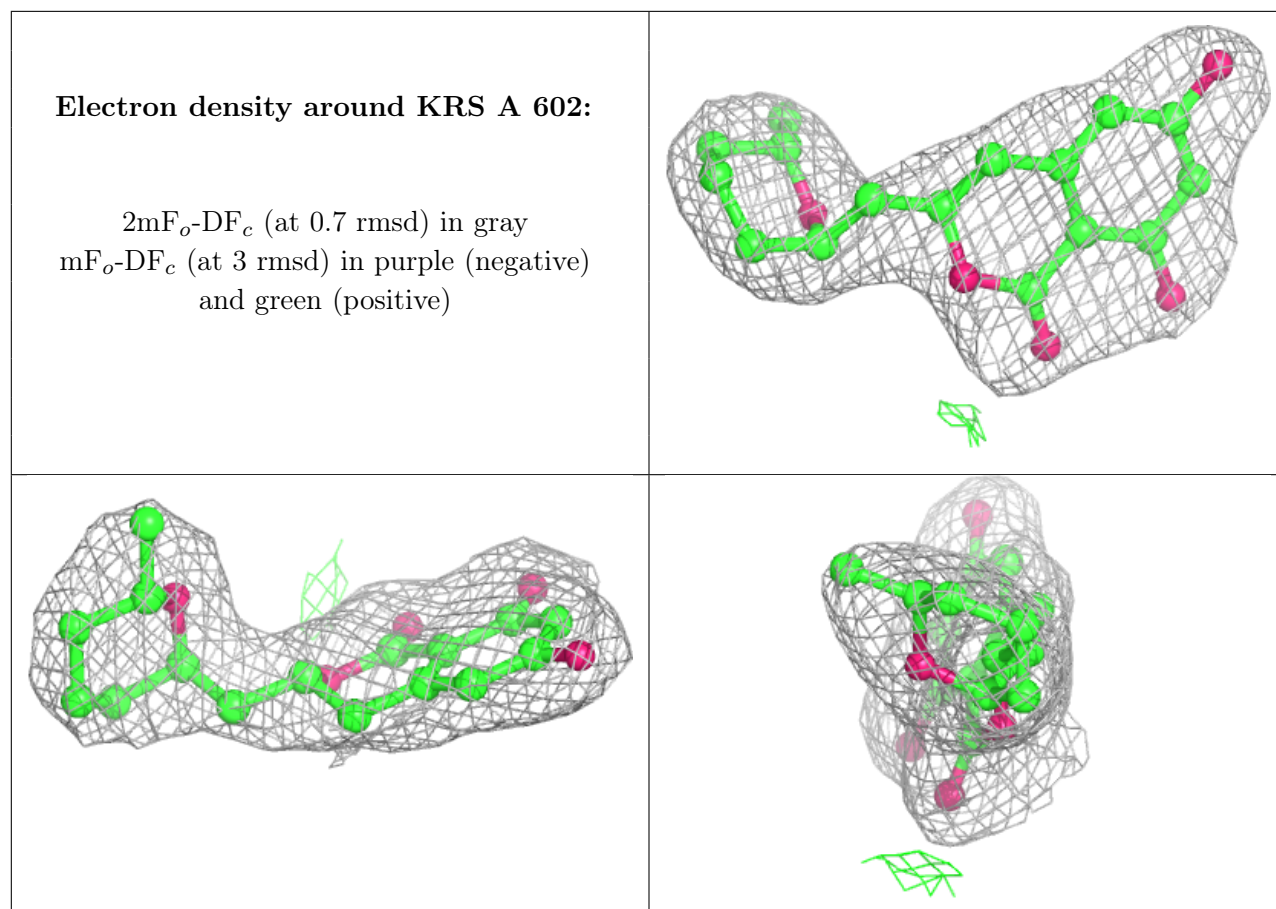
6.5   Other polymers (i)

There are no such residues in this entry.