Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 10:16 PM JST

PDB ID	:	7XJW
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:

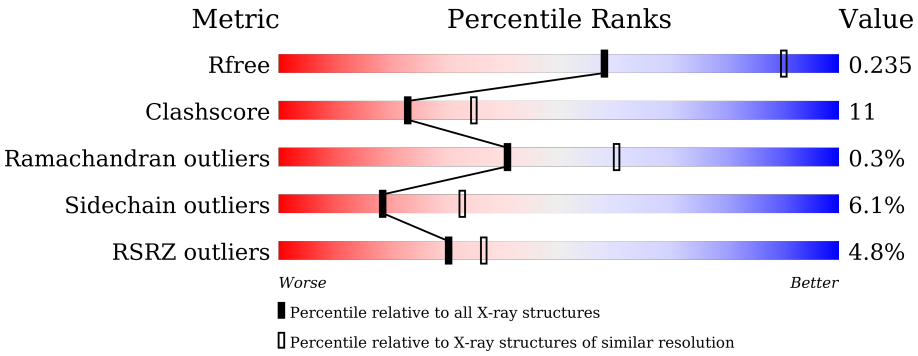
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 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}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	302	82% 16%
1	B	302	78% 20%
1	C	302	73% 25%
1	D	302	5% 76% 21%
1	E	302	73% 24%
1	F	302	6% 74% 22%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	302	7% 72% 25%
1	H	302	14% 63% 28% 5%

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	K36	H	401	-	-	-	X

2 Entry composition (i)

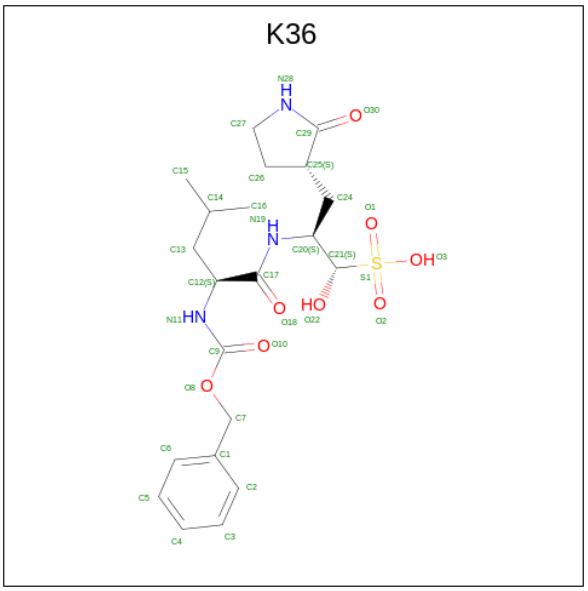
There are 3 unique types of molecules in this entry. The entry contains 18564 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-oxopyrrolidin-3-yl]propane-1-sulfonic acid (three-letter code: K36) (formula: $C_{21}H_{31}N_3O_8S$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

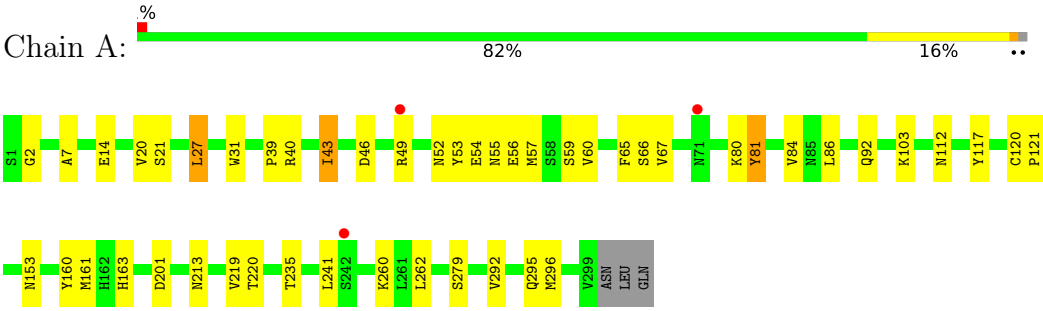
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	13	Total O 13 13	0	0
3	F	14	Total O 14 14	0	0
3	G	9	Total O 9 9	0	0
3	H	10	Total O 10 10	0	0

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.

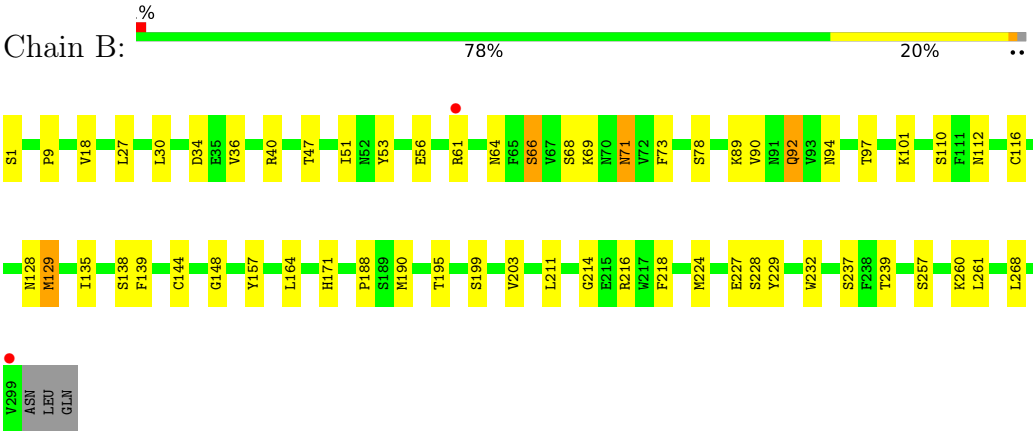
• Molecule 1: ORF1a polyprotein

Chain A:



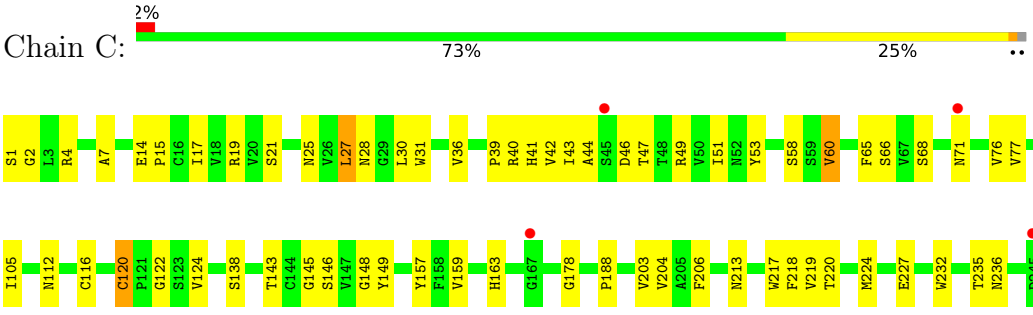
• Molecule 1: ORF1a polyprotein

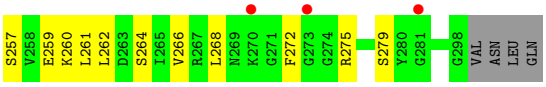
Chain B:



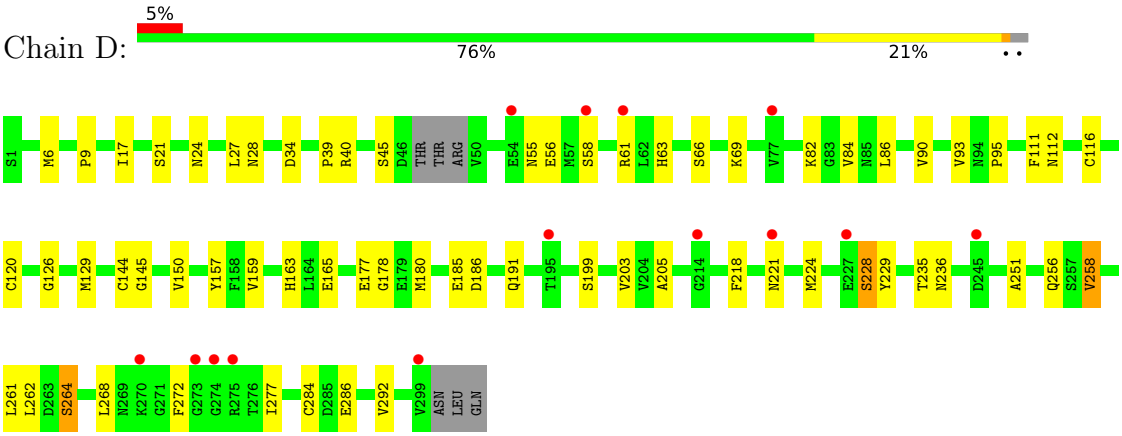
• Molecule 1: ORF1a polyprotein

Chain C:

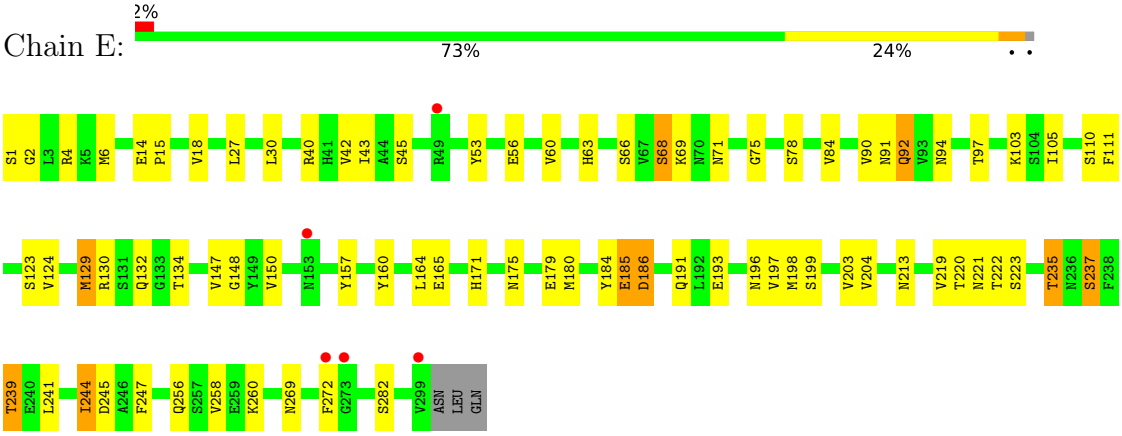




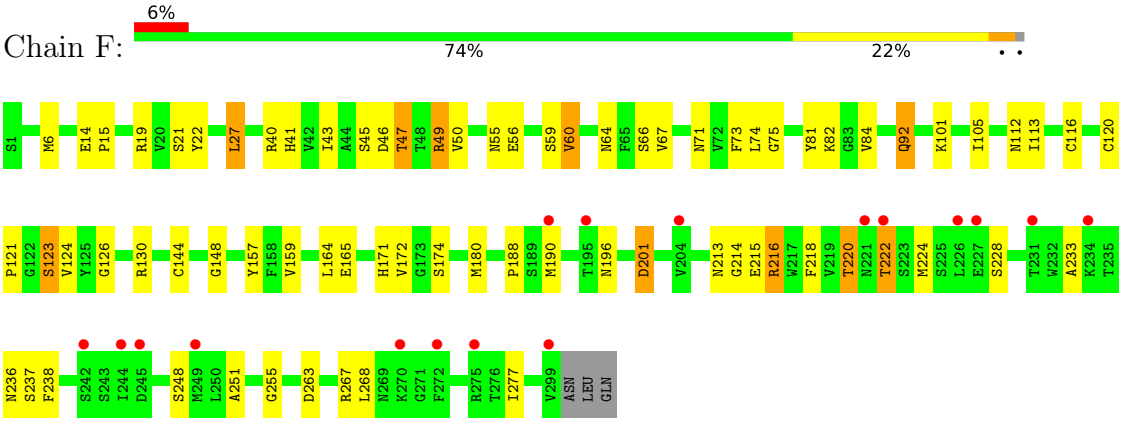
• Molecule 1: ORF1a polyprotein



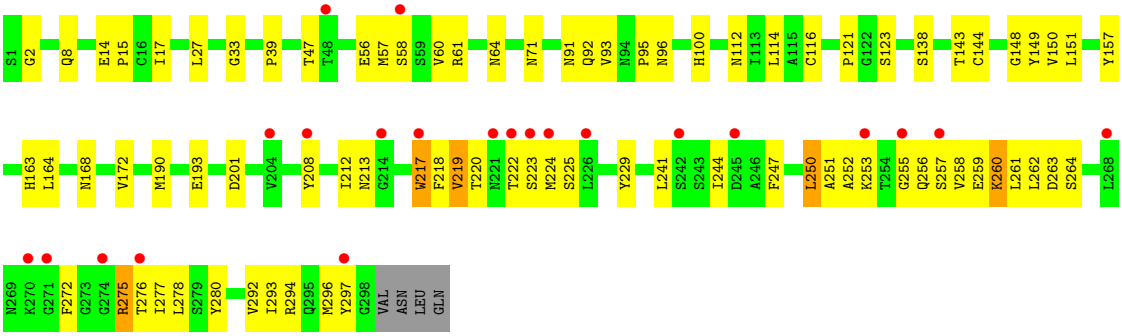
• Molecule 1: ORF1a polyprotein



• Molecule 1: ORF1a polyprotein

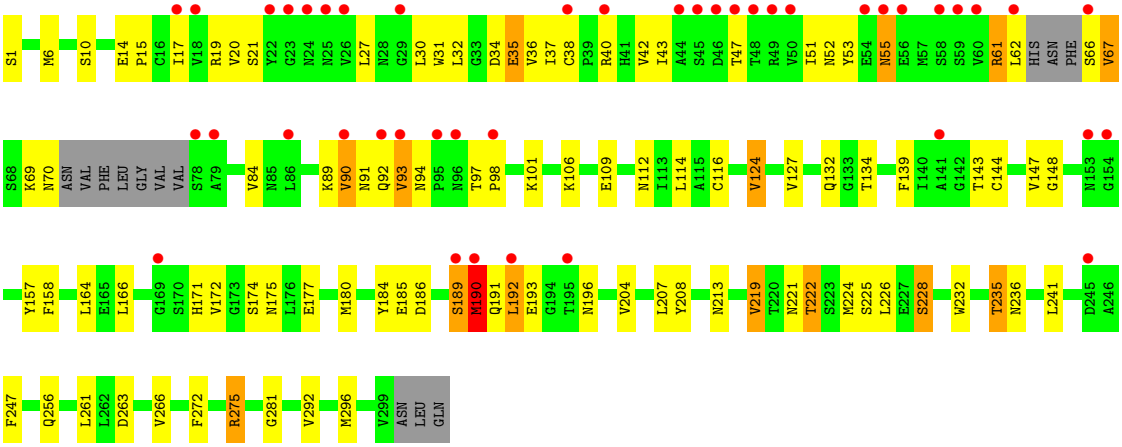


• Molecule 1: ORF1a polyprotein



• Molecule 1: ORF1a polyprotein

Chain H:



4 Data and refinement statistics (i)

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 27.81 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.4 (27.82-2.75) 96.5 (27.81-2.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.08%)	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)	0.31 , 49.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.75	0/2338	0.77	0/3164
1	B	0.73	0/2338	0.75	0/3164
1	C	0.77	0/2331	0.78	0/3154
1	D	0.70	0/2312	0.73	0/3127
1	E	0.74	0/2338	0.76	0/3164
1	F	0.73	0/2338	0.75	0/3164
1	G	0.72	0/2331	0.75	0/3154
1	H	0.74	0/2252	0.75	0/3043
All	All	0.73	0/18578	0.75	0/25134

There are no bond length outliers.

There are no bond angle outliers.

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	30	0
1	B	2293	0	2253	35	0
1	C	2286	0	2243	57	0
1	D	2268	0	2225	41	0
1	E	2293	0	2252	53	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2293	0	2253	53	0
1	G	2286	0	2243	77	0
1	H	2212	0	2172	83	0
2	A	29	0	29	1	0
2	B	29	0	29	7	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	417	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 11.

All (417) 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:H:20:VAL:HG22	1:H:67:VAL:CG2	1.93	0.98
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:B:144:CYS:HG	2:B:401:K36:C21	1.70	0.90
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:B:144:CYS:SG	2:B:401:K36:O22	2.23	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:224:MET:HE2	1:D:228:SER:C	2.09	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:E:75:GLY:H	1:E:91:ASN:ND2	1.88	0.72
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:D:224:MET:HE2	1:D:229:TYR:N	2.05	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:C:217:TRP:CE3	1:C:275:ARG:NH1	2.60	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LYS:HG2	1:D:177:GLU:O	1.96	0.66
1:H:47:THR:HG23	2:H:401:K36:H13	1.78	0.65
1:H:189:SER:C	1:H:190:MET:HG3	2.17	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:F:224:MET:HE2	1:F:228:SER:OG	1.96	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:G:57:MET:C	1:G:60:VAL:HG23	2.17	0.63
1:F:74:LEU:CD2	1:F:92:GLN:HG3	2.26	0.63
1:E:84:VAL:HG21	1:E:180:MET:HE1	1.80	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:E:123:SER:HB2	1:F:6:MET:HB3	1.82	0.61
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:H:189:SER:C	1:H:190:MET:CG	2.68	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: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:F:224:MET:CE	1:F:228:SER:OG	2.50	0.59
1:A:2:GLY:H	1:A:213:ASN:ND2	1.99	0.59
1:G:57:MET:HA	1:G:60:VAL:CG2	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:224:MET:HE2	1:F:228:SER:C	2.24	0.58
1:C:7:ALA:HB1	1:C:124:VAL:HG12	1.86	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: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: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
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:G:100:HIS:CG	1:G:100:HIS:O	2.60	0.56
1:H:62:LEU:HD13	1:H:62:LEU:C	2.26	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: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:F:130:ARG:HB3	1:F:196:ASN:OD1	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:166:LEU:N	1:H:166:LEU:HD23	2.24	0.52
1:F:164:LEU:C	1:F:164:LEU:HD12	2.29	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:222:THR:HB	1:F:263:ASP:CG	2.31	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
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: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: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: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:D:235:THR:C	1:D:236:ASN:HD22	2.16	0.49
1:G:39:PRO:HB3	1:G:163:HIS:CE1	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:C:27:LEU:C	1:C:27:LEU:HD12	2.34	0.47
1:A:27:LEU:CD2	1:A:39:PRO:HG2	2.40	0.47
1:D:224:MET:HE2	1:D:228:SER:HB2	1.95	0.47
1:F:75:GLY:N	1:F:92:GLN:NE2	2.61	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:G:217:TRP:CD1	1:G:217:TRP:C	2.88	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:D:224:MET:CE	1:D:228:SER:HB2	2.47	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:G:95:PRO:HG2	1:G:96:ASN:ND2	2.31	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:G:47:THR:O	1:G:47:THR:CG2	2.65	0.45
1:G:224:MET:HE1	1:G:229:TYR:HA	1.99	0.45
1:E:220:THR:O	1:E:260:LYS:CE	2.65	0.45
1:C:65:PHE:CB	1:C:76:VAL:HG21	2.46	0.45
1:C:143:THR:O	1:C:146:SER:OG	2.31	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:225:SER:HB3	1:H:228:SER:HG	1.72	0.44
1:E:164:LEU:HD12	1:E:164:LEU:C	2.38	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: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:D:180:MET:HE3	1:D:186:ASP:HB3	2.00	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:A:295:GLN:HB3	1:A:296:MET:HE3	2.00	0.43
1:B:224:MET:HE2	1:B:228:SER:C	2.39	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:H:62:LEU:C	1:H:62:LEU:CD1	2.86	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: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:H:42:VAL:HG13	1:H:43:ILE:HG13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:HD11	1:B:261:LEU:HD21	2.01	0.43
1:E:40:ARG:NE	1:E:186:ASP:OD1	2.46	0.43
1:F:165:GLU:OE1	2:F:401:K36:N28	2.52	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:G:212:ILE:HD13	1:G:297:TYR:HH	1.79	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: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: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:15:PRO:O	1:E:69:LYS:NZ	2.44	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: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: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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:138:SER:HB3	1:D:6:MET:HE3	2.01	0.41
1:E:241:LEU:HD11	1:E:247:PHE:HE2	1.85	0.41
1:A:14:GLU:CD	1:B:9:PRO:HB3	2.40	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:224:MET:CE	1:G:229:TYR:HA	2.51	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:D:224:MET:CE	1:D:228:SER:C	2.85	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:84:VAL:CG1	1:H:186:ASP:CG	2.90	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:D:150:VAL:HG22	1:D:159:VAL:HG11	2.04	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:E:129:MET:HE2	1:E:134:THR:O	2.21	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 (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	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%)	41	60
1	D	292/302 (97%)	269 (92%)	22 (8%)	1 (0%)	41	60
1	E	297/302 (98%)	277 (93%)	19 (6%)	1 (0%)	41	60
1	F	297/302 (98%)	280 (94%)	16 (5%)	1 (0%)	41	60
1	G	296/302 (98%)	269 (91%)	27 (9%)	0	100	100
1	H	283/302 (94%)	251 (89%)	29 (10%)	3 (1%)	14	25
All	All	2355/2416 (98%)	2177 (92%)	171 (7%)	7 (0%)	41	60

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 (i)

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%)	243 (95%)	12 (5%)	26 45
1	B	255/258 (99%)	239 (94%)	16 (6%)	18 31
1	C	254/258 (98%)	245 (96%)	9 (4%)	36 56
1	D	252/258 (98%)	244 (97%)	8 (3%)	39 59
1	E	255/258 (99%)	234 (92%)	21 (8%)	11 20
1	F	255/258 (99%)	233 (91%)	22 (9%)	10 18
1	G	254/258 (98%)	241 (95%)	13 (5%)	24 41
1	H	246/258 (95%)	224 (91%)	22 (9%)	9 17
All	All	2026/2064 (98%)	1903 (94%)	123 (6%)	18 33

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	43	ILE
1	A	54	GLU
1	A	59	SER
1	A	80	LYS
1	A	81	TYR
1	A	103	LYS
1	A	121	PRO
1	A	153	ASN
1	A	219	VAL
1	A	235	THR
1	A	279	SER
1	B	1	SER
1	B	27	LEU
1	B	66	SER
1	B	68	SER
1	B	71	ASN
1	B	92	GLN
1	B	123	SER
1	B	124	VAL
1	B	129	MET
1	B	138	SER
1	B	190	MET
1	B	195	THR
1	B	227	GLU
1	B	237	SER
1	B	239	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	279	SER
1	C	1	SER
1	C	27	LEU
1	C	58	SER
1	C	60	VAL
1	C	71	ASN
1	C	120	CYS
1	C	227	GLU
1	C	235	THR
1	C	272	PHE
1	D	27	LEU
1	D	45	SER
1	D	69	LYS
1	D	112	ASN
1	D	129	MET
1	D	221	ASN
1	D	228	SER
1	D	264	SER
1	E	45	SER
1	E	60	VAL
1	E	63	HIS
1	E	68	SER
1	E	78	SER
1	E	90	VAL
1	E	92	GLN
1	E	110	SER
1	E	124	VAL
1	E	129	MET
1	E	185	GLU
1	E	186	ASP
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	F	27	LEU
1	F	41	HIS
1	F	45	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	46	ASP
1	F	47	THR
1	F	49	ARG
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	190	MET
1	F	201	ASP
1	F	216	ARG
1	F	220	THR
1	F	222	THR
1	F	236	ASN
1	F	237	SER
1	F	248	SER
1	G	58	SER
1	G	71	ASN
1	G	150	VAL
1	G	190	MET
1	G	217	TRP
1	G	219	VAL
1	G	223	SER
1	G	225	SER
1	G	250	LEU
1	G	260	LYS
1	G	263	ASP
1	G	275	ARG
1	G	278	LEU
1	H	35	GLU
1	H	38	CYS
1	H	55	ASN
1	H	67	VAL
1	H	90	VAL
1	H	91	ASN
1	H	93	VAL
1	H	97	THR
1	H	124	VAL
1	H	127	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	174	SER
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
1	H	275	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	163	HIS
1	A	213	ASN
1	B	64	ASN
1	B	71	ASN
1	B	92	GLN
1	B	128	ASN
1	B	132	GLN
1	C	55	ASN
1	C	63	HIS
1	C	92	GLN
1	C	213	ASN
1	D	63	HIS
1	D	221	ASN
1	D	236	ASN
1	E	55	ASN
1	E	91	ASN
1	E	92	GLN
1	E	213	ASN
1	E	269	ASN
1	F	85	ASN
1	F	92	GLN
1	F	171	HIS
1	F	236	ASN
1	G	41	HIS
1	G	55	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	64	ASN
1	G	96	ASN
1	G	236	ASN
1	G	256	GLN
1	H	70	ASN
1	H	132	GLN
1	H	221	ASN
1	H	236	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	3.80	7 (23%)	37,39,47	1.70	7 (18%)
2	K36	C	401	1	30,30,34	3.49	8 (26%)	37,39,47	2.04	11 (29%)
2	K36	E	401	1	30,30,34	3.74	9 (30%)	37,39,47	1.89	10 (27%)
2	K36	D	401	-	30,30,34	3.82	8 (26%)	37,39,47	1.73	8 (21%)
2	K36	A	401	1	30,30,34	3.48	8 (26%)	37,39,47	2.04	11 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	K36	G	401	1	30,30,34	3.48	6 (20%)	37,39,47	1.91	10 (27%)
2	K36	H	401	-	30,30,34	3.48	8 (26%)	37,39,47	2.05	11 (29%)
2	K36	B	401	-	30,30,34	3.50	10 (33%)	37,39,47	2.00	10 (27%)

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

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	401	K36	C29-N28	16.37	1.51	1.33
2	E	401	K36	C29-N28	16.26	1.50	1.33
2	G	401	K36	C29-N28	15.43	1.50	1.33
2	D	401	K36	C29-N28	15.39	1.50	1.33
2	C	401	K36	C29-N28	15.10	1.49	1.33
2	A	401	K36	C29-N28	15.05	1.49	1.33
2	H	401	K36	C29-N28	15.02	1.49	1.33
2	B	401	K36	C29-N28	14.37	1.48	1.33
2	F	401	K36	C9-N11	6.80	1.51	1.34
2	D	401	K36	C17-N19	6.72	1.48	1.34
2	D	401	K36	C25-C29	-6.48	1.44	1.52
2	E	401	K36	C9-N11	6.16	1.49	1.34
2	D	401	K36	C9-N11	6.09	1.49	1.34
2	B	401	K36	C17-N19	5.96	1.47	1.34
2	E	401	K36	O8-C9	5.95	1.46	1.35
2	B	401	K36	C9-N11	5.93	1.49	1.34
2	F	401	K36	C17-N19	5.87	1.47	1.34
2	C	401	K36	C9-N11	5.80	1.49	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	K36	C9-N11	5.80	1.49	1.34
2	A	401	K36	C9-N11	5.77	1.48	1.34
2	H	401	K36	C9-N11	5.75	1.48	1.34
2	C	401	K36	C17-N19	5.67	1.46	1.34
2	A	401	K36	C17-N19	5.66	1.46	1.34
2	H	401	K36	C17-N19	5.66	1.46	1.34
2	G	401	K36	C17-N19	5.37	1.45	1.34
2	D	401	K36	O8-C9	5.15	1.45	1.35
2	B	401	K36	O8-C9	5.10	1.45	1.35
2	F	401	K36	C25-C29	-4.58	1.46	1.52
2	F	401	K36	O8-C9	4.46	1.43	1.35
2	E	401	K36	C17-N19	4.45	1.43	1.34
2	G	401	K36	O8-C9	4.26	1.43	1.35
2	G	401	K36	C24-C25	3.99	1.63	1.53
2	B	401	K36	C25-C29	-3.96	1.47	1.52
2	C	401	K36	O8-C9	3.61	1.42	1.35
2	A	401	K36	O8-C9	3.60	1.42	1.35
2	H	401	K36	O8-C9	3.59	1.42	1.35
2	A	401	K36	C24-C25	3.35	1.61	1.53
2	C	401	K36	C24-C25	3.35	1.61	1.53
2	H	401	K36	C24-C25	3.32	1.61	1.53
2	E	401	K36	C25-C29	-3.12	1.48	1.52
2	D	401	K36	C27-N28	-3.04	1.39	1.46
2	H	401	K36	C25-C29	-2.94	1.48	1.52
2	C	401	K36	C25-C29	-2.90	1.48	1.52
2	A	401	K36	C25-C29	-2.89	1.48	1.52
2	E	401	K36	O30-C29	-2.88	1.17	1.23
2	B	401	K36	C7-C1	2.76	1.57	1.50
2	F	401	K36	C27-N28	-2.71	1.40	1.46
2	F	401	K36	C24-C25	2.69	1.60	1.53
2	E	401	K36	C24-C25	2.63	1.59	1.53
2	E	401	K36	C12-N11	-2.61	1.40	1.45
2	B	401	K36	C3-C2	2.49	1.44	1.38
2	D	401	K36	C21-C20	-2.46	1.48	1.52
2	H	401	K36	C27-N28	-2.44	1.41	1.46
2	A	401	K36	C27-N28	-2.43	1.41	1.46
2	C	401	K36	C27-N28	-2.42	1.41	1.46
2	B	401	K36	C21-C20	-2.38	1.48	1.52
2	G	401	K36	C12-N11	-2.34	1.40	1.45
2	C	401	K36	C21-C20	-2.29	1.48	1.52
2	H	401	K36	C21-C20	-2.28	1.48	1.52
2	A	401	K36	C21-C20	-2.26	1.48	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	K36	C3-C2	2.25	1.43	1.38
2	B	401	K36	C5-C6	2.19	1.43	1.38
2	B	401	K36	C24-C25	2.17	1.58	1.53
2	E	401	K36	C7-C1	2.02	1.55	1.50

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	401	K36	O8-C9-N11	5.97	122.64	110.50
2	C	401	K36	O10-C9-N11	-5.86	115.25	124.85
2	B	401	K36	O8-C9-N11	5.86	122.40	110.50
2	A	401	K36	O10-C9-N11	-5.85	115.26	124.85
2	H	401	K36	O10-C9-N11	-5.85	115.26	124.85
2	F	401	K36	O8-C9-N11	5.27	121.21	110.50
2	H	401	K36	O8-C9-N11	5.26	121.20	110.50
2	A	401	K36	O8-C9-N11	5.24	121.15	110.50
2	C	401	K36	O8-C9-N11	5.22	121.11	110.50
2	D	401	K36	O8-C9-N11	5.15	120.96	110.50
2	H	401	K36	O8-C9-O10	-5.13	114.40	124.25
2	A	401	K36	O8-C9-O10	-5.11	114.45	124.25
2	C	401	K36	O8-C9-O10	-5.07	114.51	124.25
2	B	401	K36	O10-C9-N11	-4.92	116.78	124.85
2	G	401	K36	O10-C9-N11	-4.76	117.04	124.85
2	E	401	K36	O10-C9-N11	-4.56	117.37	124.85
2	D	401	K36	O10-C9-N11	-4.01	118.28	124.85
2	G	401	K36	O8-C9-O10	-3.86	116.85	124.25
2	B	401	K36	C20-N19-C17	-3.84	117.08	123.20
2	G	401	K36	C20-N19-C17	-3.79	117.16	123.20
2	G	401	K36	C7-O8-C9	-3.78	107.48	115.93
2	F	401	K36	O8-C9-O10	-3.77	117.01	124.25
2	D	401	K36	C20-N19-C17	-3.62	117.43	123.20
2	B	401	K36	C12-C17-N19	3.23	123.79	116.70
2	C	401	K36	C27-N28-C29	-3.20	107.56	113.84
2	A	401	K36	C27-N28-C29	-3.19	107.58	113.84
2	H	401	K36	C27-N28-C29	-3.18	107.59	113.84
2	B	401	K36	O8-C9-O10	-3.16	118.18	124.25
2	E	401	K36	C27-N28-C29	-3.16	107.64	113.84
2	G	401	K36	C26-C27-N28	3.11	107.98	103.43
2	D	401	K36	O8-C9-O10	-3.04	118.42	124.25
2	D	401	K36	C27-N28-C29	-3.01	107.93	113.84
2	F	401	K36	C26-C27-N28	2.98	107.80	103.43
2	F	401	K36	C21-C20-N19	2.97	116.26	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	K36	C27-N28-C29	-2.90	108.14	113.84
2	G	401	K36	C24-C20-C21	2.85	115.61	111.65
2	G	401	K36	C27-N28-C29	-2.74	108.45	113.84
2	F	401	K36	C24-C25-C26	-2.72	107.31	117.31
2	B	401	K36	C26-C27-N28	2.70	107.39	103.43
2	G	401	K36	O8-C9-N11	2.70	115.99	110.50
2	E	401	K36	C26-C27-N28	2.67	107.34	103.43
2	A	401	K36	C21-C20-N19	-2.56	103.87	109.60
2	C	401	K36	C21-C20-N19	-2.56	103.87	109.60
2	E	401	K36	O8-C9-O10	-2.56	119.35	124.25
2	H	401	K36	C21-C20-N19	-2.55	103.88	109.60
2	H	401	K36	C7-O8-C9	-2.54	110.26	115.93
2	C	401	K36	C7-O8-C9	-2.54	110.26	115.93
2	A	401	K36	C7-O8-C9	-2.54	110.26	115.93
2	E	401	K36	C20-N19-C17	-2.50	119.21	123.20
2	E	401	K36	C21-C20-N19	-2.50	104.00	109.60
2	F	401	K36	C26-C25-C29	2.49	106.11	102.88
2	D	401	K36	C27-C26-C25	-2.42	101.83	105.75
2	B	401	K36	C24-C25-C29	-2.39	107.63	112.89
2	E	401	K36	O18-C17-N19	-2.35	118.58	122.93
2	B	401	K36	O18-C17-N19	-2.34	118.59	122.93
2	C	401	K36	C12-N11-C9	-2.34	115.19	120.90
2	H	401	K36	C6-C1-C2	2.33	121.83	118.17
2	A	401	K36	C6-C1-C2	2.32	121.82	118.17
2	C	401	K36	C6-C1-C2	2.32	121.81	118.17
2	A	401	K36	C12-N11-C9	-2.32	115.25	120.90
2	H	401	K36	C12-N11-C9	-2.30	115.29	120.90
2	C	401	K36	C24-C25-C26	-2.28	108.94	117.31
2	A	401	K36	C27-C26-C25	-2.28	102.07	105.75
2	A	401	K36	C24-C25-C26	-2.27	108.96	117.31
2	C	401	K36	C27-C26-C25	-2.26	102.09	105.75
2	H	401	K36	C24-C25-C26	-2.26	109.00	117.31
2	H	401	K36	C27-C26-C25	-2.26	102.09	105.75
2	E	401	K36	C24-C25-C26	-2.22	109.17	117.31
2	G	401	K36	C6-C1-C2	2.21	121.63	118.17
2	F	401	K36	C27-N28-C29	-2.20	109.52	113.84
2	C	401	K36	C26-C27-N28	2.17	106.60	103.43
2	A	401	K36	C26-C27-N28	2.17	106.60	103.43
2	H	401	K36	C26-C27-N28	2.16	106.60	103.43
2	G	401	K36	C26-C25-C29	2.12	105.64	102.88
2	B	401	K36	C26-C25-C29	2.11	105.63	102.88
2	E	401	K36	C7-O8-C9	-2.07	111.32	115.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	K36	C21-C20-N19	2.06	114.23	109.60
2	D	401	K36	C24-C25-C29	-2.05	108.39	112.89

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	O10-C9-O8-C7
2	A	401	K36	N11-C9-O8-C7
2	A	401	K36	C24-C20-C21-O22
2	B	401	K36	N19-C20-C21-O22
2	B	401	K36	C24-C20-C21-O22
2	C	401	K36	O10-C9-O8-C7
2	C	401	K36	N11-C9-O8-C7
2	C	401	K36	C24-C20-C21-O22
2	D	401	K36	O10-C9-O8-C7
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	N19-C20-C21-O22
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	O10-C9-O8-C7
2	H	401	K36	N11-C9-O8-C7
2	H	401	K36	C24-C20-C21-O22
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	401	K36	N19-C20-C21-O22
2	C	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
2	F	401	K36	C17-C12-C13-C14
2	B	401	K36	C12-C13-C14-C16
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	A	401	K36	C1-C7-O8-C9
2	C	401	K36	C1-C7-O8-C9
2	H	401	K36	C1-C7-O8-C9
2	E	401	K36	C12-C13-C14-C15
2	G	401	K36	C1-C7-O8-C9
2	E	401	K36	C1-C7-O8-C9
2	D	401	K36	C12-C13-C14-C15

There are no ring outliers.

7 monomers are involved in 25 short contacts:

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

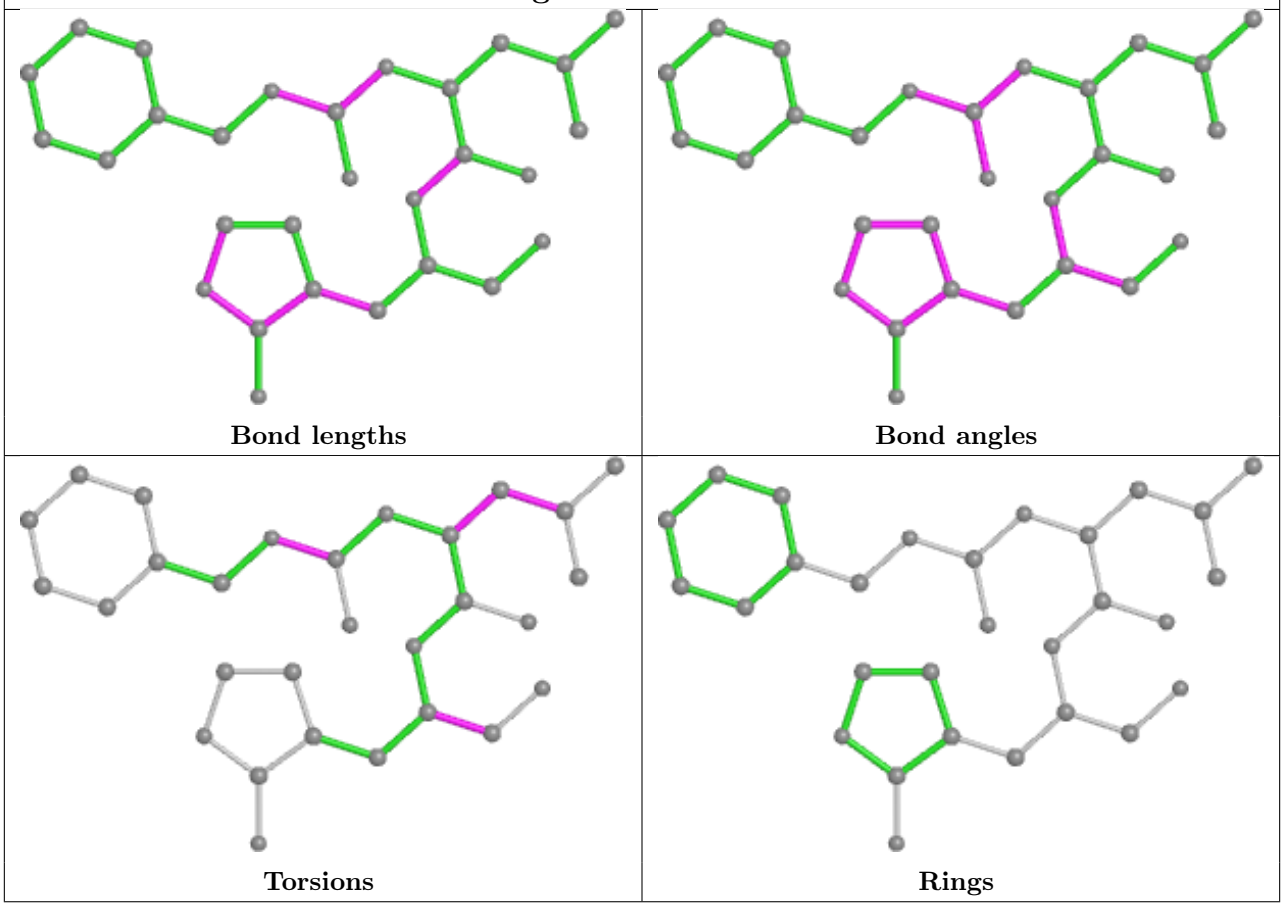
Continued on next page...

Continued from previous page...

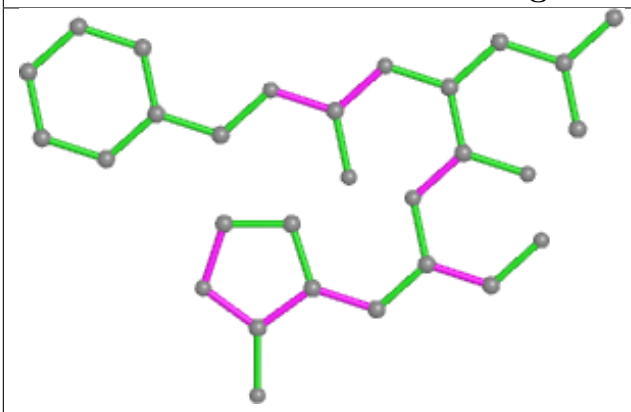
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	401	K36	1	0
2	H	401	K36	5	0
2	B	401	K36	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

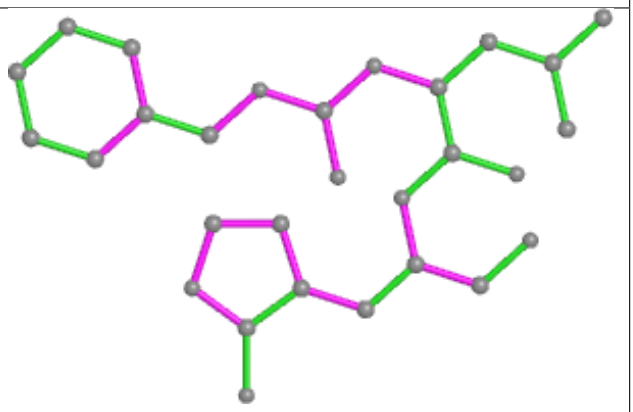
Ligand K36 F 401



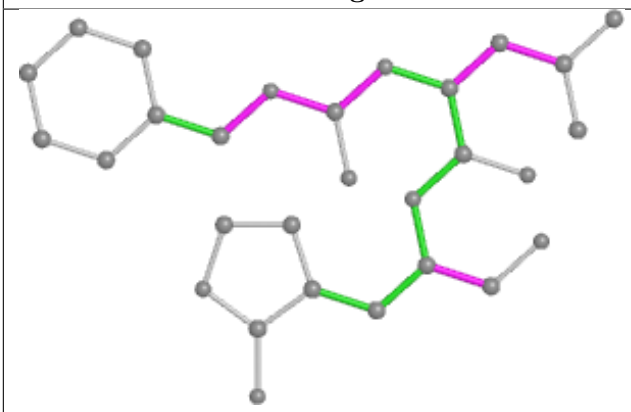
Ligand K36 C 401



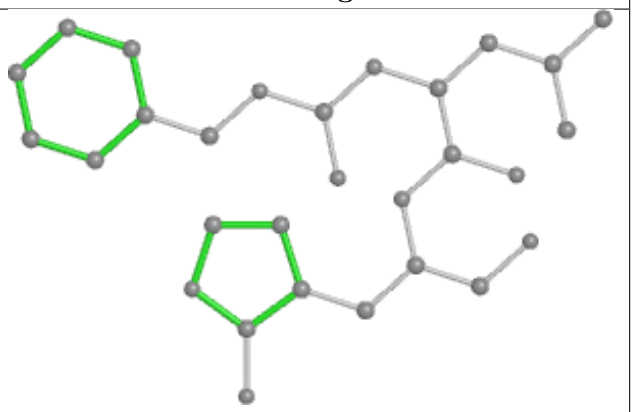
Bond lengths



Bond angles

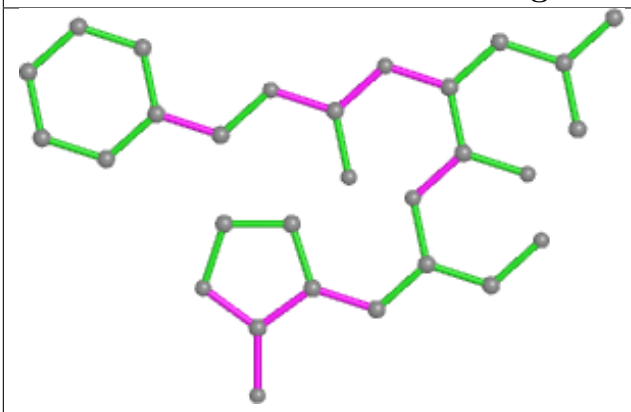


Torsions

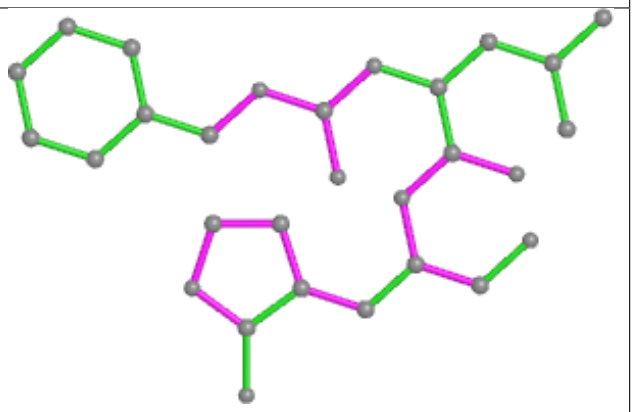


Rings

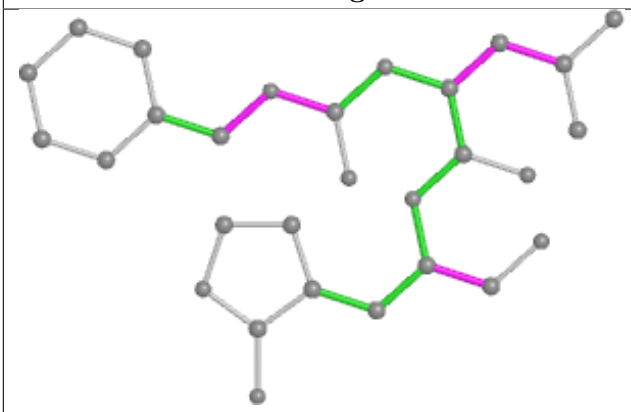
Ligand K36 E 401



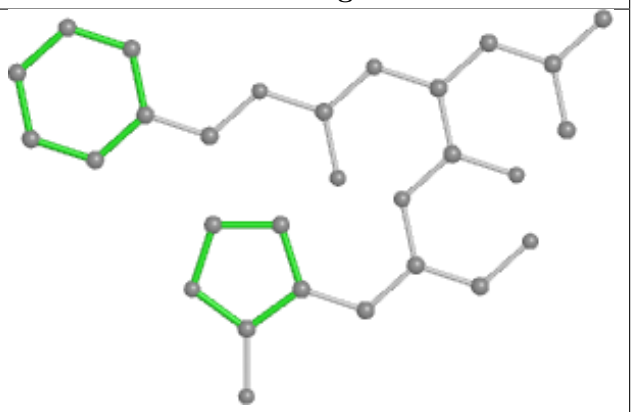
Bond lengths



Bond angles

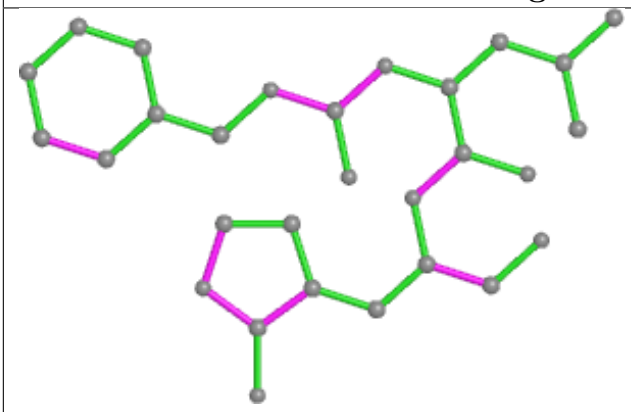


Torsions

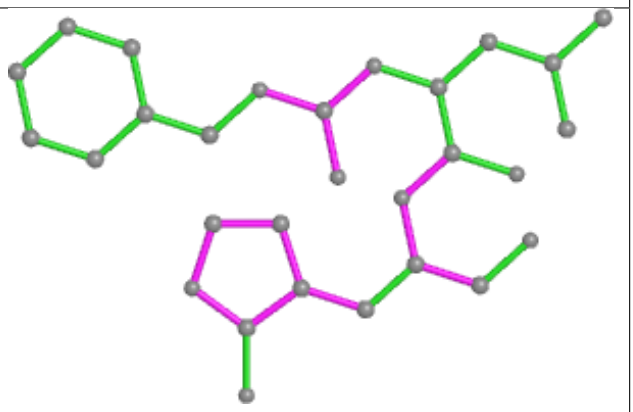


Rings

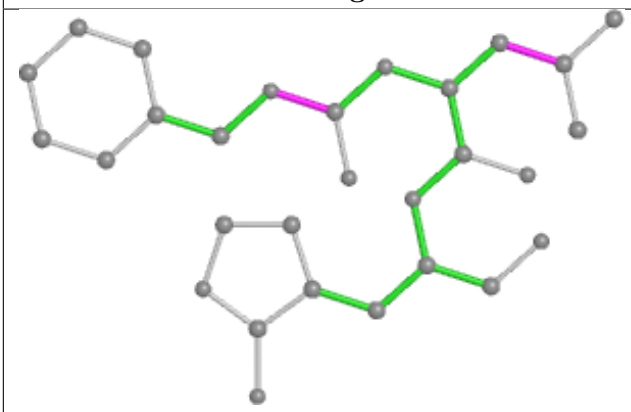
Ligand K36 D 401



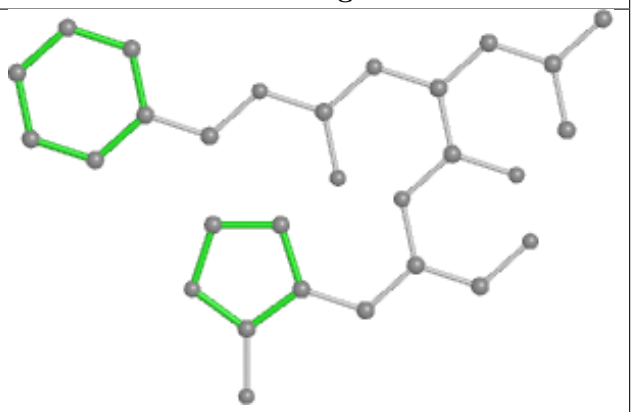
Bond lengths



Bond angles

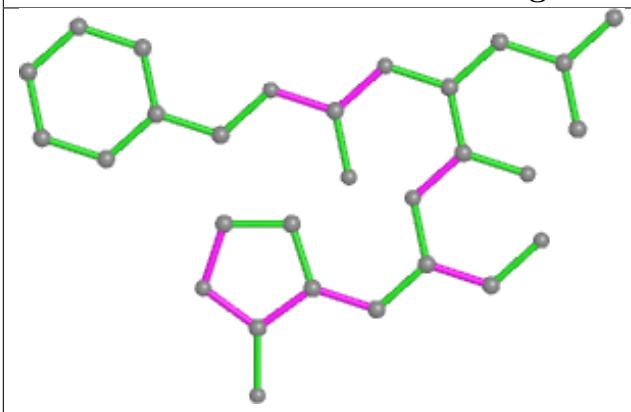


Torsions

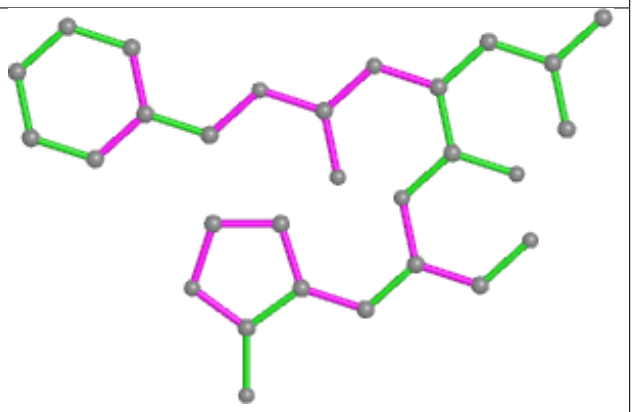


Rings

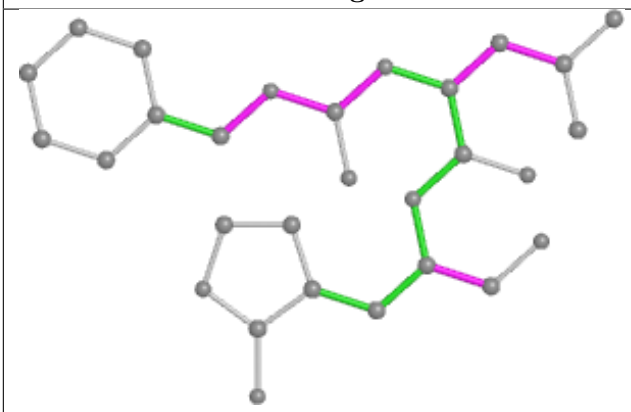
Ligand K36 A 401



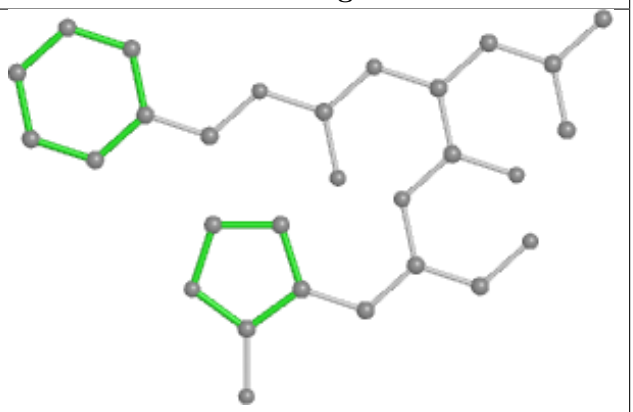
Bond lengths



Bond angles

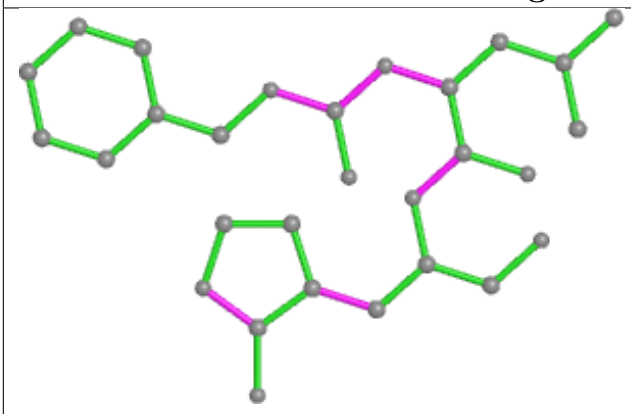


Torsions

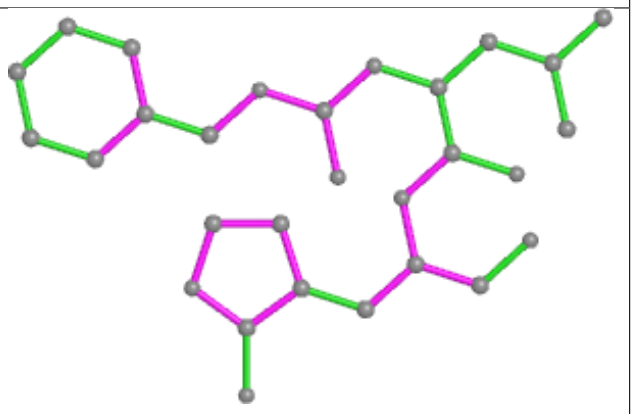


Rings

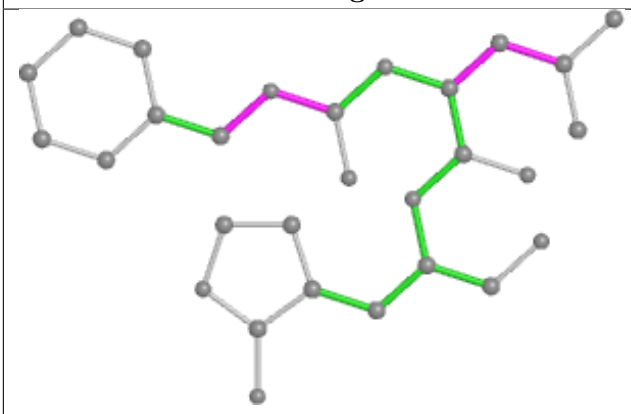
Ligand K36 G 401



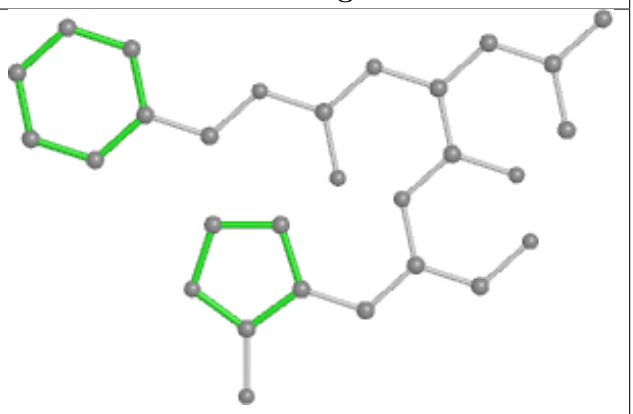
Bond lengths



Bond angles

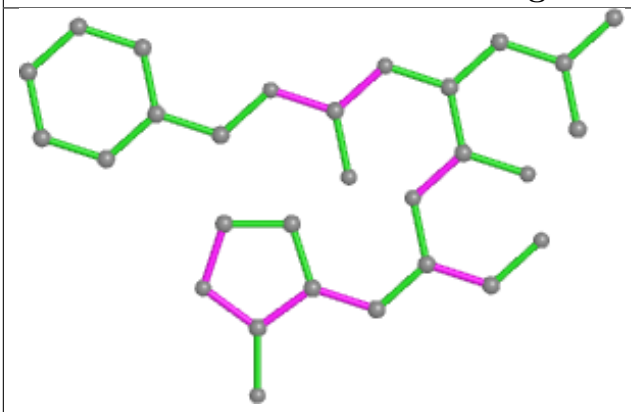


Torsions

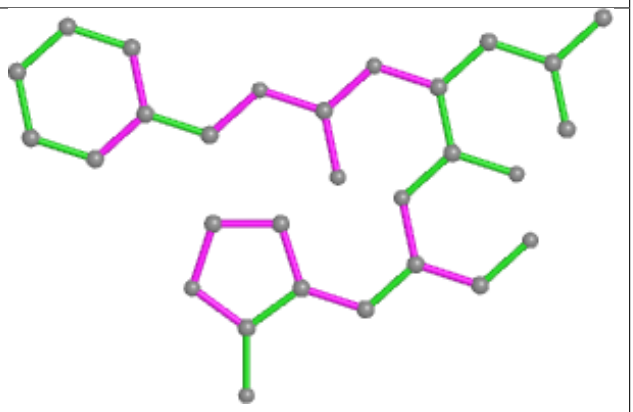


Rings

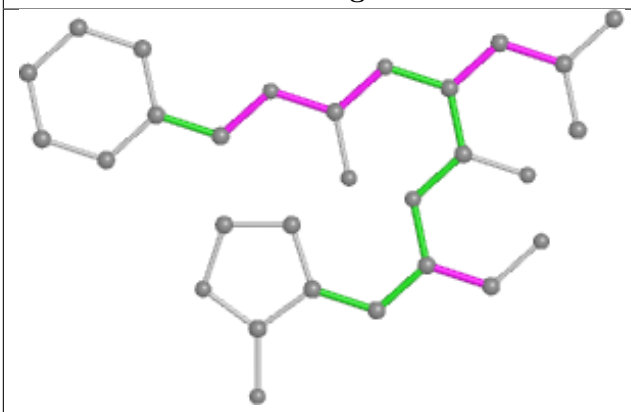
Ligand K36 H 401



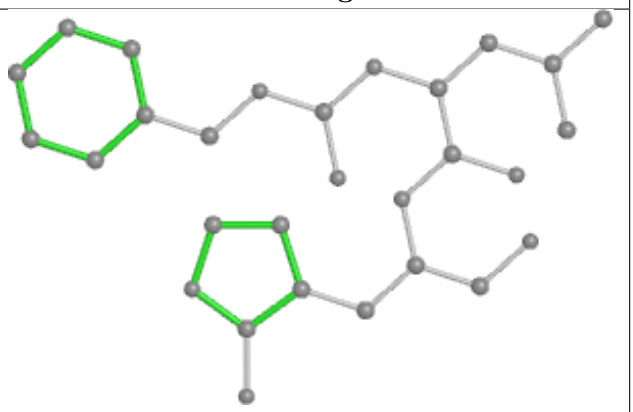
Bond lengths



Bond angles

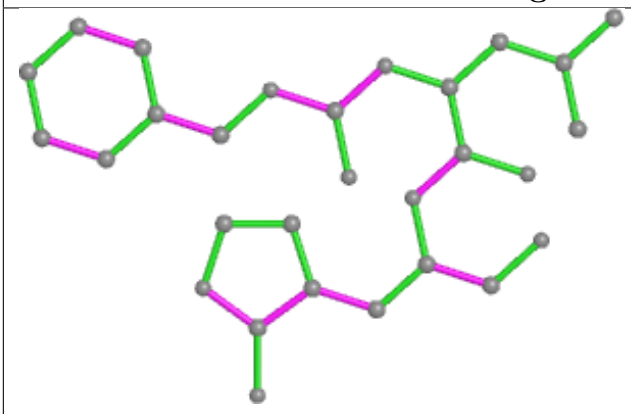


Torsions

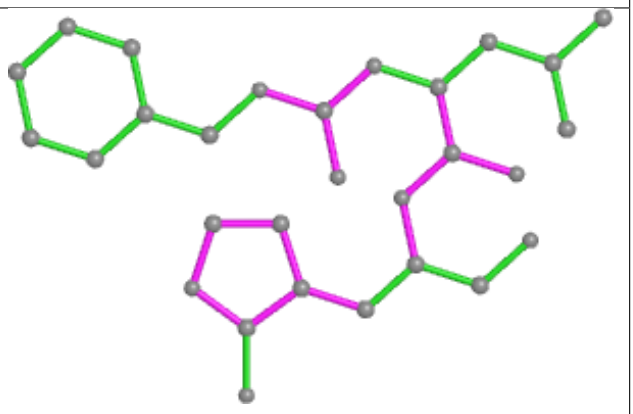


Rings

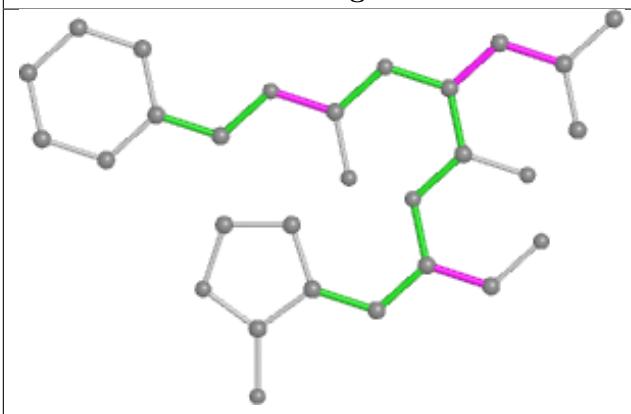
Ligand K36 B 401



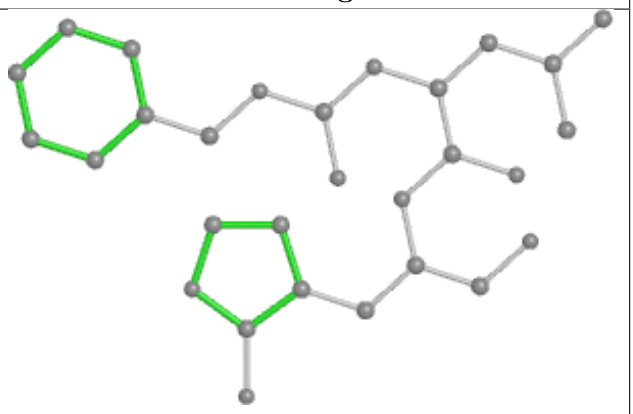
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	-0.22	3 (1%) 82 87	15, 38, 66, 88	0
1	B	299/302 (99%)	-0.06	3 (1%) 82 87	16, 43, 71, 87	0
1	C	298/302 (98%)	0.04	7 (2%) 60 69	18, 45, 71, 94	0
1	D	296/302 (98%)	0.23	14 (4%) 31 37	25, 59, 99, 118	0
1	E	299/302 (99%)	0.13	5 (1%) 70 78	23, 51, 85, 112	0
1	F	299/302 (99%)	0.30	17 (5%) 23 28	22, 50, 108, 136	0
1	G	298/302 (98%)	0.29	22 (7%) 14 17	22, 55, 118, 139	0
1	H	289/302 (95%)	0.73	43 (14%) 2 2	25, 66, 123, 153	0
All	All	2377/2416 (98%)	0.18	114 (4%) 30 36	15, 50, 102, 153	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	22	TYR	5.7
1	H	58	SER	5.3
1	F	242	SER	4.6
1	D	61	ARG	4.6
1	H	56	GLU	4.5
1	F	227	GLU	4.5
1	G	271	GLY	4.3
1	H	54	GLU	4.3
1	D	195	THR	4.3
1	H	50	VAL	4.3
1	H	95	PRO	4.2
1	H	45	SER	4.1
1	H	90	VAL	4.0
1	D	58	SER	4.0
1	G	242	SER	4.0
1	G	217	TRP	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	195	THR	3.9
1	G	270	LYS	3.9
1	F	249	MET	3.9
1	H	190	MET	3.9
1	H	24	ASN	3.9
1	B	274	GLY	3.8
1	G	274	GLY	3.7
1	D	77	VAL	3.6
1	H	153	ASN	3.5
1	F	245	ASP	3.5
1	C	245	ASP	3.4
1	D	270	LYS	3.4
1	H	92	GLN	3.3
1	H	47	THR	3.2
1	H	60	VAL	3.2
1	D	273	GLY	3.2
1	C	71	ASN	3.2
1	G	221	ASN	3.2
1	H	154	GLY	3.2
1	F	270	LYS	3.2
1	C	270	LYS	3.1
1	E	272	PHE	3.1
1	H	48	THR	3.1
1	F	195	THR	3.0
1	D	299	VAL	3.0
1	H	192	LEU	3.0
1	H	78	SER	2.9
1	G	224	MET	2.9
1	D	245	ASP	2.9
1	G	245	ASP	2.9
1	H	26	VAL	2.9
1	E	273	GLY	2.8
1	D	275	ARG	2.8
1	H	46	ASP	2.8
1	F	299	VAL	2.8
1	D	221	ASN	2.8
1	F	275	ARG	2.8
1	H	62	LEU	2.7
1	H	38	CYS	2.7
1	D	274	GLY	2.7
1	B	299	VAL	2.7
1	H	25	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	45	SER	2.6
1	G	255	GLY	2.6
1	F	204	VAL	2.6
1	F	190	MET	2.6
1	G	214	GLY	2.6
1	G	223	SER	2.6
1	G	257	SER	2.6
1	G	297	TYR	2.5
1	E	153	ASN	2.5
1	H	59	SER	2.5
1	A	49	ARG	2.5
1	F	226	LEU	2.5
1	F	221	ASN	2.5
1	H	29	GLY	2.5
1	H	18	VAL	2.5
1	B	61	ARG	2.5
1	H	245	ASP	2.5
1	D	227	GLU	2.4
1	A	71	ASN	2.4
1	H	55	ASN	2.4
1	F	222	THR	2.4
1	H	79	ALA	2.4
1	H	93	VAL	2.4
1	D	214	GLY	2.4
1	H	169	GLY	2.4
1	H	96	ASN	2.4
1	G	222	THR	2.3
1	H	66	SER	2.3
1	F	231	THR	2.3
1	C	167	GLY	2.3
1	H	23	GLY	2.3
1	G	48	THR	2.3
1	H	49	ARG	2.3
1	H	98	PRO	2.3
1	H	189	SER	2.3
1	G	208	TYR	2.3
1	F	272	PHE	2.2
1	G	226	LEU	2.2
1	H	86	LEU	2.2
1	D	54	GLU	2.2
1	F	244	ILE	2.2
1	H	44	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	40	ARG	2.2
1	E	299	VAL	2.2
1	G	276	THR	2.1
1	H	141	ALA	2.1
1	C	281	GLY	2.1
1	G	58	SER	2.1
1	G	204	VAL	2.1
1	E	49	ARG	2.1
1	C	273	GLY	2.1
1	G	253	LYS	2.0
1	H	17	ILE	2.0
1	F	234	LYS	2.0
1	G	268	LEU	2.0
1	A	242	SER	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 monosaccharides in this entry.

6.4 Ligands (i)

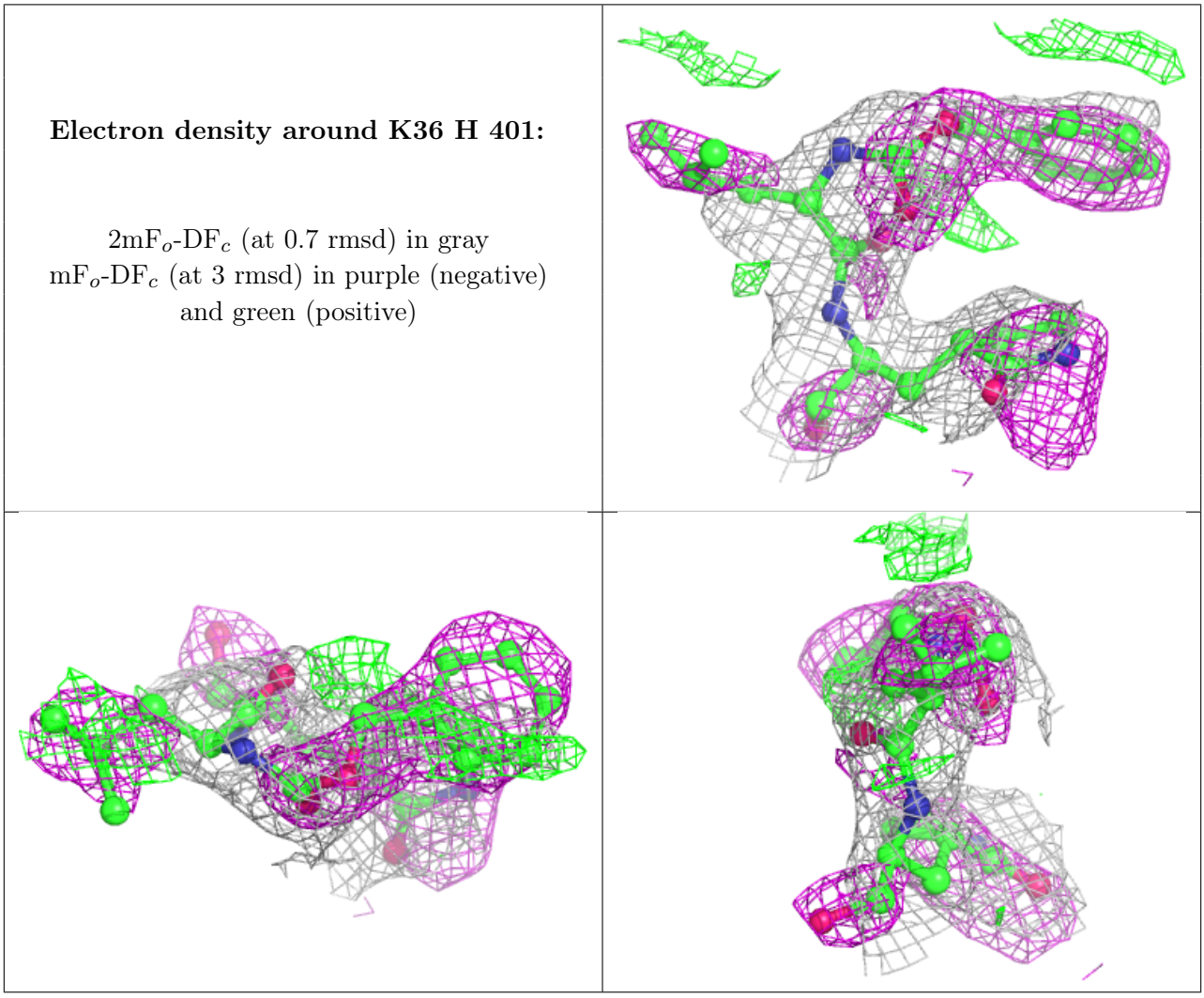
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.69	0.51	31,40,46,47	0
2	K36	C	401	29/33	0.85	0.26	31,40,46,47	0
2	K36	F	401	29/33	0.89	0.19	31,39,49,53	0
2	K36	A	401	29/33	0.94	0.17	31,40,46,47	0
2	K36	D	401	29/33	0.94	0.19	42,53,72,79	0
2	K36	G	401	29/33	0.95	0.18	26,46,50,54	0
2	K36	B	401	29/33	0.95	0.17	17,27,76,77	0
2	K36	E	401	29/33	0.96	0.15	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.

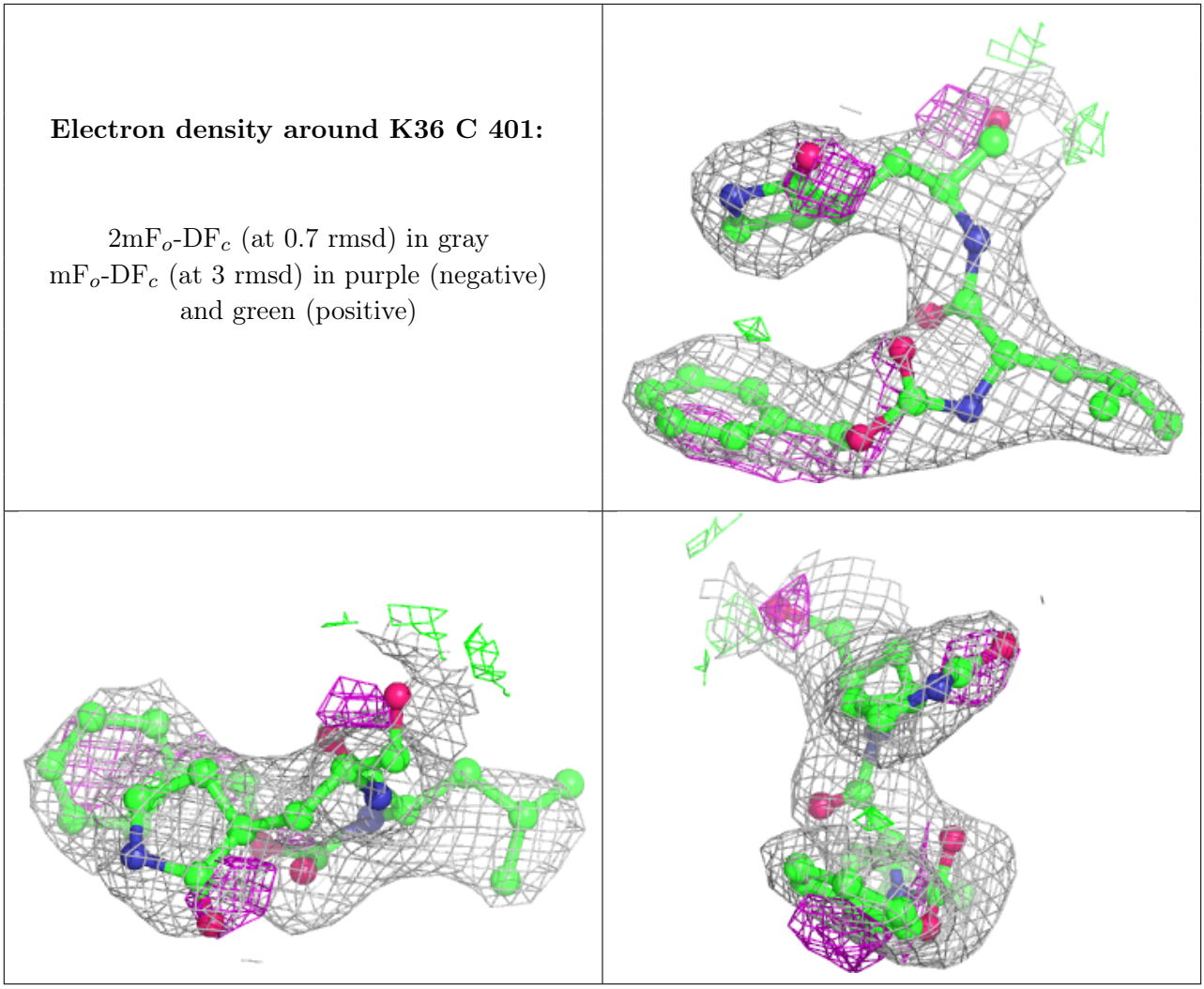
Electron density around K36 H 401:

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



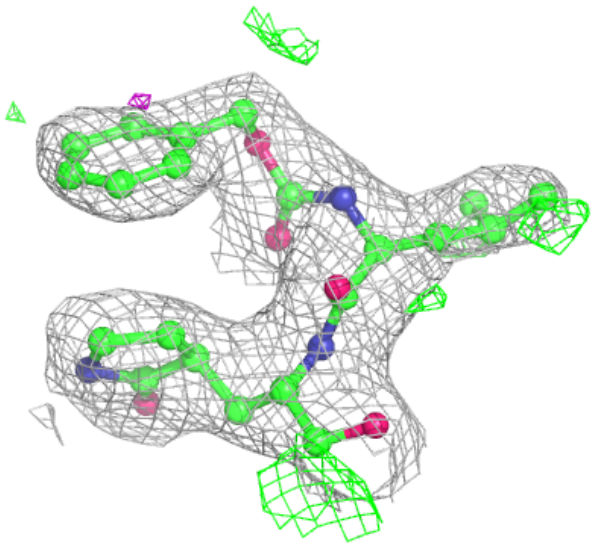
Electron density around K36 C 401:

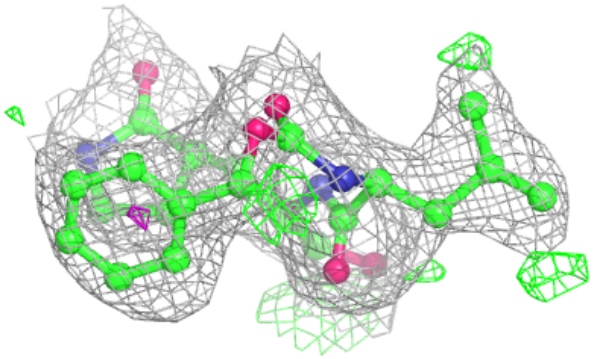
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

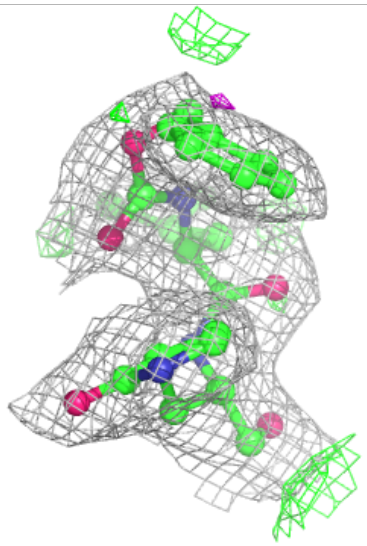


Electron density around K36 F 401:

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

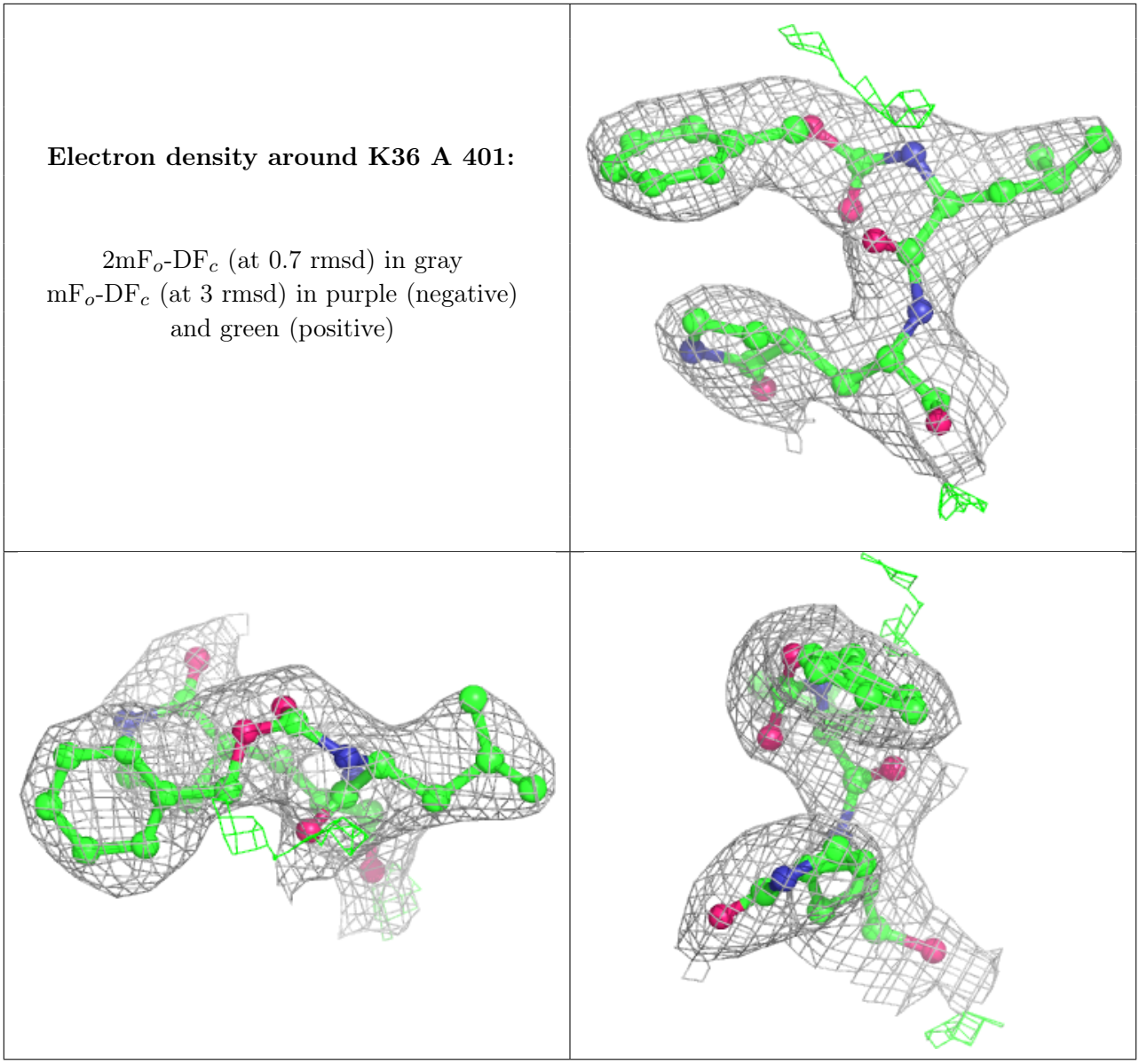






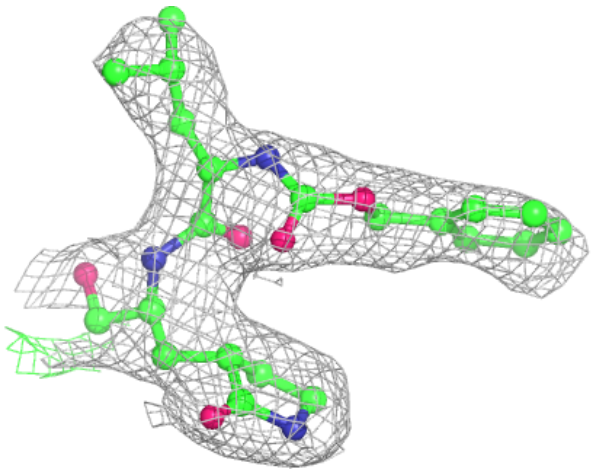
Electron density around K36 A 401:

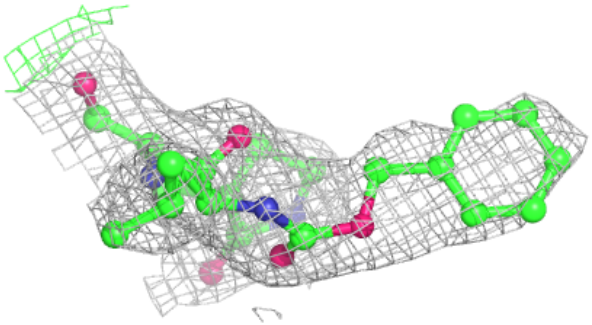
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around K36 D 401:

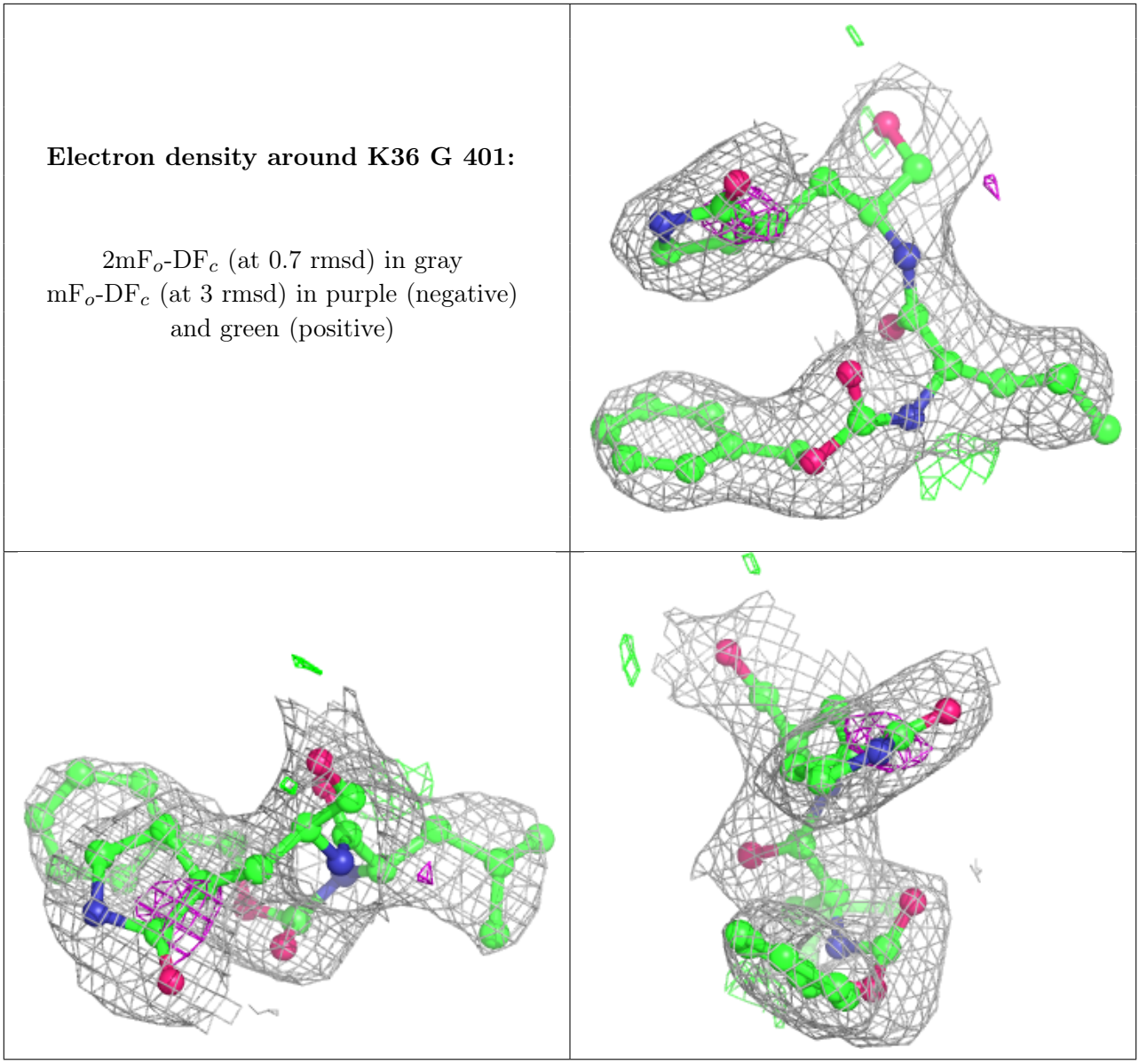
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





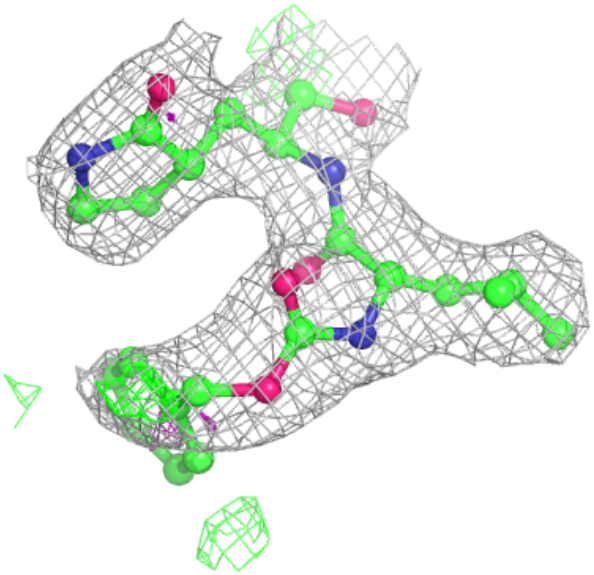
Electron density around K36 G 401:

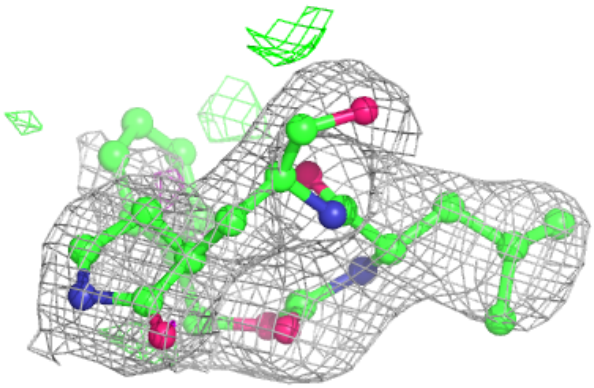
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

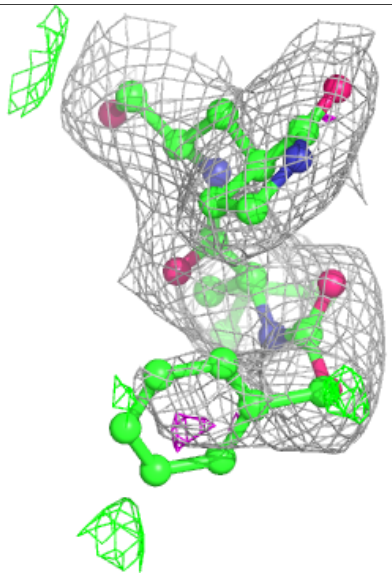


Electron density around K36 B 401:

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

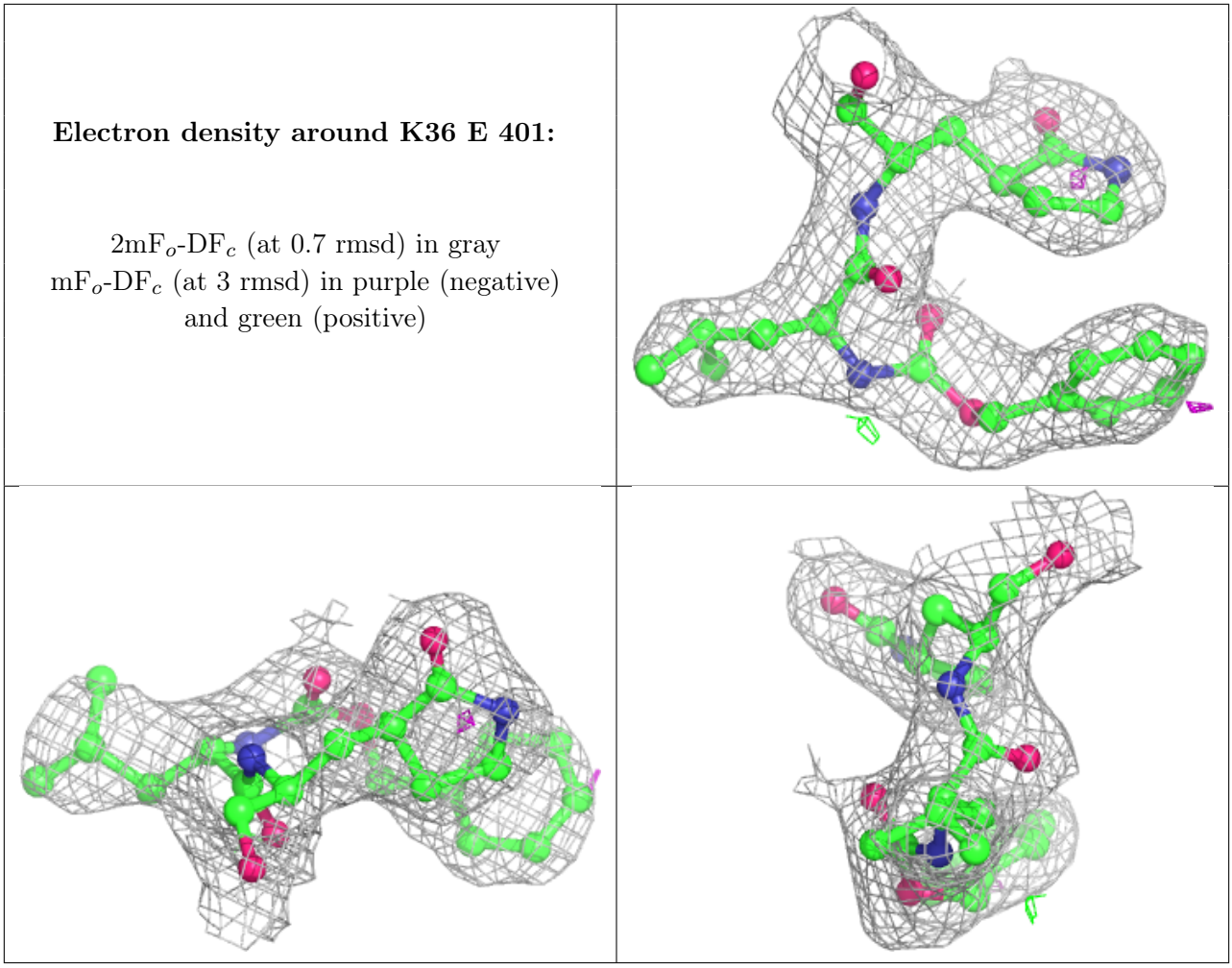






Electron density around K36 E 401:

$2mF_o$-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.