



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:33 AM UTC

PDB ID : 7XJW / pdb_00007xjw
Title : Crystal structure of canine coronavirus main protease in complex with GC376
Authors : Wang, Y.C.; Yang, C.S.; Hou, M.H.; Tsai, C.L.; Chiu, Y.F.; Chen, Y.
Deposited on : 2022-04-18
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

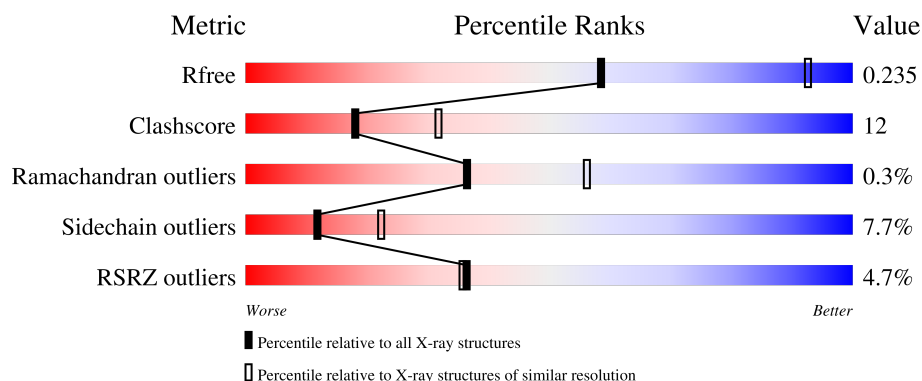
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	302	79% 19% ..
1	B	302	76% 22% ..
1	C	302	69% 28% ..
1	D	302	74% 22% ..
1	E	302	70% 25% ..

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Mol	Chain	Length	Quality of chain
1	F	302	
1	G	302	
1	H	302	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	K36	C	401	X	-	-	-

2 Entry composition

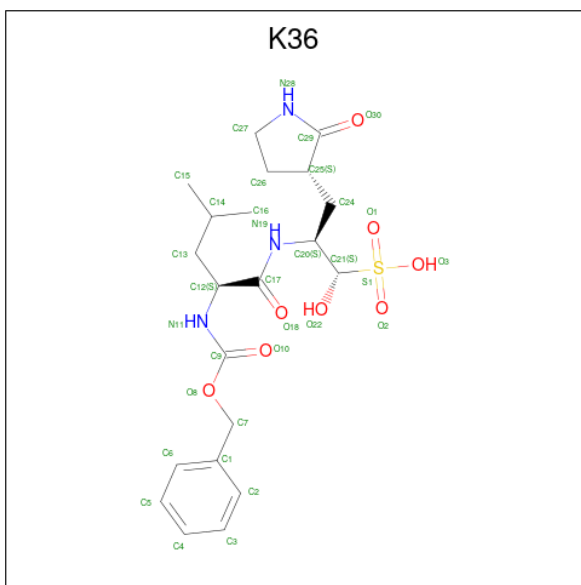
There are 3 unique types of molecules in this entry. The entry contains 18564 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ORF1a polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2293	1447	388	442	16			
1	B	299	Total	C	N	O	S	0	0	0
			2293	1447	388	442	16			
1	C	298	Total	C	N	O	S	0	0	0
			2286	1442	387	441	16			
1	D	296	Total	C	N	O	S	0	0	0
			2268	1433	382	437	16			
1	E	299	Total	C	N	O	S	0	0	0
			2293	1447	388	442	16			
1	F	299	Total	C	N	O	S	0	0	0
			2293	1447	388	442	16			
1	G	298	Total	C	N	O	S	0	0	0
			2286	1442	387	441	16			
1	H	289	Total	C	N	O	S	0	0	0
			2212	1392	374	430	16			

- Molecule 2 is (1S,2S)-2-({N-[(benzyloxy)carbonyl]-L-leucyl}amino)-1-hydroxy-3-[(3S)-2-oxo pyrrolidin-3-yl]propane-1-sulfonic acid (CCD ID: K36) (formula: C₂₁H₃₁N₃O₈S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 29	C 21	N 3	O 5	0	0
2	B	1	Total 29	C 21	N 3	O 5	0	0
2	C	1	Total 29	C 21	N 3	O 5	0	0
2	D	1	Total 29	C 21	N 3	O 5	0	0
2	E	1	Total 29	C 21	N 3	O 5	0	0
2	F	1	Total 29	C 21	N 3	O 5	0	0
2	G	1	Total 29	C 21	N 3	O 5	0	0
2	H	1	Total 29	C 21	N 3	O 5	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	B	20	Total O 20 20	0	0
3	C	10	Total O 10 10	0	0
3	D	9	Total O 9 9	0	0

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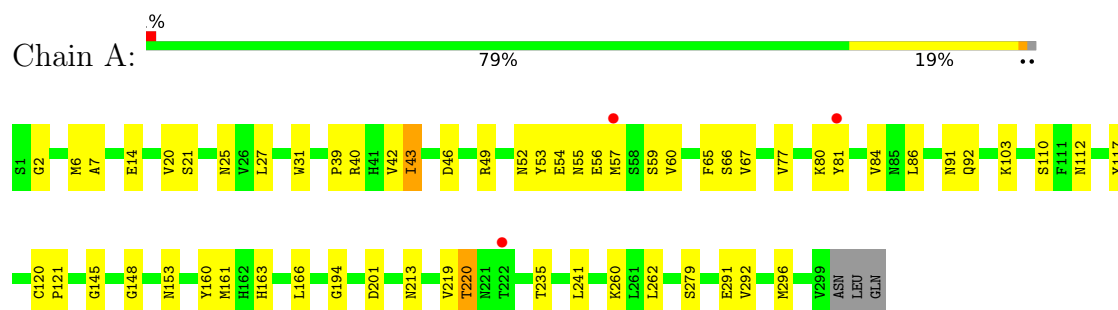
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	13	Total 13	O 13	0	0
3	F	14	Total 14	O 14	0	0
3	G	9	Total 9	O 9	0	0
3	H	10	Total 10	O 10	0	0

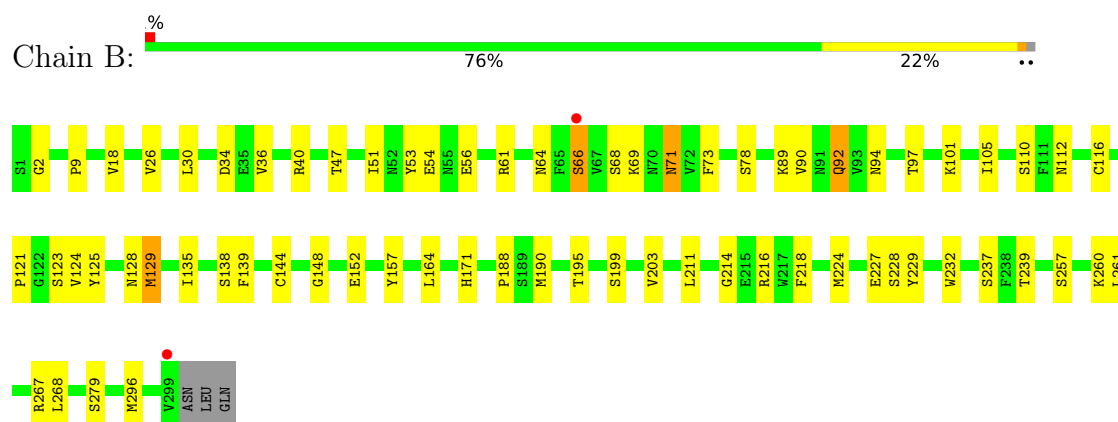
3 Residue-property plots [i](#)

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

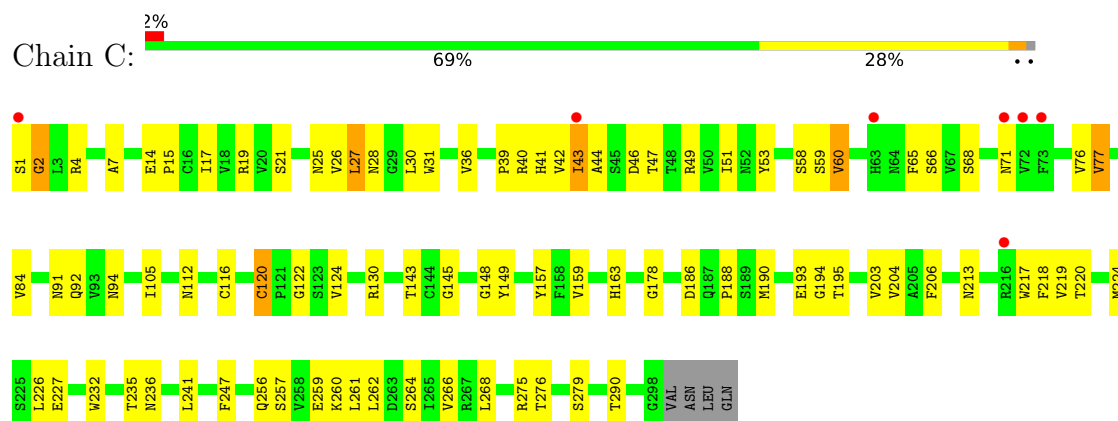
• Molecule 1: ORF1a polypeptide



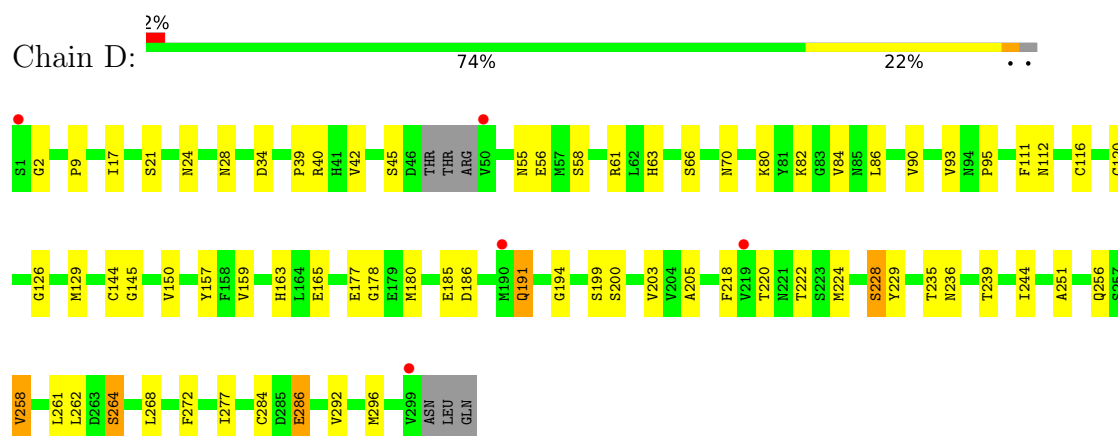
• Molecule 1: ORF1a polypeptide



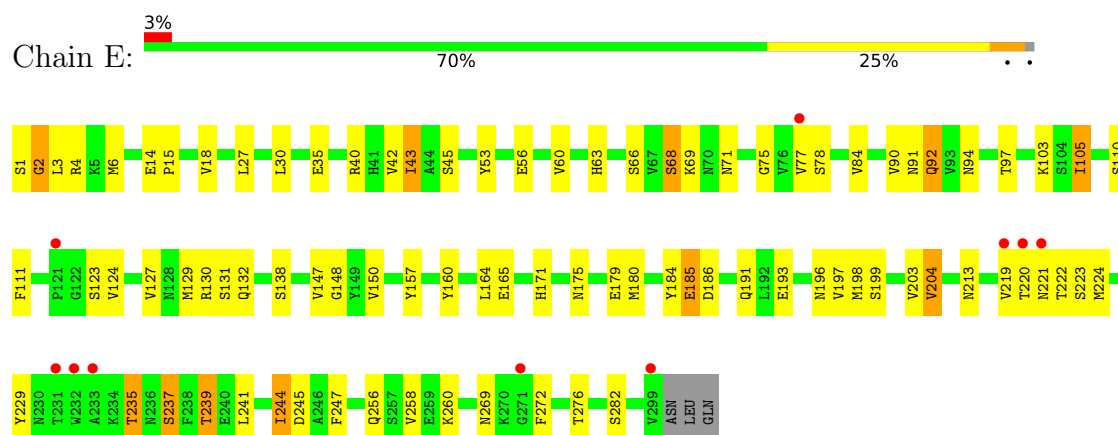
• Molecule 1: ORF1a polypeptide



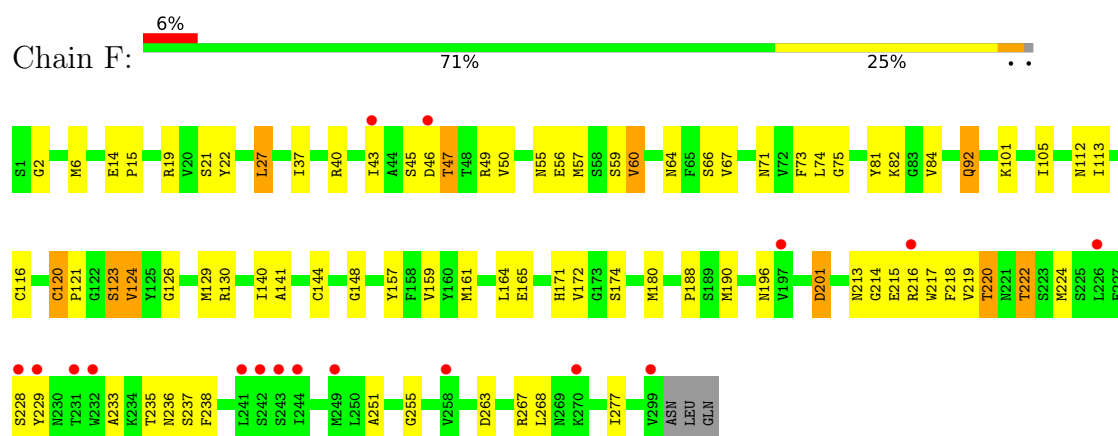
- Molecule 1: ORF1a polypeptide



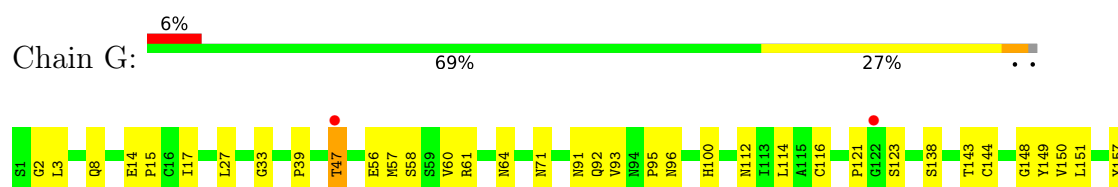
- Molecule 1: ORF1a polypeptide

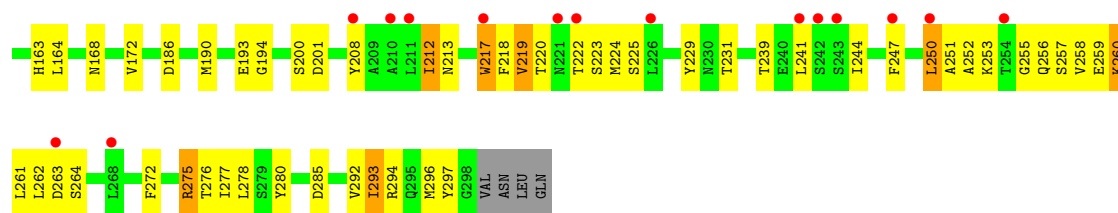


- Molecule 1: ORF1a polypeptide

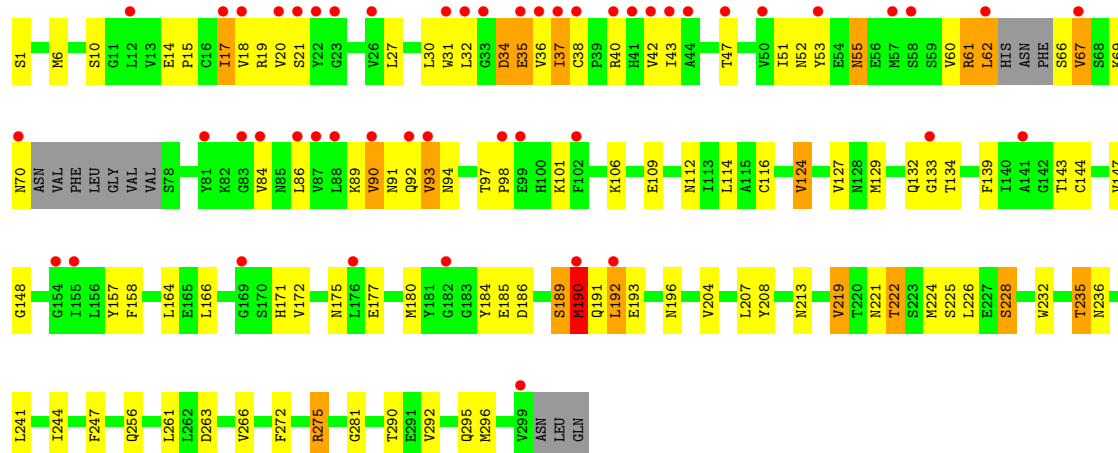


- Molecule 1: ORF1a polypeptide





● Molecule 1: ORF1a polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	156.97Å 125.75Å 160.42Å 90.00° 97.47° 90.00°	Depositor
Resolution (Å)	27.82 – 2.75 27.82 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.4 (27.82-2.75) 96.4 (27.82-2.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.76Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.213 , 0.233 0.215 , 0.235	Depositor DCC
R_{free} test set	3926 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18564	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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: K36

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	1.10	0/2338	1.37	3/3164 (0.1%)
1	B	1.08	0/2338	1.35	1/3164 (0.0%)
1	C	1.14	0/2331	1.39	3/3154 (0.1%)
1	D	1.07	0/2312	1.36	3/3127 (0.1%)
1	E	1.11	1/2338 (0.0%)	1.40	1/3164 (0.0%)
1	F	1.10	0/2338	1.38	1/3164 (0.0%)
1	G	1.06	0/2331	1.37	1/3154 (0.0%)
1	H	1.11	0/2252	1.37	0/3043
All	All	1.10	1/18578 (0.0%)	1.37	13/25134 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	127	VAL	C-O	5.54	1.29	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	GLY	CA-C-O	-6.45	117.78	122.23
1	C	2	GLY	CA-C-O	-6.38	117.48	122.52
1	A	194	GLY	CA-C-O	-6.27	117.94	122.45
1	D	70	ASN	CB-CA-C	-5.99	109.09	117.23
1	E	2	GLY	CA-C-O	-5.97	118.15	122.45
1	D	2	GLY	CA-C-O	-5.95	118.12	122.23
1	F	2	GLY	CA-C-O	-5.41	118.55	122.45
1	A	166	LEU	CA-C-N	5.37	126.06	119.99
1	A	166	LEU	C-N-CA	5.37	126.06	119.99
1	G	194	GLY	CA-C-O	-5.35	118.74	122.22
1	C	186	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	2	GLY	CA-C-O	-5.13	118.69	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	GLY	CA-C-O	-5.09	118.17	122.29

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	2293	0	2252	33	0
1	B	2293	0	2253	36	0
1	C	2286	0	2243	58	0
1	D	2268	0	2225	47	0
1	E	2293	0	2252	58	0
1	F	2293	0	2253	63	0
1	G	2286	0	2243	80	0
1	H	2212	0	2172	85	0
2	A	29	0	29	1	0
2	B	29	0	29	6	0
2	C	29	0	29	2	0
2	D	29	0	29	5	0
2	E	29	0	29	0	0
2	F	29	0	29	4	0
2	G	29	0	29	1	0
2	H	29	0	29	5	0
3	A	23	0	0	0	0
3	B	20	0	0	0	0
3	C	10	0	0	1	0
3	D	9	0	0	2	0
3	E	13	0	0	0	0
3	F	14	0	0	0	0
3	G	9	0	0	0	0
3	H	10	0	0	0	0
All	All	18564	0	18125	447	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 12.

All (447) 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:H:144:CYS:SG	2:H:401:K36:C21	2.01	1.48
1:B:144:CYS:SG	2:B:401:K36:C21	2.10	1.39
1:D:144:CYS:SG	2:D:401:K36:C21	2.20	1.28
1:G:244:ILE:HG23	1:G:258:VAL:HG21	1.37	1.07
1:H:225:SER:HB3	1:H:228:SER:OG	1.54	1.05
1:F:144:CYS:SG	2:F:401:K36:C21	2.45	1.04
1:H:20:VAL:HG22	1:H:67:VAL:HG22	1.39	1.02
1:F:224:MET:HE3	1:F:228:SER:OG	1.61	0.98
1:H:20:VAL:HG22	1:H:67:VAL:CG2	1.93	0.98
1:B:144:CYS:SG	2:B:401:K36:O22	2.23	0.96
1:G:244:ILE:HG23	1:G:258:VAL:CG2	1.95	0.96
1:F:74:LEU:HA	1:F:92:GLN:NE2	1.83	0.93
1:C:2:GLY:H	1:C:213:ASN:HD21	1.11	0.89
1:F:74:LEU:HD22	1:F:92:GLN:HG3	1.54	0.89
1:G:277:ILE:O	1:G:280:TYR:HB2	1.75	0.86
1:H:32:LEU:HD22	1:H:98:PRO:HD2	1.58	0.85
1:H:32:LEU:O	1:H:35:GLU:HG3	1.78	0.84
1:H:32:LEU:CD2	1:H:98:PRO:HD2	2.09	0.83
1:A:2:GLY:H	1:A:213:ASN:HD21	1.22	0.82
1:C:2:GLY:H	1:C:213:ASN:ND2	1.77	0.82
1:G:212:ILE:HD13	1:G:297:TYR:OH	1.82	0.79
1:H:30:LEU:O	1:H:36:VAL:HA	1.82	0.79
1:G:208:TYR:CE1	1:G:261:LEU:HD12	2.18	0.79
1:H:14:GLU:O	1:H:17:ILE:CD1	2.32	0.78
1:D:120:CYS:SG	3:D:503:HOH:O	2.42	0.77
1:G:224:MET:HE2	1:G:229:TYR:HA	1.65	0.77
1:H:222:THR:HB	1:H:263:ASP:OD2	1.83	0.77
1:C:220:THR:O	1:C:260:LYS:HE3	1.85	0.76
1:H:219:VAL:HG21	1:H:256:GLN:OE1	1.86	0.76
1:H:184:TYR:OH	1:H:193:GLU:HA	1.87	0.74
1:C:2:GLY:N	1:C:213:ASN:HD21	1.86	0.73
1:C:4:ARG:NH1	1:D:126:GLY:O	2.21	0.73
1:H:132:GLN:HE21	1:H:196:ASN:H	1.33	0.73
1:H:189:SER:O	1:H:190:MET:HG2	1.89	0.73
1:H:90:VAL:CG2	1:H:92:GLN:O	2.37	0.72
1:H:112:ASN:O	1:H:148:GLY:HA2	1.90	0.72
1:F:74:LEU:HA	1:F:92:GLN:HE21	1.53	0.72
1:E:4:ARG:NH1	1:F:126:GLY:O	2.23	0.72
1:F:224:MET:HE2	1:F:229:TYR:HA	1.69	0.72
1:E:75:GLY:H	1:E:91:ASN:ND2	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:198:MET:O	1:E:239:THR:HG23	1.89	0.71
1:A:27:LEU:HD22	1:A:39:PRO:HG2	1.71	0.71
1:C:43:ILE:CD1	1:C:60:VAL:HG21	2.20	0.71
1:G:208:TYR:HD2	1:G:250:LEU:HD13	1.55	0.70
1:C:21:SER:OG	1:C:66:SER:HB3	1.91	0.70
1:G:219:VAL:HG21	1:G:256:GLN:NE2	2.07	0.69
1:D:224:MET:HE3	1:D:228:SER:HB2	1.73	0.69
1:C:217:TRP:CE3	1:C:275:ARG:NH1	2.60	0.69
1:H:189:SER:C	1:H:190:MET:HG3	2.17	0.69
1:H:14:GLU:O	1:H:17:ILE:HD13	1.92	0.68
1:C:44:ALA:CB	1:C:51:ILE:HD13	2.23	0.68
1:H:27:LEU:HB2	1:H:144:CYS:O	1.94	0.68
1:F:22:TYR:CE2	1:F:64:ASN:HB2	2.29	0.68
1:G:57:MET:C	1:G:60:VAL:HG23	2.17	0.67
1:F:214:GLY:O	1:F:216:ARG:NH1	2.28	0.67
1:G:57:MET:O	1:G:60:VAL:HG23	1.94	0.67
1:E:165:GLU:OE1	1:E:171:HIS:NE2	2.28	0.67
1:H:272:PHE:O	1:H:275:ARG:NH1	2.27	0.67
1:D:82:LYS:HG2	1:D:177:GLU:O	1.96	0.66
1:H:189:SER:C	1:H:190:MET:CG	2.68	0.65
1:H:47:THR:HG23	2:H:401:K36:H13	1.78	0.65
1:H:90:VAL:HG23	1:H:92:GLN:O	1.97	0.65
1:D:218:PHE:HB2	1:D:268:LEU:HD11	1.79	0.64
1:F:74:LEU:CA	1:F:92:GLN:HE21	2.09	0.64
1:F:75:GLY:H	1:F:92:GLN:NE2	1.94	0.64
1:E:2:GLY:H	1:E:213:ASN:HD21	1.44	0.64
1:H:40:ARG:HG3	1:H:53:TYR:HE1	1.62	0.64
1:C:112:ASN:O	1:C:148:GLY:HA2	1.98	0.64
1:E:244:ILE:HG13	1:E:258:VAL:HG21	1.80	0.63
1:G:208:TYR:CE1	1:G:261:LEU:CD1	2.82	0.63
1:G:61:ARG:HB2	1:G:64:ASN:ND2	2.13	0.63
1:H:189:SER:O	1:H:190:MET:CG	2.46	0.63
1:F:74:LEU:CD2	1:F:92:GLN:HG3	2.26	0.63
1:F:224:MET:HE3	1:F:228:SER:HG	1.63	0.62
1:B:144:CYS:SG	2:B:401:K36:C20	2.86	0.62
1:G:56:GLU:O	1:G:60:VAL:HG22	1.99	0.62
1:C:46:ASP:OD2	1:C:49:ARG:HG3	2.00	0.62
1:F:21:SER:OG	1:F:66:SER:HB3	2.00	0.62
1:D:296:MET:HE2	1:D:296:MET:HA	1.81	0.62
1:D:224:MET:HE2	1:D:229:TYR:HA	1.82	0.61
1:E:123:SER:HB2	1:F:6:MET:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:THR:HG23	1:F:267:ARG:NH2	2.14	0.61
1:H:34:ASP:O	1:H:89:LYS:HG2	2.01	0.61
1:H:34:ASP:OD2	1:H:93:VAL:HB	2.01	0.61
1:H:55:ASN:N	1:H:55:ASN:OD1	2.33	0.61
1:D:224:MET:HE2	1:D:229:TYR:N	2.16	0.61
1:G:208:TYR:CD2	1:G:250:LEU:HD22	2.35	0.60
1:G:212:ILE:CD1	1:G:297:TYR:OH	2.49	0.60
1:C:122:GLY:O	1:D:9:PRO:HD3	2.01	0.60
1:H:62:LEU:HD13	1:H:62:LEU:C	2.26	0.60
1:C:218:PHE:HB2	1:C:268:LEU:HD11	1.84	0.60
1:D:144:CYS:SG	2:D:401:K36:C20	2.88	0.60
1:H:17:ILE:HD12	1:H:17:ILE:N	2.15	0.60
1:F:116:CYS:SG	1:F:121:PRO:HA	2.41	0.60
1:H:164:LEU:HB3	2:H:401:K36:H11	1.83	0.60
1:E:220:THR:O	1:E:260:LYS:HE3	2.02	0.59
1:E:199:SER:O	1:E:203:VAL:HG23	2.02	0.59
1:D:84:VAL:HG11	1:D:180:MET:HE2	1.84	0.59
1:A:2:GLY:H	1:A:213:ASN:ND2	1.99	0.59
1:E:224:MET:HE2	1:E:229:TYR:HA	1.85	0.59
1:G:57:MET:HA	1:G:60:VAL:CG2	2.32	0.59
1:F:43:ILE:HG22	1:F:56:GLU:HB3	1.85	0.59
1:E:1:SER:O	1:F:171:HIS:HE1	1.86	0.59
1:D:56:GLU:HA	1:D:56:GLU:OE2	2.01	0.58
1:D:224:MET:HE3	1:D:228:SER:CB	2.33	0.58
1:C:7:ALA:HB1	1:C:124:VAL:HG12	1.86	0.58
1:F:224:MET:HE2	1:F:229:TYR:CA	2.33	0.58
1:H:37:ILE:N	1:H:37:ILE:HD12	2.18	0.58
1:C:44:ALA:HB1	1:C:51:ILE:HD13	1.85	0.58
1:H:69:LYS:HE2	1:H:70:ASN:HD22	1.69	0.57
1:H:32:LEU:CD2	1:H:98:PRO:CD	2.80	0.57
1:C:84:VAL:HG22	1:C:178:GLY:O	2.05	0.57
1:H:292:VAL:O	1:H:296:MET:HG2	2.04	0.57
1:D:284:CYS:SG	1:D:286:GLU:HB2	2.44	0.57
1:F:75:GLY:H	1:F:92:GLN:HE22	1.51	0.56
1:G:208:TYR:CG	1:G:250:LEU:HD22	2.40	0.56
1:F:164:LEU:C	1:F:164:LEU:HD12	2.29	0.56
1:C:217:TRP:CE3	1:C:275:ARG:CZ	2.88	0.56
1:E:30:LEU:HD13	1:E:147:VAL:HG21	1.87	0.56
1:B:296:MET:HE2	1:B:296:MET:HA	1.86	0.56
1:G:2:GLY:H	1:G:213:ASN:HD21	1.52	0.56
1:H:20:VAL:CG2	1:H:67:VAL:HG22	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:THR:HA	1:B:51:ILE:HD11	1.86	0.56
1:C:43:ILE:HD11	1:C:60:VAL:HG21	1.86	0.56
1:G:244:ILE:CG2	1:G:258:VAL:CG2	2.77	0.56
2:B:401:K36:H25	2:B:401:K36:H30	1.86	0.56
1:D:224:MET:HE2	1:D:229:TYR:CA	2.35	0.56
1:F:222:THR:HB	1:F:263:ASP:CG	2.31	0.56
1:G:100:HIS:CG	1:G:100:HIS:O	2.60	0.56
1:C:44:ALA:HB2	1:C:51:ILE:HD13	1.87	0.55
1:D:24:ASN:HB2	3:D:506:HOH:O	2.06	0.55
1:D:185:GLU:O	1:D:191:GLN:NE2	2.39	0.55
1:G:164:LEU:HG	1:G:172:VAL:HB	1.89	0.55
1:E:40:ARG:HG3	1:E:53:TYR:CE1	2.41	0.55
1:E:130:ARG:HB3	1:E:196:ASN:OD1	2.06	0.55
1:G:241:LEU:HD22	1:G:262:LEU:HD21	1.87	0.55
1:E:84:VAL:HG11	1:E:180:MET:HE2	1.89	0.55
1:B:71:ASN:CB	1:E:92:GLN:HE22	2.19	0.55
1:G:116:CYS:O	1:G:143:THR:HA	2.07	0.55
1:H:32:LEU:HD11	1:H:158:PHE:CE2	2.42	0.55
1:E:197:VAL:HG12	1:E:239:THR:HG22	1.89	0.55
1:B:164:LEU:HB3	2:B:401:K36:H11	1.89	0.55
1:C:14:GLU:HB2	1:C:15:PRO:HD3	1.89	0.55
1:A:292:VAL:O	1:A:296:MET:HG2	2.07	0.54
1:C:219:VAL:HG11	1:C:256:GLN:OE1	2.07	0.54
1:H:61:ARG:HB3	1:H:61:ARG:CZ	2.37	0.54
1:D:224:MET:HE2	1:D:228:SER:C	2.32	0.54
1:F:130:ARG:HB3	1:F:196:ASN:OD1	2.08	0.54
1:F:22:TYR:CE2	1:F:64:ASN:CB	2.91	0.54
1:F:43:ILE:HD13	1:F:60:VAL:HG21	1.88	0.54
1:H:40:ARG:HG3	1:H:53:TYR:CE1	2.42	0.54
1:E:14:GLU:N	1:E:15:PRO:CD	2.70	0.54
1:F:144:CYS:SG	2:F:401:K36:O22	2.65	0.54
1:D:235:THR:C	1:D:236:ASN:HD22	2.16	0.54
1:G:292:VAL:O	1:G:296:MET:HG3	2.08	0.54
1:H:47:THR:HG23	2:H:401:K36:C16	2.38	0.53
1:H:272:PHE:CD2	1:H:281:GLY:O	2.61	0.53
1:A:2:GLY:N	1:A:213:ASN:HD21	2.01	0.53
1:A:43:ILE:HD11	1:A:65:PHE:CZ	2.43	0.53
1:F:201:ASP:OD2	1:F:201:ASP:N	2.41	0.53
1:G:123:SER:OG	1:H:6:MET:SD	2.61	0.53
1:C:224:MET:O	1:C:259:GLU:HB3	2.08	0.53
1:G:219:VAL:HG11	1:G:256:GLN:HE22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ASP:O	1:B:90:VAL:HG22	2.09	0.53
1:D:61:ARG:HB3	1:D:63:HIS:CE1	2.43	0.53
1:B:47:THR:O	1:B:188:PRO:HG3	2.08	0.53
1:C:65:PHE:HB3	1:C:76:VAL:HG21	1.89	0.53
1:E:75:GLY:N	1:E:91:ASN:ND2	2.55	0.53
1:H:175:ASN:ND2	1:H:177:GLU:HB2	2.23	0.53
1:G:100:HIS:O	1:G:100:HIS:CD2	2.62	0.53
1:C:259:GLU:OE2	1:C:259:GLU:N	2.31	0.53
1:A:39:PRO:HB3	1:A:163:HIS:CE1	2.43	0.52
1:C:7:ALA:CB	1:C:124:VAL:HG12	2.38	0.52
1:G:168:ASN:ND2	1:G:193:GLU:OE2	2.40	0.52
1:C:27:LEU:C	1:C:27:LEU:HD12	2.34	0.52
1:C:31:TRP:CE2	1:C:94:ASN:HB2	2.44	0.52
1:G:220:THR:HG22	1:G:222:THR:HG23	1.90	0.52
1:C:261:LEU:O	1:C:264:SER:HB2	2.10	0.52
1:E:43:ILE:CG2	1:E:56:GLU:HB3	2.40	0.52
1:F:101:LYS:O	1:F:157:TYR:HA	2.09	0.52
1:H:139:PHE:HB2	1:H:171:HIS:CD2	2.45	0.52
1:D:17:ILE:HG21	1:D:116:CYS:SG	2.50	0.52
1:H:21:SER:OG	1:H:66:SER:HB2	2.10	0.52
1:H:129:MET:HE2	1:H:133:GLY:C	2.34	0.52
1:H:166:LEU:N	1:H:166:LEU:HD23	2.24	0.52
1:G:114:LEU:HD11	1:G:121:PRO:HB3	1.92	0.52
1:C:25:ASN:ND2	1:C:42:VAL:O	2.29	0.52
1:G:217:TRP:NE1	1:G:275:ARG:HD2	2.25	0.52
1:E:138:SER:HB3	1:F:6:MET:HE1	1.92	0.51
1:E:219:VAL:HG11	1:E:256:GLN:NE2	2.25	0.51
1:F:218:PHE:HB2	1:F:268:LEU:HD11	1.92	0.51
1:B:92:GLN:NE2	1:E:71:ASN:HD22	2.08	0.51
1:G:56:GLU:O	1:G:60:VAL:CG2	2.59	0.51
1:E:185:GLU:N	1:E:191:GLN:OE1	2.33	0.51
1:G:57:MET:HA	1:G:60:VAL:HG21	1.92	0.51
1:G:208:TYR:CD1	1:G:261:LEU:CD1	2.93	0.51
1:D:272:PHE:CE2	1:D:277:ILE:HG13	2.46	0.51
1:D:84:VAL:HG22	1:D:178:GLY:O	2.10	0.51
1:G:138:SER:HB3	1:H:6:MET:CE	2.41	0.51
1:F:215:GLU:OE2	1:F:277:ILE:HA	2.10	0.51
1:B:214:GLY:O	1:B:216:ARG:HG3	2.11	0.51
1:C:217:TRP:CZ3	1:C:275:ARG:CZ	2.94	0.51
1:G:292:VAL:O	1:G:296:MET:CG	2.59	0.51
1:H:185:GLU:N	1:H:191:GLN:OE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:GLU:O	1:A:60:VAL:HG23	2.11	0.51
1:D:34:ASP:O	1:D:90:VAL:HG22	2.11	0.51
1:G:208:TYR:CD2	1:G:250:LEU:HD13	2.42	0.51
1:G:217:TRP:CD1	1:G:217:TRP:C	2.88	0.50
1:G:201:ASP:OD1	1:G:241:LEU:HD12	2.11	0.50
1:H:14:GLU:O	1:H:17:ILE:HD12	2.09	0.50
1:E:27:LEU:HD21	1:E:42:VAL:HB	1.93	0.50
1:E:15:PRO:O	1:E:69:LYS:NZ	2.44	0.50
1:G:224:MET:O	1:G:259:GLU:HB3	2.11	0.50
1:H:51:ILE:HG22	1:H:52:ASN:N	2.26	0.50
1:D:224:MET:CE	1:D:228:SER:C	2.85	0.50
1:D:205:ALA:O	1:D:292:VAL:HG21	2.12	0.50
1:G:277:ILE:O	1:G:280:TYR:N	2.45	0.50
1:A:40:ARG:HD3	1:A:84:VAL:HA	1.94	0.49
1:C:40:ARG:HG3	1:C:53:TYR:CE1	2.47	0.49
1:D:39:PRO:HB3	1:D:163:HIS:CE1	2.46	0.49
1:D:111:PHE:CB	1:D:150:VAL:HG13	2.42	0.49
1:D:251:ALA:HA	1:D:256:GLN:O	2.13	0.49
1:G:39:PRO:HB3	1:G:163:HIS:CE1	2.48	0.49
1:E:164:LEU:HD12	1:E:164:LEU:C	2.38	0.49
1:B:112:ASN:O	1:B:148:GLY:HA2	2.12	0.49
1:C:262:LEU:O	1:C:266:VAL:HG23	2.13	0.49
1:D:144:CYS:CB	2:D:401:K36:C21	2.91	0.49
1:C:232:TRP:CD1	1:C:236:ASN:OD1	2.66	0.48
1:A:46:ASP:OD2	1:A:49:ARG:HG3	2.13	0.48
1:C:31:TRP:CD2	1:C:94:ASN:HB2	2.48	0.48
1:E:18:VAL:HG12	1:E:69:LYS:HB2	1.96	0.48
1:F:47:THR:O	1:F:188:PRO:HG3	2.13	0.48
1:E:75:GLY:HA3	1:E:91:ASN:HD22	1.78	0.48
1:F:14:GLU:HB2	1:F:15:PRO:HD3	1.95	0.48
1:D:199:SER:O	1:D:203:VAL:HG23	2.13	0.48
1:E:84:VAL:HG21	1:E:180:MET:HE2	1.96	0.48
1:E:272:PHE:CE1	1:E:282:SER:HA	2.48	0.48
1:H:14:GLU:N	1:H:15:PRO:CD	2.77	0.48
1:H:62:LEU:C	1:H:62:LEU:CD1	2.86	0.48
1:A:145:GLY:HA2	1:A:161:MET:HG3	1.95	0.48
1:B:73:PHE:CD1	1:E:68:SER:HB2	2.48	0.48
1:C:47:THR:O	1:C:188:PRO:HG3	2.13	0.48
1:H:204:VAL:HG12	1:H:247:PHE:CE1	2.48	0.48
1:B:110:SER:OG	1:B:128:ASN:ND2	2.45	0.48
1:C:39:PRO:HB3	1:C:163:HIS:CE1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:CYS:HB3	3:C:509:HOH:O	2.14	0.48
1:G:272:PHE:CE2	1:G:277:ILE:CD1	2.97	0.48
1:H:31:TRP:CH2	1:H:94:ASN:HA	2.49	0.48
1:C:2:GLY:N	1:C:213:ASN:ND2	2.52	0.48
1:B:199:SER:O	1:B:203:VAL:HG23	2.13	0.48
1:G:244:ILE:HG22	1:G:244:ILE:O	2.14	0.48
1:C:17:ILE:HG21	1:C:116:CYS:SG	2.53	0.47
1:A:27:LEU:CD2	1:A:39:PRO:HG2	2.40	0.47
1:F:75:GLY:N	1:F:92:GLN:NE2	2.61	0.47
1:G:224:MET:HE2	1:G:229:TYR:CA	2.41	0.47
1:H:180:MET:CE	1:H:186:ASP:HB3	2.44	0.47
1:F:27:LEU:HB2	1:F:144:CYS:O	2.14	0.47
1:H:207:LEU:HB3	1:H:261:LEU:HD22	1.96	0.47
1:D:28:ASN:O	1:D:145:GLY:HA3	2.15	0.47
1:H:17:ILE:HD12	1:H:17:ILE:H	1.79	0.47
1:A:112:ASN:O	1:A:148:GLY:HA2	2.13	0.47
1:A:241:LEU:HD22	1:A:262:LEU:HD21	1.97	0.47
1:B:129:MET:CE	1:B:135:ILE:HG23	2.45	0.47
1:E:94:ASN:HB3	1:E:97:THR:OG1	2.14	0.47
1:G:217:TRP:CD1	1:G:218:PHE:N	2.83	0.47
1:H:19:ARG:O	1:H:67:VAL:HA	2.15	0.47
1:E:1:SER:O	1:F:171:HIS:CE1	2.67	0.47
1:E:2:GLY:N	1:E:213:ASN:HD21	2.11	0.47
1:B:71:ASN:HB2	1:E:92:GLN:HE22	1.79	0.47
1:E:14:GLU:N	1:E:15:PRO:HD3	2.30	0.47
1:E:235:THR:O	1:E:235:THR:OG1	2.33	0.47
1:B:73:PHE:CD1	1:E:68:SER:CB	2.98	0.47
1:E:111:PHE:HA	1:E:150:VAL:HG12	1.97	0.47
1:E:199:SER:HA	1:E:239:THR:CG2	2.45	0.47
1:A:20:VAL:HG22	1:A:67:VAL:HG22	1.96	0.46
1:A:52:ASN:ND2	1:A:55:ASN:OD1	2.48	0.46
1:H:31:TRP:CZ2	1:H:94:ASN:N	2.83	0.46
1:E:6:MET:SD	1:F:123:SER:HB2	2.55	0.46
1:C:217:TRP:HE3	1:C:275:ARG:NH1	2.13	0.46
1:A:14:GLU:CD	1:B:9:PRO:HB3	2.40	0.46
1:A:148:GLY:HA3	1:A:160:TYR:HB3	1.98	0.46
1:C:19:ARG:HB3	1:C:68:SER:OG	2.16	0.46
1:D:40:ARG:HA	1:D:86:LEU:HB2	1.98	0.46
1:G:112:ASN:O	1:G:148:GLY:HA2	2.15	0.46
1:G:293:ILE:HG22	1:G:294:ARG:N	2.30	0.46
1:E:180:MET:HG2	1:E:184:TYR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:ALA:O	1:F:255:GLY:N	2.48	0.46
1:G:208:TYR:HE1	1:G:261:LEU:HD12	1.73	0.46
1:C:77:VAL:HG23	1:C:77:VAL:O	2.15	0.46
1:G:33:GLY:O	1:G:93:VAL:HA	2.15	0.46
1:H:52:ASN:OD1	1:H:55:ASN:OD1	2.34	0.46
1:H:208:TYR:CZ	1:H:261:LEU:HD12	2.51	0.46
1:H:106:LYS:O	1:H:109:GLU:HB2	2.16	0.46
1:A:201:ASP:OD1	1:A:241:LEU:HD12	2.16	0.46
1:D:55:ASN:O	1:D:58:SER:OG	2.30	0.46
1:B:66:SER:HB3	1:E:66:SER:OG	2.16	0.45
1:B:229:TYR:O	1:B:232:TRP:N	2.49	0.45
1:F:105:ILE:HG12	1:F:159:VAL:HB	1.97	0.45
1:F:112:ASN:O	1:F:148:GLY:HA2	2.15	0.45
1:C:149:TYR:HA	1:C:157:TYR:O	2.16	0.45
1:F:213:ASN:N	1:F:213:ASN:HD22	2.14	0.45
1:G:27:LEU:HB2	1:G:144:CYS:O	2.16	0.45
1:C:257:SER:O	1:C:260:LYS:HB2	2.17	0.45
1:F:37:ILE:O	1:F:161:MET:HE1	2.16	0.45
1:G:95:PRO:HG2	1:G:96:ASN:ND2	2.31	0.45
1:A:6:MET:HE2	1:B:125:TYR:CE1	2.51	0.45
1:F:40:ARG:HB2	1:F:81:TYR:CE1	2.51	0.45
1:G:91:ASN:OD1	1:G:92:GLN:HG3	2.17	0.45
1:H:114:LEU:CD1	1:H:124:VAL:HG13	2.46	0.45
1:F:224:MET:HE2	1:F:228:SER:C	2.42	0.45
1:G:47:THR:O	1:G:47:THR:CG2	2.65	0.45
1:H:84:VAL:CG1	1:H:186:ASP:CG	2.90	0.45
1:B:224:MET:HE2	1:B:228:SER:C	2.41	0.45
1:D:220:THR:OG1	1:D:222:THR:OG1	2.31	0.45
1:E:220:THR:O	1:E:260:LYS:CE	2.65	0.45
1:F:66:SER:HG	1:F:73:PHE:HE2	1.65	0.45
1:C:65:PHE:CB	1:C:76:VAL:HG21	2.46	0.45
1:G:217:TRP:CG	1:G:275:ARG:NH2	2.85	0.45
1:G:272:PHE:CE2	1:G:277:ILE:HD12	2.51	0.45
1:C:27:LEU:C	1:C:27:LEU:CD1	2.90	0.44
1:C:41:HIS:CD2	2:C:401:K36:H8	2.52	0.44
1:F:47:THR:O	1:F:47:THR:CG2	2.65	0.44
1:G:252:ALA:O	1:G:255:GLY:N	2.50	0.44
1:G:247:PHE:O	1:G:251:ALA:HB2	2.18	0.44
1:H:166:LEU:HD21	1:H:172:VAL:HG21	1.99	0.44
1:C:232:TRP:NE1	1:C:236:ASN:OD1	2.50	0.44
1:F:120:CYS:O	1:F:121:PRO:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:225:SER:HB3	1:H:228:SER:HG	1.72	0.44
1:G:253:LYS:HB3	1:G:297:TYR:OH	2.17	0.44
1:H:116:CYS:O	1:H:143:THR:HA	2.17	0.44
1:A:25:ASN:HD22	1:A:42:VAL:C	2.25	0.44
1:A:40:ARG:NH2	1:A:53:TYR:CD2	2.86	0.44
1:D:150:VAL:HG23	1:D:157:TYR:HB2	1.99	0.44
1:A:7:ALA:HA	1:A:112:ASN:OD1	2.17	0.44
1:A:21:SER:OG	1:A:66:SER:HB3	2.17	0.44
1:A:86:LEU:HD12	1:A:86:LEU:HA	1.84	0.44
1:B:61:ARG:HB2	1:B:64:ASN:ND2	2.33	0.44
1:C:204:VAL:HG12	1:C:247:PHE:CE1	2.52	0.44
1:A:31:TRP:HZ2	1:A:92:GLN:HG2	1.83	0.44
1:A:57:MET:SD	1:A:81:TYR:HE1	2.41	0.44
1:G:2:GLY:N	1:G:213:ASN:HD21	2.16	0.43
2:A:401:K36:O10	2:A:401:K36:C17	2.65	0.43
1:H:101:LYS:O	1:H:157:TYR:HA	2.18	0.43
1:H:192:LEU:HD22	1:H:192:LEU:HA	1.76	0.43
1:C:116:CYS:O	1:C:143:THR:HA	2.17	0.43
1:G:220:THR:HG22	1:G:222:THR:H	1.83	0.43
1:G:257:SER:O	1:G:260:LYS:HG2	2.19	0.43
1:B:101:LYS:O	1:B:157:TYR:HA	2.18	0.43
1:C:28:ASN:O	1:C:145:GLY:HA3	2.18	0.43
1:G:200:SER:H	1:G:239:THR:HG1	1.66	0.43
1:F:140:ILE:O	1:F:141:ALA:C	2.61	0.43
1:G:261:LEU:HA	1:G:264:SER:OG	2.18	0.43
1:H:134:THR:HG21	1:H:193:GLU:HG3	2.00	0.43
1:H:185:GLU:O	1:H:191:GLN:NE2	2.50	0.43
1:F:217:TRP:CE3	1:F:217:TRP:C	2.97	0.43
1:F:233:ALA:HB1	1:F:238:PHE:O	2.18	0.43
1:G:276:THR:HA	1:G:280:TYR:O	2.19	0.43
1:A:43:ILE:CD1	1:A:86:LEU:HD21	2.49	0.43
2:H:401:K36:C17	2:H:401:K36:O10	2.65	0.43
1:B:257:SER:O	1:B:260:LYS:HB2	2.19	0.43
1:D:165:GLU:OE1	2:D:401:K36:N28	2.52	0.43
1:G:8:GLN:HB3	1:G:151:LEU:HD12	2.00	0.43
2:B:401:K36:H11	2:B:401:K36:H5	1.74	0.43
1:E:131:SER:HG	1:E:197:VAL:H	1.66	0.43
1:H:42:VAL:HG13	1:H:43:ILE:HG13	2.00	0.43
1:B:211:LEU:HD11	1:B:261:LEU:HD21	2.01	0.43
1:C:130:ARG:HH11	1:C:193:GLU:CD	2.25	0.43
1:E:40:ARG:NE	1:E:186:ASP:OD1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:GLU:OE1	2:F:401:K36:N28	2.52	0.43
1:F:224:MET:HE2	1:F:229:TYR:N	2.34	0.43
1:H:34:ASP:O	1:H:89:LYS:CG	2.66	0.43
2:C:401:K36:C17	2:C:401:K36:O10	2.65	0.42
1:H:31:TRP:HA	1:H:35:GLU:O	2.19	0.42
1:A:110:SER:OG	1:A:291:GLU:OE2	2.29	0.42
1:E:132:GLN:HG3	1:E:193:GLU:O	2.19	0.42
1:H:235:THR:O	1:H:235:THR:OG1	2.34	0.42
1:E:27:LEU:C	1:E:27:LEU:HD12	2.45	0.42
1:B:78:SER:HB3	1:B:89:LYS:HB2	2.01	0.42
1:D:261:LEU:HA	1:D:264:SER:OG	2.20	0.42
1:F:164:LEU:CD1	1:F:172:VAL:HB	2.49	0.42
1:G:17:ILE:HG21	1:G:116:CYS:SG	2.59	0.42
1:G:217:TRP:CD1	1:G:275:ARG:CZ	3.02	0.42
1:E:91:ASN:OD1	1:E:91:ASN:C	2.61	0.42
1:F:66:SER:OG	1:F:73:PHE:HE2	2.03	0.42
1:G:138:SER:HA	1:H:1:SER:O	2.19	0.42
1:C:203:VAL:O	1:C:206:PHE:HB3	2.20	0.42
1:E:148:GLY:HA3	1:E:160:TYR:HB3	2.02	0.42
1:A:220:THR:O	1:A:260:LYS:HE3	2.20	0.42
1:B:18:VAL:HG12	1:B:69:LYS:HB2	2.02	0.42
1:B:116:CYS:SG	1:B:121:PRO:HA	2.60	0.42
1:C:30:LEU:O	1:C:36:VAL:HA	2.19	0.42
1:D:21:SER:OG	1:D:66:SER:HB3	2.20	0.42
1:E:175:ASN:HD21	1:E:179:GLU:HB2	1.84	0.42
1:G:220:THR:CG2	1:G:222:THR:HG23	2.49	0.42
1:H:147:VAL:CG1	1:H:158:PHE:HD1	2.32	0.42
1:A:57:MET:SD	1:A:81:TYR:CE1	3.13	0.42
1:D:40:ARG:C	1:D:42:VAL:H	2.26	0.42
1:E:103:LYS:HB3	1:E:157:TYR:CD2	2.54	0.42
1:G:14:GLU:N	1:G:15:PRO:CD	2.82	0.42
1:H:14:GLU:C	1:H:17:ILE:CD1	2.91	0.42
1:G:164:LEU:HD12	1:G:164:LEU:C	2.46	0.41
1:H:224:MET:SD	1:H:266:VAL:HG21	2.60	0.41
1:H:232:TRP:O	1:H:236:ASN:OD1	2.37	0.41
1:E:164:LEU:HD12	1:E:165:GLU:N	2.35	0.41
1:F:49:ARG:HG2	1:F:49:ARG:HH11	1.85	0.41
1:A:27:LEU:HD12	1:A:27:LEU:C	2.45	0.41
1:B:40:ARG:HG3	1:B:53:TYR:CE1	2.55	0.41
1:B:56:GLU:HA	1:B:56:GLU:OE2	2.21	0.41
1:C:27:LEU:HD21	1:C:42:VAL:HB	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:TYR:HB3	1:G:250:LEU:CD2	2.50	0.41
1:D:258:VAL:O	1:D:262:LEU:HG	2.20	0.41
1:G:149:TYR:HA	1:G:157:TYR:O	2.20	0.41
1:G:241:LEU:HD12	1:G:241:LEU:HA	1.84	0.41
1:E:199:SER:HA	1:E:239:THR:HG23	2.02	0.41
1:F:174:SER:HA	1:F:180:MET:HA	2.01	0.41
1:G:186:ASP:CG	1:G:186:ASP:O	2.64	0.41
1:D:180:MET:HE1	1:D:186:ASP:HB3	2.02	0.41
1:C:19:ARG:N	1:C:68:SER:O	2.49	0.41
1:D:144:CYS:SG	2:D:401:K36:N19	2.94	0.41
1:G:244:ILE:HG21	1:G:258:VAL:HB	2.03	0.41
1:G:275:ARG:HH21	1:G:275:ARG:HB2	1.84	0.41
1:E:241:LEU:HD11	1:E:247:PHE:HE2	1.85	0.41
1:D:200:SER:H	1:D:239:THR:HG1	1.65	0.41
1:E:105:ILE:HD13	1:E:105:ILE:HA	1.89	0.41
1:E:204:VAL:HG12	1:E:247:PHE:CE1	2.56	0.41
1:F:113:ILE:O	1:F:124:VAL:HA	2.21	0.41
1:B:139:PHE:HB2	1:B:171:HIS:CD2	2.56	0.41
1:B:218:PHE:HB2	1:B:268:LEU:HD11	2.02	0.41
1:F:40:ARG:HG2	1:F:84:VAL:O	2.21	0.41
1:F:164:LEU:HB3	2:F:401:K36:H11	2.03	0.41
1:B:30:LEU:O	1:B:36:VAL:HA	2.21	0.40
1:G:285:ASP:OD1	1:G:285:ASP:C	2.64	0.40
1:H:84:VAL:HG12	1:H:84:VAL:O	2.21	0.40
1:H:10:SER:OG	1:H:14:GLU:HG3	2.21	0.40
1:F:19:ARG:O	1:F:67:VAL:HA	2.21	0.40
2:G:401:K36:H11	2:G:401:K36:H5	1.87	0.40
1:H:114:LEU:HD13	1:H:124:VAL:HG13	2.02	0.40
1:B:94:ASN:HB3	1:B:97:THR:OG1	2.21	0.40
1:C:91:ASN:CG	1:C:92:GLN:HE21	2.29	0.40
1:D:150:VAL:HG22	1:D:159:VAL:HG11	2.04	0.40
1:F:57:MET:HE2	1:F:81:TYR:CE2	2.57	0.40
1:A:117:TYR:O	1:A:120:CYS:HB2	2.21	0.40
1:C:105:ILE:HG12	1:C:159:VAL:HB	2.03	0.40
1:D:93:VAL:O	1:D:95:PRO:HD3	2.22	0.40
1:F:43:ILE:HD13	1:F:60:VAL:CG2	2.52	0.40
1:G:244:ILE:CG2	1:G:258:VAL:HB	2.51	0.40
1:H:204:VAL:CG1	1:H:247:PHE:CE1	3.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	297/302 (98%)	281 (95%)	16 (5%)	0	100	100
1	B	297/302 (98%)	273 (92%)	24 (8%)	0	100	100
1	C	296/302 (98%)	277 (94%)	18 (6%)	1 (0%)	36	56
1	D	292/302 (97%)	269 (92%)	22 (8%)	1 (0%)	36	56
1	E	297/302 (98%)	277 (93%)	19 (6%)	1 (0%)	36	56
1	F	297/302 (98%)	280 (94%)	16 (5%)	1 (0%)	36	56
1	G	296/302 (98%)	269 (91%)	27 (9%)	0	100	100
1	H	283/302 (94%)	251 (89%)	29 (10%)	3 (1%)	11	22
All	All	2355/2416 (98%)	2177 (92%)	171 (7%)	7 (0%)	36	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	190	MET
1	H	189	SER
1	E	237	SER
1	C	279	SER
1	H	61	ARG
1	D	258	VAL
1	F	50	VAL

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	255/258 (99%)	242 (95%)	13 (5%)	21	40
1	B	255/258 (99%)	236 (92%)	19 (8%)	12	24
1	C	254/258 (98%)	236 (93%)	18 (7%)	13	25
1	D	252/258 (98%)	243 (96%)	9 (4%)	31	55
1	E	255/258 (99%)	228 (89%)	27 (11%)	6	13
1	F	255/258 (99%)	233 (91%)	22 (9%)	10	18
1	G	254/258 (98%)	236 (93%)	18 (7%)	13	25
1	H	246/258 (95%)	215 (87%)	31 (13%)	4	8
All	All	2026/2064 (98%)	1869 (92%)	157 (8%)	12	22

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	54	GLU
1	A	59	SER
1	A	77	VAL
1	A	80	LYS
1	A	91	ASN
1	A	103	LYS
1	A	121	PRO
1	A	153	ASN
1	A	219	VAL
1	A	220	THR
1	A	235	THR
1	A	279	SER
1	B	26	VAL
1	B	54	GLU
1	B	66	SER
1	B	68	SER
1	B	71	ASN
1	B	92	GLN
1	B	105	ILE
1	B	123	SER
1	B	124	VAL
1	B	129	MET
1	B	138	SER
1	B	152	GLU
1	B	190	MET
1	B	195	THR

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Mol	Chain	Res	Type
1	B	227	GLU
1	B	237	SER
1	B	239	THR
1	B	267	ARG
1	B	279	SER
1	C	1	SER
1	C	26	VAL
1	C	27	LEU
1	C	43	ILE
1	C	58	SER
1	C	59	SER
1	C	60	VAL
1	C	71	ASN
1	C	77	VAL
1	C	120	CYS
1	C	190	MET
1	C	195	THR
1	C	226	LEU
1	C	227	GLU
1	C	235	THR
1	C	241	LEU
1	C	276	THR
1	C	290	THR
1	D	45	SER
1	D	80	LYS
1	D	112	ASN
1	D	129	MET
1	D	191	GLN
1	D	228	SER
1	D	244	ILE
1	D	264	SER
1	D	286	GLU
1	E	3	LEU
1	E	35	GLU
1	E	43	ILE
1	E	45	SER
1	E	60	VAL
1	E	63	HIS
1	E	68	SER
1	E	77	VAL
1	E	78	SER
1	E	90	VAL

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Mol	Chain	Res	Type
1	E	92	GLN
1	E	105	ILE
1	E	110	SER
1	E	124	VAL
1	E	129	MET
1	E	185	GLU
1	E	204	VAL
1	E	221	ASN
1	E	222	THR
1	E	223	SER
1	E	235	THR
1	E	237	SER
1	E	239	THR
1	E	244	ILE
1	E	245	ASP
1	E	269	ASN
1	E	276	THR
1	F	27	LEU
1	F	45	SER
1	F	46	ASP
1	F	47	THR
1	F	55	ASN
1	F	59	SER
1	F	60	VAL
1	F	71	ASN
1	F	82	LYS
1	F	92	GLN
1	F	120	CYS
1	F	123	SER
1	F	124	VAL
1	F	129	MET
1	F	190	MET
1	F	201	ASP
1	F	219	VAL
1	F	220	THR
1	F	222	THR
1	F	235	THR
1	F	236	ASN
1	F	237	SER
1	G	3	LEU
1	G	47	THR
1	G	58	SER

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Mol	Chain	Res	Type
1	G	71	ASN
1	G	150	VAL
1	G	190	MET
1	G	212	ILE
1	G	217	TRP
1	G	219	VAL
1	G	223	SER
1	G	225	SER
1	G	231	THR
1	G	250	LEU
1	G	260	LYS
1	G	263	ASP
1	G	275	ARG
1	G	278	LEU
1	G	293	ILE
1	H	17	ILE
1	H	18	VAL
1	H	34	ASP
1	H	35	GLU
1	H	37	ILE
1	H	38	CYS
1	H	55	ASN
1	H	60	VAL
1	H	62	LEU
1	H	67	VAL
1	H	86	LEU
1	H	90	VAL
1	H	91	ASN
1	H	93	VAL
1	H	97	THR
1	H	124	VAL
1	H	127	VAL
1	H	190	MET
1	H	192	LEU
1	H	213	ASN
1	H	219	VAL
1	H	221	ASN
1	H	222	THR
1	H	226	LEU
1	H	228	SER
1	H	235	THR
1	H	241	LEU

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Mol	Chain	Res	Type
1	H	244	ILE
1	H	275	ARG
1	H	290	THR
1	H	295	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	52	ASN
1	A	92	GLN
1	A	163	HIS
1	A	213	ASN
1	A	230	ASN
1	B	64	ASN
1	B	71	ASN
1	B	92	GLN
1	B	128	ASN
1	C	52	ASN
1	C	55	ASN
1	C	63	HIS
1	C	71	ASN
1	C	92	GLN
1	C	213	ASN
1	D	55	ASN
1	D	63	HIS
1	D	196	ASN
1	D	221	ASN
1	D	236	ASN
1	E	24	ASN
1	E	55	ASN
1	E	91	ASN
1	E	92	GLN
1	E	213	ASN
1	E	236	ASN
1	E	269	ASN
1	F	55	ASN
1	F	92	GLN
1	F	171	HIS
1	F	236	ASN
1	G	41	HIS
1	G	55	ASN

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Mol	Chain	Res	Type
1	G	94	ASN
1	G	96	ASN
1	G	230	ASN
1	G	236	ASN
1	G	256	GLN
1	G	269	ASN
1	H	41	HIS
1	H	70	ASN
1	H	132	GLN
1	H	221	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	K36	F	401	-	30,30,34	3.77	9 (30%)	35,39,47	1.61	5 (14%)
2	K36	E	401	1	30,30,34	3.74	10 (33%)	35,39,47	1.84	8 (22%)
2	K36	H	401	-	30,30,34	3.47	6 (20%)	35,39,47	2.03	9 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	K36	B	401	-	30,30,34	3.49	9 (30%)	35,39,47	1.95	9 (25%)
2	K36	C	401	1	30,30,34	3.49	6 (20%)	35,39,47	2.02	9 (25%)
2	K36	G	401	1	30,30,34	3.51	6 (20%)	35,39,47	1.85	9 (25%)
2	K36	D	401	-	30,30,34	3.71	11 (36%)	35,39,47	1.72	9 (25%)
2	K36	A	401	1	30,30,34	3.48	6 (20%)	35,39,47	2.03	9 (25%)

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	K36	F	401	-	-	7/27/37/45	0/2/2/2
2	K36	E	401	1	-	8/27/37/45	0/2/2/2
2	K36	H	401	-	-	10/27/37/45	0/2/2/2
2	K36	C	401	1	1/1/7/12	10/27/37/45	0/2/2/2
2	K36	B	401	-	-	8/27/37/45	0/2/2/2
2	K36	G	401	1	-	7/27/37/45	0/2/2/2
2	K36	D	401	-	-	4/27/37/45	0/2/2/2
2	K36	A	401	1	-	10/27/37/45	0/2/2/2

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	K36	C29-N28	16.49	1.51	1.33
2	E	401	K36	C29-N28	16.37	1.50	1.33
2	G	401	K36	C29-N28	15.54	1.50	1.33
2	D	401	K36	C29-N28	15.50	1.50	1.33
2	C	401	K36	C29-N28	15.21	1.49	1.33
2	A	401	K36	C29-N28	15.16	1.49	1.33
2	H	401	K36	C29-N28	15.13	1.49	1.33
2	B	401	K36	C29-N28	14.47	1.48	1.33
2	D	401	K36	C17-N19	6.90	1.48	1.34
2	F	401	K36	C9-N11	6.72	1.51	1.34
2	B	401	K36	C17-N19	6.12	1.47	1.34
2	E	401	K36	C9-N11	6.09	1.49	1.34
2	F	401	K36	C17-N19	6.03	1.47	1.34
2	D	401	K36	C9-N11	6.03	1.49	1.34
2	B	401	K36	C9-N11	5.86	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	K36	C17-N19	5.82	1.46	1.34
2	A	401	K36	C17-N19	5.81	1.46	1.34
2	H	401	K36	C17-N19	5.81	1.46	1.34
2	C	401	K36	C9-N11	5.74	1.49	1.34
2	G	401	K36	C9-N11	5.73	1.49	1.34
2	E	401	K36	O8-C9	5.72	1.46	1.35
2	A	401	K36	C9-N11	5.70	1.48	1.34
2	H	401	K36	C9-N11	5.69	1.48	1.34
2	G	401	K36	C17-N19	5.51	1.45	1.34
2	D	401	K36	O8-C9	4.95	1.45	1.35
2	B	401	K36	O8-C9	4.90	1.45	1.35
2	E	401	K36	C17-N19	4.57	1.43	1.34
2	F	401	K36	O8-C9	4.28	1.43	1.35
2	G	401	K36	C24-C25	4.13	1.63	1.53
2	G	401	K36	O8-C9	4.09	1.43	1.35
2	A	401	K36	C24-C25	3.48	1.61	1.53
2	C	401	K36	C24-C25	3.47	1.61	1.53
2	C	401	K36	O8-C9	3.47	1.42	1.35
2	A	401	K36	O8-C9	3.45	1.42	1.35
2	H	401	K36	O8-C9	3.45	1.42	1.35
2	H	401	K36	C24-C25	3.44	1.61	1.53
2	D	401	K36	C25-C29	-3.17	1.44	1.52
2	B	401	K36	C3-C2	3.08	1.44	1.38
2	D	401	K36	C27-N28	-3.01	1.39	1.46
2	E	401	K36	O30-C29	-2.98	1.17	1.23
2	F	401	K36	C24-C25	2.80	1.60	1.53
2	B	401	K36	C7-C1	2.78	1.57	1.50
2	D	401	K36	C3-C2	2.78	1.43	1.38
2	E	401	K36	C24-C25	2.75	1.59	1.53
2	B	401	K36	C5-C6	2.70	1.43	1.38
2	F	401	K36	C27-N28	-2.67	1.40	1.46
2	E	401	K36	C12-N11	-2.65	1.40	1.45
2	F	401	K36	C5-C6	2.40	1.43	1.38
2	H	401	K36	C27-N28	-2.40	1.41	1.46
2	A	401	K36	C27-N28	-2.40	1.41	1.46
2	C	401	K36	C27-N28	-2.38	1.41	1.46
2	G	401	K36	C12-N11	-2.37	1.40	1.45
2	D	401	K36	C5-C6	2.34	1.42	1.38
2	B	401	K36	C24-C25	2.27	1.58	1.53
2	F	401	K36	C3-C2	2.24	1.42	1.38
2	F	401	K36	C25-C29	-2.23	1.46	1.52
2	D	401	K36	C21-C20	-2.10	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	K36	C5-C6	2.07	1.42	1.38
2	E	401	K36	C5-C4	2.05	1.42	1.38
2	E	401	K36	C7-C1	2.04	1.55	1.50
2	B	401	K36	C21-C20	-2.04	1.48	1.52
2	D	401	K36	C24-C25	2.02	1.58	1.53
2	D	401	K36	C7-C1	2.00	1.55	1.50

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	K36	O10-C9-N11	-5.87	115.25	124.86
2	A	401	K36	O10-C9-N11	-5.86	115.26	124.86
2	H	401	K36	O10-C9-N11	-5.86	115.26	124.86
2	E	401	K36	O8-C9-N11	5.70	122.64	110.45
2	B	401	K36	O8-C9-N11	5.59	122.40	110.45
2	H	401	K36	O8-C9-O10	-5.14	114.40	124.26
2	A	401	K36	O8-C9-O10	-5.12	114.45	124.26
2	C	401	K36	O8-C9-O10	-5.08	114.51	124.26
2	F	401	K36	O8-C9-N11	5.03	121.21	110.45
2	H	401	K36	O8-C9-N11	5.03	121.20	110.45
2	A	401	K36	O8-C9-N11	5.00	121.15	110.45
2	C	401	K36	O8-C9-N11	4.98	121.11	110.45
2	B	401	K36	O10-C9-N11	-4.93	116.78	124.86
2	D	401	K36	O8-C9-N11	4.91	120.96	110.45
2	G	401	K36	O10-C9-N11	-4.77	117.04	124.86
2	E	401	K36	O10-C9-N11	-4.57	117.37	124.86
2	D	401	K36	O10-C9-N11	-4.02	118.28	124.86
2	G	401	K36	O8-C9-O10	-3.87	116.85	124.26
2	B	401	K36	C20-N19-C17	-3.86	117.08	123.29
2	G	401	K36	C20-N19-C17	-3.81	117.16	123.29
2	F	401	K36	O8-C9-O10	-3.78	117.01	124.26
2	G	401	K36	C7-O8-C9	-3.75	107.48	115.93
2	D	401	K36	C20-N19-C17	-3.64	117.43	123.29
2	B	401	K36	C12-C17-N19	3.36	123.79	116.63
2	B	401	K36	O8-C9-O10	-3.17	118.18	124.26
2	F	401	K36	C21-C20-N19	3.10	116.26	109.63
2	D	401	K36	O8-C9-O10	-3.05	118.42	124.26
2	C	401	K36	C27-N28-C29	-2.94	107.56	113.79
2	A	401	K36	C27-N28-C29	-2.93	107.58	113.79
2	H	401	K36	C27-N28-C29	-2.92	107.59	113.79
2	E	401	K36	C27-N28-C29	-2.90	107.64	113.79
2	D	401	K36	C27-N28-C29	-2.76	107.93	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	K36	C21-C20-N19	-2.70	103.87	109.63
2	C	401	K36	C21-C20-N19	-2.70	103.87	109.63
2	H	401	K36	C21-C20-N19	-2.69	103.88	109.63
2	B	401	K36	C27-N28-C29	-2.66	108.14	113.79
2	E	401	K36	C21-C20-N19	-2.64	104.00	109.63
2	D	401	K36	C27-C26-C25	-2.61	101.83	105.69
2	G	401	K36	O8-C9-N11	2.59	115.99	110.45
2	E	401	K36	O8-C9-O10	-2.56	119.35	124.26
2	E	401	K36	C20-N19-C17	-2.53	119.21	123.29
2	H	401	K36	C7-O8-C9	-2.52	110.26	115.93
2	C	401	K36	C7-O8-C9	-2.52	110.26	115.93
2	A	401	K36	C7-O8-C9	-2.52	110.26	115.93
2	G	401	K36	C27-N28-C29	-2.52	108.45	113.79
2	A	401	K36	C27-C26-C25	-2.45	102.07	105.69
2	E	401	K36	O18-C17-N19	-2.45	118.58	122.96
2	B	401	K36	O18-C17-N19	-2.44	118.59	122.96
2	C	401	K36	C27-C26-C25	-2.44	102.09	105.69
2	H	401	K36	C27-C26-C25	-2.44	102.09	105.69
2	H	401	K36	C6-C1-C2	2.42	121.83	118.23
2	A	401	K36	C6-C1-C2	2.41	121.82	118.23
2	C	401	K36	C6-C1-C2	2.41	121.81	118.23
2	B	401	K36	C24-C25-C29	-2.40	107.63	112.81
2	F	401	K36	C26-C25-C29	2.37	106.11	102.87
2	C	401	K36	C12-N11-C9	-2.31	115.19	120.93
2	G	401	K36	C6-C1-C2	2.29	121.63	118.23
2	A	401	K36	C12-N11-C9	-2.28	115.25	120.93
2	H	401	K36	C12-N11-C9	-2.27	115.29	120.93
2	D	401	K36	C21-C20-N19	2.15	114.23	109.63
2	G	401	K36	C24-C20-C21	2.08	115.61	111.30
2	E	401	K36	C7-O8-C9	-2.05	111.32	115.93
2	D	401	K36	C24-C25-C29	-2.04	108.39	112.81
2	G	401	K36	C26-C25-C29	2.02	105.64	102.87
2	F	401	K36	C27-N28-C29	-2.01	109.52	113.79
2	B	401	K36	C26-C25-C29	2.01	105.63	102.87
2	D	401	K36	C12-C17-N19	2.00	120.89	116.63

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	401	K36	C21

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	K36	N11-C9-O8-C7
2	A	401	K36	C24-C20-C21-O22
2	B	401	K36	C24-C20-C21-O22
2	C	401	K36	N11-C9-O8-C7
2	C	401	K36	C24-C20-C21-O22
2	D	401	K36	N11-C9-O8-C7
2	E	401	K36	O10-C9-O8-C7
2	E	401	K36	N11-C9-O8-C7
2	E	401	K36	N19-C20-C21-O22
2	E	401	K36	C24-C20-C21-O22
2	F	401	K36	O10-C9-O8-C7
2	F	401	K36	N11-C9-O8-C7
2	F	401	K36	C24-C20-C21-O22
2	G	401	K36	O10-C9-O8-C7
2	G	401	K36	N11-C9-O8-C7
2	H	401	K36	N11-C9-O8-C7
2	H	401	K36	C24-C20-C21-O22
2	A	401	K36	O10-C9-O8-C7
2	C	401	K36	O10-C9-O8-C7
2	D	401	K36	O10-C9-O8-C7
2	H	401	K36	O10-C9-O8-C7
2	B	401	K36	O10-C9-O8-C7
2	B	401	K36	N11-C9-O8-C7
2	G	401	K36	N11-C12-C13-C14
2	E	401	K36	N11-C12-C13-C14
2	E	401	K36	C17-C12-C13-C14
2	G	401	K36	C17-C12-C13-C14
2	B	401	K36	C12-C13-C14-C15
2	G	401	K36	C12-C13-C14-C15
2	A	401	K36	N19-C20-C21-O22
2	B	401	K36	N19-C20-C21-O22
2	C	401	K36	N19-C20-C21-O22
2	F	401	K36	N19-C20-C21-O22
2	H	401	K36	N19-C20-C21-O22
2	A	401	K36	C12-C13-C14-C15
2	C	401	K36	C12-C13-C14-C15
2	H	401	K36	C12-C13-C14-C15
2	F	401	K36	N11-C12-C13-C14
2	F	401	K36	C12-C13-C14-C15
2	A	401	K36	O8-C9-N11-C12
2	H	401	K36	O8-C9-N11-C12
2	C	401	K36	O8-C9-N11-C12
2	B	401	K36	N11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
2	B	401	K36	C12-C13-C14-C16
2	F	401	K36	C17-C12-C13-C14
2	G	401	K36	C12-C13-C14-C16
2	A	401	K36	N11-C12-C13-C14
2	C	401	K36	N11-C12-C13-C14
2	H	401	K36	N11-C12-C13-C14
2	A	401	K36	C17-C12-C13-C14
2	C	401	K36	C17-C12-C13-C14
2	H	401	K36	C17-C12-C13-C14
2	B	401	K36	C17-C12-C13-C14
2	C	401	K36	C12-C13-C14-C16
2	A	401	K36	C12-C13-C14-C16
2	H	401	K36	C12-C13-C14-C16
2	D	401	K36	C12-C13-C14-C16
2	E	401	K36	C12-C13-C14-C15
2	A	401	K36	C1-C7-O8-C9
2	C	401	K36	C1-C7-O8-C9
2	H	401	K36	C1-C7-O8-C9
2	G	401	K36	C1-C7-O8-C9
2	D	401	K36	C12-C13-C14-C15
2	E	401	K36	C1-C7-O8-C9

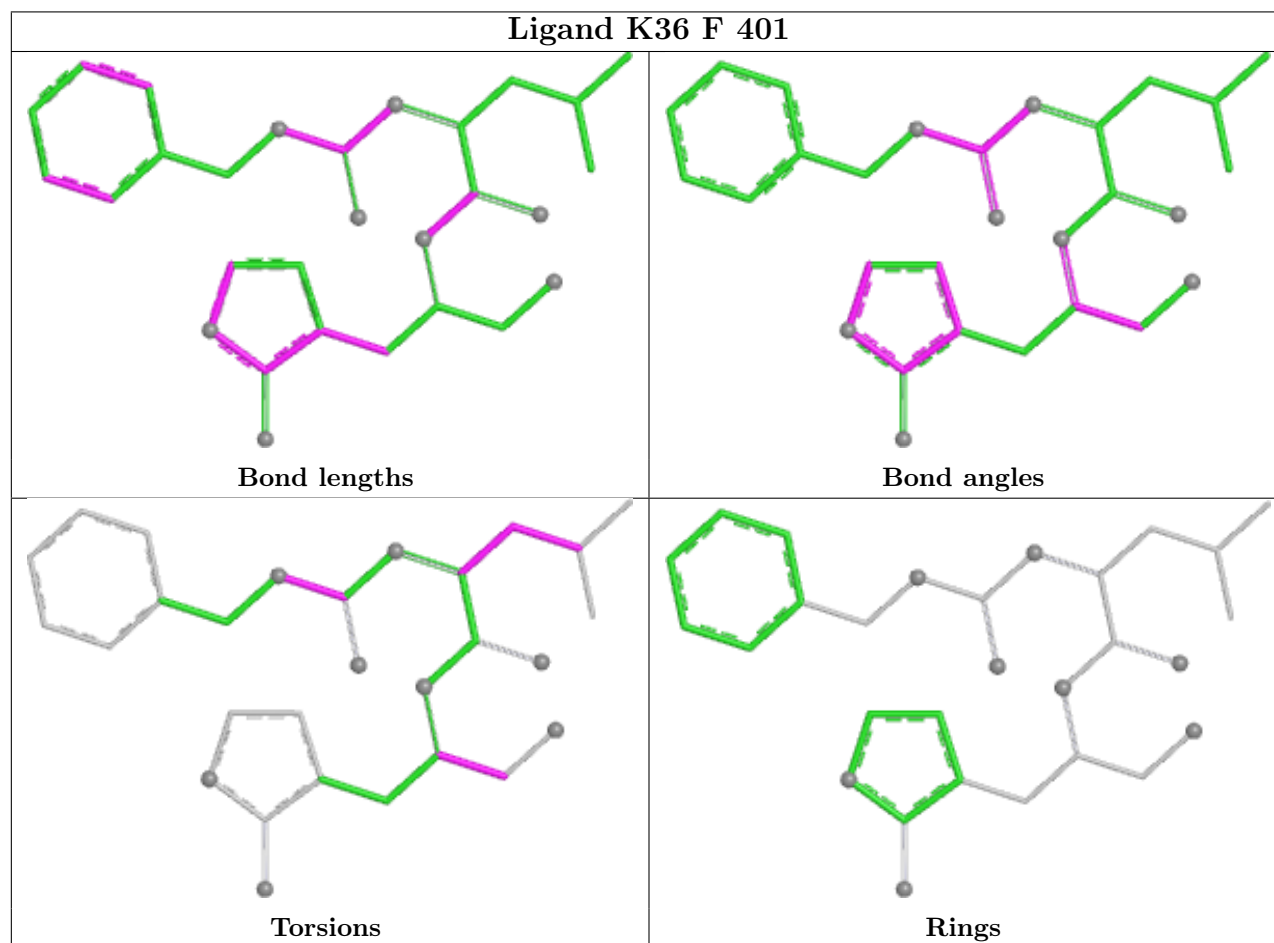
There are no ring outliers.

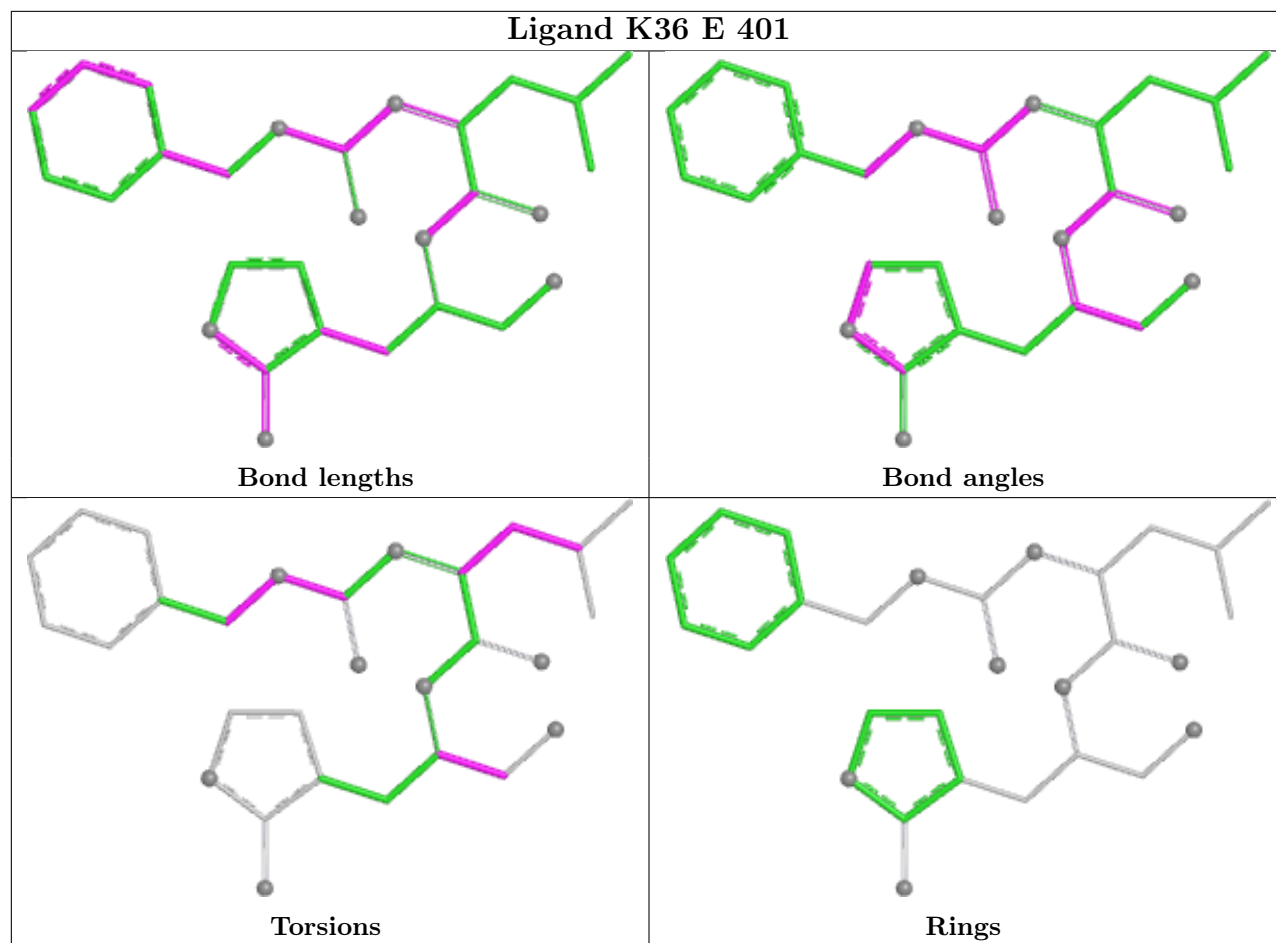
7 monomers are involved in 24 short contacts:

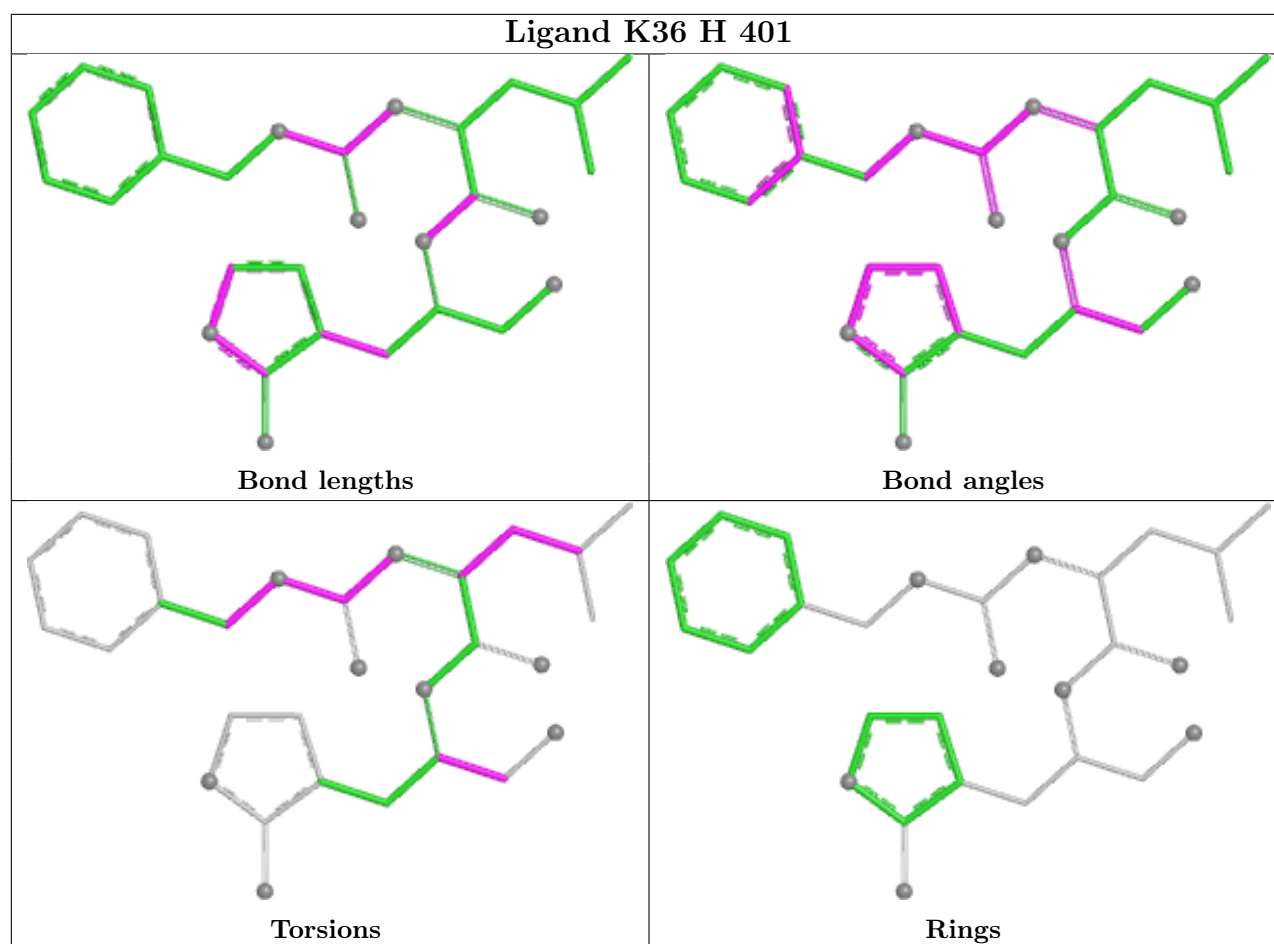
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	K36	4	0
2	H	401	K36	5	0
2	B	401	K36	6	0
2	C	401	K36	2	0
2	G	401	K36	1	0
2	D	401	K36	5	0
2	A	401	K36	1	0

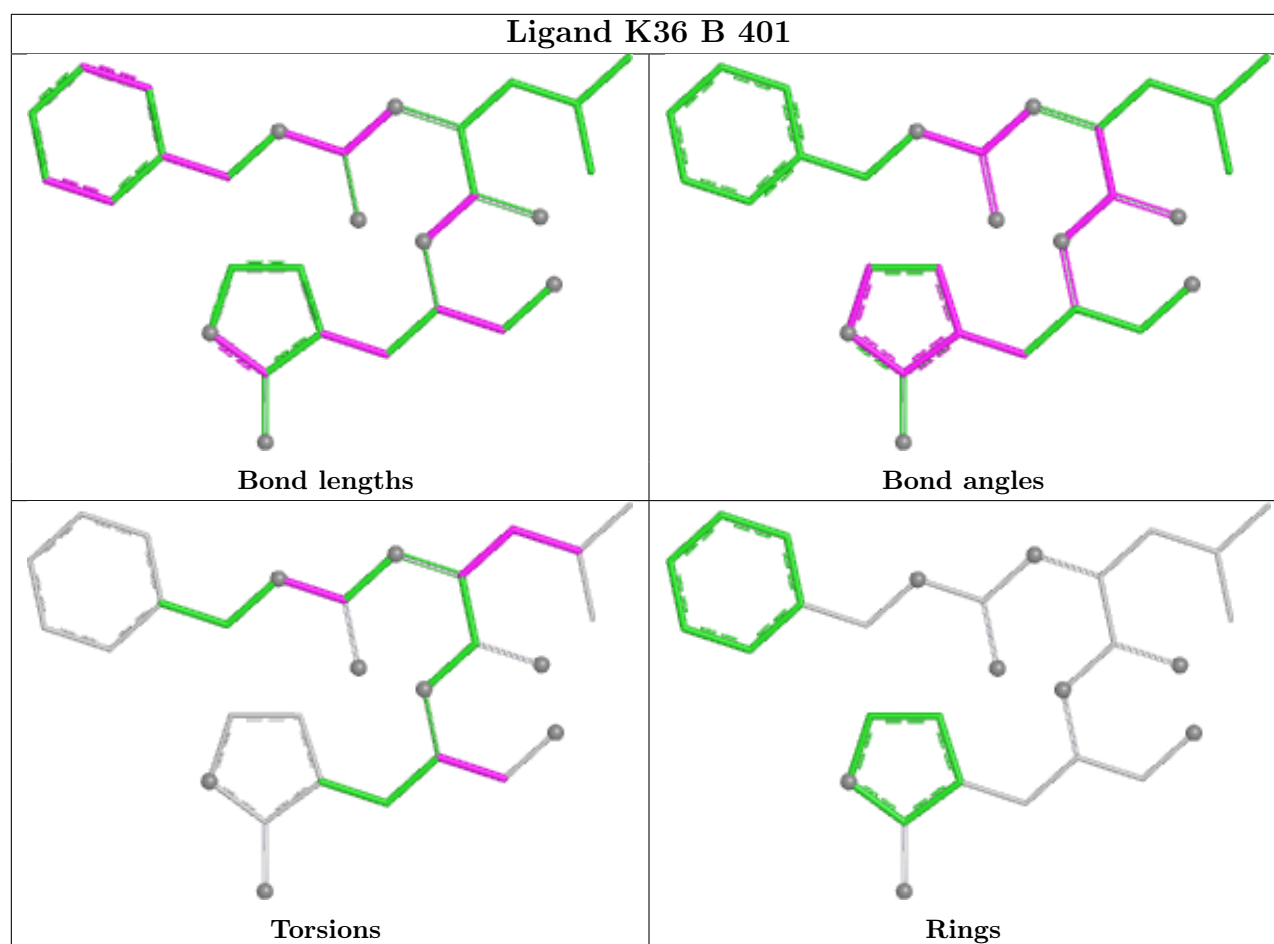
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

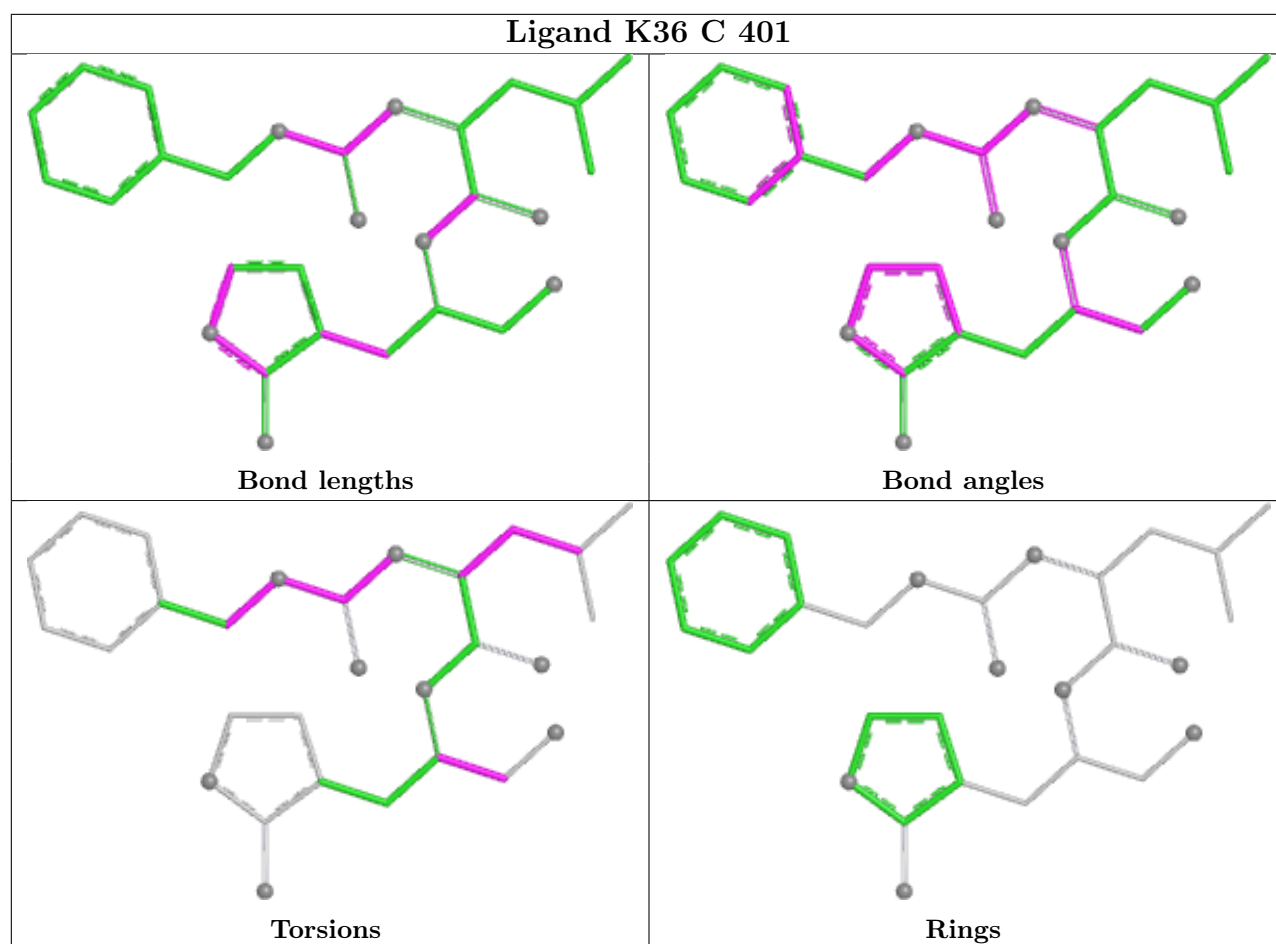
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

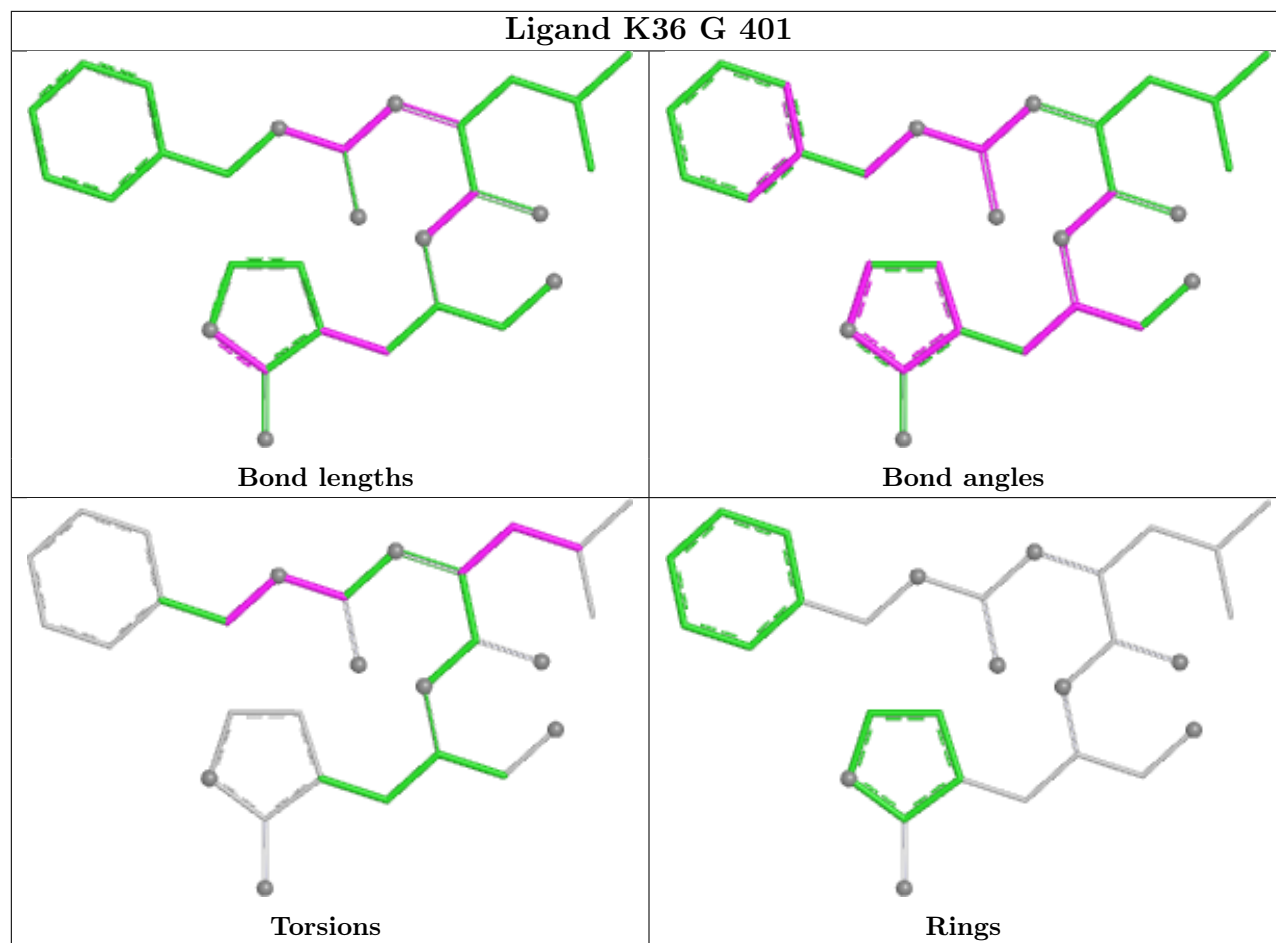


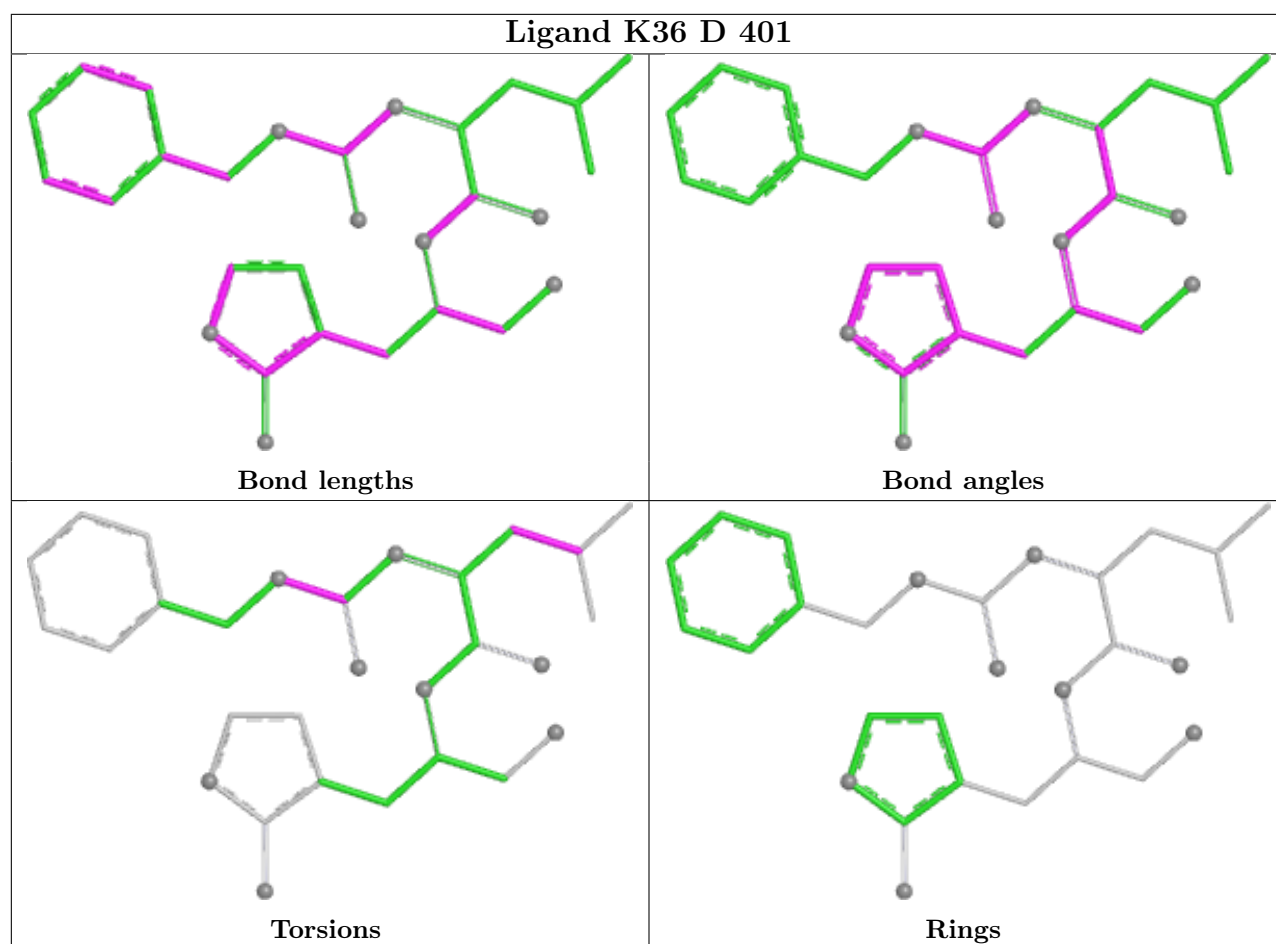


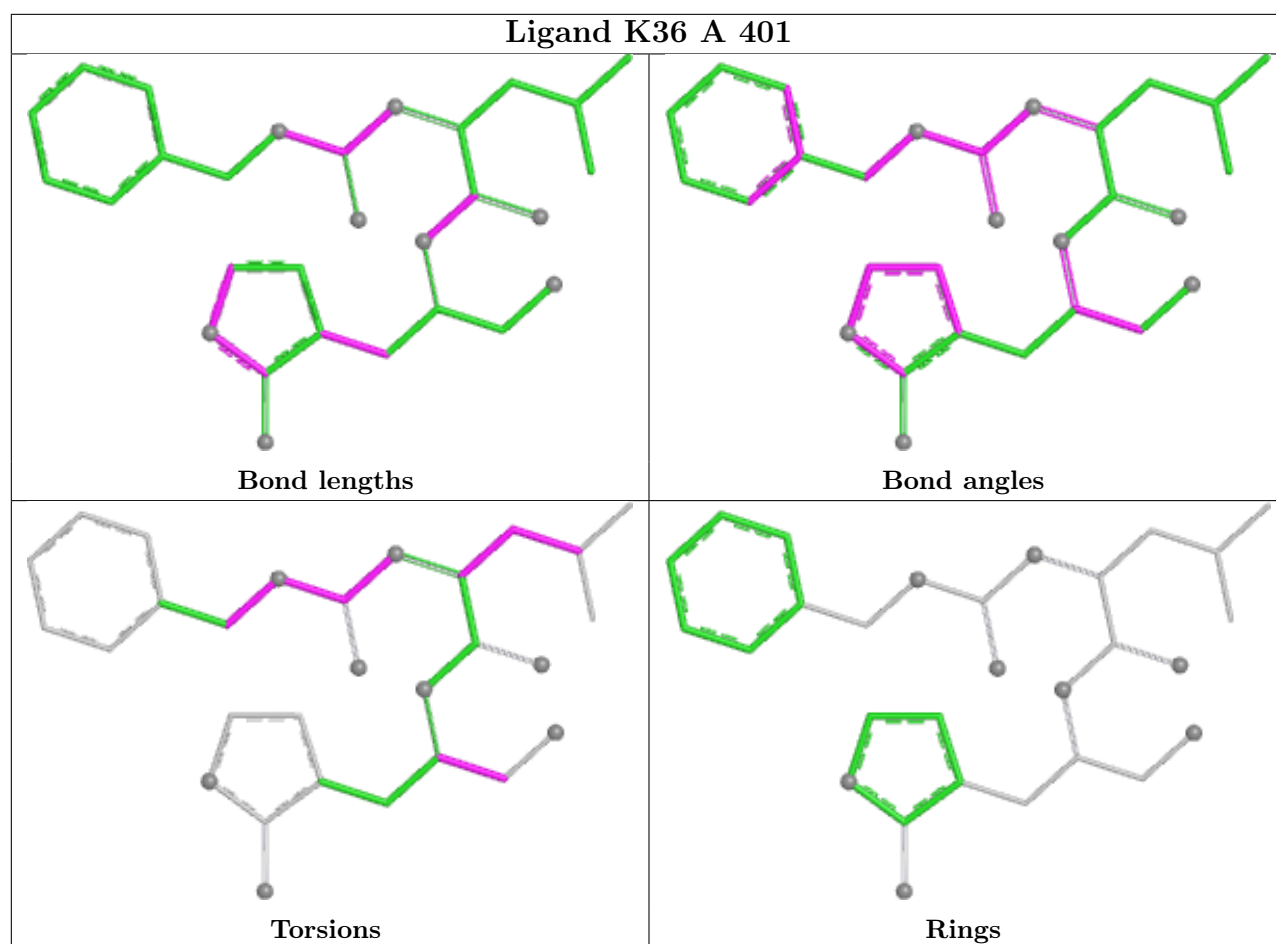












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	299/302 (99%)	-0.13	3 (1%) 79 79	15, 38, 66, 88	0
1	B	299/302 (99%)	-0.04	2 (0%) 84 84	16, 43, 71, 87	0
1	C	298/302 (98%)	0.21	7 (2%) 61 59	18, 45, 71, 94	0
1	D	296/302 (98%)	0.41	5 (1%) 69 67	25, 59, 99, 118	0
1	E	299/302 (99%)	0.31	10 (3%) 49 47	23, 51, 85, 112	0
1	F	299/302 (99%)	0.38	17 (5%) 29 29	22, 50, 108, 136	0
1	G	298/302 (98%)	0.50	17 (5%) 29 29	22, 55, 118, 139	0
1	H	289/302 (95%)	0.91	50 (17%) 4 3	25, 66, 123, 153	0
All	All	2377/2416 (98%)	0.32	111 (4%) 36 36	15, 50, 102, 153	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	86	LEU	5.0
1	F	242	SER	4.2
1	H	93	VAL	4.2
1	H	41	HIS	4.2
1	H	81	TYR	4.2
1	H	154	GLY	3.8
1	H	18	VAL	3.8
1	H	102	PHE	3.7
1	H	47	THR	3.7
1	G	208	TYR	3.6
1	H	44	ALA	3.5
1	H	20	VAL	3.5
1	A	81	TYR	3.5
1	H	38	CYS	3.4
1	G	222	THR	3.3
1	F	299	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	244	ILE	3.3
1	H	40	ARG	3.3
1	A	57	MET	3.3
1	H	87	VAL	3.3
1	G	226	LEU	3.2
1	F	270	LYS	3.2
1	H	50	VAL	3.2
1	C	1	SER	3.1
1	H	36	VAL	3.1
1	G	243	SER	3.1
1	H	299	VAL	3.1
1	F	216	ARG	3.1
1	G	242	SER	3.1
1	C	71	ASN	3.0
1	H	84	VAL	3.0
1	H	22	TYR	3.0
1	H	12	LEU	2.9
1	D	1	SER	2.9
1	H	43	ILE	2.9
1	E	299	VAL	2.9
1	H	21	SER	2.8
1	E	231	THR	2.8
1	G	217	TRP	2.8
1	D	50	VAL	2.8
1	F	258	VAL	2.8
1	H	26	VAL	2.8
1	G	122	GLY	2.7
1	G	221	ASN	2.7
1	H	62	LEU	2.7
1	E	221	ASN	2.7
1	D	299	VAL	2.7
1	H	88	LEU	2.6
1	H	169	GLY	2.6
1	H	141	ALA	2.6
1	H	98	PRO	2.6
1	C	73	PHE	2.6
1	H	53	TYR	2.5
1	H	42	VAL	2.5
1	G	247	PHE	2.5
1	F	228	SER	2.5
1	F	46	ASP	2.5
1	G	241	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	176	LEU	2.5
1	E	77	VAL	2.5
1	F	232	TRP	2.5
1	F	241	LEU	2.5
1	H	33	GLY	2.5
1	G	211	LEU	2.4
1	F	243	SER	2.4
1	H	58	SER	2.4
1	H	90	VAL	2.4
1	H	35	GLU	2.4
1	H	57	MET	2.4
1	C	72	VAL	2.4
1	G	250	LEU	2.4
1	E	271	GLY	2.4
1	H	83	GLY	2.4
1	E	232	TRP	2.4
1	H	192	LEU	2.3
1	G	210	ALA	2.3
1	F	43	ILE	2.3
1	F	231	THR	2.3
1	H	37	ILE	2.3
1	F	249	MET	2.3
1	H	31	TRP	2.3
1	H	182	GLY	2.3
1	G	47	THR	2.3
1	B	66	SER	2.3
1	B	299	VAL	2.3
1	D	219	VAL	2.2
1	E	219	VAL	2.2
1	H	155	ILE	2.2
1	H	17	ILE	2.2
1	G	254	THR	2.2
1	H	99	GLU	2.2
1	F	229	TYR	2.2
1	H	70	ASN	2.2
1	H	133	GLY	2.2
1	E	220	THR	2.2
1	H	92	GLN	2.2
1	H	23	GLY	2.2
1	E	233	ALA	2.1
1	F	226	LEU	2.1
1	G	268	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	32	LEU	2.1
1	F	197	VAL	2.1
1	H	190	MET	2.1
1	G	263	ASP	2.1
1	C	63	HIS	2.1
1	C	216	ARG	2.1
1	E	121	PRO	2.1
1	C	43	ILE	2.1
1	H	67	VAL	2.1
1	A	222	THR	2.0
1	D	190	MET	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](#)

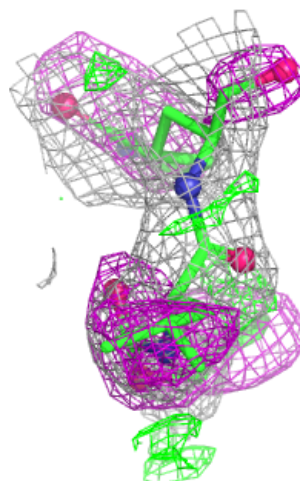
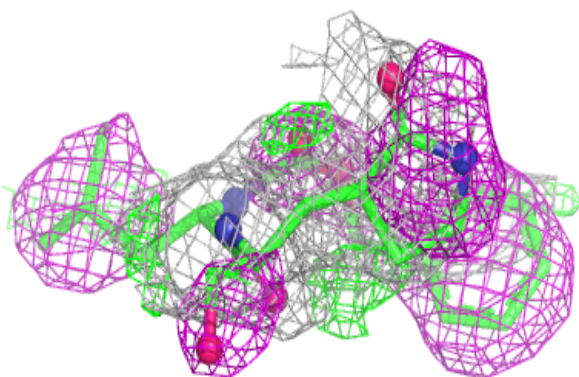
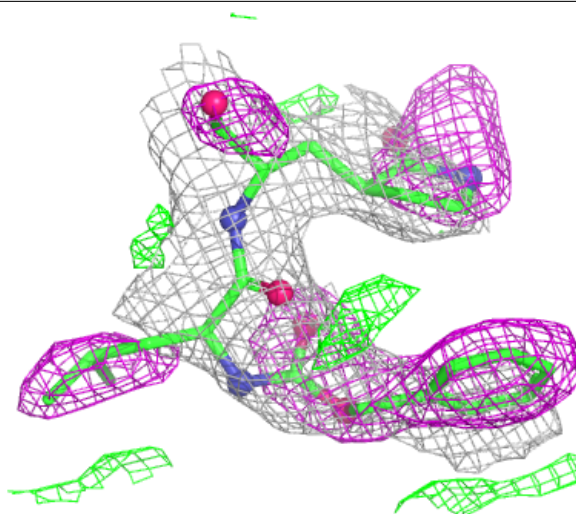
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	K36	H	401	29/33	0.58	0.18	31,40,46,47	0
2	K36	C	401	29/33	0.86	0.15	31,40,46,47	0
2	K36	F	401	29/33	0.90	0.11	31,39,49,53	0
2	K36	D	401	29/33	0.93	0.11	42,53,72,79	0
2	K36	G	401	29/33	0.94	0.09	26,46,50,54	0
2	K36	B	401	29/33	0.95	0.10	17,27,76,77	0
2	K36	A	401	29/33	0.95	0.07	31,40,46,47	0
2	K36	E	401	29/33	0.96	0.07	26,34,41,46	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.

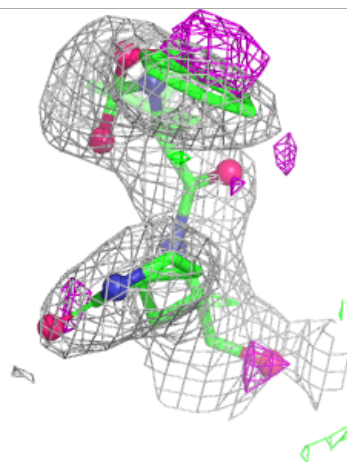
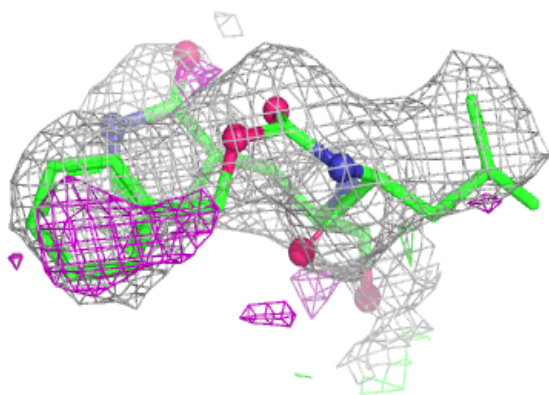
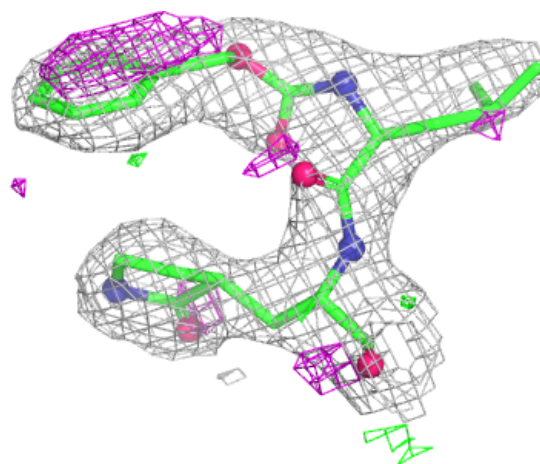
Electron density around K36 H 401:

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



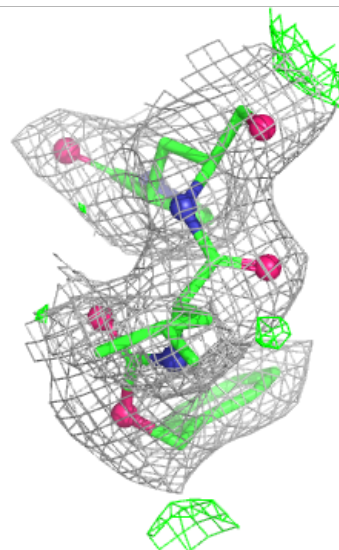
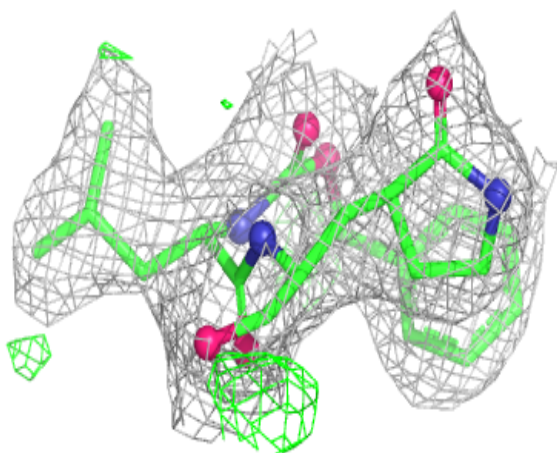
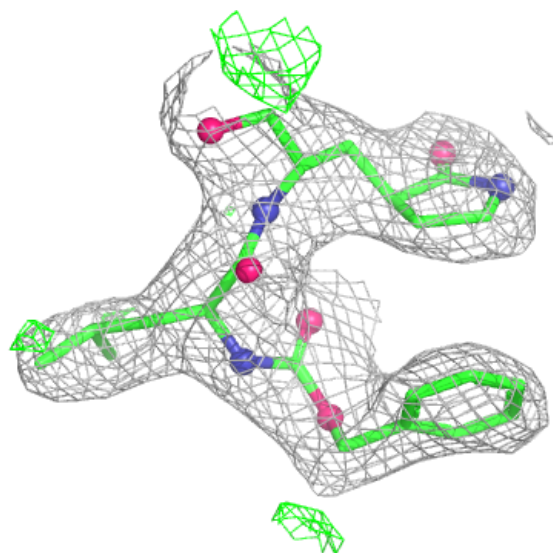
Electron density around K36 C 401:

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



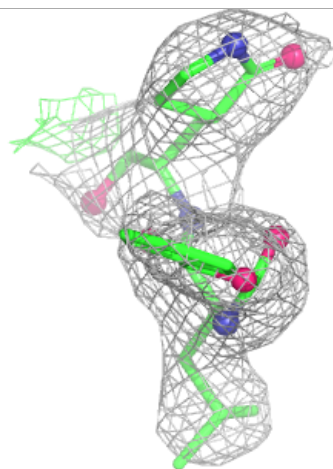
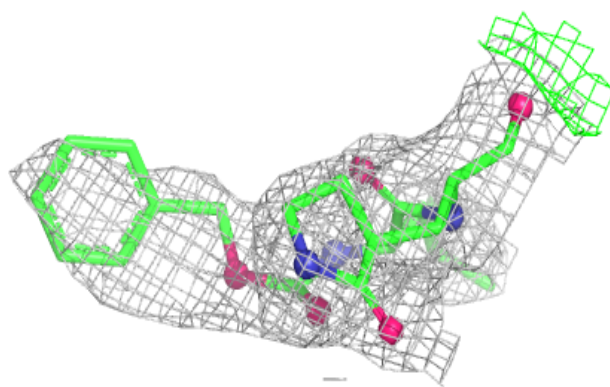
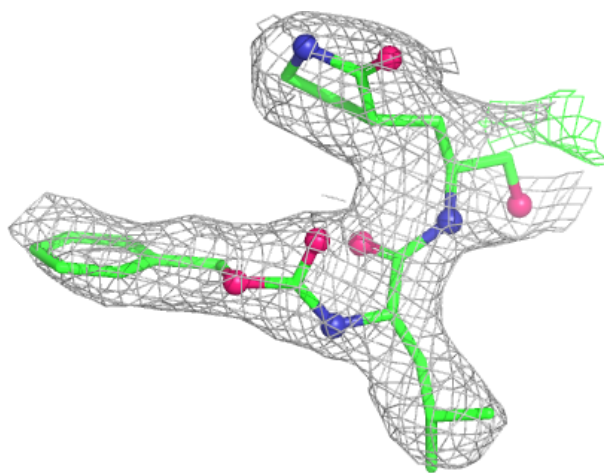
Electron density around K36 F 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



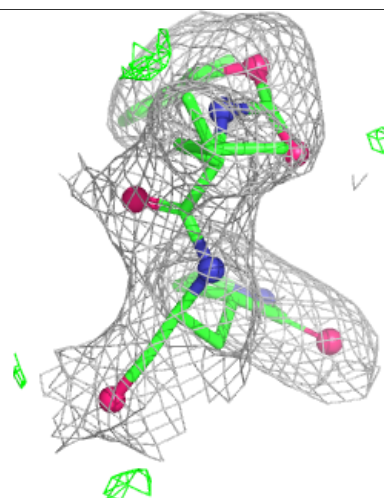
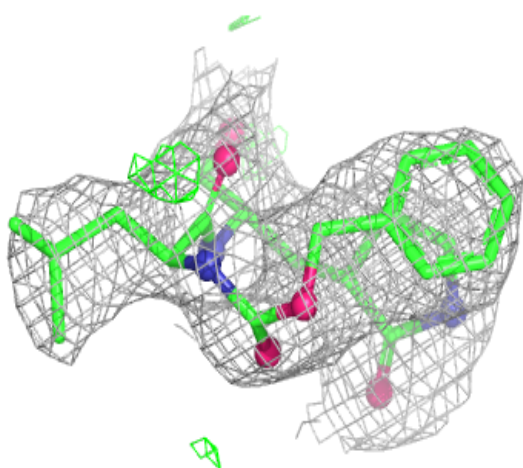
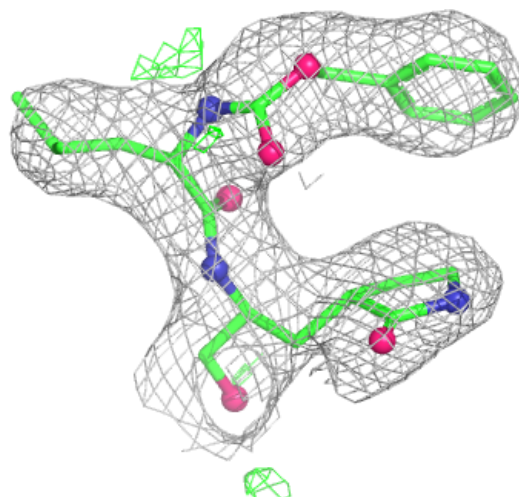
Electron density around K36 D 401:

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and green (positive)



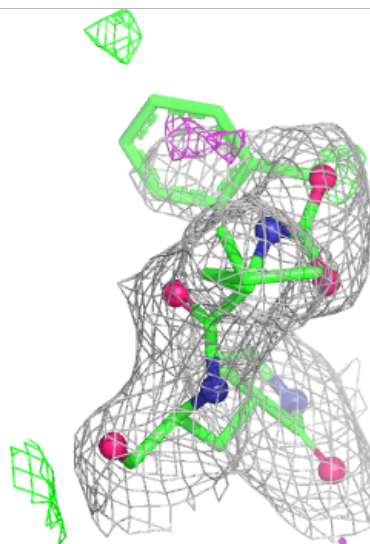
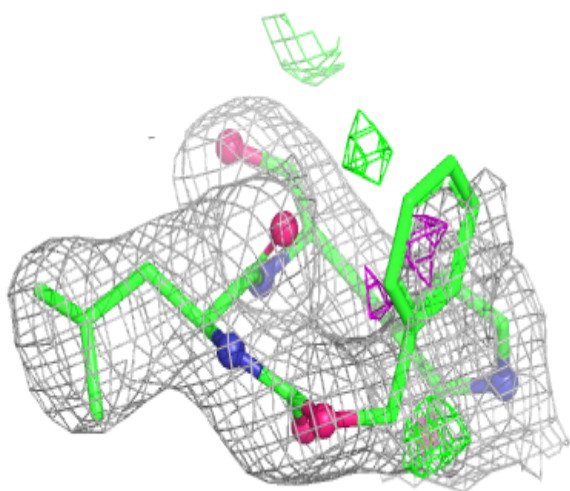
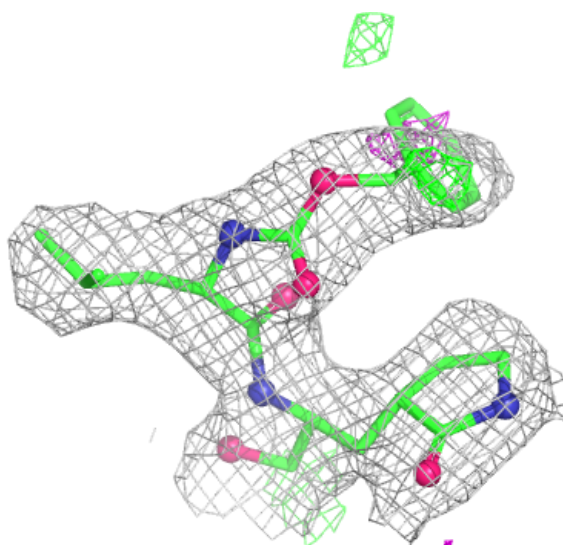
Electron density around K36 G 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



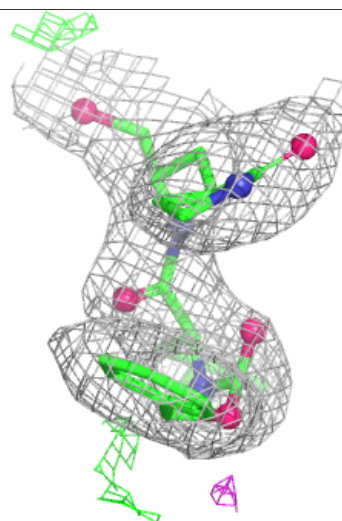
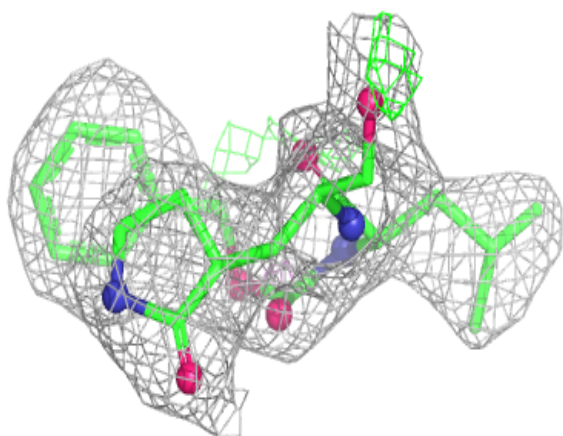
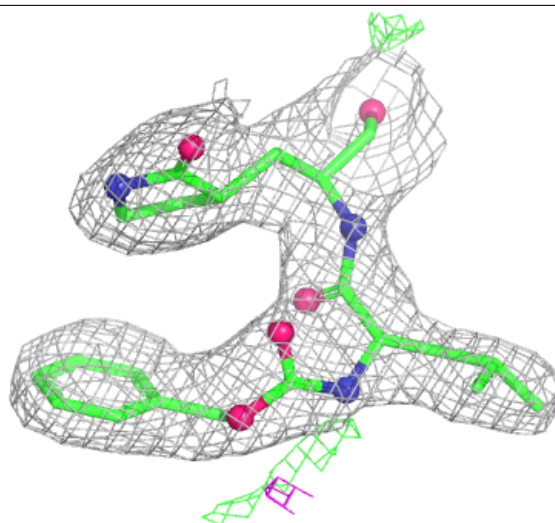
Electron density around K36 B 401:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



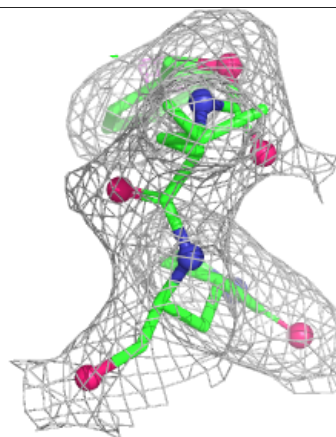
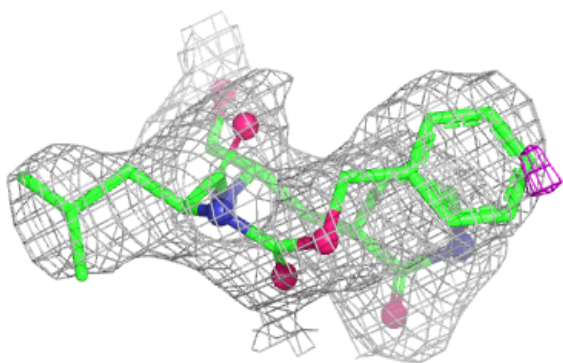
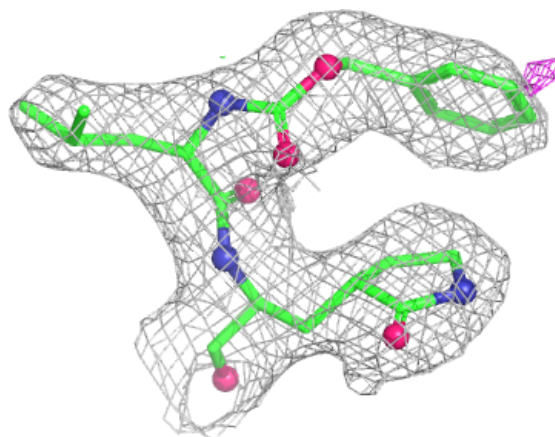
Electron density around K36 A 401:

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



Electron density around K36 E 401:

$2mF_o-DF_c$ (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.