



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:09 AM UTC

PDB ID : 6SP4 / pdb_00006sp4
Title : KEAP1 IN COMPLEX WITH COMPOUND 23
Authors : Ontoria, J.M.; Biancofiore, I.; Fezzardi, P.; Torrente de Haro, E.; Colarusso, S.; Bianchi, E.; Andreini, M.; Patsilidakos, A.; Summa, V.; Pacifici, R.; Munoz-Sanjuan, I.; Park, L.; Bresciani, A.; Dominguez, C.; Toledo-Sherman, L.; Harper, S.
Deposited on : 2019-08-30
Resolution : 2.59 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](#) ①) were used in the production of this report:

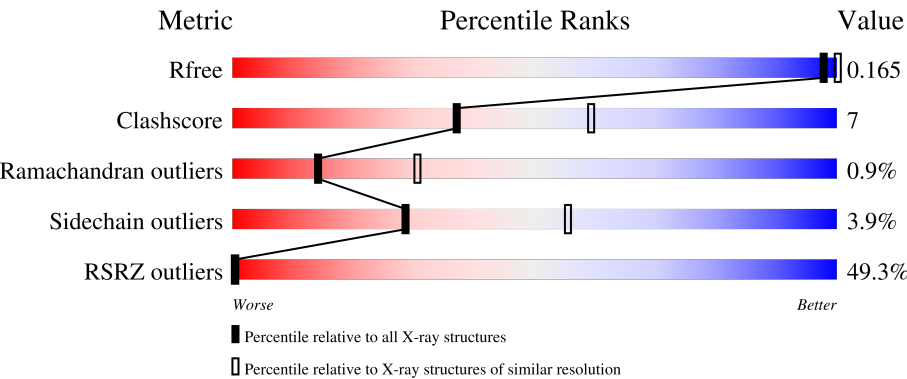
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	293	34% 75% 20%
1	B	293	48% 90% 7%
1	C	293	35% 78% 15%
1	D	293	53% 80% 16%
1	E	293	63% 80% 16%

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Mol	Chain	Length	Quality of chain
1	F	293	53% 89% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13531 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2181	1357	396	413	15			
1	B	285	Total	C	N	O	S	0	0	0
			2185	1359	397	414	15			
1	C	284	Total	C	N	O	S	0	0	0
			2181	1357	396	413	15			
1	D	284	Total	C	N	O	S	0	0	0
			2181	1357	396	413	15			
1	E	284	Total	C	N	O	S	0	0	0
			2181	1357	396	413	15			
1	F	286	Total	C	N	O	S	0	0	0
			2192	1364	398	415	15			

There are 36 discrepancies between the modelled and reference sequences:

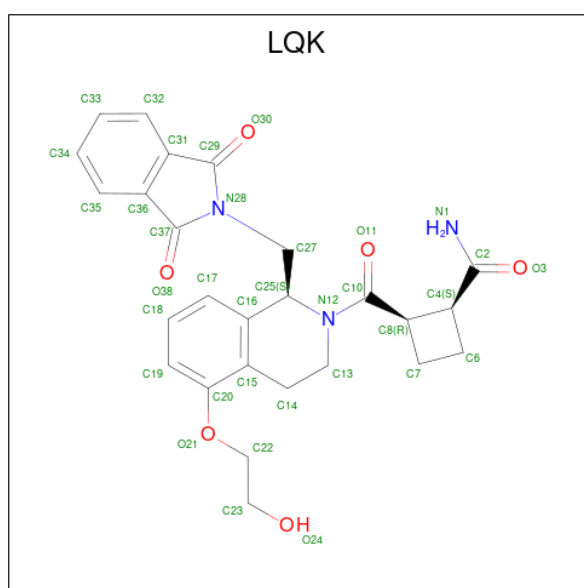
Chain	Residue	Modelled	Actual	Comment	Reference
A	317	GLY	-	expression tag	UNP Q14145
A	318	SER	-	expression tag	UNP Q14145
A	319	HIS	-	expression tag	UNP Q14145
A	320	MET	-	expression tag	UNP Q14145
A	540	ALA	GLU	conflict	UNP Q14145
A	542	ALA	GLU	conflict	UNP Q14145
B	317	GLY	-	expression tag	UNP Q14145
B	318	SER	-	expression tag	UNP Q14145
B	319	HIS	-	expression tag	UNP Q14145
B	320	MET	-	expression tag	UNP Q14145
B	540	ALA	GLU	conflict	UNP Q14145
B	542	ALA	GLU	conflict	UNP Q14145
C	317	GLY	-	expression tag	UNP Q14145
C	318	SER	-	expression tag	UNP Q14145
C	319	HIS	-	expression tag	UNP Q14145
C	320	MET	-	expression tag	UNP Q14145
C	540	ALA	GLU	conflict	UNP Q14145

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Chain	Residue	Modelled	Actual	Comment	Reference
C	542	ALA	GLU	conflict	UNP Q14145
D	317	GLY	-	expression tag	UNP Q14145
D	318	SER	-	expression tag	UNP Q14145
D	319	HIS	-	expression tag	UNP Q14145
D	320	MET	-	expression tag	UNP Q14145
D	540	ALA	GLU	conflict	UNP Q14145
D	542	ALA	GLU	conflict	UNP Q14145
E	317	GLY	-	expression tag	UNP Q14145
E	318	SER	-	expression tag	UNP Q14145
E	319	HIS	-	expression tag	UNP Q14145
E	320	MET	-	expression tag	UNP Q14145
E	540	ALA	GLU	conflict	UNP Q14145
E	542	ALA	GLU	conflict	UNP Q14145
F	317	GLY	-	expression tag	UNP Q14145
F	318	SER	-	expression tag	UNP Q14145
F	319	HIS	-	expression tag	UNP Q14145
F	320	MET	-	expression tag	UNP Q14145
F	540	ALA	GLU	conflict	UNP Q14145
F	542	ALA	GLU	conflict	UNP Q14145

- Molecule 2 is (1 {S},2 {R})-2-[[[(1 {S})-1-[[1,3-bis(oxidanylidene)isoindol-2-yl]methyl]-5-(2-hydroxyethoxy)-3,4-dihydro-1 {H}-isoquinolin-2-yl]carbonyl]cyclobutane-1-carboxamide (CCD ID: LQK) (formula: C₂₆H₂₇N₃O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	26	3	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			35	26	3	6		
2	C	1	Total	C	N	O	0	0
			35	26	3	6		
2	D	1	Total	C	N	O	0	0
			35	26	3	6		
2	E	1	Total	C	N	O	0	0
			35	26	3	6		
2	F	1	Total	C	N	O	0	0
			35	26	3	6		

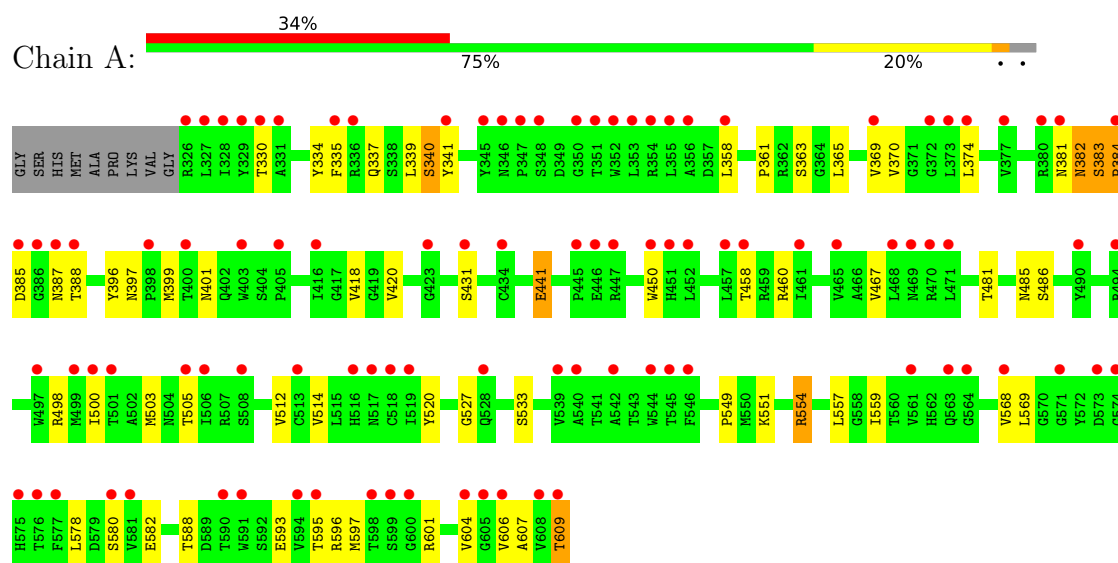
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	27	Total	O	0	0
			27	27		
3	C	39	Total	O	0	0
			39	39		
3	D	34	Total	O	0	0
			34	34		
3	E	41	Total	O	0	0
			41	41		
3	F	37	Total	O	0	0
			37	37		

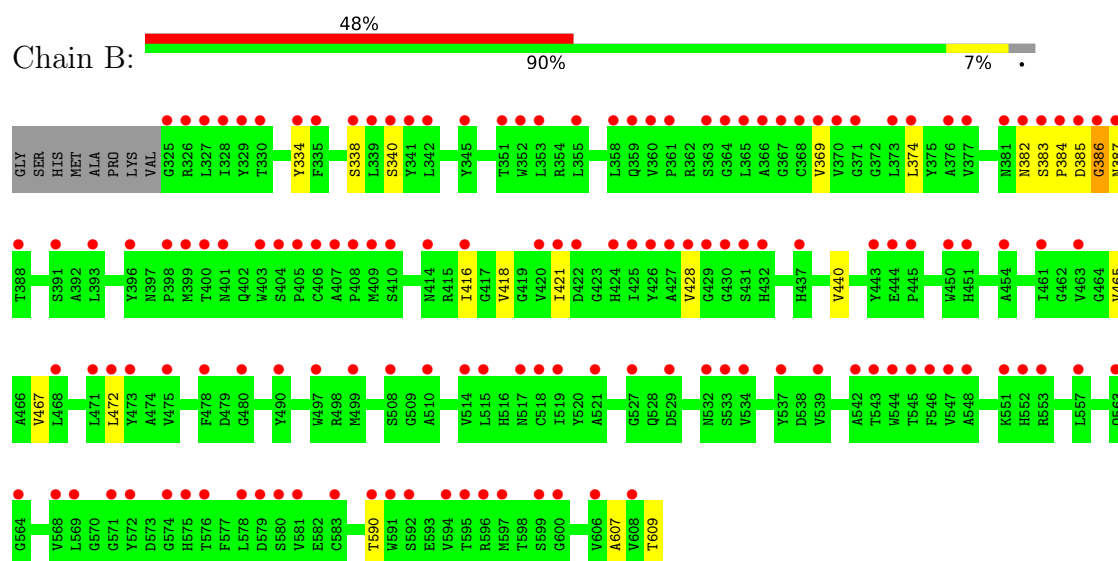
3 Residue-property plots

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.

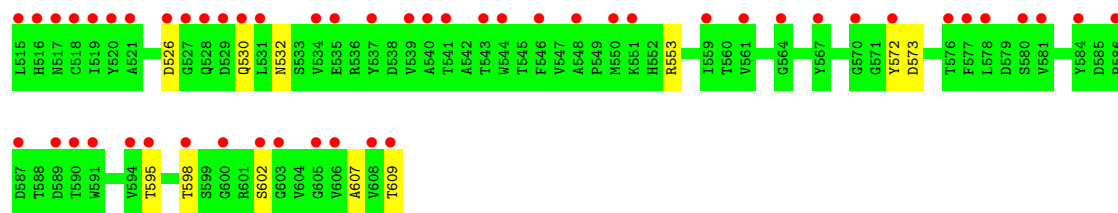
• Molecule 1: Kelch-like ECH-associated protein 1



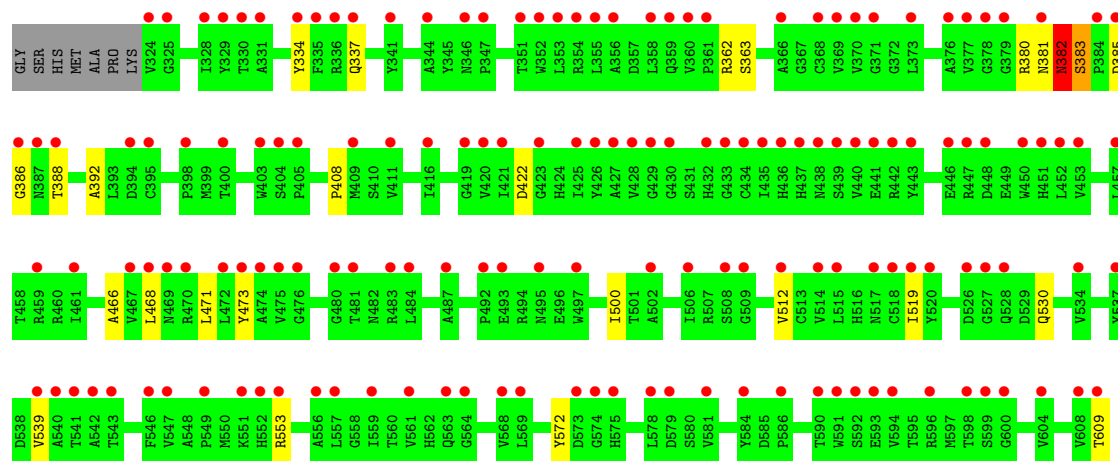
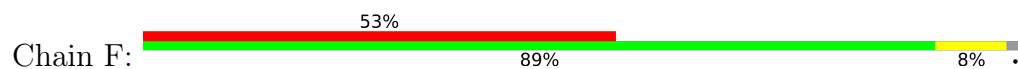
• Molecule 1: Kelch-like ECH-associated protein 1



• Molecule 1: Kelch-like ECH-associated protein 1



● Molecule 1: Kelch-like ECH-associated protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.45Å 91.88Å 112.31Å 90.00° 119.89° 90.00°	Depositor
Resolution (Å)	47.99 – 2.59 47.99 – 2.59	Depositor EDS
% Data completeness (in resolution range)	96.6 (47.99-2.59) 97.2 (47.99-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.175 , 0.225 0.175 , 0.165	Depositor DCC
R_{free} test set	898 reflections (1.46%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.875	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.260 for l,k,-h-l 0.260 for -h-l,k,h 0.296 for -h-l,-k,l 0.238 for h,-k,-h-l 0.358 for l,-k,h	Xtriage
Reported twinning fraction	0.381 for H, K, L 0.152 for H+L, -K, -L 0.231 for L, -K, H 0.110 for L, K, -H-L 0.036 for -H-L, K, H 0.090 for -H, -K, H+L	Depositor
Outliers	4 of 59516 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	13531	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.19% 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: LQK

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	0.58	0/2234	0.81	1/3043 (0.0%)
1	B	0.60	0/2238	0.78	0/3048
1	C	0.59	0/2234	0.83	1/3043 (0.0%)
1	D	0.58	0/2234	0.77	1/3043 (0.0%)
1	E	0.55	0/2234	0.76	0/3043
1	F	0.58	0/2245	0.80	3/3058 (0.1%)
All	All	0.58	0/13419	0.79	6/18278 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	362	ARG	N-CA-C	5.79	117.64	108.79
1	A	554	ARG	N-CA-C	5.75	117.14	108.46
1	F	382	ASN	N-CA-C	5.36	122.20	110.80
1	F	385	ASP	N-CA-C	-5.22	105.50	111.14
1	C	385	ASP	N-CA-C	-5.02	100.28	108.67
1	D	477	GLY	N-CA-C	5.00	117.79	110.63

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	2181	0	2078	44	0
1	B	2185	0	2081	14	0
1	C	2181	0	2078	37	0
1	D	2181	0	2078	33	0
1	E	2181	0	2078	45	0
1	F	2192	0	2090	22	0
2	A	35	0	0	1	0
2	B	35	0	0	0	0
2	C	35	0	0	0	0
2	D	35	0	0	1	0
2	E	35	0	0	0	0
2	F	35	0	0	0	0
3	A	42	0	0	0	0
3	B	27	0	0	0	0
3	C	39	0	0	3	0
3	D	34	0	0	1	0
3	E	41	0	0	1	0
3	F	37	0	0	1	0
All	All	13531	0	12483	183	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 7.

All (183) 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:E:329:TYR:CE1	1:E:344:ALA:HB2	1.86	1.11
1:E:329:TYR:HE1	1:E:344:ALA:HB2	1.42	0.81
1:E:355:LEU:HD23	1:E:396:TYR:OH	1.80	0.81
1:C:422:ASP:OD2	1:C:470:ARG:NH2	2.13	0.80
1:C:385:ASP:HB2	1:D:380:ARG:CZ	2.13	0.78
1:F:337:GLN:NE2	1:F:382:ASN:OD1	2.19	0.74
1:F:572:TYR:OH	3:F:801:HOH:O	2.05	0.74
1:E:329:TYR:CE1	1:E:344:ALA:CB	2.70	0.73
1:E:377:VAL:HG22	1:E:393:LEU:HD13	1.70	0.73
1:C:366:ALA:HB3	1:C:418:VAL:HG23	1.70	0.71
1:C:593:GLU:OE2	1:C:596:ARG:NH2	2.24	0.69
1:E:506:ILE:HB	1:E:526:ASP:HB2	1.74	0.69
1:C:334:TYR:OH	3:C:801:HOH:O	2.11	0.68
1:C:385:ASP:HB2	1:D:380:ARG:NH2	2.09	0.67
1:A:385:ASP:HA	1:B:382:ASN:ND2	2.10	0.67
1:C:385:ASP:N	1:D:380:ARG:HH22	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:530:GLN:O	1:F:553:ARG:NH1	2.29	0.66
1:A:460:ARG:NH1	1:A:486:SER:OG	2.27	0.66
1:D:468:LEU:HD11	1:D:517:ASN:HA	1.78	0.66
1:C:485:ASN:HB3	1:C:506:ILE:HG12	1.79	0.65
1:E:352:TRP:C	1:E:353:LEU:HD12	2.22	0.65
1:E:369:VAL:HG23	1:E:607:ALA:HB1	1.79	0.64
1:B:369:VAL:HG23	1:B:607:ALA:HB1	1.81	0.63
1:C:366:ALA:HB3	1:C:418:VAL:CG2	2.29	0.63
1:E:355:LEU:HD23	1:E:396:TYR:CZ	2.34	0.63
1:E:385:ASP:HA	1:F:380:ARG:HH21	1.63	0.62
1:A:383:SER:HB3	1:A:385:ASP:H	1.65	0.62
1:C:366:ALA:CB	1:C:418:VAL:HG23	2.29	0.62
1:C:525:TYR:OH	3:C:802:HOH:O	2.12	0.62
1:C:505:THR:HG21	3:C:831:HOH:O	2.00	0.62
1:A:383:SER:HB3	1:A:385:ASP:N	2.15	0.61
1:C:468:LEU:HD11	1:C:517:ASN:HA	1.82	0.61
1:D:424:HIS:CD2	1:D:444:GLU:HB3	2.36	0.61
1:B:428:VAL:HG22	1:B:440:VAL:HG13	1.84	0.60
1:D:380:ARG:NE	1:D:388:THR:OG1	2.34	0.60
1:E:385:ASP:HA	1:F:380:ARG:NH2	2.17	0.60
1:A:339:LEU:HD12	1:A:601:ARG:HD3	1.84	0.59
1:A:385:ASP:HB3	1:B:334:TYR:OH	2.04	0.58
1:E:374:LEU:HD13	1:E:607:ALA:HB3	1.85	0.58
1:D:576:THR:HG22	1:D:577:PHE:H	1.69	0.58
1:C:384:PRO:C	1:D:380:ARG:HH12	2.12	0.57
1:F:468:LEU:CD1	1:F:539:VAL:HG21	2.35	0.57
1:C:431:SER:HB3	1:C:461:ILE:HG21	1.85	0.57
1:C:505:THR:OG1	1:C:535:GLU:OE2	2.22	0.57
1:C:466:ALA:HB1	1:C:514:VAL:HG23	1.85	0.57
1:A:582:GLU:HG2	1:A:593:GLU:HG2	1.87	0.56
1:E:382:ASN:O	1:E:382:ASN:ND2	2.38	0.56
1:F:382:ASN:HD22	1:F:383:SER:H	1.54	0.56
1:A:330:THR:HG23	1:A:604:VAL:HB	1.88	0.56
1:A:441:GLU:HG3	1:A:450:TRP:CE3	2.41	0.55
1:B:374:LEU:HD13	1:B:607:ALA:HB3	1.89	0.55
1:F:382:ASN:ND2	1:F:383:SER:H	2.04	0.55
1:E:530:GLN:HG2	1:E:573:ASP:HA	1.89	0.55
1:D:333:GLY:O	1:D:363:SER:HB3	2.06	0.55
1:A:512:VAL:HG13	1:A:520:TYR:O	2.07	0.55
1:F:337:GLN:HE21	1:F:382:ASN:CB	2.20	0.55
1:A:383:SER:CB	1:A:384:PRO:HA	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:572:TYR:CE2	1:C:574:GLY:HA2	2.43	0.54
1:E:335:PHE:CD2	1:E:336:ARG:HG2	2.42	0.54
1:E:377:VAL:CG2	1:E:393:LEU:HD13	2.38	0.54
1:A:361:PRO:HG2	1:A:382:ASN:HB2	1.89	0.54
1:E:530:GLN:N	1:E:530:GLN:OE1	2.40	0.54
1:A:384:PRO:O	1:B:382:ASN:ND2	2.40	0.54
1:C:493:GLU:N	1:C:493:GLU:OE2	2.40	0.53
1:A:588:THR:HG21	1:D:387:ASN:ND2	2.23	0.53
1:C:412:PRO:O	1:C:432:HIS:HB2	2.09	0.53
1:C:387:ASN:N	1:C:387:ASN:OD1	2.42	0.52
1:A:385:ASP:HA	1:B:382:ASN:HD21	1.71	0.52
1:C:416:ILE:HG12	1:C:417:GLY:N	2.24	0.52
1:A:551:LYS:NZ	1:C:576:THR:OG1	2.43	0.52
1:E:343:GLU:OE2	1:E:598:THR:HG21	2.10	0.52
1:E:380:ARG:HG2	1:E:388:THR:HB	1.92	0.51
1:D:460:ARG:NH1	1:D:484:LEU:HD13	2.25	0.51
1:D:381:ASN:N	1:D:388:THR:O	2.44	0.51
1:A:369:VAL:HG23	1:A:607:ALA:HB1	1.92	0.51
1:F:468:LEU:HD23	1:F:468:LEU:O	2.10	0.50
1:C:335:PHE:O	1:C:336:ARG:HB3	2.11	0.50
1:E:483:ARG:NH2	3:E:801:HOH:O	2.44	0.50
1:B:385:ASP:OD1	1:B:386:GLY:N	2.45	0.50
1:E:329:TYR:CD1	1:E:344:ALA:HB2	2.40	0.49
1:D:430:GLY:O	1:D:461:ILE:HG22	2.12	0.49
1:A:397:ASN:O	1:A:401:ASN:N	2.43	0.49
1:E:327:LEU:HD23	1:E:345:TYR:O	2.12	0.49
1:D:575:HIS:N	1:D:575:HIS:CD2	2.81	0.49
1:D:438:ASN:HB3	1:D:459:ARG:HG2	1.95	0.49
1:A:604:VAL:HG23	1:A:606:VAL:HG23	1.95	0.49
1:C:421:ILE:HD11	1:C:472:LEU:HB2	1.95	0.49
1:D:377:VAL:HG22	1:D:393:LEU:HD12	1.95	0.49
1:E:334:TYR:N	1:E:602:SER:O	2.45	0.48
1:B:428:VAL:HG21	1:B:472:LEU:HD21	1.95	0.48
1:E:369:VAL:HG23	1:E:607:ALA:CB	2.43	0.48
1:A:554:ARG:NH2	1:A:582:GLU:OE2	2.47	0.48
1:A:334:TYR:HB2	1:A:363:SER:CB	2.42	0.48
1:D:443:TYR:OH	1:D:448:ASP:OD1	2.22	0.48
1:A:578:LEU:HD22	1:A:580:SER:HB3	1.93	0.48
1:D:443:TYR:HA	1:D:449:GLU:O	2.13	0.48
1:E:466:ALA:HB1	1:E:514:VAL:HG23	1.95	0.48
1:A:369:VAL:HG11	1:A:609:THR:CG2	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:THR:OG1	1:A:596:ARG:N	2.47	0.48
1:F:380:ARG:CZ	1:F:388:THR:HG21	2.43	0.48
1:D:446:GLU:O	1:D:447:ARG:HB2	2.14	0.48
1:E:530:GLN:HG2	1:E:572:TYR:O	2.13	0.47
1:C:369:VAL:HG21	1:C:609:THR:HB	1.96	0.47
1:E:389:ASP:OD2	1:E:433:GLY:N	2.47	0.47
1:E:327:LEU:HD21	1:E:346:ASN:HB2	1.96	0.47
1:E:369:VAL:HG11	1:E:609:THR:HB	1.96	0.47
1:D:600:GLY:HA3	3:D:830:HOH:O	2.14	0.47
1:E:380:ARG:HG2	1:E:388:THR:CB	2.44	0.47
1:F:468:LEU:HD21	1:F:473:TYR:CE1	2.48	0.47
1:B:421:ILE:HD11	1:B:472:LEU:HB2	1.96	0.47
1:D:380:ARG:CZ	1:D:388:THR:OG1	2.62	0.47
1:A:339:LEU:HB3	1:A:341:TYR:CD2	2.50	0.47
1:F:468:LEU:HD13	1:F:519:ILE:HD11	1.96	0.47
1:E:506:ILE:O	1:E:526:ASP:HB3	2.15	0.47
1:A:365:LEU:O	2:A:701:LQK:O24	2.32	0.46
1:A:369:VAL:HG11	1:A:609:THR:HG21	1.97	0.46
1:C:338:SER:HB2	1:C:382:ASN:HD22	1.79	0.46
1:C:352:TRP:NE1	1:C:596:ARG:O	2.48	0.46
1:E:532:ASN:OD1	1:E:553:ARG:NH1	2.49	0.46
1:C:381:ASN:N	1:C:388:THR:O	2.43	0.46
1:C:385:ASP:C	1:C:387:ASN:N	2.73	0.46
1:D:554:ARG:HA	1:D:573:ASP:HA	1.97	0.45
1:A:559:ILE:HG13	1:A:568:VAL:HG12	1.99	0.45
1:C:374:LEU:CD1	1:C:607:ALA:HB3	2.47	0.45
1:A:339:LEU:HB3	1:A:341:TYR:CE2	2.52	0.45
1:F:468:LEU:HD11	1:F:539:VAL:HG21	1.98	0.45
1:C:560:THR:HG21	1:C:608:VAL:HG23	1.99	0.45
1:E:353:LEU:HD12	1:E:353:LEU:N	2.32	0.45
1:D:383:SER:N	1:D:384:PRO:HA	2.32	0.45
1:F:468:LEU:HD22	1:F:473:TYR:CD1	2.52	0.45
1:D:335:PHE:C	1:D:337:GLN:H	2.25	0.44
1:F:468:LEU:HD21	1:F:473:TYR:HE1	1.81	0.44
1:A:396:TYR:OH	1:A:401:ASN:ND2	2.50	0.44
1:E:335:PHE:CE2	1:E:336:ARG:HG2	2.53	0.44
1:B:467:VAL:CG2	1:B:472:LEU:HD12	2.48	0.44
1:C:465:VAL:HG11	1:C:472:LEU:HD11	1.99	0.44
1:D:362:ARG:NH1	1:D:390:SER:OG	2.50	0.44
1:D:383:SER:HB3	1:D:384:PRO:C	2.42	0.44
1:E:381:ASN:OD1	1:E:382:ASN:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:468:LEU:HD23	1:F:468:LEU:H	1.83	0.43
1:A:335:PHE:C	1:A:337:GLN:H	2.25	0.43
2:D:701:LQK:C10	2:D:701:LQK:C29	2.96	0.43
1:E:382:ASN:O	1:E:383:SER:C	2.61	0.43
1:F:473:TYR:HE2	1:F:500:ILE:HD13	1.84	0.43
1:E:338:SER:HB2	1:E:382:ASN:HB2	2.01	0.43
1:A:340:SER:O	1:A:358:LEU:N	2.46	0.43
1:A:580:SER:OG	1:A:593:GLU:OE2	2.29	0.43
1:D:576:THR:HG22	1:D:577:PHE:N	2.33	0.43
1:E:340:SER:OG	1:E:361:PRO:HG3	2.19	0.43
1:A:334:TYR:HB2	1:A:363:SER:HB3	2.01	0.42
1:E:366:ALA:HB1	1:E:418:VAL:CG1	2.49	0.42
1:A:370:VAL:HG22	1:A:420:VAL:HG11	2.01	0.42
1:A:467:VAL:O	1:A:514:VAL:HG21	2.19	0.42
1:E:385:ASP:CB	1:F:334:TYR:HE2	2.31	0.42
1:A:374:LEU:CD1	1:A:607:ALA:HB3	2.50	0.42
1:F:334:TYR:HB2	1:F:363:SER:CB	2.49	0.42
1:B:465:VAL:CG1	1:B:472:LEU:HD11	2.50	0.42
1:A:569:LEU:HD23	1:A:597:MET:HE3	2.02	0.42
1:B:338:SER:OG	1:B:382:ASN:HB2	2.19	0.42
1:F:392:ALA:HA	1:F:408:PRO:HB3	2.01	0.41
1:D:416:ILE:HG12	1:D:417:GLY:N	2.35	0.41
1:E:345:TYR:CE1	1:E:595:THR:HG21	2.56	0.41
1:F:466:ALA:HB2	1:F:512:VAL:HG12	2.03	0.41
1:D:383:SER:HB3	1:D:385:ASP:O	2.19	0.41
1:A:557:LEU:HD12	1:A:568:VAL:HB	2.01	0.41
1:C:385:ASP:O	1:C:386:GLY:C	2.64	0.41
1:A:381:ASN:HB2	1:A:388:THR:CG2	2.50	0.41
1:D:443:TYR:HB2	1:D:450:TRP:CE3	2.55	0.41
1:A:383:SER:HB3	1:A:384:PRO:CA	2.51	0.41
1:D:335:PHE:HA	1:D:577:PHE:CE1	2.55	0.41
1:B:338:SER:CB	1:B:382:ASN:HB2	2.51	0.41
1:D:384:PRO:O	1:D:385:ASP:CB	2.69	0.41
1:D:463:VAL:HG23	1:D:476:GLY:O	2.21	0.41
1:E:466:ALA:CB	1:E:514:VAL:HG23	2.51	0.41
1:E:468:LEU:HB2	1:E:514:VAL:HG21	2.03	0.41
1:E:530:GLN:O	1:E:553:ARG:HD3	2.21	0.41
1:C:504:ASN:OD1	1:C:504:ASN:N	2.53	0.41
1:A:330:THR:HG23	1:A:604:VAL:CB	2.50	0.40
1:A:533:SER:HA	1:A:549:PRO:HB3	2.03	0.40
1:C:385:ASP:HB3	1:C:386:GLY:H	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:GLN:O	1:E:339:LEU:HD13	2.21	0.40
1:A:485:ASN:HA	1:A:503:MET:HE3	2.03	0.40
1:C:416:ILE:HD11	1:C:427:ALA:HB1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	282/293 (96%)	262 (93%)	16 (6%)	4 (1%)	9	19
1	B	283/293 (97%)	265 (94%)	15 (5%)	3 (1%)	11	25
1	C	282/293 (96%)	263 (93%)	18 (6%)	1 (0%)	30	51
1	D	282/293 (96%)	258 (92%)	21 (7%)	3 (1%)	11	25
1	E	282/293 (96%)	258 (92%)	22 (8%)	2 (1%)	18	38
1	F	284/293 (97%)	265 (93%)	16 (6%)	3 (1%)	11	25
All	All	1695/1758 (96%)	1571 (93%)	108 (6%)	16 (1%)	14	30

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	SER
1	B	383	SER
1	C	381	ASN
1	B	386	GLY
1	D	481	THR
1	E	335	PHE
1	F	382	ASN
1	D	385	ASP
1	E	341	TYR

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Mol	Chain	Res	Type
1	F	381	ASN
1	D	574	GLY
1	A	527	GLY
1	B	384	PRO
1	F	386	GLY
1	A	500	ILE
1	A	384	PRO

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	229/235 (97%)	217 (95%)	12 (5%)	21	44
1	B	229/235 (97%)	223 (97%)	6 (3%)	40	68
1	C	229/235 (97%)	211 (92%)	18 (8%)	11	26
1	D	229/235 (97%)	220 (96%)	9 (4%)	28	55
1	E	229/235 (97%)	225 (98%)	4 (2%)	53	78
1	F	230/235 (98%)	225 (98%)	5 (2%)	45	72
All	All	1375/1410 (98%)	1321 (96%)	54 (4%)	28	55

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	SER
1	A	382	ASN
1	A	387	ASN
1	A	399	MET
1	A	418	VAL
1	A	431	SER
1	A	441	GLU
1	A	458	THR
1	A	481	THR
1	A	498	ARG
1	A	505	THR

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Mol	Chain	Res	Type
1	A	609	THR
1	B	340	SER
1	B	387	ASN
1	B	416	ILE
1	B	418	VAL
1	B	590	THR
1	B	609	THR
1	C	330	THR
1	C	353	LEU
1	C	365	LEU
1	C	382	ASN
1	C	387	ASN
1	C	418	VAL
1	C	421	ILE
1	C	458	THR
1	C	463	VAL
1	C	481	THR
1	C	485	ASN
1	C	504	ASN
1	C	505	THR
1	C	517	ASN
1	C	530	GLN
1	C	593	GLU
1	C	596	ARG
1	C	604	VAL
1	D	340	SER
1	D	418	VAL
1	D	444	GLU
1	D	448	ASP
1	D	458	THR
1	D	461	ILE
1	D	493	GLU
1	D	530	GLN
1	D	604	VAL
1	E	327	LEU
1	E	339	LEU
1	E	394	ASP
1	E	495	ASN
1	F	382	ASN
1	F	383	SER
1	F	422	ASP
1	F	471	LEU

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Mol	Chain	Res	Type
1	F	609	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	ASN
1	A	401	ASN
1	A	432	HIS
1	A	469	ASN
1	B	382	ASN
1	B	387	ASN
1	B	401	ASN
1	B	451	HIS
1	B	495	ASN
1	B	575	HIS
1	C	359	GLN
1	C	382	ASN
1	C	424	HIS
1	C	485	ASN
1	C	562	HIS
1	D	382	ASN
1	D	424	HIS
1	D	517	ASN
1	D	575	HIS
1	E	382	ASN
1	E	387	ASN
1	E	482	ASN
1	E	528	GLN
1	E	575	HIS
1	F	337	GLN
1	F	382	ASN
1	F	552	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	LQK	B	701	-	38,39,39	1.16	2 (5%)	51,57,57	1.58	14 (27%)
2	LQK	A	701	-	38,39,39	1.05	2 (5%)	51,57,57	1.73	12 (23%)
2	LQK	E	701	-	38,39,39	1.08	2 (5%)	51,57,57	1.50	13 (25%)
2	LQK	D	701	-	38,39,39	1.08	2 (5%)	51,57,57	1.57	14 (27%)
2	LQK	F	701	-	38,39,39	1.02	2 (5%)	51,57,57	1.53	13 (25%)
2	LQK	C	701	-	38,39,39	1.11	2 (5%)	51,57,57	1.54	12 (23%)

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	LQK	B	701	-	-	3/19/58/58	0/5/5/5
2	LQK	A	701	-	-	4/19/58/58	0/5/5/5
2	LQK	E	701	-	-	4/19/58/58	0/5/5/5
2	LQK	D	701	-	-	5/19/58/58	0/5/5/5
2	LQK	F	701	-	-	3/19/58/58	0/5/5/5
2	LQK	C	701	-	-	5/19/58/58	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	LQK	C37-N28	-4.36	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	LQK	C37-N28	-4.31	1.34	1.39
2	C	701	LQK	C37-N28	-4.23	1.34	1.39
2	F	701	LQK	C37-N28	-3.76	1.35	1.39
2	C	701	LQK	C29-N28	-3.69	1.35	1.39
2	D	701	LQK	C37-N28	-3.66	1.35	1.39
2	A	701	LQK	C37-N28	-3.65	1.35	1.39
2	A	701	LQK	C29-N28	-3.51	1.35	1.39
2	B	701	LQK	C29-N28	-3.46	1.35	1.39
2	D	701	LQK	C29-N28	-3.36	1.35	1.39
2	F	701	LQK	C29-N28	-3.35	1.35	1.39
2	E	701	LQK	C29-N28	-3.07	1.36	1.39

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	LQK	C31-C29-N28	4.07	108.89	105.88
2	C	701	LQK	O21-C20-C15	3.87	121.15	115.75
2	F	701	LQK	C31-C29-N28	3.61	108.55	105.88
2	A	701	LQK	C36-C37-N28	3.60	108.54	105.88
2	A	701	LQK	C7-C6-C4	-3.58	85.35	88.94
2	C	701	LQK	C36-C37-N28	3.33	108.35	105.88
2	D	701	LQK	C36-C37-N28	3.32	108.34	105.88
2	D	701	LQK	C4-C2-N1	3.30	121.15	116.42
2	A	701	LQK	C35-C36-C37	3.25	135.04	129.59
2	D	701	LQK	C31-C29-N28	3.23	108.27	105.88
2	E	701	LQK	O21-C20-C15	3.15	120.14	115.75
2	C	701	LQK	C31-C29-N28	3.11	108.18	105.88
2	F	701	LQK	C35-C36-C37	3.10	134.80	129.59
2	F	701	LQK	C36-C37-N28	3.10	108.17	105.88
2	D	701	LQK	O30-C29-N28	3.08	127.91	124.79
2	B	701	LQK	C32-C31-C29	3.04	134.69	129.59
2	D	701	LQK	O21-C20-C15	2.95	119.86	115.75
2	C	701	LQK	C32-C31-C29	2.94	134.52	129.59
2	A	701	LQK	O30-C29-N28	2.91	127.73	124.79
2	E	701	LQK	C36-C37-N28	2.87	108.01	105.88
2	A	701	LQK	C22-O21-C20	2.87	124.61	117.69
2	B	701	LQK	C36-C37-N28	2.82	107.97	105.88
2	C	701	LQK	C35-C36-C37	2.80	134.29	129.59
2	A	701	LQK	C31-C36-C37	-2.78	105.83	108.26
2	A	701	LQK	O30-C29-C31	-2.73	123.37	128.66
2	D	701	LQK	C35-C36-C37	2.73	134.16	129.59
2	E	701	LQK	O30-C29-N28	2.71	127.53	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	LQK	C4-C2-N1	2.68	120.26	116.42
2	D	701	LQK	O3-C2-N1	-2.67	118.33	123.04
2	B	701	LQK	C22-O21-C20	2.67	124.12	117.69
2	C	701	LQK	O3-C2-N1	-2.66	118.34	123.04
2	E	701	LQK	C31-C29-N28	2.64	107.84	105.88
2	E	701	LQK	C32-C31-C29	2.63	134.01	129.59
2	A	701	LQK	C8-C10-N12	2.62	123.55	118.85
2	C	701	LQK	C31-C36-C37	-2.61	105.97	108.26
2	F	701	LQK	C31-C36-C37	-2.59	105.99	108.26
2	D	701	LQK	C31-C36-C37	-2.57	106.01	108.26
2	E	701	LQK	C35-C36-C37	2.56	133.88	129.59
2	E	701	LQK	C36-C31-C29	-2.53	106.04	108.26
2	D	701	LQK	O30-C29-C31	-2.51	123.79	128.66
2	B	701	LQK	C36-C31-C29	-2.49	106.08	108.26
2	B	701	LQK	O30-C29-N28	2.48	127.30	124.79
2	C	701	LQK	C36-C31-C29	-2.46	106.11	108.26
2	B	701	LQK	C7-C6-C4	-2.45	86.48	88.94
2	E	701	LQK	C7-C6-C4	-2.41	86.53	88.94
2	F	701	LQK	C14-C13-N12	-2.37	106.18	109.40
2	F	701	LQK	C32-C31-C29	2.37	133.57	129.59
2	F	701	LQK	C36-C31-C29	-2.37	106.19	108.26
2	E	701	LQK	O3-C2-N1	-2.35	118.89	123.04
2	B	701	LQK	C4-C2-N1	2.34	119.78	116.42
2	D	701	LQK	C32-C31-C29	2.33	133.50	129.59
2	F	701	LQK	O3-C2-N1	-2.33	118.93	123.04
2	E	701	LQK	C14-C13-N12	-2.30	106.28	109.40
2	A	701	LQK	C32-C31-C29	2.30	133.45	129.59
2	C	701	LQK	O21-C20-C19	-2.28	118.97	123.95
2	A	701	LQK	C36-C31-C29	-2.26	106.28	108.26
2	D	701	LQK	O11-C10-C8	-2.25	117.88	121.85
2	D	701	LQK	C36-C31-C29	-2.25	106.29	108.26
2	C	701	LQK	O11-C10-C8	-2.24	117.90	121.85
2	B	701	LQK	C17-C16-C15	2.22	122.04	119.33
2	F	701	LQK	C7-C8-C10	-2.22	112.38	117.94
2	F	701	LQK	O30-C29-N28	2.20	127.02	124.79
2	F	701	LQK	O30-C29-C31	-2.19	124.42	128.66
2	B	701	LQK	C31-C36-C37	-2.18	106.35	108.26
2	E	701	LQK	C31-C36-C37	-2.14	106.38	108.26
2	C	701	LQK	C7-C8-C10	-2.14	112.57	117.94
2	E	701	LQK	O11-C10-C8	-2.14	118.08	121.85
2	F	701	LQK	O11-C10-C8	-2.12	118.10	121.85
2	E	701	LQK	O30-C29-C31	-2.08	124.63	128.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	LQK	O38-C37-N28	2.08	126.89	124.79
2	B	701	LQK	C7-C8-C10	-2.08	112.73	117.94
2	B	701	LQK	O3-C2-N1	-2.07	119.38	123.04
2	A	701	LQK	O11-C10-C8	-2.07	118.19	121.85
2	D	701	LQK	C6-C7-C8	-2.04	86.90	88.94
2	F	701	LQK	O21-C20-C15	2.03	118.58	115.75
2	B	701	LQK	C35-C36-C37	2.03	132.99	129.59
2	B	701	LQK	C27-N28-C37	-2.01	121.42	123.97
2	D	701	LQK	O38-C37-N28	2.00	126.82	124.79

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	701	LQK	O21-C22-C23-O24
2	F	701	LQK	O21-C22-C23-O24
2	D	701	LQK	O21-C22-C23-O24
2	B	701	LQK	C23-C22-O21-C20
2	A	701	LQK	O11-C10-C8-C4
2	C	701	LQK	O11-C10-C8-C4
2	D	701	LQK	O11-C10-C8-C4
2	C	701	LQK	N12-C10-C8-C4
2	D	701	LQK	N12-C10-C8-C4
2	F	701	LQK	C19-C20-O21-C22
2	D	701	LQK	C19-C20-O21-C22
2	A	701	LQK	O21-C22-C23-O24
2	C	701	LQK	C19-C20-O21-C22
2	E	701	LQK	C19-C20-O21-C22
2	F	701	LQK	C15-C20-O21-C22
2	A	701	LQK	C23-C22-O21-C20
2	D	701	LQK	C15-C20-O21-C22
2	C	701	LQK	C15-C20-O21-C22
2	E	701	LQK	C15-C20-O21-C22
2	B	701	LQK	O11-C10-C8-C4
2	E	701	LQK	O11-C10-C8-C4
2	A	701	LQK	N12-C10-C8-C4
2	B	701	LQK	N12-C10-C8-C4
2	E	701	LQK	N12-C10-C8-C4

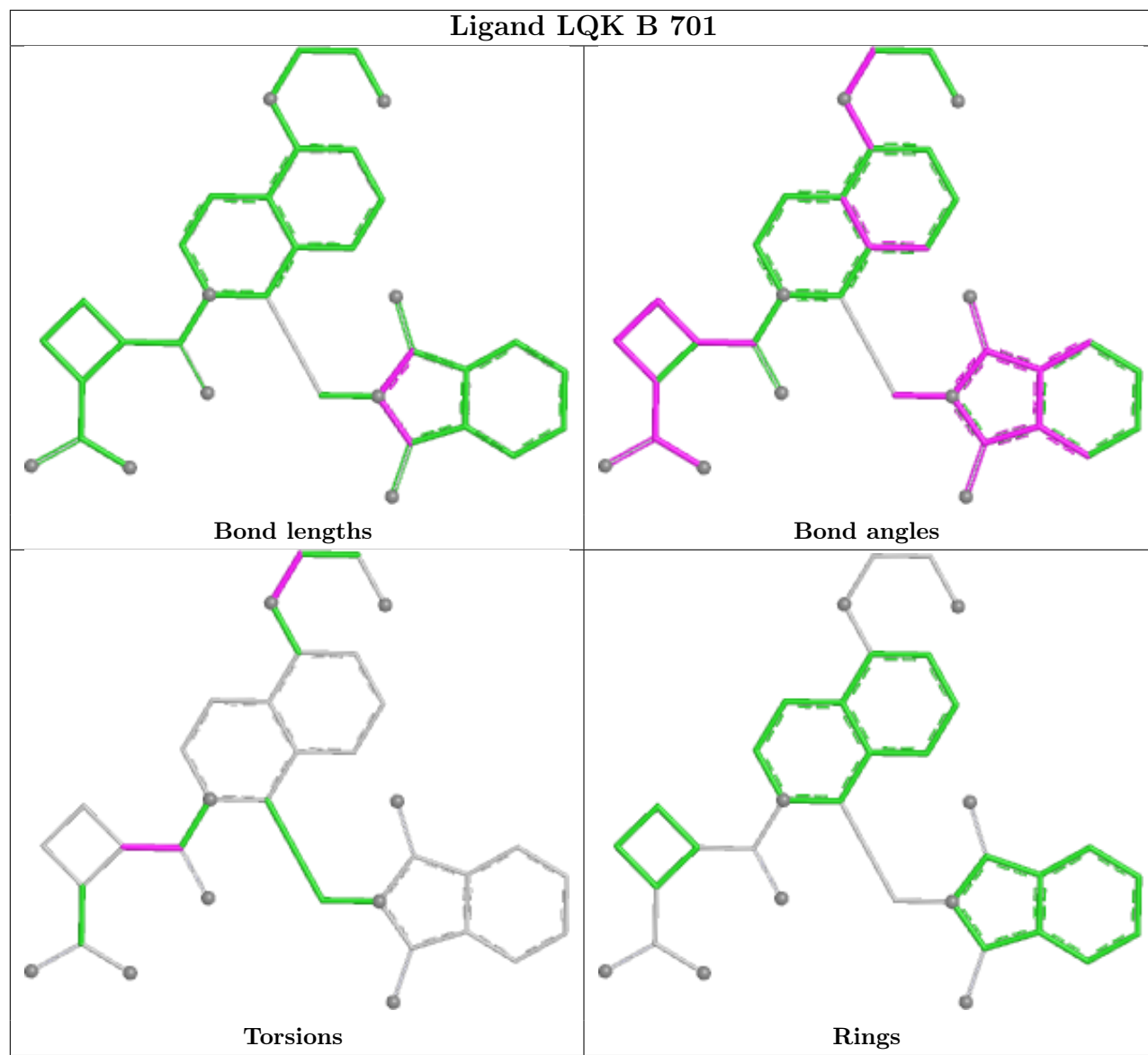
There are no ring outliers.

2 monomers are involved in 2 short contacts:

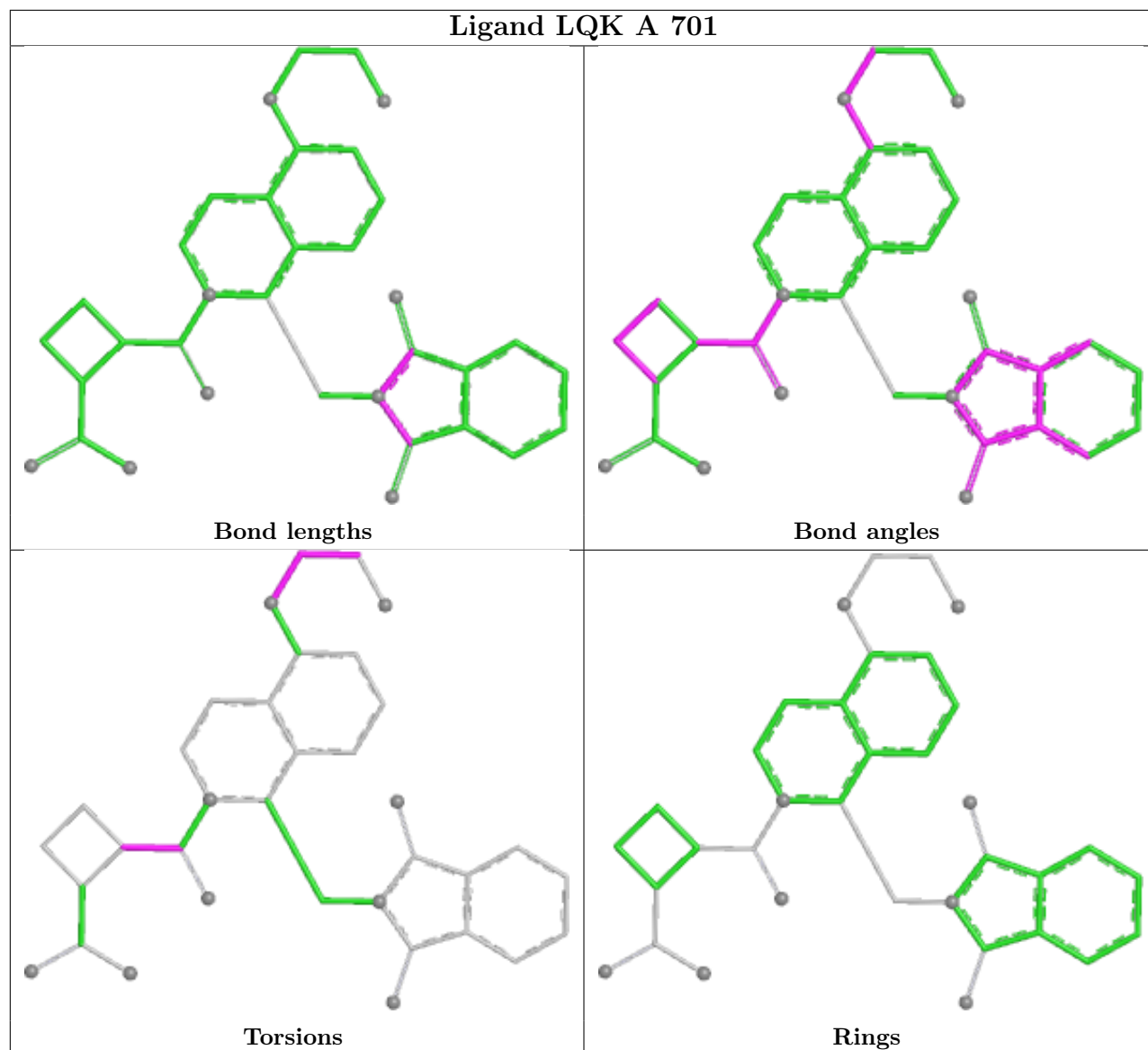
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	LQK	1	0
2	D	701	LQK	1	0

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.

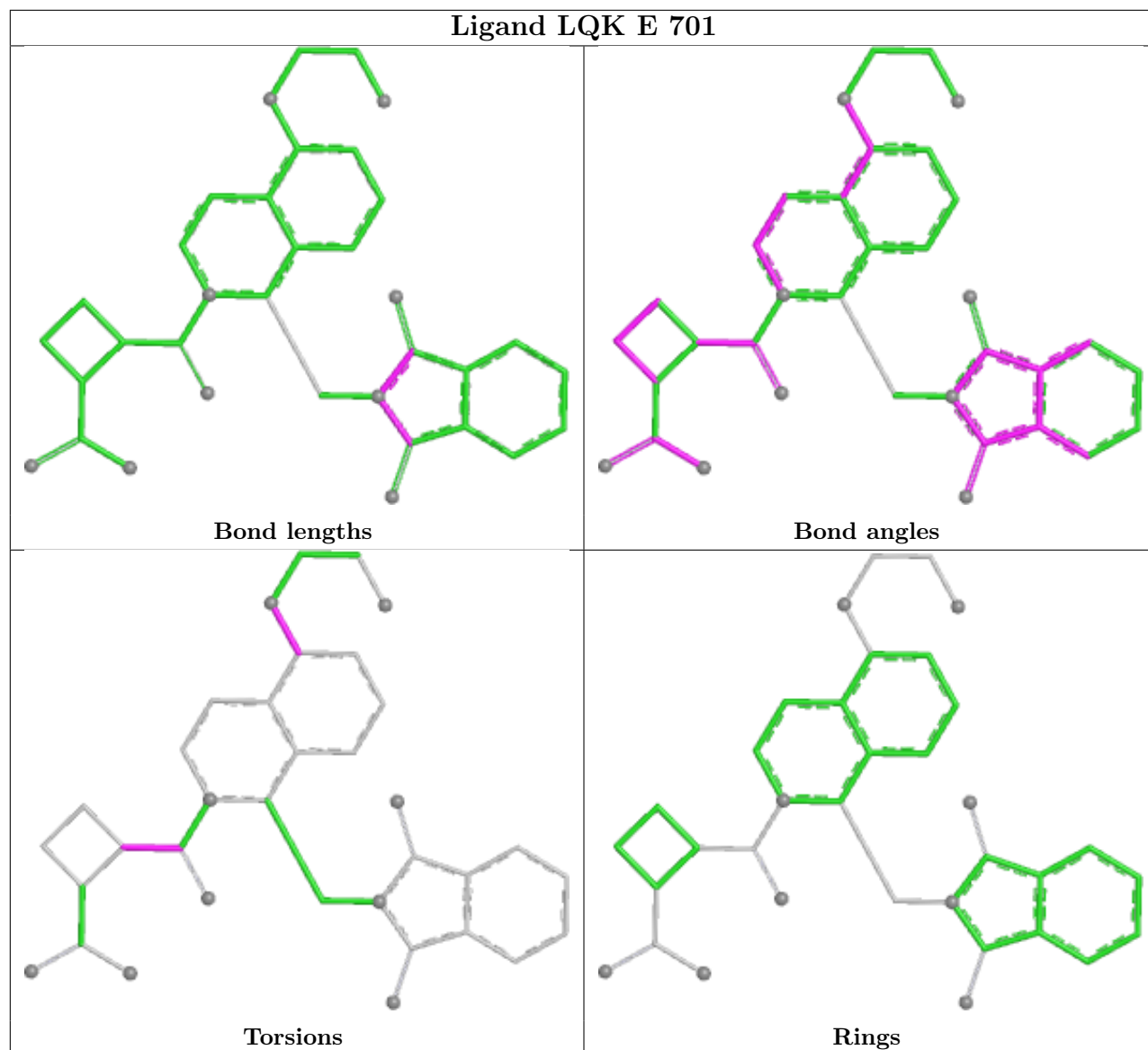
Ligand LQK B 701

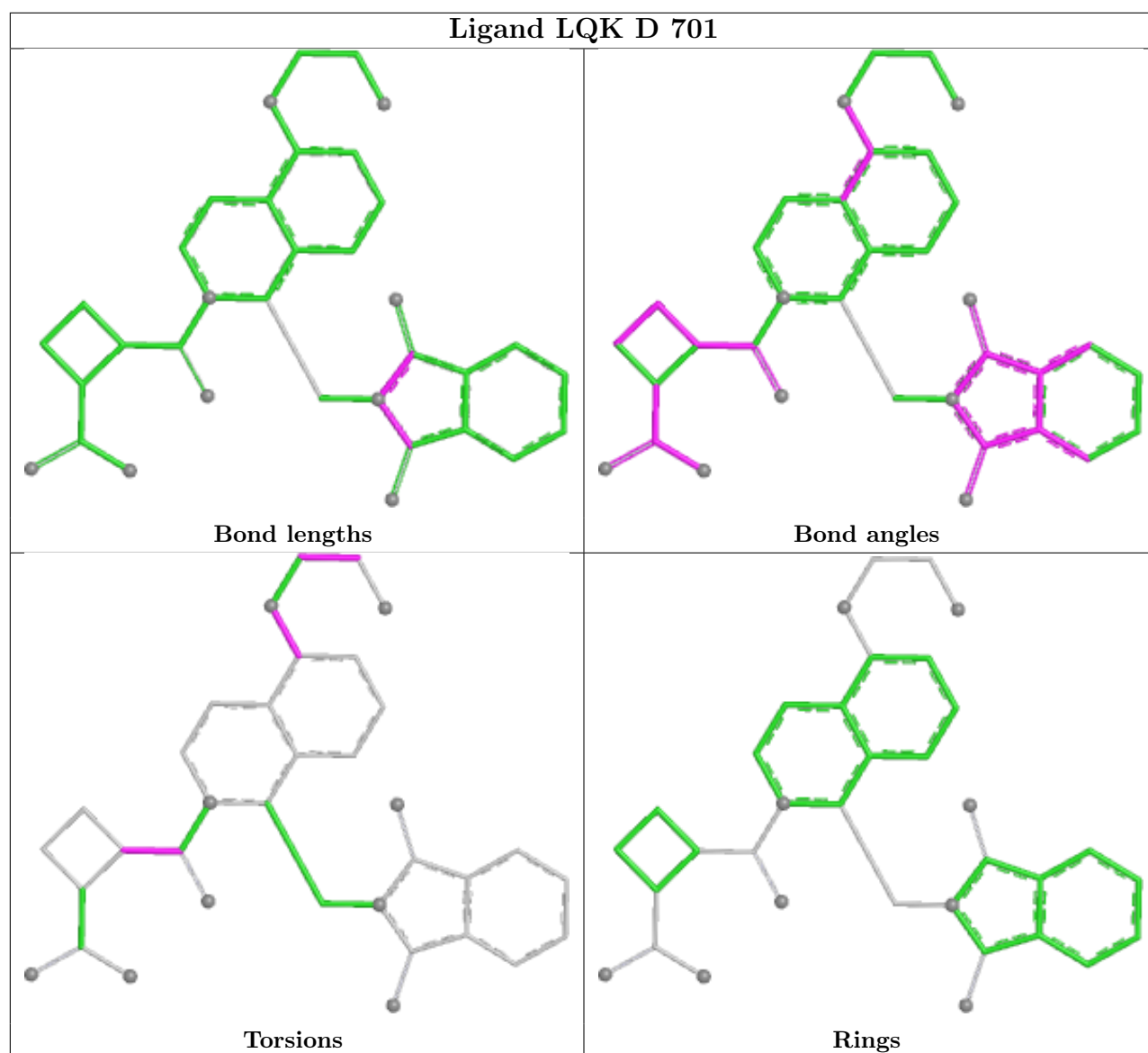


Ligand LQK A 701

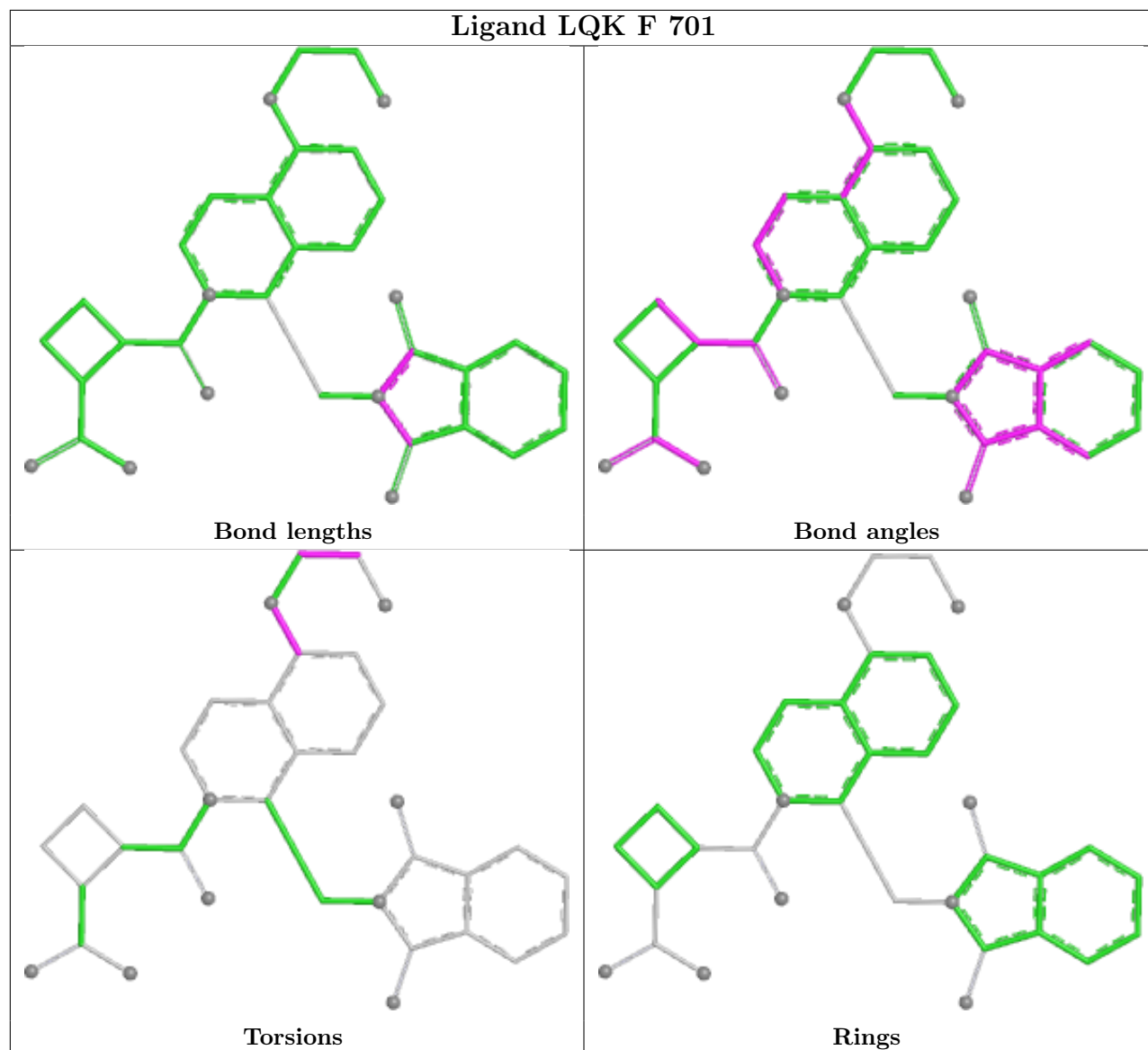


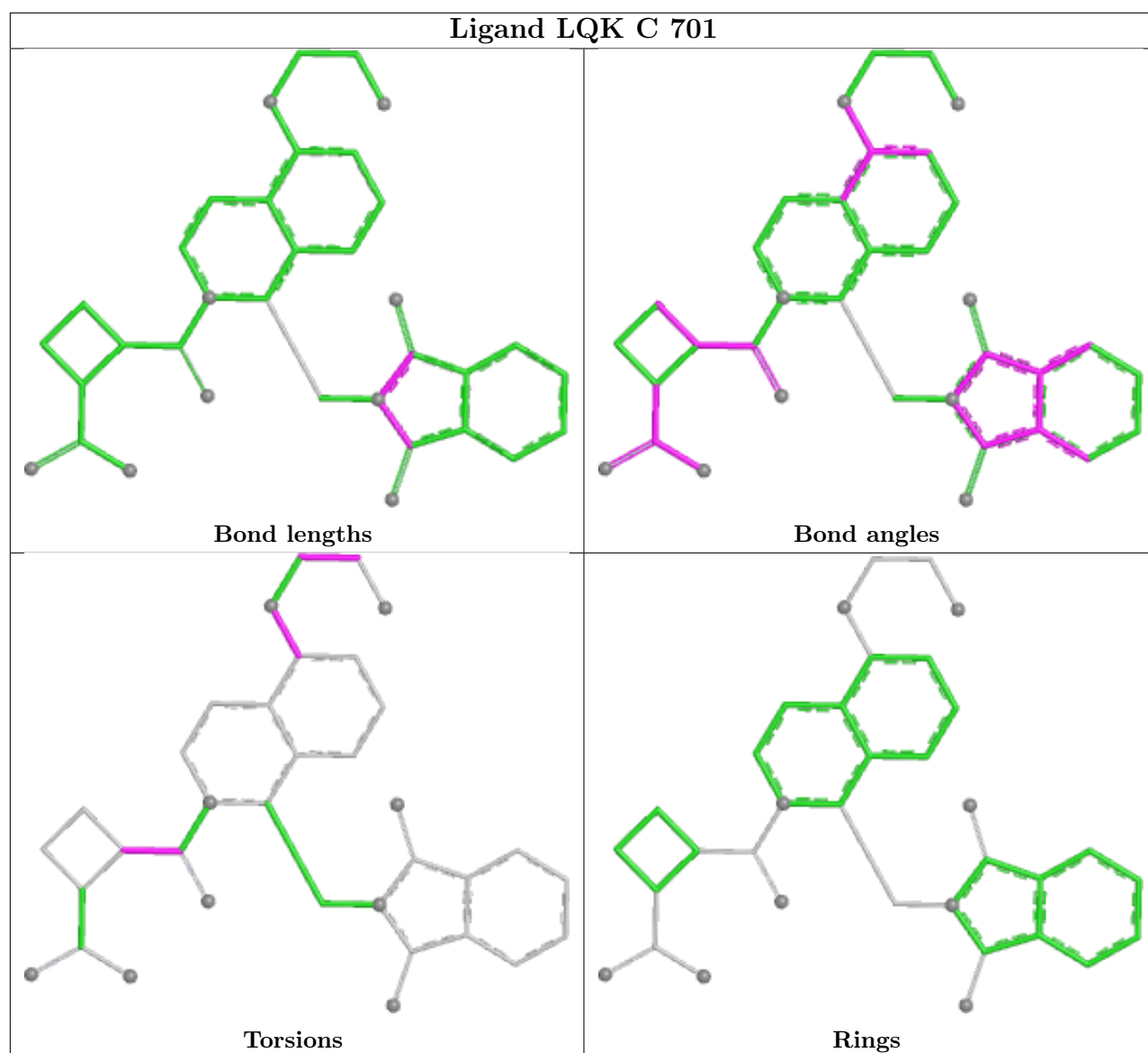
Ligand LQK E 701





Ligand LQK F 701





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	284/293 (96%)	1.72	100 (35%) 1 1	8, 53, 88, 121	0
1	B	285/293 (97%)	2.19	142 (49%) 0 0	15, 65, 98, 129	0
1	C	284/293 (96%)	1.73	103 (36%) 1 0	12, 54, 82, 109	0
1	D	284/293 (96%)	2.24	155 (54%) 0 0	24, 66, 96, 112	0
1	E	284/293 (96%)	2.55	186 (65%) 0 0	36, 75, 106, 130	0
1	F	286/293 (97%)	2.24	155 (54%) 0 0	31, 68, 95, 137	0
All	All	1707/1758 (97%)	2.11	841 (49%) 0 0	8, 63, 98, 137	0

All (841) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	514	VAL	8.4
1	E	461	ILE	8.1
1	D	502	ALA	7.6
1	D	446	GLU	7.1
1	A	398	PRO	6.8
1	F	420	VAL	6.6
1	D	381	ASN	6.3
1	E	431	SER	6.2
1	E	514	VAL	5.9
1	E	329	TYR	5.7
1	B	329	TYR	5.6
1	F	423	GLY	5.6
1	B	387	ASN	5.6
1	A	386	GLY	5.5
1	D	570	GLY	5.5
1	E	502	ALA	5.5
1	E	372	GLY	5.5
1	D	575	HIS	5.5
1	F	421	ILE	5.4

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Mol	Chain	Res	Type	RSRZ
1	F	369	VAL	5.4
1	D	423	GLY	5.4
1	E	384	PRO	5.3
1	B	421	ILE	5.2
1	E	335	PHE	5.1
1	B	444	GLU	5.1
1	C	384	PRO	5.1
1	A	352	TRP	5.1
1	E	511	GLY	5.1
1	E	403	TRP	5.0
1	B	497	TRP	5.0
1	E	351	THR	5.0
1	E	519	ILE	5.0
1	B	367	GLY	5.0
1	E	537	TYR	4.9
1	D	545	THR	4.9
1	B	517	ASN	4.9
1	E	365	LEU	4.9
1	F	519	ILE	4.8
1	B	443	TYR	4.8
1	A	353	LEU	4.8
1	C	555	SER	4.8
1	B	581	VAL	4.8
1	E	505	THR	4.8
1	B	407	ALA	4.8
1	D	544	TRP	4.8
1	F	330	THR	4.7
1	F	609	THR	4.7
1	D	546	PHE	4.7
1	C	486	SER	4.7
1	E	584	TYR	4.7
1	E	421	ILE	4.7
1	B	386	GLY	4.6
1	D	528	GLN	4.6
1	C	544	TRP	4.6
1	C	594	VAL	4.6
1	D	599	SER	4.5
1	B	427	ALA	4.5
1	E	520	TYR	4.5
1	F	468	LEU	4.5
1	F	506	ILE	4.5
1	F	387	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	408	PRO	4.5
1	F	404	SER	4.5
1	C	569	LEU	4.5
1	F	386	GLY	4.4
1	A	335	PHE	4.4
1	A	369	VAL	4.4
1	A	546	PHE	4.4
1	D	426	TYR	4.4
1	E	418	VAL	4.4
1	B	352	TRP	4.4
1	F	596	ARG	4.4
1	D	584	TYR	4.4
1	E	334	TYR	4.4
1	B	583	CYS	4.4
1	B	338	SER	4.4
1	F	347	PRO	4.4
1	B	383	SER	4.3
1	D	471	LEU	4.3
1	E	373	LEU	4.3
1	F	474	ALA	4.3
1	F	405	PRO	4.3
1	D	467	VAL	4.3
1	F	579	ASP	4.3
1	F	551	LYS	4.3
1	E	426	TYR	4.2
1	E	405	PRO	4.2
1	E	408	PRO	4.2
1	B	430	GLY	4.2
1	E	414	ASN	4.2
1	E	510	ALA	4.2
1	B	580	SER	4.2
1	E	381	ASN	4.2
1	B	571	GLY	4.1
1	F	377	VAL	4.1
1	F	563	GLN	4.1
1	C	514	VAL	4.1
1	E	452	LEU	4.1
1	B	385	ASP	4.1
1	C	572	TYR	4.1
1	A	609	THR	4.1
1	B	328	ILE	4.0
1	F	574	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	411	VAL	4.0
1	F	378	GLY	4.0
1	D	452	LEU	4.0
1	E	472	LEU	4.0
1	F	428	VAL	4.0
1	B	563	GLN	4.0
1	F	549	PRO	4.0
1	D	414	ASN	4.0
1	D	374	LEU	4.0
1	F	427	ALA	3.9
1	D	489	CYS	3.9
1	E	513	CYS	3.9
1	E	499	MET	3.9
1	C	425	ILE	3.9
1	E	328	ILE	3.9
1	B	339	LEU	3.9
1	B	374	LEU	3.9
1	B	388	THR	3.9
1	E	397	ASN	3.9
1	B	360	VAL	3.9
1	B	384	PRO	3.9
1	F	443	TYR	3.9
1	E	379	GLY	3.9
1	C	519	ILE	3.9
1	F	368	CYS	3.9
1	D	468	LEU	3.9
1	A	539	VAL	3.9
1	D	403	TRP	3.9
1	E	564	GLY	3.9
1	B	445	PRO	3.9
1	D	534	VAL	3.9
1	F	450	TRP	3.8
1	E	540	ALA	3.8
1	C	526	ASP	3.8
1	C	564	GLY	3.8
1	F	381	ASN	3.8
1	D	405	PRO	3.8
1	F	514	VAL	3.8
1	C	502	ALA	3.8
1	E	473	TYR	3.8
1	E	504	ASN	3.8
1	A	351	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	501	THR	3.7
1	F	599	SER	3.7
1	D	539	VAL	3.7
1	E	577	PHE	3.7
1	A	497	TRP	3.7
1	E	450	TRP	3.7
1	E	567	TYR	3.7
1	A	528	GLN	3.7
1	F	432	HIS	3.7
1	F	600	GLY	3.7
1	F	569	LEU	3.7
1	C	445	PRO	3.7
1	A	387	ASN	3.7
1	E	398	PRO	3.7
1	D	450	TRP	3.7
1	D	548	ALA	3.7
1	A	518	CYS	3.7
1	C	385	ASP	3.7
1	F	534	VAL	3.6
1	F	452	LEU	3.6
1	E	506	ILE	3.6
1	D	445	PRO	3.6
1	F	329	TYR	3.6
1	F	575	HIS	3.6
1	A	377	VAL	3.6
1	E	425	ILE	3.6
1	B	381	ASN	3.6
1	D	352	TRP	3.6
1	E	392	ALA	3.6
1	E	451	HIS	3.6
1	C	345	TYR	3.6
1	D	443	TYR	3.6
1	E	541	THR	3.6
1	F	543	THR	3.6
1	B	553	ARG	3.6
1	A	373	LEU	3.6
1	A	542	ALA	3.6
1	C	548	ALA	3.6
1	D	344	ALA	3.6
1	D	361	PRO	3.6
1	D	535	GLU	3.5
1	B	426	TYR	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	467	VAL	3.5
1	E	595	THR	3.5
1	B	342	LEU	3.5
1	B	358	LEU	3.5
1	B	569	LEU	3.5
1	D	578	LEU	3.5
1	D	448	ASP	3.5
1	B	551	LYS	3.5
1	E	535	GLU	3.5
1	F	354	ARG	3.5
1	E	345	TYR	3.5
1	E	375	TYR	3.5
1	E	546	PHE	3.5
1	D	573	ASP	3.5
1	D	353	LEU	3.5
1	E	353	LEU	3.5
1	A	385	ASP	3.5
1	A	354	ARG	3.5
1	F	388	THR	3.5
1	E	374	LEU	3.5
1	F	437	HIS	3.5
1	F	430	GLY	3.4
1	E	580	SER	3.4
1	E	440	VAL	3.4
1	F	475	VAL	3.4
1	B	355	LEU	3.4
1	E	427	ALA	3.4
1	F	434	CYS	3.4
1	D	520	TYR	3.4
1	B	399	MET	3.4
1	D	388	THR	3.4
1	F	360	VAL	3.4
1	F	581	VAL	3.4
1	F	608	VAL	3.4
1	A	423	GLY	3.4
1	E	404	SER	3.4
1	B	578	LEU	3.4
1	D	547	VAL	3.4
1	F	355	LEU	3.4
1	F	594	VAL	3.4
1	A	372	GLY	3.4
1	A	574	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	336	ARG	3.4
1	D	431	SER	3.4
1	D	517	ASN	3.3
1	B	428	VAL	3.3
1	E	369	VAL	3.3
1	F	480	GLY	3.3
1	D	466	ALA	3.3
1	D	519	ILE	3.3
1	E	518	CYS	3.3
1	F	426	TYR	3.3
1	E	385	ASP	3.3
1	D	549	PRO	3.3
1	F	492	PRO	3.3
1	B	475	VAL	3.3
1	F	331	ALA	3.3
1	D	550	MET	3.3
1	B	546	PHE	3.3
1	B	518	CYS	3.3
1	C	531	LEU	3.3
1	A	447	ARG	3.3
1	C	447	ARG	3.3
1	B	595	THR	3.3
1	D	543	THR	3.3
1	F	509	GLY	3.3
1	F	564	GLY	3.3
1	D	500	ILE	3.3
1	C	363	SER	3.3
1	E	422	ASP	3.3
1	C	484	LEU	3.3
1	C	557	LEU	3.3
1	E	453	VAL	3.3
1	A	605	GLY	3.3
1	E	528	GLN	3.2
1	C	482	ASN	3.2
1	E	485	ASN	3.2
1	A	405	PRO	3.2
1	F	353	LEU	3.2
1	C	360	VAL	3.2
1	C	543	THR	3.2
1	B	425	ILE	3.2
1	F	502	ALA	3.2
1	F	528	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	515	LEU	3.2
1	D	342	LEU	3.2
1	F	398	PRO	3.2
1	B	330	THR	3.2
1	C	328	ILE	3.2
1	C	331	ALA	3.2
1	A	403	TRP	3.2
1	F	442	ARG	3.2
1	E	492	PRO	3.2
1	B	432	HIS	3.2
1	E	490	TYR	3.2
1	D	600	GLY	3.2
1	A	416	ILE	3.2
1	C	500	ILE	3.2
1	D	394	ASP	3.2
1	B	361	PRO	3.2
1	B	424	HIS	3.2
1	D	516	HIS	3.2
1	F	469	ASN	3.2
1	A	604	VAL	3.2
1	B	568	VAL	3.2
1	D	428	VAL	3.2
1	E	423	GLY	3.2
1	E	462	GLY	3.2
1	E	395	CYS	3.2
1	E	454	ALA	3.1
1	E	413	ARG	3.1
1	F	352	TRP	3.1
1	A	431	SER	3.1
1	F	384	PRO	3.1
1	D	597	MET	3.1
1	E	387	ASN	3.1
1	B	574	GLY	3.1
1	C	465	VAL	3.1
1	D	480	GLY	3.1
1	E	527	GLY	3.1
1	F	370	VAL	3.1
1	A	374	LEU	3.1
1	C	373	LEU	3.1
1	C	428	VAL	3.1
1	D	574	GLY	3.1
1	E	475	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	501	THR	3.1
1	C	506	ILE	3.1
1	A	384	PRO	3.1
1	C	516	HIS	3.1
1	E	445	PRO	3.1
1	E	383	SER	3.1
1	E	508	SER	3.1
1	C	547	VAL	3.1
1	E	360	VAL	3.1
1	B	345	TYR	3.1
1	D	329	TYR	3.1
1	D	396	TYR	3.1
1	C	602	SER	3.1
1	D	404	SER	3.1
1	A	600	GLY	3.1
1	E	419	GLY	3.1
1	E	509	GLY	3.1
1	C	539	VAL	3.1
1	D	454	ALA	3.0
1	B	575	HIS	3.0
1	D	492	PRO	3.0
1	A	327	LEU	3.0
1	D	457	LEU	3.0
1	E	410	SER	3.0
1	A	380	ARG	3.0
1	B	325	GLY	3.0
1	D	594	VAL	3.0
1	A	576	THR	3.0
1	D	537	TYR	3.0
1	E	503	MET	3.0
1	B	529	ASP	3.0
1	D	553	ARG	3.0
1	B	404	SER	3.0
1	D	486	SER	3.0
1	E	350	GLY	3.0
1	E	480	GLY	3.0
1	B	591	TRP	3.0
1	E	539	VAL	3.0
1	E	543	THR	3.0
1	C	446	GLU	3.0
1	E	361	PRO	3.0
1	C	353	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	523	GLY	3.0
1	B	409	MET	3.0
1	E	497	TRP	3.0
1	A	451	HIS	3.0
1	D	384	PRO	3.0
1	C	468	LEU	3.0
1	D	326	ARG	3.0
1	F	439	SER	3.0
1	B	564	GLY	3.0
1	D	524	GLY	3.0
1	A	581	VAL	2.9
1	A	358	LEU	2.9
1	B	359	GLN	2.9
1	D	371	GLY	2.9
1	B	353	LEU	2.9
1	B	334	TYR	2.9
1	A	517	ASN	2.9
1	A	513	CYS	2.9
1	C	518	CYS	2.9
1	D	506	ILE	2.9
1	E	432	HIS	2.9
1	E	436	HIS	2.9
1	E	534	VAL	2.9
1	E	561	VAL	2.9
1	A	595	THR	2.9
1	D	576	THR	2.9
1	B	548	ALA	2.9
1	E	551	LYS	2.9
1	F	540	ALA	2.9
1	E	393	LEU	2.9
1	F	591	TRP	2.9
1	B	490	TYR	2.9
1	D	592	SER	2.9
1	F	517	ASN	2.9
1	A	461	ILE	2.9
1	F	461	ILE	2.9
1	B	368	CYS	2.9
1	C	395	CYS	2.9
1	B	400	THR	2.9
1	C	607	ALA	2.9
1	B	597	MET	2.9
1	E	399	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	520	TYR	2.9
1	B	340	SER	2.8
1	E	435	ILE	2.8
1	E	420	VAL	2.8
1	A	400	THR	2.8
1	C	541	THR	2.8
1	E	394	ASP	2.8
1	E	544	TRP	2.8
1	C	329	TYR	2.8
1	C	442	ARG	2.8
1	D	447	ARG	2.8
1	F	419	GLY	2.8
1	E	517	ASN	2.8
1	F	481	THR	2.8
1	A	331	ALA	2.8
1	B	366	ALA	2.8
1	E	327	LEU	2.8
1	F	336	ARG	2.8
1	F	341	TYR	2.8
1	A	348	SER	2.8
1	B	363	SER	2.8
1	B	599	SER	2.8
1	B	376	ALA	2.8
1	D	357	ASP	2.8
1	D	459	ARG	2.8
1	B	478	PHE	2.8
1	E	386	GLY	2.8
1	E	570	GLY	2.8
1	F	371	GLY	2.8
1	A	329	TYR	2.8
1	A	345	TYR	2.8
1	B	473	TYR	2.8
1	D	532	ASN	2.8
1	E	482	ASN	2.8
1	F	547	VAL	2.8
1	B	472	LEU	2.8
1	D	505	THR	2.8
1	E	468	LEU	2.8
1	E	515	LEU	2.8
1	E	590	THR	2.8
1	F	376	ALA	2.8
1	D	518	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	596	ARG	2.8
1	C	326	ARG	2.8
1	D	577	PHE	2.8
1	B	414	ASN	2.7
1	E	606	VAL	2.7
1	E	330	THR	2.7
1	E	331	ALA	2.7
1	C	470	ARG	2.7
1	C	359	GLN	2.7
1	E	589	ASP	2.7
1	F	416	ILE	2.7
1	F	495	ASN	2.7
1	B	508	SER	2.7
1	C	525	TYR	2.7
1	E	391	SER	2.7
1	A	330	THR	2.7
1	A	505	THR	2.7
1	B	499	MET	2.7
1	B	576	THR	2.7
1	E	376	ALA	2.7
1	E	470	ARG	2.7
1	E	359	GLN	2.7
1	D	435	ILE	2.7
1	A	580	SER	2.7
1	B	369	VAL	2.7
1	E	594	VAL	2.7
1	B	373	LEU	2.7
1	D	393	LEU	2.7
1	F	537	TYR	2.7
1	C	545	THR	2.7
1	F	446	GLU	2.7
1	F	359	GLN	2.7
1	F	451	HIS	2.7
1	A	434	CYS	2.7
1	B	527	GLY	2.7
1	F	409	MET	2.7
1	E	390	SER	2.7
1	A	446	GLU	2.7
1	D	341	TYR	2.7
1	E	449	GLU	2.7
1	F	334	TYR	2.7
1	A	540	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	598	THR	2.7
1	A	563	GLN	2.7
1	C	563	GLN	2.7
1	A	575	HIS	2.7
1	B	552	HIS	2.7
1	A	350	GLY	2.6
1	E	371	GLY	2.6
1	F	328	ILE	2.6
1	F	467	VAL	2.6
1	E	338	SER	2.6
1	A	501	THR	2.6
1	F	552	HIS	2.6
1	A	573	ASP	2.6
1	D	526	ASP	2.6
1	F	335	PHE	2.6
1	A	494	ARG	2.6
1	D	380	ARG	2.6
1	D	442	ARG	2.6
1	A	471	LEU	2.6
1	C	568	VAL	2.6
1	F	568	VAL	2.6
1	C	510	ALA	2.6
1	D	359	GLN	2.6
1	D	598	THR	2.6
1	A	516	HIS	2.6
1	F	403	TRP	2.6
1	B	429	GLY	2.6
1	F	385	ASP	2.6
1	F	435	ILE	2.6
1	D	475	VAL	2.6
1	D	606	VAL	2.6
1	E	469	ASN	2.6
1	F	411	VAL	2.6
1	E	602	SER	2.6
1	D	400	THR	2.6
1	F	590	THR	2.6
1	E	352	TRP	2.6
1	A	571	GLY	2.6
1	D	538	ASP	2.6
1	F	448	ASP	2.6
1	D	399	MET	2.6
1	E	500	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	468	LEU	2.6
1	A	606	VAL	2.6
1	B	420	VAL	2.6
1	D	440	VAL	2.6
1	D	501	THR	2.6
1	E	388	THR	2.6
1	A	470	ARG	2.5
1	F	470	ARG	2.5
1	C	352	TRP	2.5
1	D	497	TRP	2.5
1	B	579	ASP	2.5
1	F	361	PRO	2.5
1	F	433	GLY	2.5
1	D	416	ILE	2.5
1	A	381	ASN	2.5
1	A	508	SER	2.5
1	E	439	SER	2.5
1	E	481	THR	2.5
1	E	362	ARG	2.5
1	D	398	PRO	2.5
1	D	358	LEU	2.5
1	D	373	LEU	2.5
1	B	370	VAL	2.5
1	E	424	HIS	2.5
1	F	324	VAL	2.5
1	F	453	VAL	2.5
1	C	466	ALA	2.5
1	A	545	THR	2.5
1	D	351	THR	2.5
1	F	395	CYS	2.5
1	F	400	THR	2.5
1	F	592	SER	2.5
1	F	518	CYS	2.5
1	E	455	PRO	2.5
1	F	473	TYR	2.5
1	C	511	GLY	2.5
1	C	524	GLY	2.5
1	D	364	GLY	2.5
1	D	386	GLY	2.5
1	E	603	GLY	2.5
1	B	519	ILE	2.5
1	F	559	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	365	LEU	2.5
1	E	342	LEU	2.5
1	B	382	ASN	2.5
1	C	414	ASN	2.5
1	E	495	ASN	2.5
1	D	340	SER	2.5
1	B	480	GLY	2.5
1	E	341	TYR	2.5
1	E	572	TYR	2.5
1	A	519	ILE	2.5
1	F	573	ASP	2.5
1	A	452	LEU	2.5
1	A	450	TRP	2.5
1	C	528	GLN	2.5
1	E	512	VAL	2.5
1	D	470	ARG	2.5
1	D	521	ALA	2.5
1	E	521	ALA	2.5
1	F	556	ALA	2.5
1	A	499	MET	2.5
1	B	543	THR	2.5
1	F	541	THR	2.5
1	D	372	GLY	2.4
1	D	493	GLU	2.4
1	F	584	TYR	2.4
1	D	569	LEU	2.4
1	C	577	PHE	2.4
1	D	514	VAL	2.4
1	B	542	ALA	2.4
1	F	366	ALA	2.4
1	A	388	THR	2.4
1	E	400	THR	2.4
1	F	508	SER	2.4
1	B	398	PRO	2.4
1	D	417	GLY	2.4
1	E	368	CYS	2.4
1	A	506	ILE	2.4
1	B	416	ILE	2.4
1	B	437	HIS	2.4
1	D	451	HIS	2.4
1	C	403	TRP	2.4
1	D	469	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	438	ASN	2.4
1	E	548	ALA	2.4
1	F	351	THR	2.4
1	B	405	PRO	2.4
1	C	586	PRO	2.4
1	F	557	LEU	2.4
1	F	459	ARG	2.4
1	B	537	TYR	2.4
1	C	473	TYR	2.4
1	D	490	TYR	2.4
1	B	450	TRP	2.4
1	B	521	ALA	2.4
1	D	356	ALA	2.4
1	F	487	ALA	2.4
1	D	496	GLU	2.4
1	F	441	GLU	2.4
1	C	386	GLY	2.4
1	E	416	ILE	2.4
1	A	326	ARG	2.4
1	E	484	LEU	2.4
1	E	494	ARG	2.4
1	F	484	LEU	2.4
1	B	572	TYR	2.4
1	C	520	TYR	2.4
1	E	443	TYR	2.4
1	A	594	VAL	2.4
1	A	608	VAL	2.4
1	D	568	VAL	2.4
1	F	440	VAL	2.4
1	F	539	VAL	2.4
1	B	532	ASN	2.4
1	D	582	GLU	2.4
1	A	445	PRO	2.3
1	A	590	THR	2.3
1	D	363	SER	2.3
1	F	429	GLY	2.3
1	F	476	GLY	2.3
1	D	461	ILE	2.3
1	E	526	ASP	2.3
1	E	531	LEU	2.3
1	E	559	ILE	2.3
1	F	553	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	394	ASP	2.3
1	A	341	TYR	2.3
1	B	341	TYR	2.3
1	B	401	ASN	2.3
1	C	517	ASN	2.3
1	D	487	ALA	2.3
1	E	407	ALA	2.3
1	F	356	ALA	2.3
1	F	497	TRP	2.3
1	B	391	SER	2.3
1	B	600	GLY	2.3
1	D	354	ARG	2.3
1	B	557	LEU	2.3
1	F	373	LEU	2.3
1	C	589	ASP	2.3
1	E	587	ASP	2.3
1	B	406	CYS	2.3
1	A	568	VAL	2.3
1	B	594	VAL	2.3
1	C	608	VAL	2.3
1	D	345	TYR	2.3
1	D	370	VAL	2.3
1	D	453	VAL	2.3
1	C	361	PRO	2.3
1	D	540	ALA	2.3
1	C	330	THR	2.3
1	A	591	TRP	2.3
1	D	419	GLY	2.3
1	E	600	GLY	2.3
1	C	515	LEU	2.3
1	C	566	ILE	2.3
1	E	389	ASP	2.3
1	E	581	VAL	2.3
1	F	593	GLU	2.3
1	D	473	TYR	2.3
1	C	474	ALA	2.3
1	C	540	ALA	2.3
1	C	556	ALA	2.3
1	D	458	THR	2.3
1	B	451	HIS	2.3
1	F	527	GLY	2.3
1	B	468	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	544	TRP	2.3
1	D	499	MET	2.3
1	A	465	VAL	2.3
1	A	561	VAL	2.3
1	B	463	VAL	2.3
1	C	492	PRO	2.3
1	D	542	ALA	2.2
1	B	364	GLY	2.2
1	B	533	SER	2.2
1	B	592	SER	2.2
1	C	592	SER	2.2
1	D	328	ILE	2.2
1	E	339	LEU	2.2
1	B	608	VAL	2.2
1	D	336	ARG	2.2
1	F	561	VAL	2.2
1	C	382	ASN	2.2
1	E	474	ALA	2.2
1	A	490	TYR	2.2
1	C	537	TYR	2.2
1	A	458	THR	2.2
1	A	598	THR	2.2
1	D	595	THR	2.2
1	E	609	THR	2.2
1	D	422	ASP	2.2
1	F	493	GLU	2.2
1	C	553	ARG	2.2
1	A	577	PHE	2.2
1	F	546	PHE	2.2
1	D	377	VAL	2.2
1	F	586	PRO	2.2
1	B	454	ALA	2.2
1	F	344	ALA	2.2
1	F	346	ASN	2.2
1	C	575	HIS	2.2
1	A	564	GLY	2.2
1	B	371	GLY	2.2
1	F	379	GLY	2.2
1	B	461	ILE	2.2
1	B	410	SER	2.2
1	C	348	SER	2.2
1	D	555	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	587	ASP	2.2
1	E	444	GLU	2.2
1	B	403	TRP	2.2
1	E	483	ARG	2.2
1	A	356	ALA	2.2
1	D	382	ASN	2.2
1	D	427	ALA	2.2
1	D	563	GLN	2.2
1	B	351	THR	2.2
1	B	393	LEU	2.2
1	E	457	LEU	2.2
1	E	578	LEU	2.2
1	A	500	ILE	2.2
1	D	444	GLU	2.2
1	E	326	ARG	2.2
1	F	447	ARG	2.2
1	C	497	TRP	2.2
1	E	412	PRO	2.2
1	E	591	TRP	2.2
1	C	546	PHE	2.2
1	B	539	VAL	2.1
1	D	456	MET	2.1
1	B	327	LEU	2.1
1	B	471	LEU	2.1
1	B	545	THR	2.1
1	B	590	THR	2.1
1	C	374	LEU	2.1
1	D	355	LEU	2.1
1	F	515	LEU	2.1
1	D	596	ARG	2.1
1	B	534	VAL	2.1
1	E	456	MET	2.1
1	C	376	ALA	2.1
1	C	542	ALA	2.1
1	C	401	ASN	2.1
1	C	588	THR	2.1
1	C	609	THR	2.1
1	D	477	GLY	2.1
1	E	598	THR	2.1
1	E	605	GLY	2.1
1	F	457	LEU	2.1
1	C	421	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	436	HIS	2.1
1	A	544	TRP	2.1
1	A	346	ASN	2.1
1	D	438	ASN	2.1
1	C	355	LEU	2.1
1	C	400	THR	2.1
1	D	378	GLY	2.1
1	F	358	LEU	2.1
1	E	498	ARG	2.1
1	A	328	ILE	2.1
1	F	425	ILE	2.1
1	E	529	ASP	2.1
1	F	526	ASP	2.1
1	A	347	PRO	2.1
1	E	586	PRO	2.1
1	E	409	MET	2.1
1	E	437	HIS	2.1
1	E	516	HIS	2.1
1	B	335	PHE	2.1
1	E	530	GLN	2.1
1	E	463	VAL	2.1
1	E	465	VAL	2.1
1	E	608	VAL	2.1
1	F	604	VAL	2.1
1	A	469	ASN	2.1
1	C	358	LEU	2.1
1	D	472	LEU	2.1
1	D	504	ASN	2.1
1	F	483	ARG	2.1
1	C	458	THR	2.1
1	D	541	THR	2.1
1	C	461	ILE	2.1
1	B	396	TYR	2.1
1	B	422	ASP	2.1
1	B	431	SER	2.1
1	D	533	SER	2.1
1	C	503	MET	2.1
1	D	424	HIS	2.1
1	B	547	VAL	2.0
1	C	453	VAL	2.0
1	C	475	VAL	2.0
1	D	581	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	510	ALA	2.0
1	D	536	ARG	2.0
1	E	447	ARG	2.0
1	A	457	LEU	2.0
1	C	471	LEU	2.0
1	F	578	LEU	2.0
1	C	429	GLY	2.0
1	C	593	GLU	2.0
1	F	325	GLY	2.0
1	E	576	THR	2.0
1	A	599	SER	2.0
1	E	550	MET	2.0
1	F	337	GLN	2.0
1	A	336	ARG	2.0
1	B	326	ARG	2.0
1	B	377	VAL	2.0
1	B	606	VAL	2.0
1	F	512	VAL	2.0
1	A	355	LEU	2.0
1	E	466	ALA	2.0
1	F	472	LEU	2.0
1	F	542	ALA	2.0
1	E	438	ASN	2.0
1	E	396	TYR	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](#)

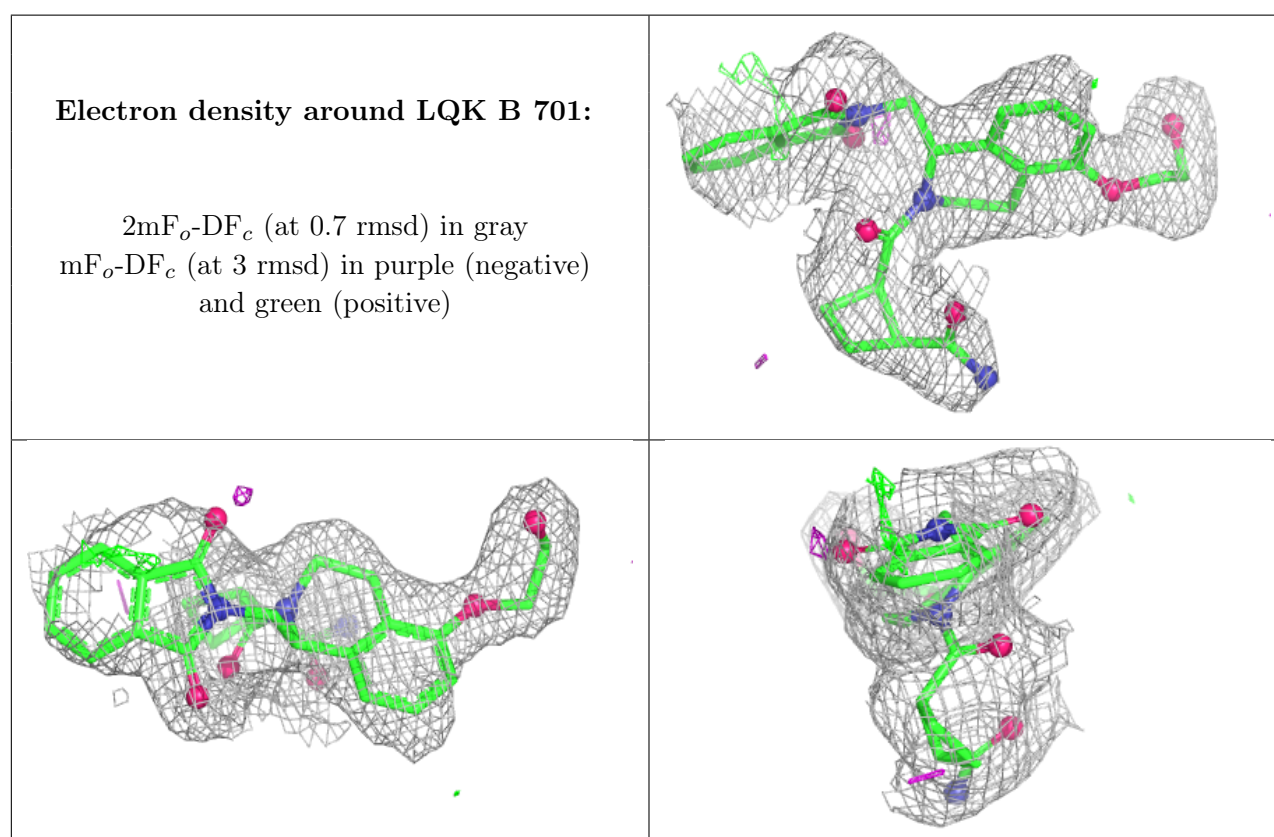
There are no oligosaccharides in this entry.

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.

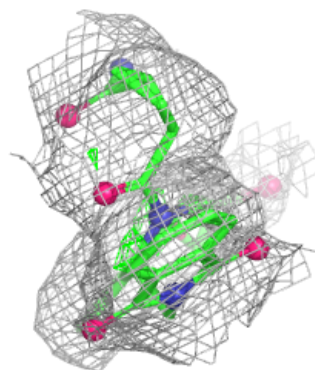
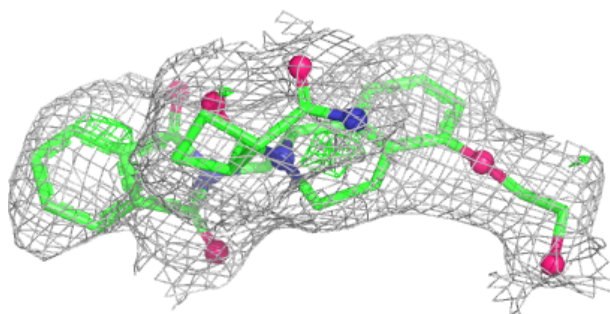
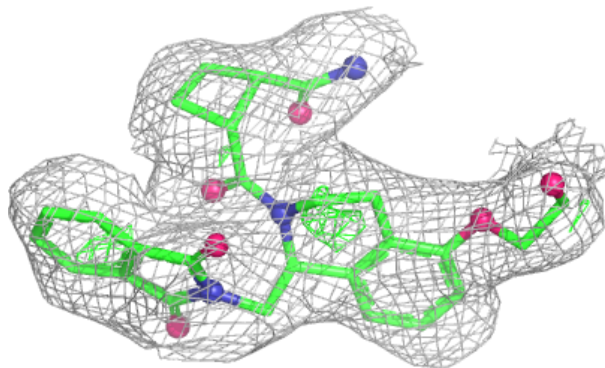
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LQK	B	701	35/35	0.82	0.19	40,57,83,87	0
2	LQK	D	701	35/35	0.84	0.18	41,57,75,81	0
2	LQK	A	701	35/35	0.85	0.19	49,65,87,93	0
2	LQK	C	701	35/35	0.86	0.15	32,51,74,78	0
2	LQK	E	701	35/35	0.86	0.14	33,56,71,77	0
2	LQK	F	701	35/35	0.89	0.14	39,47,62,72	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.

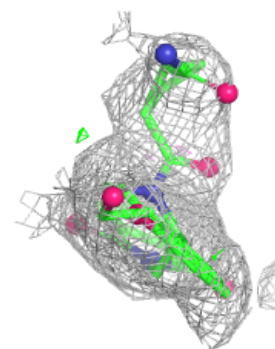
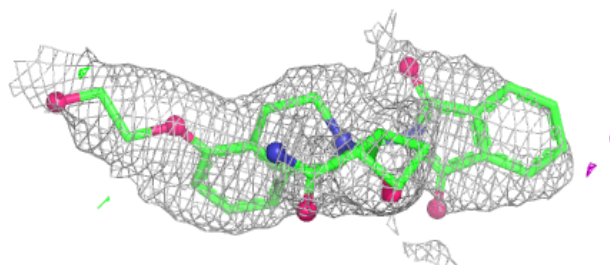
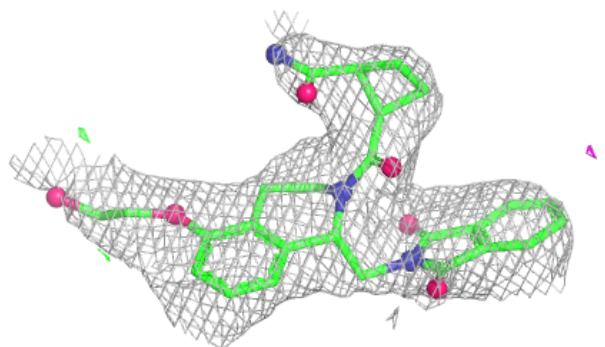


Electron density around LQK D 701:

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

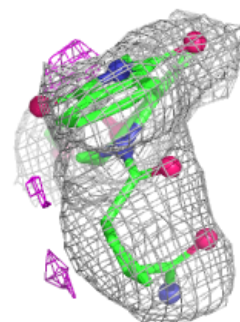
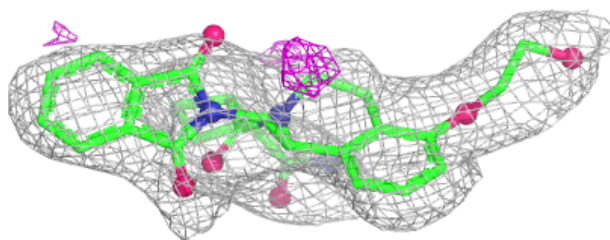
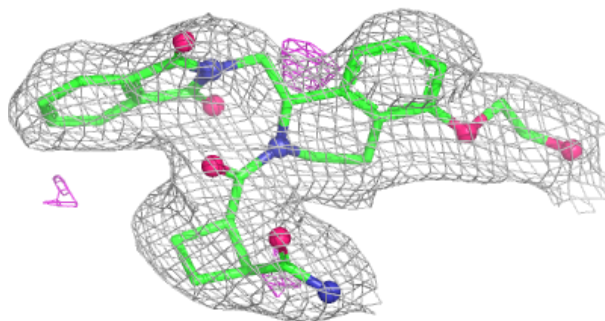
**Electron density around LQK A 701:**

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

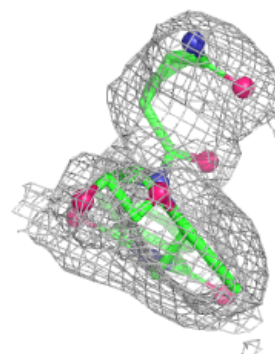
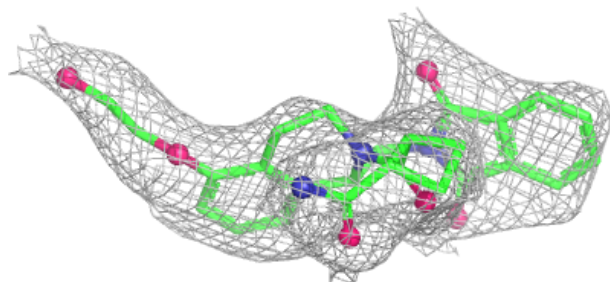
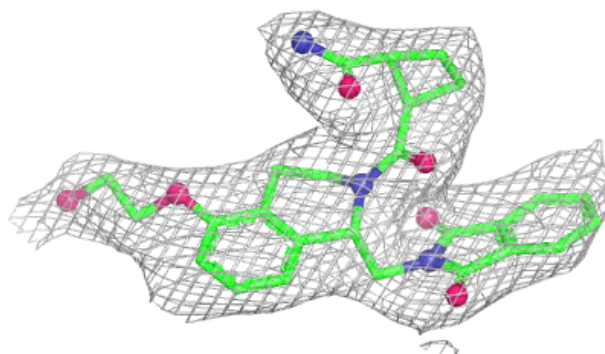


Electron density around LQK C 701:

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

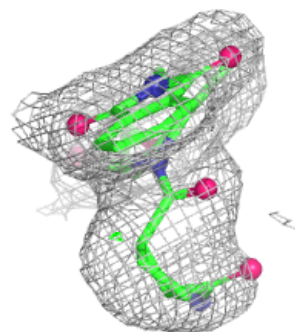
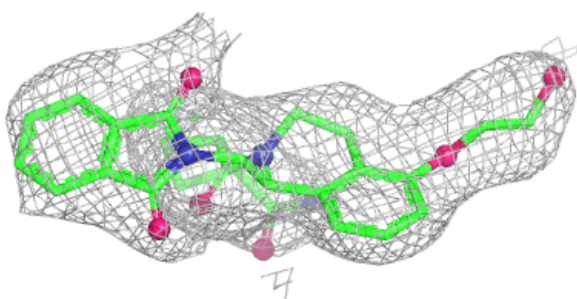
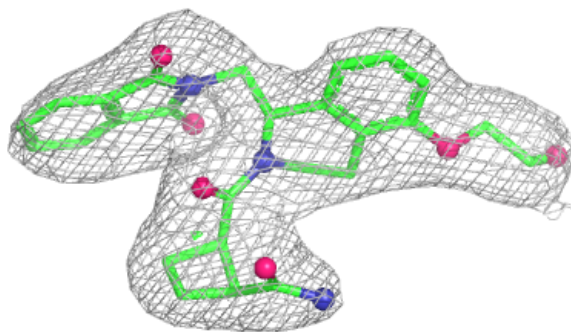
**Electron density around LQK E 701:**

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



Electron density around LQK F 701:

$2mF_o - DF_c$ (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.