



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2025 – 04:09 PM EDT

PDB ID : 9O0U / pdb\_00009o0u  
Title : Crystal structure of CRAF/MEK1 complex with PLX4720 and CH5126766  
Authors : Jang, D.M.; Eck, M.J.  
Deposited on : 2025-04-03  
Resolution : 2.91 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](mailto: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>.

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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 : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
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) : 2.46

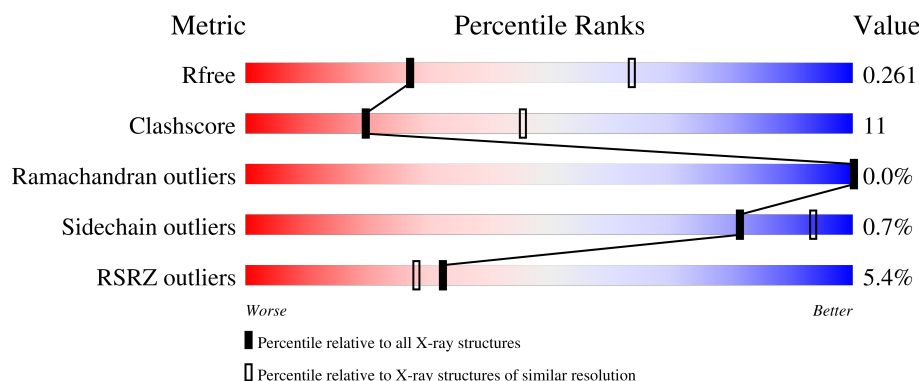
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.91 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))
$R_{free}$	164625	2797 (2.94-2.90)
Clashscore	180529	3049 (2.94-2.90)
Ramachandran outliers	177936	2981 (2.94-2.90)
Sidechain outliers	177891	2983 (2.94-2.90)
RSRZ outliers	164620	2799 (2.94-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	280	<div> <div>2%</div> <div>80% 15% 5%</div> </div>
1	C	280	<div> <div>5%</div> <div>76% 18% 6%</div> </div>
1	E	280	<div> <div>2%</div> <div>78% 15% 8%</div> </div>
1	G	280	<div> <div>2%</div> <div>83% 11% 5%</div> </div>
2	B	395	<div> <div>2%</div> <div>62% 19% 18%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	395	
2	F	395	
2	H	395	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18804 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 RAF proto-oncogene serine/threonine-protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	1	0
			2146	1374	369	389	14			
1	C	264	Total	C	N	O	S	0	0	0
			2115	1355	362	384	14			
1	E	258	Total	C	N	O	S	0	0	0
			2075	1332	355	374	14			
1	G	265	Total	C	N	O	S	0	1	0
			2135	1368	366	387	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	336	SER	-	expression tag	UNP P04049
A	340	ASP	TYR	engineered mutation	UNP P04049
A	341	ASP	TYR	engineered mutation	UNP P04049
C	336	SER	-	expression tag	UNP P04049
C	340	ASP	TYR	engineered mutation	UNP P04049
C	341	ASP	TYR	engineered mutation	UNP P04049
E	336	SER	-	expression tag	UNP P04049
E	340	ASP	TYR	engineered mutation	UNP P04049
E	341	ASP	TYR	engineered mutation	UNP P04049
G	336	SER	-	expression tag	UNP P04049
G	340	ASP	TYR	engineered mutation	UNP P04049
G	341	ASP	TYR	engineered mutation	UNP P04049

- Molecule 2 is a protein called Dual specificity mitogen-activated protein kinase kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	322	Total	C	N	O	S	0	0	0
			2532	1618	430	467	17			
2	D	317	Total	C	N	O	S	0	0	0
			2477	1584	416	462	15			

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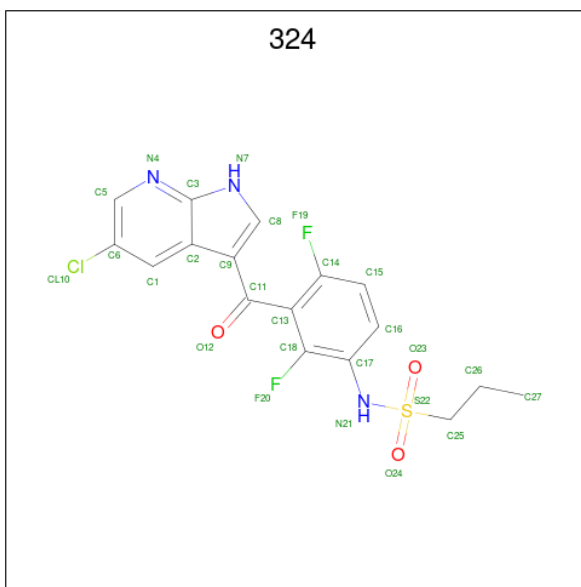
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	322	Total	C	N	O	S	0	0	0
			2522	1613	427	465	17			
2	H	315	Total	C	N	O	S	0	0	0
			2487	1591	422	459	15			

There are 16 discrepancies between the modelled and reference sequences:

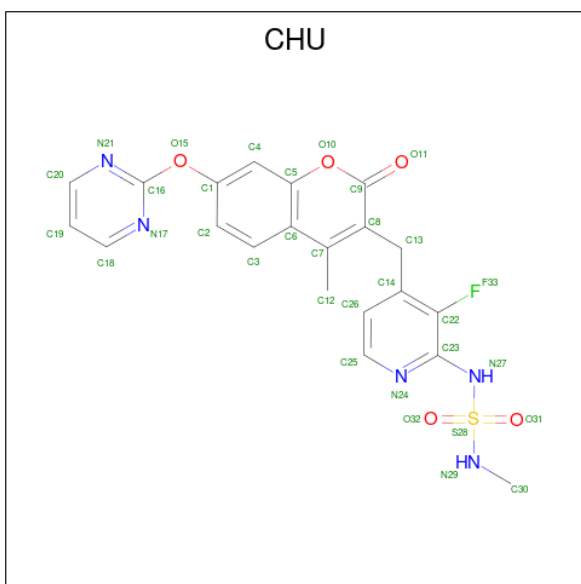
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q02750
B	0	GLY	-	expression tag	UNP Q02750
B	218	ALA	SER	engineered mutation	UNP Q02750
B	222	ALA	SER	engineered mutation	UNP Q02750
D	-1	GLY	-	expression tag	UNP Q02750
D	0	GLY	-	expression tag	UNP Q02750
D	218	ALA	SER	engineered mutation	UNP Q02750
D	222	ALA	SER	engineered mutation	UNP Q02750
F	-1	GLY	-	expression tag	UNP Q02750
F	0	GLY	-	expression tag	UNP Q02750
F	218	ALA	SER	engineered mutation	UNP Q02750
F	222	ALA	SER	engineered mutation	UNP Q02750
H	-1	GLY	-	expression tag	UNP Q02750
H	0	GLY	-	expression tag	UNP Q02750
H	218	ALA	SER	engineered mutation	UNP Q02750
H	222	ALA	SER	engineered mutation	UNP Q02750

- Molecule 3 is N-{3-[(5-chloro-1H-pyrrolo[2,3-b]pyridin-3-yl)carbonyl]-2,4-difluorophenyl}propane-1-sulfonamide (CCD ID: 324) (formula: C<sub>17</sub>H<sub>14</sub>ClF<sub>2</sub>N<sub>3</sub>O<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



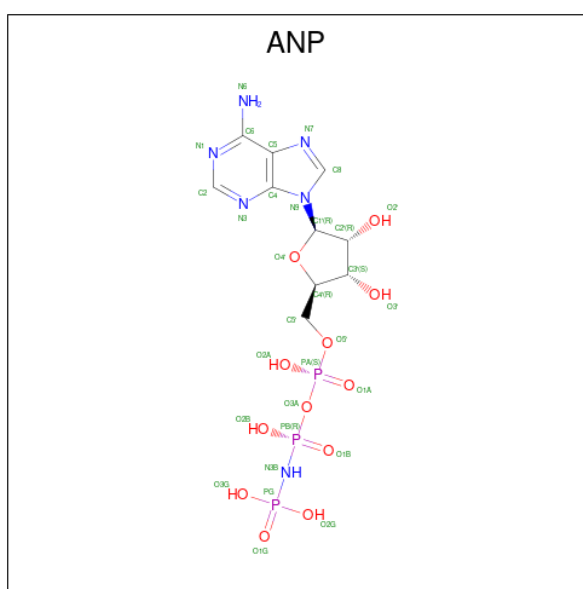
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	S	0	0
			27	17	1	2	3	3	1		
3	C	1	Total	C	Cl	F	N	O	S	0	0
			27	17	1	2	3	3	1		
3	E	1	Total	C	Cl	F	N	O	S	0	0
			27	17	1	2	3	3	1		
3	G	1	Total	C	Cl	F	N	O	S	0	0
			27	17	1	2	3	3	1		

- Molecule 4 is N-(3-fluoro-4-{[4-methyl-2-oxo-7-(pyrimidin-2-yloxy)-2H-chromen-3-yl]methyl}pyridin-2-yl)-N'-methylsulfuric diamide (CCD ID: CHU) (formula:  $C_{21}H_{18}FN_5O_5S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	S	
			33	21	1	5	5	1	0
4	D	1	Total	C	F	N	O	S	
			33	21	1	5	5	1	0
4	F	1	Total	C	F	N	O	S	
			33	21	1	5	5	1	0
4	H	1	Total	C	F	N	O	S	
			33	21	1	5	5	1	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	H	1	Total	C	N	O	P		
			31	10	6	12	3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	13	Total 13 O	0	0
6	B	6	Total 6 O	0	0
6	C	7	Total 7 O	0	0
6	D	1	Total 1 O	0	0

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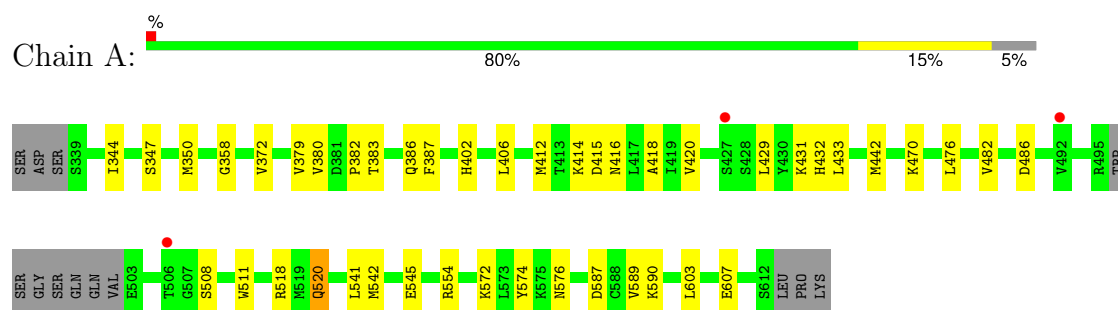
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	6	Total 6	O 6	0	0
6	F	1	Total 1	O 1	0	0
6	G	9	Total 9	O 9	0	0
6	H	1	Total 1	O 1	0	0



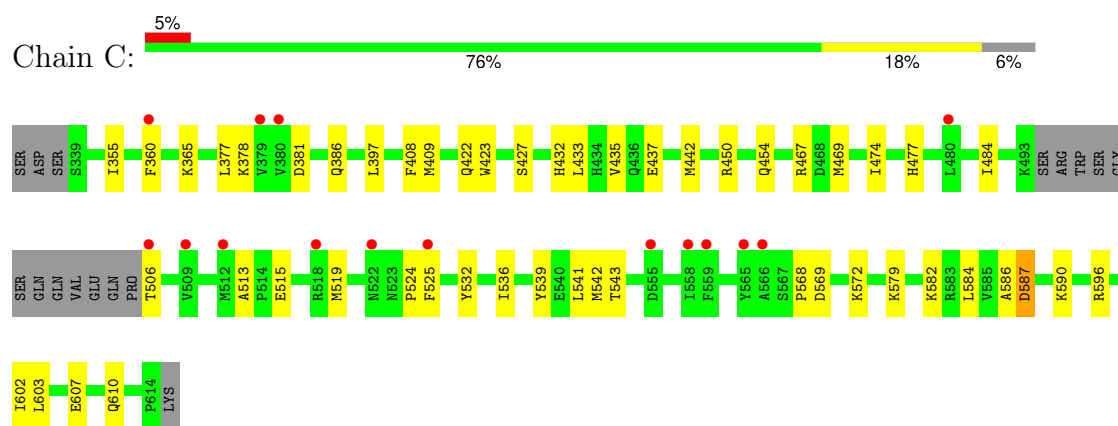
### 3 Residue-property plots [i](#)

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.

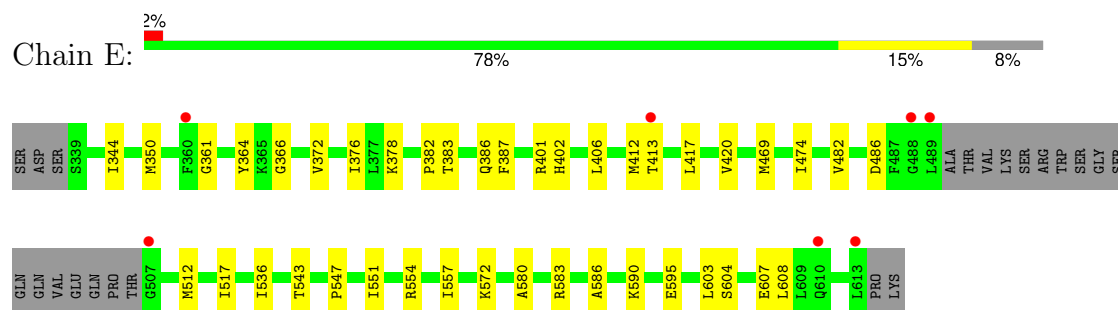
- Molecule 1: RAF proto-oncogene serine/threonine-protein kinase



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- Molecule 1: RAF proto-oncogene serine/threonine-protein kinase

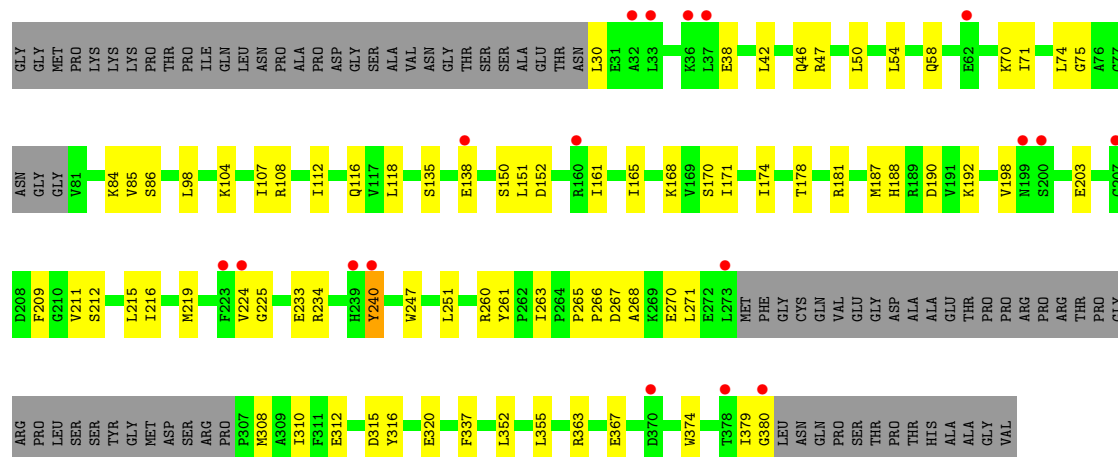
Chain G:

- Molecule 2: Dual specificity mitogen-activated protein kinase kinase 1

Chain B:

- Molecule 2: Dual specificity mitogen-activated protein kinase kinase 1

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	180.99Å 180.99Å 367.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.10 – 2.91 46.10 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.10-2.91) 99.8 (46.10-2.91)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, $R_{free}$	0.230 , 0.264 0.228 , 0.261	Depositor DCC
$R_{free}$ test set	3912 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.4	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 57.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18804	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.29% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: 324, CHU, ANP

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	0.20	0/2196	0.51	0/2964
1	C	0.28	0/2161	0.59	0/2918
1	E	0.21	0/2121	0.51	0/2862
1	G	0.25	0/2182	0.55	0/2947
2	B	0.31	0/2580	0.60	3/3471 (0.1%)
2	D	0.54	0/2524	0.84	0/3400
2	F	0.42	0/2570	0.70	1/3459 (0.0%)
2	H	0.33	0/2533	0.63	0/3408
All	All	0.34	0/18867	0.63	4/25429 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	32	ALA	N-CA-C	-5.99	105.46	112.89
2	B	261	TYR	CB-CA-C	5.68	118.53	109.62
2	B	263	ILE	N-CA-CB	5.38	114.13	110.52
2	F	223	PHE	CA-CB-CG	5.36	119.16	113.80

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	2146	0	2151	40	0
1	C	2115	0	2125	39	0
1	E	2075	0	2080	37	0
1	G	2135	0	2144	27	0
2	B	2532	0	2574	54	0
2	D	2477	0	2504	121	0
2	F	2522	0	2559	79	0
2	H	2487	0	2535	52	0
3	A	27	0	14	2	0
3	C	27	0	14	0	0
3	E	27	0	14	2	0
3	G	27	0	14	0	0
4	B	33	0	18	1	0
4	D	33	0	18	1	0
4	F	33	0	18	0	0
4	H	33	0	18	1	0
5	H	31	0	13	1	0
6	A	13	0	0	1	0
6	B	6	0	0	3	0
6	C	7	0	0	2	0
6	D	1	0	0	0	0
6	E	6	0	0	1	0
6	F	1	0	0	0	0
6	G	9	0	0	1	0
6	H	1	0	0	0	0
All	All	18804	0	18813	424	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 (424) 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:A:415:ASP:HA	1:E:583:ARG:HH22	1.36	0.90
2:D:181:ARG:HD2	2:D:242:VAL:HG21	1.54	0.89
1:C:469:MET:HE1	1:C:474:ILE:HD11	1.60	0.84
1:C:506:THR:HB	2:D:224:VAL:HG11	1.58	0.83
1:E:382:PRO:HB2	1:E:387:PHE:CE1	2.15	0.82
2:D:251:LEU:HD21	2:D:263:ILE:HD11	1.62	0.80
2:F:90:SER:HB2	2:F:92:LEU:HD13	1.65	0.78
2:D:74:LEU:HD21	2:D:84:LYS:HB2	1.66	0.78
1:A:415:ASP:HA	1:E:583:ARG:NH2	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:ASN:ND2	2:D:201:ARG:HG3	2.01	0.76
2:F:337:PHE:CE1	2:F:355:LEU:HD12	2.21	0.76
2:F:31:GLU:HA	2:F:34:GLN:HB2	1.68	0.75
2:B:170:SER:O	2:B:174:ILE:HG13	1.86	0.75
2:F:364:SER:HA	2:F:367:GLU:HG2	1.69	0.75
1:C:584:LEU:HD21	1:C:602:ILE:HG23	1.67	0.75
1:A:382:PRO:HB2	1:A:387:PHE:CE1	2.21	0.74
2:D:151:LEU:HD21	2:D:198:VAL:HG13	1.69	0.74
2:H:260:ARG:HD3	2:H:266:PRO:HG3	1.69	0.74
2:D:87:HIS:HB2	2:D:94:MET:HE1	1.71	0.71
1:A:412:MET:HE1	1:E:608:LEU:HD11	1.71	0.71
2:D:333:GLU:HB2	2:D:363:ARG:HH22	1.55	0.71
1:C:539:TYR:HE1	1:C:543:THR:HG21	1.54	0.71
1:A:358:GLY:HA3	6:A:806:HOH:O	1.89	0.71
1:E:551:ILE:HD11	1:E:557:ILE:HG12	1.72	0.70
2:F:361:ILE:HD12	2:F:362:LYS:N	2.05	0.70
2:D:325:LEU:HD13	2:D:335:GLN:HA	1.74	0.70
2:D:171:ILE:HD11	2:D:361:ILE:HB	1.74	0.69
2:B:308:MET:HE3	2:B:313:LEU:HD23	1.73	0.69
2:F:355:LEU:O	2:F:361:ILE:HG12	1.93	0.69
2:H:74:LEU:HD21	2:H:84:LYS:HB2	1.75	0.68
2:D:127:VAL:HG11	2:D:197:LEU:HD12	1.75	0.68
2:H:174:ILE:HG23	2:H:352:LEU:HD22	1.75	0.68
1:G:554:ARG:NH2	2:H:225:GLY:H	1.91	0.67
1:C:539:TYR:CE2	1:C:568:PRO:HB3	2.29	0.67
2:D:351:ASP:HB3	2:D:354:GLN:HG2	1.76	0.67
1:E:486:ASP:H	3:E:701:324:HN21	1.39	0.67
2:B:267:ASP:HB3	2:B:270:GLU:HG3	1.75	0.67
2:D:191:VAL:HB	2:D:248:SER:HB2	1.76	0.67
2:D:166:LEU:HA	2:D:169:VAL:HG22	1.78	0.66
2:D:269:LYS:O	2:D:273:LEU:HD23	1.95	0.66
2:F:87:HIS:CE1	2:F:89:PRO:HG2	2.31	0.66
2:H:215:LEU:O	2:H:219:MET:HG3	1.96	0.66
2:B:74:LEU:HD11	2:B:84:LYS:HB2	1.78	0.66
2:F:252:SER:O	2:F:256:MET:HG3	1.95	0.66
2:D:60:VAL:HG12	2:D:90:SER:HB3	1.78	0.66
2:D:76:ALA:HA	2:D:81:VAL:HA	1.78	0.66
2:D:261:TYR:HE2	2:D:313:LEU:HD13	1.60	0.65
1:C:397:LEU:HB3	1:C:408:PHE:HB2	1.77	0.65
2:H:42:LEU:HD21	2:H:50:LEU:HD12	1.79	0.65
2:F:118:LEU:HD21	2:F:211:VAL:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:554:ARG:CZ	2:H:225:GLY:H	2.11	0.64
1:G:505:PRO:HB2	1:G:512:MET:HE2	1.78	0.64
1:A:520:GLN:HE21	1:A:520:GLN:HA	1.63	0.64
2:D:235:LEU:HD11	2:D:314:LEU:HD22	1.80	0.64
2:H:187:MET:HE1	2:H:240:TYR:HB2	1.81	0.63
1:A:414:LYS:HB3	1:E:583:ARG:HH12	1.64	0.63
2:H:190:ASP:OD1	2:H:192:LYS:HE3	1.98	0.63
1:E:469:MET:HE3	1:E:474:ILE:HD11	1.80	0.62
2:F:251:LEU:HD11	2:F:262:PRO:HG2	1.80	0.62
2:H:118:LEU:HD21	2:H:211:VAL:HG21	1.80	0.62
1:C:539:TYR:CE1	1:C:543:THR:HG21	2.32	0.62
2:D:199:ASN:HD21	2:D:201:ARG:HG3	1.65	0.62
1:G:554:ARG:NE	2:H:224:VAL:HA	2.15	0.62
1:C:467:ARG:HD2	1:C:525:PHE:CG	2.35	0.61
2:F:157:LYS:HD2	2:F:379:ILE:HG22	1.82	0.61
1:A:415:ASP:CA	1:E:583:ARG:HH22	2.13	0.61
1:A:508:SER:HA	6:B:501:HOH:O	2.00	0.61
1:E:383:THR:OG1	1:E:386:GLN:HG3	2.01	0.61
2:H:170:SER:O	2:H:174:ILE:HG13	2.00	0.61
2:D:47:ARG:HB2	2:D:47:ARG:CZ	2.30	0.60
2:F:263:ILE:O	2:F:265:PRO:HD3	2.01	0.60
2:H:209:PHE:CE1	4:H:401:CHU:H11	2.36	0.60
2:H:266:PRO:HB2	2:H:271:LEU:HD22	1.81	0.60
2:D:47:ARG:HB2	2:D:47:ARG:NH1	2.15	0.60
1:E:364:TYR:CE1	1:E:376:ILE:HD12	2.36	0.60
2:D:191:VAL:HB	2:D:248:SER:CB	2.32	0.60
2:B:363:ARG:O	2:B:367:GLU:HG3	2.02	0.60
2:D:153:GLN:O	2:D:157:LYS:HG3	2.02	0.60
1:C:435:VAL:HG13	2:D:104:LYS:HA	1.84	0.59
2:D:250:GLY:O	2:D:254:VAL:HG23	2.02	0.59
2:B:260:ARG:HD2	2:B:274:MET:HE1	1.85	0.59
1:C:360:PHE:O	1:C:377:LEU:HD12	2.03	0.59
2:D:267:ASP:O	2:D:271:LEU:HD22	2.03	0.58
2:H:188:HIS:CD2	2:H:209:PHE:HB3	2.38	0.58
2:D:69:GLU:HB2	2:D:88:LYS:CE	2.33	0.58
2:D:247:TRP:CZ3	2:D:251:LEU:HD22	2.38	0.58
2:H:75:GLY:HA3	5:H:402:ANP:H4'	1.85	0.58
2:D:78:ASN:HD21	2:D:194:SER:HB3	1.68	0.58
2:F:223:PHE:HD1	2:F:224:VAL:H	1.51	0.58
2:D:199:ASN:ND2	2:D:201:ARG:CG	2.66	0.57
2:D:129:PHE:HE1	2:D:141:ILE:HG23	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:382:PRO:HB2	1:E:387:PHE:HE1	1.64	0.57
1:A:415:ASP:O	1:A:416:ASN:ND2	2.38	0.57
2:B:247:TRP:CZ3	2:B:251:LEU:HD22	2.39	0.57
2:D:351:ASP:HB3	2:D:354:GLN:CG	2.35	0.57
2:D:69:GLU:HB2	2:D:88:LYS:HE3	1.87	0.57
2:D:90:SER:HB2	2:D:92:LEU:HD13	1.87	0.57
2:F:87:HIS:HB2	2:F:94:MET:HE2	1.85	0.57
2:F:230:MET:HE1	2:F:234:ARG:HB3	1.87	0.57
1:G:563:ARG:HH21	2:H:315:ASP:CG	2.13	0.57
1:E:590:LYS:HE3	1:E:595:GLU:HB3	1.87	0.56
2:D:263:ILE:HB	2:D:264:PRO:HD3	1.87	0.56
2:F:265:PRO:HG2	2:F:316:TYR:OH	2.05	0.56
1:G:384:PRO:HA	1:G:387:PHE:HD2	1.70	0.56
1:A:406:LEU:HD21	3:A:701:324:H8	1.87	0.56
2:H:135:SER:O	2:H:138:GLU:HG3	2.06	0.56
2:B:215:LEU:O	2:B:219:MET:HG3	2.05	0.56
2:B:263:ILE:O	2:B:265:PRO:HD3	2.06	0.56
2:D:53:PHE:HE1	2:D:130:TYR:CZ	2.23	0.56
2:D:125:TYR:C	2:D:126:ILE:HD12	2.31	0.56
2:H:50:LEU:O	2:H:54:LEU:HG	2.05	0.56
2:D:69:GLU:O	2:D:85:VAL:HG23	2.06	0.55
2:F:170:SER:O	2:F:174:ILE:HG13	2.05	0.55
1:A:379:VAL:HG12	1:A:382:PRO:HG3	1.88	0.55
1:E:406:LEU:HD21	3:E:701:324:H8	1.88	0.55
1:A:372:VAL:HG21	1:A:420:VAL:CG1	2.36	0.55
2:D:263:ILE:O	2:D:265:PRO:HD3	2.07	0.55
1:G:379:VAL:HG11	1:G:382:PRO:HA	1.89	0.55
1:A:574:TYR:HB3	1:A:576:ASN:OD1	2.07	0.54
2:B:190:ASP:OD1	2:B:192:LYS:HE3	2.07	0.54
2:F:74:LEU:HD21	2:F:84:LYS:HB2	1.89	0.54
2:D:181:ARG:O	2:D:185:LYS:HD3	2.07	0.54
2:B:40:LEU:HB3	2:B:42:LEU:HD13	1.90	0.54
1:E:543:THR:HG22	1:E:572:LYS:C	2.33	0.54
1:C:539:TYR:CD2	1:C:568:PRO:HB3	2.43	0.54
1:C:543:THR:HG22	1:C:572:LYS:O	2.08	0.54
2:D:129:PHE:HZ	2:D:132:ALA:HB2	1.74	0.53
1:C:355:ILE:HG13	1:C:423:TRP:HH2	1.72	0.53
1:G:397:LEU:HB3	1:G:408:PHE:HB2	1.90	0.53
2:B:87:HIS:HB2	2:B:94:MET:HE3	1.90	0.53
1:C:579:LYS:HD3	1:C:582:LYS:NZ	2.24	0.53
2:F:191:VAL:HB	2:F:248:SER:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518[A]:ARG:HB3	1:A:520:GLN:HG2	1.91	0.53
2:B:374:TRP:O	2:B:378:THR:HG22	2.09	0.53
2:F:73:GLU:HG2	2:F:83:PHE:CE1	2.43	0.53
2:F:165:ILE:HG21	2:F:374:TRP:CZ3	2.44	0.53
2:F:362:LYS:O	2:F:365:ASP:OD1	2.27	0.53
1:E:361:GLY:HA2	1:E:378:LYS:HG2	1.90	0.52
2:D:198:VAL:HG11	2:D:371:PHE:HZ	1.74	0.52
2:H:337:PHE:CE1	2:H:355:LEU:HD22	2.45	0.52
2:F:262:PRO:O	2:F:263:ILE:C	2.52	0.52
2:H:247:TRP:CZ3	2:H:251:LEU:HD22	2.43	0.52
1:C:513:ALA:HA	1:C:532:TYR:CD2	2.44	0.52
1:E:580:ALA:HA	1:E:583:ARG:HH21	1.75	0.52
1:C:519:MET:SD	1:C:524:PRO:HG3	2.50	0.52
2:D:379:ILE:HG13	2:D:380:GLY:N	2.24	0.52
2:F:31:GLU:O	2:F:35:LYS:N	2.43	0.52
2:F:379:ILE:HG13	2:F:380:GLY:N	2.25	0.51
1:E:536:ILE:HG23	1:E:547:PRO:HG3	1.90	0.51
2:B:353:LYS:H	2:B:353:LYS:HD2	1.74	0.51
2:D:188:HIS:ND1	2:D:209:PHE:HB3	2.26	0.51
2:H:71:ILE:HD11	2:H:86:SER:HB2	1.92	0.51
2:H:30:LEU:HD22	2:H:58:GLN:NE2	2.25	0.51
2:B:118:LEU:HD21	2:B:211:VAL:HG21	1.92	0.51
1:A:603:LEU:O	1:A:607:GLU:HG3	2.11	0.51
1:C:442:MET:HE1	1:C:542:MET:SD	2.50	0.51
2:B:209:PHE:CE2	4:B:401:CHU:H11	2.45	0.51
2:F:356:MET:O	2:F:356:MET:HG3	2.11	0.51
2:F:361:ILE:HD12	2:F:362:LYS:HG3	1.92	0.51
1:A:545:GLU:OE2	1:A:572:LYS:NZ	2.43	0.51
2:H:104:LYS:HG3	2:H:107:ILE:HG12	1.93	0.51
1:A:432:HIS:CD2	1:A:476:LEU:HD12	2.46	0.50
1:E:372:VAL:CG2	1:E:420:VAL:HG13	2.42	0.50
1:A:486:ASP:H	3:A:701:324:HN21	1.60	0.50
2:H:98:LEU:HD12	2:H:138:GLU:CD	2.37	0.50
2:D:101:LEU:HD13	2:D:103:ILE:HG12	1.93	0.50
2:H:168:LYS:HA	2:H:171:ILE:HD12	1.94	0.50
1:A:372:VAL:CG2	1:A:420:VAL:CG1	2.90	0.50
1:A:372:VAL:CG2	1:A:420:VAL:HG13	2.41	0.50
1:A:554:ARG:HD3	2:B:224:VAL:HA	1.93	0.50
2:B:352:LEU:HA	2:B:355:LEU:HD12	1.93	0.50
1:C:586:ALA:O	1:C:590:LYS:HG3	2.12	0.50
1:A:350:MET:HB3	1:G:350:MET:HE1	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:344:ILE:O	1:E:412:MET:HG2	2.12	0.50
2:D:162:PRO:HD2	2:D:165:ILE:HD12	1.92	0.50
1:G:388:GLN:HG2	1:G:391:ARG:HH21	1.76	0.50
2:D:192:LYS:HG2	2:D:229:TYR:HD2	1.77	0.49
2:D:216:ILE:HD13	4:D:401:CHU:C22	2.42	0.49
2:D:255:GLU:HB2	2:D:262:PRO:HD3	1.94	0.49
2:F:215:LEU:O	2:F:219:MET:HG3	2.12	0.49
2:F:261:TYR:CE2	2:F:263:ILE:HB	2.47	0.49
2:F:365:ASP:OD1	2:F:365:ASP:N	2.43	0.49
1:A:402:HIS:HA	1:C:409:MET:HE2	1.93	0.49
2:D:360:PHE:O	2:D:363:ARG:HB3	2.11	0.49
1:E:586:ALA:O	1:E:590:LYS:HG3	2.12	0.49
1:C:543:THR:HG22	1:C:572:LYS:C	2.36	0.49
2:D:64:LYS:HE2	2:D:66:ASP:CG	2.38	0.49
2:D:112:ILE:O	2:D:116:GLN:HG2	2.12	0.49
2:F:364:SER:HA	2:F:367:GLU:CG	2.42	0.49
1:C:427:SER:HB2	1:C:432:HIS:CD2	2.48	0.49
1:E:372:VAL:HG21	1:E:420:VAL:CG1	2.43	0.49
2:D:171:ILE:O	2:D:175:LYS:HG2	2.13	0.49
2:F:164:GLN:HB3	2:F:369:VAL:HG21	1.94	0.49
2:H:112:ILE:O	2:H:116:GLN:HG2	2.13	0.49
2:F:313:LEU:O	2:F:317:ILE:HG13	2.12	0.49
2:D:40:LEU:HB3	2:D:42:LEU:HD13	1.95	0.48
2:D:43:ASP:C	2:D:43:ASP:OD1	2.56	0.48
2:D:269:LYS:C	2:D:273:LEU:HD23	2.37	0.48
2:F:351:ASP:O	2:F:355:LEU:HD23	2.13	0.48
2:D:94:MET:HE3	2:D:94:MET:HB2	1.45	0.48
2:D:152:ASP:HB2	2:D:193:PRO:HB2	1.94	0.48
2:F:251:LEU:CD1	2:F:262:PRO:HG2	2.41	0.48
2:H:108:ARG:O	2:H:112:ILE:HG12	2.13	0.48
2:B:251:LEU:HD21	2:B:263:ILE:HD11	1.94	0.48
2:D:103:ILE:HG13	2:D:108:ARG:HG3	1.96	0.48
2:D:314:LEU:O	2:D:318:VAL:HG23	2.12	0.48
1:E:590:LYS:CE	1:E:595:GLU:HB3	2.43	0.48
1:C:454:GLN:HG3	1:C:603:LEU:HD11	1.96	0.48
1:C:515:GLU:OE2	1:C:596:ARG:NH2	2.46	0.48
2:F:135:SER:HB3	2:F:138:GLU:OE2	2.14	0.48
2:H:363:ARG:O	2:H:367:GLU:HG3	2.13	0.48
2:H:379:ILE:HG13	2:H:380:GLY:N	2.29	0.48
2:B:230:MET:CE	6:B:506:HOH:O	2.61	0.48
2:F:350:ALA:HB1	2:F:355:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:316:TYR:CD2	2:H:320:GLU:HG3	2.49	0.48
1:A:587:ASP:HA	1:A:590:LYS:HE2	1.96	0.47
2:F:362:LYS:C	2:F:365:ASP:OD1	2.57	0.47
2:D:64:LYS:HG3	2:D:66:ASP:H	1.79	0.47
2:F:310:ILE:O	2:F:314:LEU:HG	2.14	0.47
2:D:200:SER:O	2:D:372:ALA:HB1	2.13	0.47
2:D:263:ILE:HG13	2:D:317:ILE:HD11	1.96	0.47
1:C:437:GLU:OE2	2:D:104:LYS:NZ	2.47	0.47
1:G:387:PHE:CD1	1:G:417:LEU:HD11	2.49	0.47
1:A:545:GLU:OE2	1:A:572:LYS:HD3	2.14	0.47
2:D:228:SER:CB	2:D:314:LEU:HD21	2.44	0.47
1:E:382:PRO:HA	1:E:386:GLN:OE1	2.15	0.47
1:G:474:ILE:HG23	1:G:482:VAL:HG13	1.96	0.47
2:H:263:ILE:O	2:H:265:PRO:HD3	2.15	0.47
1:A:429:LEU:HD21	1:A:541:LEU:HD21	1.97	0.47
1:C:467:ARG:HD2	1:C:525:PHE:CD1	2.49	0.47
2:D:74:LEU:HD12	2:D:82:VAL:HG12	1.97	0.47
2:D:333:GLU:HB2	2:D:363:ARG:NH2	2.28	0.47
2:F:95:ALA:HB3	2:F:143:MET:HG3	1.97	0.47
2:H:261:TYR:CE2	2:H:263:ILE:HB	2.50	0.47
1:A:470:LYS:HB3	1:A:511:TRP:CD2	2.49	0.47
2:F:110:GLN:OE1	2:F:214:GLN:HG3	2.15	0.47
2:F:151:LEU:HD13	2:F:256:MET:HE1	1.95	0.47
1:A:380:VAL:C	1:A:382:PRO:HD3	2.40	0.47
2:D:182:GLU:OE2	2:D:353:LYS:NZ	2.48	0.47
2:F:147:ASP:OD2	2:F:200:SER:HB3	2.15	0.47
2:D:87:HIS:HB2	2:D:94:MET:CE	2.42	0.46
2:B:174:ILE:O	2:B:178:THR:HG22	2.14	0.46
1:C:378:LYS:HE2	1:C:386:GLN:OE1	2.16	0.46
1:C:378:LYS:HE3	1:C:381:ASP:C	2.41	0.46
1:G:394:VAL:O	1:G:398:ARG:HG2	2.15	0.46
1:G:545:GLU:OE2	1:G:572:LYS:HD3	2.15	0.46
2:D:118:LEU:HD21	2:D:211:VAL:HG21	1.96	0.46
1:E:580:ALA:HA	1:E:583:ARG:HE	1.81	0.46
2:H:267:ASP:HB3	2:H:270:GLU:HG3	1.98	0.46
2:F:329:VAL:HG13	2:F:330:PHE:CD2	2.50	0.46
2:H:38:GLU:HA	2:H:47:ARG:HH12	1.81	0.46
2:B:108:ARG:O	2:B:112:ILE:HG12	2.15	0.46
1:E:402:HIS:HA	1:G:409:MET:HE2	1.98	0.46
1:A:350:MET:HB3	1:G:350:MET:CE	2.46	0.46
1:C:532:TYR:CZ	1:C:536:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:64:LYS:HG2	2:F:67:ASP:OD2	2.16	0.46
2:F:267:ASP:OD1	2:F:268:ALA:N	2.48	0.46
2:D:261:TYR:CD1	2:D:262:PRO:HD2	2.50	0.46
2:B:267:ASP:OD1	2:B:268:ALA:N	2.49	0.46
2:D:33:LEU:HD12	2:D:122:ASN:ND2	2.31	0.46
2:F:57:LYS:HB3	2:F:57:LYS:HE3	1.71	0.46
2:F:148:GLY:HA3	2:F:198:VAL:HG23	1.98	0.46
2:B:343:ILE:HD12	2:B:349:ARG:HA	1.98	0.45
2:D:146:MET:HG3	2:D:197:LEU:HD13	1.99	0.45
2:F:188:HIS:CD2	2:F:209:PHE:HB3	2.51	0.45
1:G:568:PRO:HG2	1:G:589:VAL:HG21	1.96	0.45
2:B:230:MET:HE1	6:B:506:HOH:O	2.15	0.45
2:B:379:ILE:HG13	2:B:380:GLY:N	2.31	0.45
1:C:422:GLN:NE2	6:C:801:HOH:O	2.42	0.45
2:F:251:LEU:HA	2:F:251:LEU:HD12	1.56	0.45
1:C:355:ILE:HG13	1:C:423:TRP:CH2	2.49	0.45
1:C:587:ASP:O	1:C:596:ARG:HG2	2.17	0.45
2:B:73:GLU:OE2	2:B:75:GLY:N	2.50	0.45
2:D:188:HIS:HE1	2:D:207:CYS:O	2.00	0.45
2:B:88:LYS:HB2	2:B:89:PRO:HD3	1.98	0.45
2:B:247:TRP:CH2	2:B:251:LEU:HD22	2.52	0.45
2:B:263:ILE:HG13	2:B:317:ILE:HD11	1.99	0.45
2:F:82:VAL:HA	2:F:96:ARG:O	2.15	0.45
2:F:324:LYS:HB2	2:F:324:LYS:NZ	2.32	0.45
1:G:469:MET:HE3	1:G:474:ILE:HD11	1.97	0.45
1:G:517:ILE:HG23	1:G:558:ILE:HG23	1.99	0.45
1:A:383:THR:HG23	1:A:386:GLN:OE1	2.16	0.45
2:D:31:GLU:HA	2:D:34:GLN:HG3	1.99	0.45
2:D:56:GLN:HB3	2:D:92:LEU:HD21	1.98	0.45
2:D:266:PRO:HG2	2:D:271:LEU:HD11	1.99	0.45
1:E:543:THR:HG22	1:E:572:LYS:O	2.17	0.45
1:E:372:VAL:HG21	1:E:420:VAL:HG13	1.99	0.45
2:B:260:ARG:HD3	2:B:266:PRO:HG3	1.99	0.45
1:C:477:HIS:CE1	6:C:801:HOH:O	2.70	0.45
1:A:412:MET:HE2	1:A:418:ALA:HB3	1.98	0.44
2:D:189:ARG:HD2	2:D:210:GLY:HA3	1.98	0.44
2:B:188:HIS:HD2	2:B:190:ASP:H	1.66	0.44
2:F:371:PHE:CE1	2:F:374:TRP:HZ3	2.36	0.44
2:F:210:GLY:HA3	2:F:216:ILE:HD11	1.98	0.44
1:G:592:VAL:HB	1:G:595:GLU:HB2	1.98	0.44
1:E:366:GLY:C	1:E:372:VAL:HG12	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:VAL:O	2:B:258:VAL:HG12	2.18	0.44
2:B:37:LEU:HD23	2:B:37:LEU:HA	1.83	0.44
2:D:67:ASP:HB3	2:D:87:HIS:CD2	2.53	0.44
2:D:336:ASP:OD1	2:D:340:LYS:HE2	2.18	0.44
2:D:129:PHE:CE1	2:D:141:ILE:HG23	2.52	0.44
2:D:343:ILE:HG21	2:D:348:GLU:O	2.17	0.44
2:D:68:PHE:HD2	2:D:85:VAL:CG2	2.30	0.44
2:D:173:VAL:HG22	2:D:177:LEU:HD11	2.00	0.44
2:D:251:LEU:HD12	2:D:251:LEU:HA	1.76	0.44
2:B:325:LEU:HD12	2:B:335:GLN:HA	2.00	0.43
2:D:374:TRP:O	2:D:378:THR:HG22	2.18	0.43
2:F:173:VAL:HG23	2:F:206:LEU:HD21	2.00	0.43
2:D:130:TYR:HE2	2:D:144:GLU:HA	1.82	0.43
2:D:175:LYS:HB3	2:D:175:LYS:HE3	1.73	0.43
2:D:200:SER:HB2	2:D:376:CYS:SG	2.58	0.43
2:H:150:SER:OG	2:H:152:ASP:HB3	2.18	0.43
2:H:165:ILE:HD12	2:H:165:ILE:H	1.82	0.43
1:A:518[B]:ARG:HB3	1:A:520:GLN:HG2	2.00	0.43
2:D:323:PRO:HG2	2:D:342:LEU:HD13	2.01	0.43
2:F:36:LYS:O	2:F:37:LEU:C	2.60	0.43
1:A:344:ILE:O	1:A:412:MET:HG2	2.18	0.43
2:B:251:LEU:HD12	2:B:251:LEU:HA	1.73	0.43
1:C:474:ILE:CD1	1:C:484:ILE:HG12	2.48	0.43
1:E:603:LEU:O	1:E:607:GLU:HG3	2.18	0.43
2:F:168:LYS:HD3	2:F:168:LYS:HA	1.75	0.43
2:F:361:ILE:CD1	2:F:362:LYS:HG3	2.48	0.43
2:B:36:LYS:HD3	2:B:36:LYS:HA	1.78	0.43
2:B:229:TYR:CE2	2:B:255:GLU:OE1	2.71	0.43
2:D:170:SER:O	2:D:174:ILE:HG13	2.19	0.43
2:F:38:GLU:C	2:F:40:LEU:N	2.76	0.43
2:F:68:PHE:HB3	2:F:85:VAL:HG21	2.00	0.43
1:G:554:ARG:CZ	2:H:225:GLY:N	2.80	0.43
1:A:433:LEU:HD11	1:A:541:LEU:HD23	2.00	0.43
2:B:70:LYS:HE3	2:B:70:LYS:HB2	1.75	0.43
2:H:178:THR:HA	2:H:181:ARG:HG2	2.00	0.43
2:B:42:LEU:HD21	2:B:50:LEU:HD12	2.01	0.43
2:F:165:ILE:HG21	2:F:374:TRP:CH2	2.54	0.43
1:G:554:ARG:HH22	2:H:310:ILE:HG12	1.83	0.43
1:A:347:SER:HA	1:E:604:SER:OG	2.19	0.43
2:D:213:GLY:O	2:D:216:ILE:HB	2.19	0.43
2:F:353:LYS:N	2:F:353:LYS:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:343:GLU:HG2	1:G:411:TYR:HE1	1.83	0.43
1:G:554:ARG:HE	2:H:224:VAL:HA	1.84	0.43
2:B:173:VAL:HG22	2:B:206:LEU:HD21	2.00	0.42
2:D:157:LYS:HD2	2:D:379:ILE:HG22	2.01	0.42
2:F:151:LEU:HB3	2:F:256:MET:HE1	2.01	0.42
2:F:192:LYS:HB3	2:F:229:TYR:CD2	2.53	0.42
2:D:188:HIS:CD2	2:D:190:ASP:C	2.97	0.42
2:D:361:ILE:HG13	2:D:362:LYS:H	1.84	0.42
2:F:308:MET:SD	2:F:312:GLU:HB3	2.58	0.42
2:B:50:LEU:HD23	2:B:50:LEU:HA	1.84	0.42
2:B:105:PRO:HA	2:B:108:ARG:HD2	2.00	0.42
2:F:68:PHE:HD2	2:F:85:VAL:HG21	1.83	0.42
2:H:198:VAL:HA	2:H:203:GLU:O	2.19	0.42
2:F:263:ILE:HD13	2:F:263:ILE:HA	1.79	0.42
2:H:46:GLN:O	2:H:47:ARG:C	2.62	0.42
2:H:151:LEU:HD21	2:H:198:VAL:HG11	2.01	0.42
2:H:161:ILE:HD12	2:H:374:TRP:HH2	1.84	0.42
1:C:590:LYS:O	1:C:596:ARG:NH1	2.52	0.42
2:B:310:ILE:O	2:B:314:LEU:HG	2.19	0.42
2:D:263:ILE:HD12	2:D:317:ILE:HG12	2.01	0.42
2:D:87:HIS:CE1	2:D:89:PRO:HD2	2.55	0.42
1:E:413:THR:HA	1:E:417:LEU:HD23	2.01	0.42
2:B:151:LEU:HA	2:B:154:VAL:HB	2.02	0.42
2:B:314:LEU:O	2:B:318:VAL:HG23	2.20	0.42
2:F:166:LEU:HD23	2:F:166:LEU:HA	1.83	0.42
2:H:267:ASP:OD1	2:H:268:ALA:N	2.52	0.42
2:D:219:MET:HB3	2:D:219:MET:HE3	1.78	0.42
2:F:263:ILE:HG13	2:F:317:ILE:HD11	2.02	0.42
2:H:70:LYS:HA	2:H:85:VAL:HG12	2.01	0.42
2:B:262:PRO:O	2:B:263:ILE:C	2.63	0.41
1:C:569:ASP:OD1	1:C:569:ASP:C	2.61	0.41
2:D:124:PRO:HG2	2:D:125:TYR:CE2	2.54	0.41
2:F:56:GLN:C	2:F:58:GLN:N	2.78	0.41
2:F:183:LYS:HD2	2:F:183:LYS:O	2.18	0.41
1:A:382:PRO:HB2	1:A:387:PHE:CD1	2.55	0.41
2:D:151:LEU:CD1	2:D:196:ILE:HB	2.50	0.41
1:A:554:ARG:HH21	2:B:223:PHE:HB2	1.86	0.41
2:B:161:ILE:HG22	2:B:166:LEU:HG	2.01	0.41
2:D:166:LEU:HA	2:D:166:LEU:HD23	1.81	0.41
2:D:262:PRO:O	2:D:263:ILE:C	2.63	0.41
2:D:353:LYS:O	2:D:356:MET:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:ARG:NH1	6:E:802:HOH:O	2.52	0.41
2:D:71:ILE:HB	2:D:84:LYS:O	2.21	0.41
1:G:398:ARG:NH1	6:G:804:HOH:O	2.53	0.41
1:A:442:MET:HE1	1:A:542:MET:SD	2.61	0.41
1:G:543:THR:HG22	1:G:545:GLU:HG2	2.02	0.41
2:H:308:MET:HG2	2:H:312:GLU:OE1	2.20	0.41
2:B:112:ILE:O	2:B:116:GLN:HG2	2.20	0.41
2:B:261:TYR:CZ	2:B:263:ILE:HG12	2.55	0.41
1:C:365:LYS:HE2	1:C:423:TRP:NE1	2.35	0.41
2:D:37:LEU:HD23	2:D:37:LEU:HA	1.94	0.41
2:D:69:GLU:HB2	2:D:88:LYS:HE2	2.00	0.41
2:D:84:LYS:HD3	2:D:145:HIS:NE2	2.35	0.41
1:E:383:THR:HG23	1:E:386:GLN:OE1	2.21	0.41
2:D:185:LYS:HD3	2:D:185:LYS:HA	1.84	0.41
2:D:267:ASP:OD1	2:D:268:ALA:N	2.54	0.41
2:F:219:MET:HE2	2:F:219:MET:HB3	1.83	0.41
2:D:111:ILE:HD13	2:D:111:ILE:HA	1.72	0.41
2:H:212:SER:O	2:H:216:ILE:HG13	2.20	0.41
1:A:431:LYS:HE3	2:B:102:GLU:CD	2.46	0.41
2:D:101:LEU:HD12	2:D:101:LEU:O	2.21	0.41
1:E:350:MET:HE2	1:E:350:MET:HB2	1.92	0.41
2:F:73:GLU:CG	2:F:83:PHE:HE1	2.34	0.41
2:F:170:SER:HA	2:F:173:VAL:HG12	2.03	0.41
1:E:512:MET:CE	1:E:517:ILE:HG12	2.51	0.41
2:F:247:TRP:CH2	2:F:251:LEU:HD22	2.56	0.41
1:G:554:ARG:NH2	2:H:310:ILE:HG12	2.35	0.41
2:B:265:PRO:HA	2:B:266:PRO:HD3	1.96	0.40
2:D:184:HIS:O	2:D:186:ILE:HG13	2.21	0.40
1:C:450:ARG:HD3	1:C:610:GLN:OE1	2.21	0.40
2:D:68:PHE:HB3	2:D:85:VAL:HG21	2.03	0.40
2:D:118:LEU:HA	2:D:118:LEU:HD23	1.82	0.40
2:B:261:TYR:CE2	2:B:263:ILE:HB	2.56	0.40
1:C:603:LEU:O	1:C:607:GLU:HG3	2.20	0.40
2:D:64:LYS:HE2	2:D:66:ASP:OD2	2.21	0.40
2:D:325:LEU:HD23	2:D:330:PHE:CD1	2.56	0.40
2:F:125:TYR:C	2:F:126:ILE:HD12	2.47	0.40
2:F:233:GLU:HG2	2:F:234:ARG:N	2.36	0.40
1:C:433:LEU:HD11	1:C:541:LEU:HD23	2.03	0.40
2:D:215:LEU:HD12	2:D:215:LEU:HA	1.91	0.40
2:D:322:PRO:HD3	2:D:344:LYS:HE3	2.04	0.40
2:D:101:LEU:HD11	2:D:139:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:188:HIS:HA	2:D:209:PHE:CB	2.51	0.40
1:E:554:ARG:HH12	2:F:225:GLY:N	2.20	0.40
2:F:98:LEU:HD12	2:F:138:GLU:CD	2.47	0.40
2:H:118:LEU:HD23	2:H:118:LEU:HA	1.92	0.40
2:H:233:GLU:HG2	2:H:234:ARG:N	2.36	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	264/280 (94%)	253 (96%)	11 (4%)	0	100	100
1	C	260/280 (93%)	247 (95%)	13 (5%)	0	100	100
1	E	254/280 (91%)	245 (96%)	9 (4%)	0	100	100
1	G	262/280 (94%)	248 (95%)	14 (5%)	0	100	100
2	B	318/395 (80%)	301 (95%)	17 (5%)	0	100	100
2	D	313/395 (79%)	293 (94%)	20 (6%)	0	100	100
2	F	318/395 (80%)	303 (95%)	14 (4%)	1 (0%)	37	65
2	H	309/395 (78%)	297 (96%)	12 (4%)	0	100	100
All	All	2298/2700 (85%)	2187 (95%)	110 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	262	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/250 (95%)	234 (99%)	3 (1%)	65	86
1	C	234/250 (94%)	233 (100%)	1 (0%)	89	96
1	E	229/250 (92%)	228 (100%)	1 (0%)	89	96
1	G	236/250 (94%)	235 (100%)	1 (0%)	89	96
2	B	278/336 (83%)	276 (99%)	2 (1%)	81	93
2	D	271/336 (81%)	268 (99%)	3 (1%)	70	89
2	F	276/336 (82%)	274 (99%)	2 (1%)	81	93
2	H	274/336 (82%)	273 (100%)	1 (0%)	89	96
All	All	2035/2344 (87%)	2021 (99%)	14 (1%)	81	93

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	482	VAL
1	A	520	GLN
1	A	589	VAL
2	B	138	GLU
2	B	263	ILE
1	C	587	ASP
2	D	173	VAL
2	D	223	PHE
2	D	338	VAL
1	E	482	VAL
2	F	70	LYS
2	F	224	VAL
1	G	353	THR
2	H	240	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	HIS
1	A	436	GLN
1	A	466	HIS
1	A	473	ASN
1	A	520	GLN
1	A	556	GLN
2	B	188	HIS
2	B	335	GLN
1	C	460	HIS
2	D	122	ASN
2	D	164	GLN
2	D	188	HIS
2	D	199	ASN
1	E	601	GLN
2	F	34	GLN
2	F	122	ASN
2	F	145	HIS
1	G	369	HIS
1	G	422	GLN
2	H	58	GLN
2	H	100	HIS
2	H	122	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	CHU	B	401	-	35,36,36	0.70	2 (5%)	45,52,52	0.79	1 (2%)
3	324	A	701	-	28,29,29	1.12	3 (10%)	32,43,43	0.82	1 (3%)
4	CHU	H	401	-	35,36,36	0.69	2 (5%)	45,52,52	0.83	1 (2%)
3	324	E	701	-	28,29,29	1.09	3 (10%)	32,43,43	0.72	0
3	324	G	701	-	28,29,29	1.10	3 (10%)	32,43,43	0.60	0
5	ANP	H	402	-	29,33,33	1.26	5 (17%)	31,52,52	1.15	2 (6%)
4	CHU	D	401	-	35,36,36	0.69	1 (2%)	45,52,52	0.72	0
3	324	C	701	-	28,29,29	1.09	3 (10%)	32,43,43	0.64	0
4	CHU	F	401	-	35,36,36	0.70	2 (5%)	45,52,52	0.72	0

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
4	CHU	B	401	-	-	0/15/16/16	0/4/4/4
3	324	A	701	-	-	3/13/17/17	0/3/3/3
4	CHU	H	401	-	-	0/15/16/16	0/4/4/4
3	324	E	701	-	-	0/13/17/17	0/3/3/3
3	324	G	701	-	-	3/13/17/17	0/3/3/3
5	ANP	H	402	-	-	2/14/38/38	0/3/3/3
4	CHU	D	401	-	-	0/15/16/16	0/4/4/4
3	324	C	701	-	-	0/13/17/17	0/3/3/3
4	CHU	F	401	-	-	0/15/16/16	0/4/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	324	C9-C11	-4.11	1.45	1.50
3	G	701	324	C9-C11	-3.92	1.45	1.50
3	E	701	324	C9-C11	-3.89	1.45	1.50
3	C	701	324	C9-C11	-3.85	1.45	1.50
5	H	402	ANP	PG-O1G	3.25	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	402	ANP	PB-O1B	3.01	1.50	1.46
4	D	401	CHU	C8-C7	2.59	1.39	1.35
4	F	401	CHU	C8-C7	2.58	1.39	1.35
4	B	401	CHU	C8-C7	2.52	1.39	1.35
4	H	401	CHU	C8-C7	2.51	1.39	1.35
3	G	701	324	C9-C2	2.36	1.44	1.42
3	C	701	324	C9-C2	2.35	1.44	1.42
5	H	402	ANP	PB-O2B	-2.34	1.50	1.56
3	E	701	324	C9-C2	2.23	1.44	1.42
3	A	701	324	C3-N4	-2.22	1.34	1.37
3	E	701	324	C3-N4	-2.17	1.34	1.37
3	C	701	324	C3-N4	-2.16	1.34	1.37
5	H	402	ANP	PG-O2G	-2.16	1.51	1.56
5	H	402	ANP	PG-O3G	-2.15	1.51	1.56
4	F	401	CHU	C23-N27	-2.15	1.35	1.39
3	A	701	324	C9-C2	2.14	1.44	1.42
3	G	701	324	C3-N4	-2.13	1.34	1.37
4	H	401	CHU	C23-N27	-2.07	1.35	1.39
4	B	401	CHU	C23-N27	-2.07	1.35	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	402	ANP	O2B-PB-O1B	4.16	118.78	109.87
3	A	701	324	C17-N21-S22	2.59	129.87	123.58
5	H	402	ANP	C5-C6-N6	2.31	123.83	120.31
4	H	401	CHU	C16-O15-C1	2.28	124.40	118.72
4	B	401	CHU	C16-O15-C1	2.24	124.29	118.72

There are no chirality outliers.

All (8) torsion outliers are listed below:

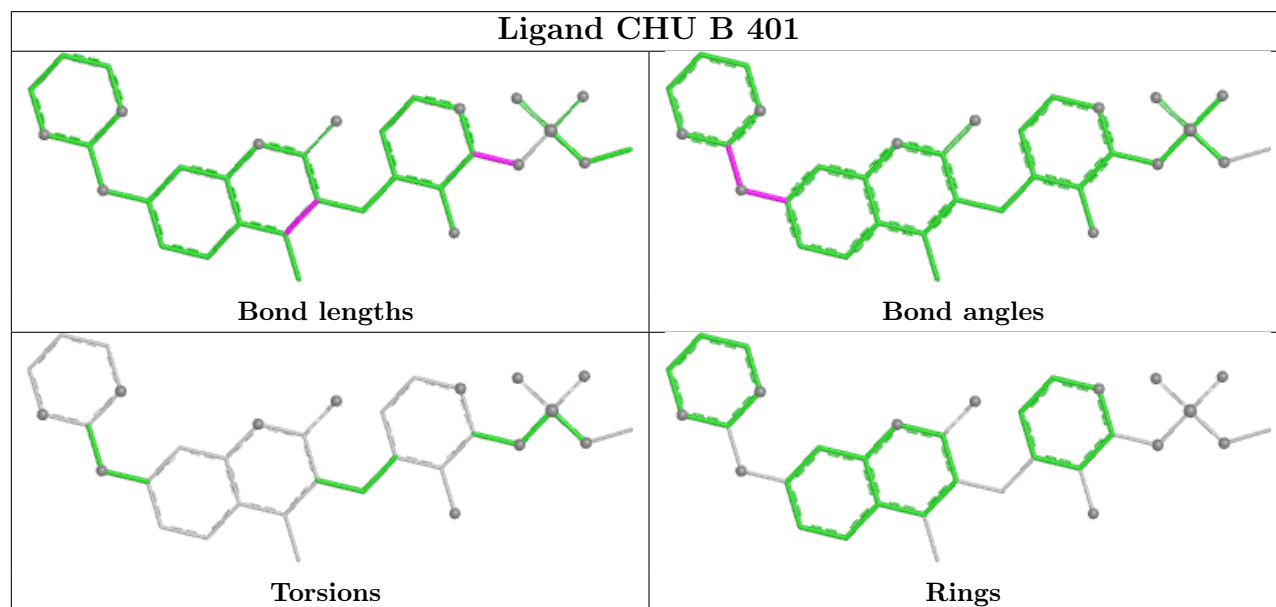
Mol	Chain	Res	Type	Atoms
5	H	402	ANP	PB-N3B-PG-O1G
5	H	402	ANP	PG-N3B-PB-O1B
3	G	701	324	C17-N21-S22-O24
3	G	701	324	S22-C25-C26-C27
3	A	701	324	C26-C25-S22-O24
3	A	701	324	C26-C25-S22-O23
3	G	701	324	C17-N21-S22-C25
3	A	701	324	C26-C25-S22-N21

There are no ring outliers.

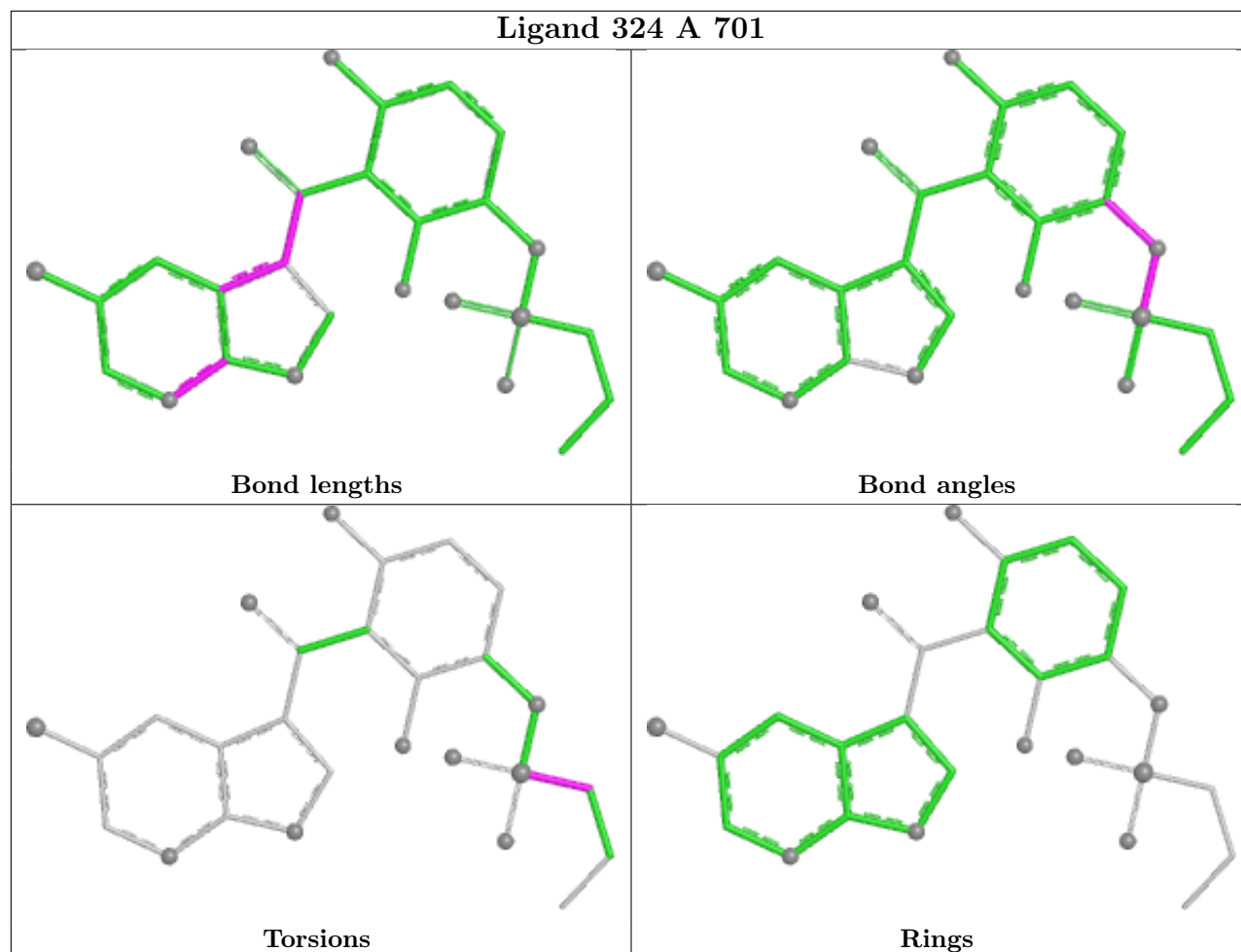
6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	CHU	1	0
3	A	701	324	2	0
4	H	401	CHU	1	0
3	E	701	324	2	0
5	H	402	ANP	1	0
4	D	401	CHU	1	0

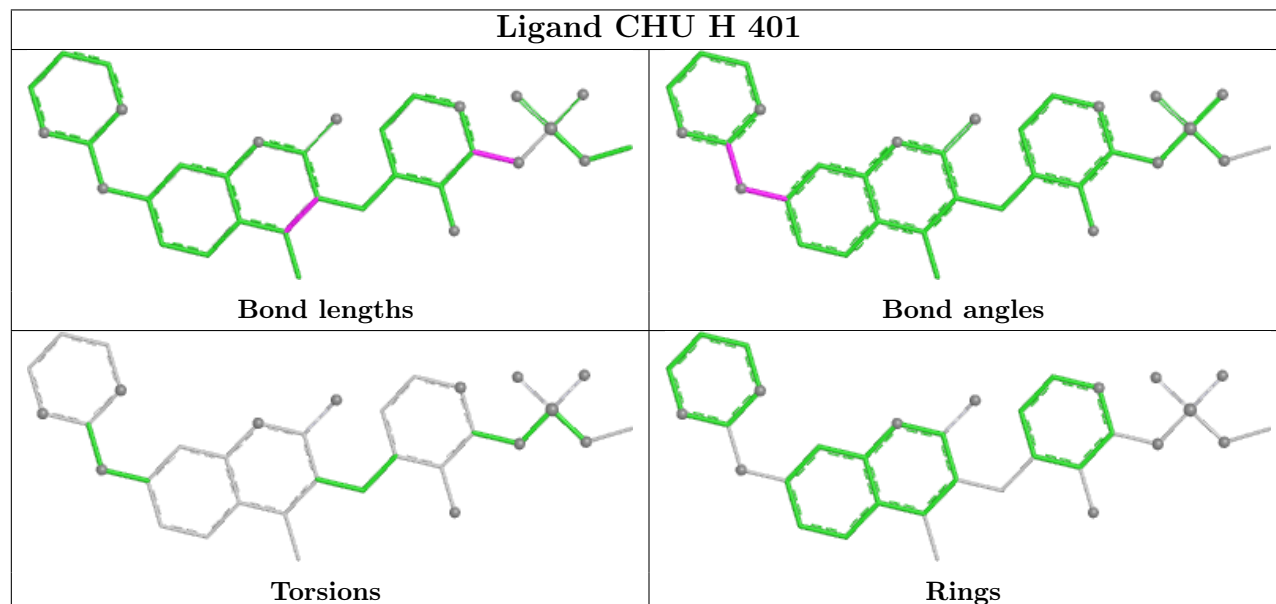
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



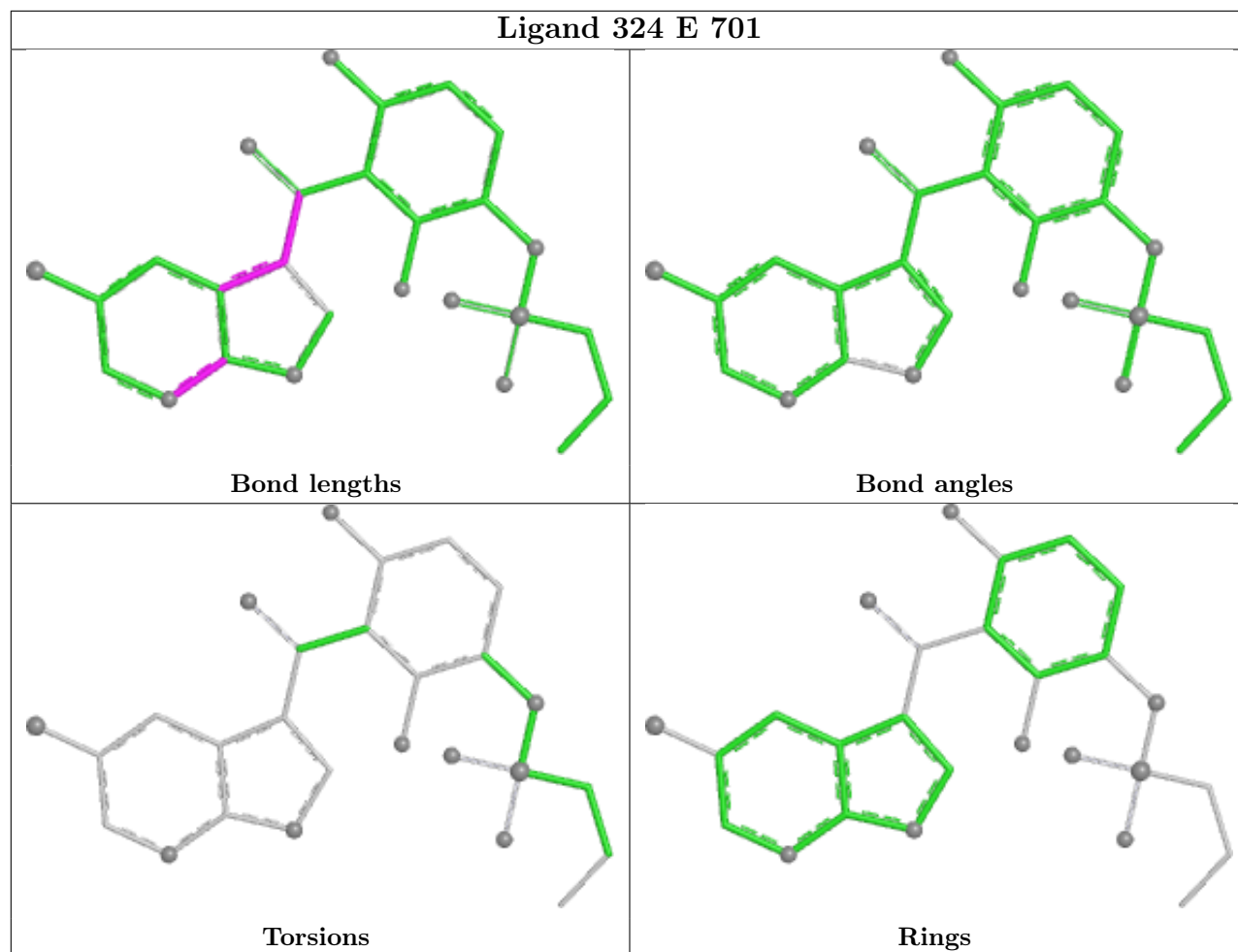
## Ligand 324 A 701



## Ligand CHU H 401

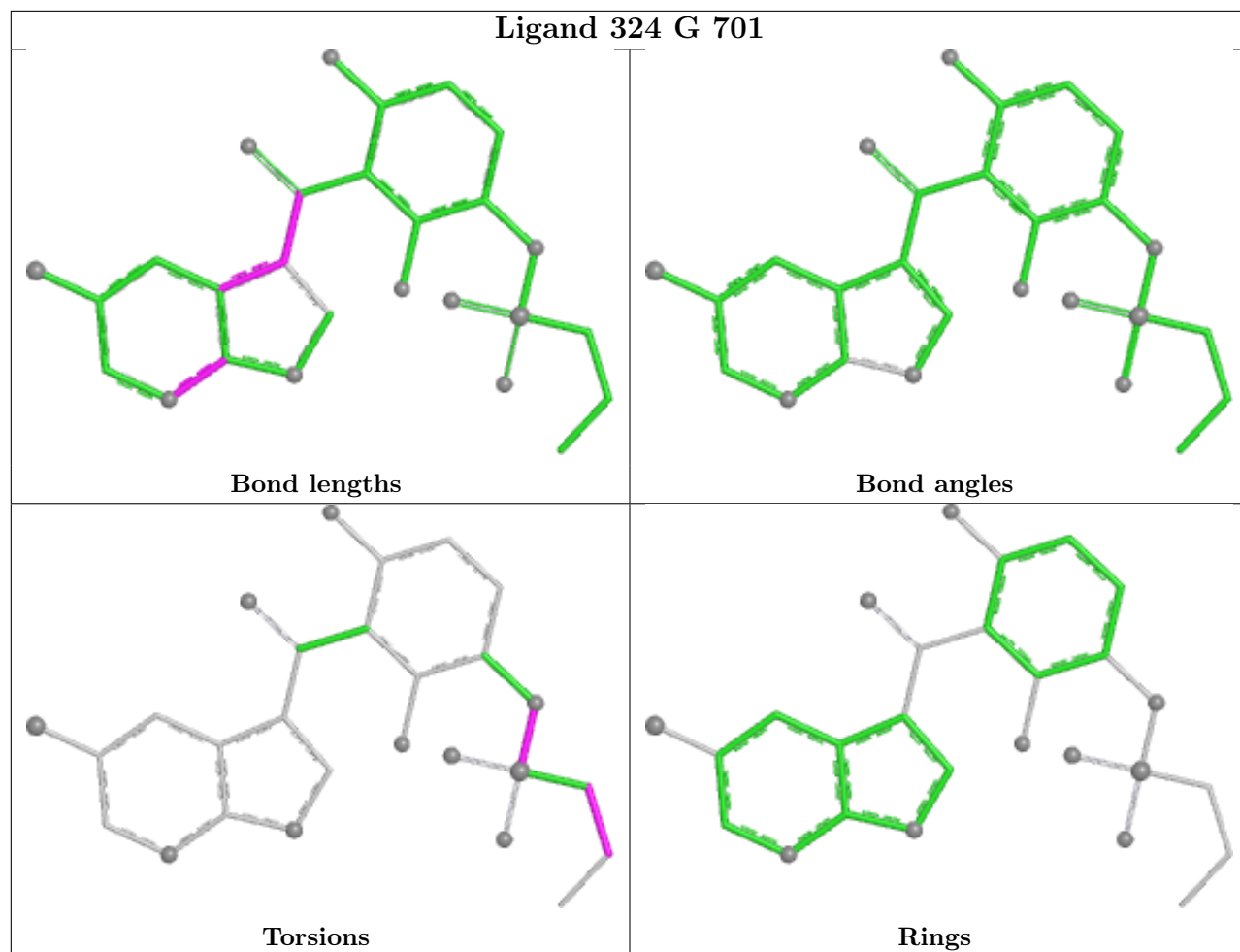


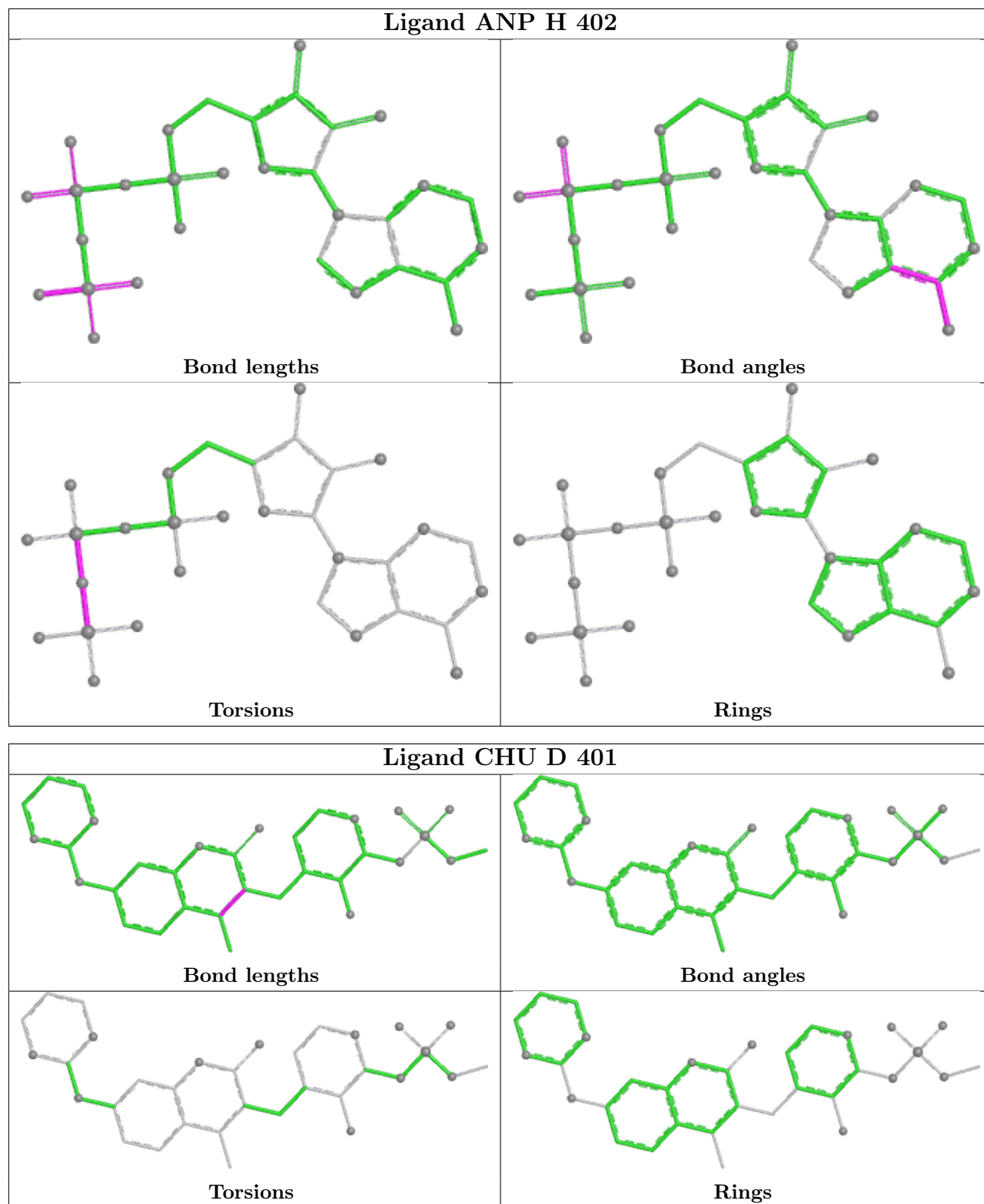
## Ligand 324 E 701

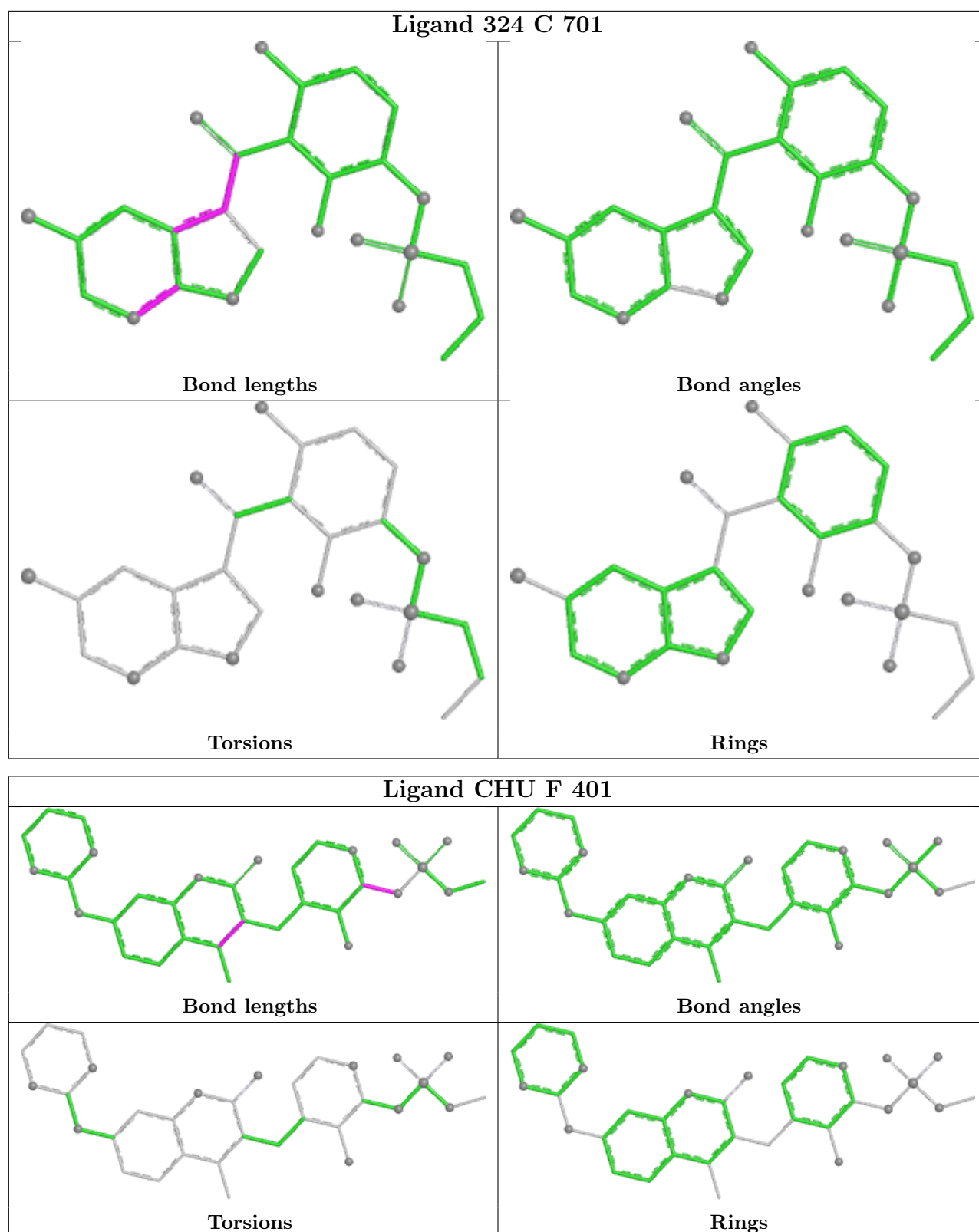




## Ligand 324 G 701







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	267/280 (95%)	-0.21	3 (1%) 77 73	31, 50, 94, 121	1 (0%)
1	C	264/280 (94%)	0.30	15 (5%) 30 27	29, 74, 112, 137	0
1	E	258/280 (92%)	-0.00	7 (2%) 56 51	34, 56, 97, 122	0
1	G	265/280 (94%)	-0.13	6 (2%) 61 55	25, 48, 107, 129	1 (0%)
2	B	322/395 (81%)	0.08	8 (2%) 58 52	36, 64, 105, 144	0
2	D	317/395 (80%)	1.16	48 (15%) 6 6	103, 140, 166, 178	0
2	F	322/395 (81%)	0.72	20 (6%) 28 24	63, 94, 140, 169	0
2	H	315/395 (79%)	0.34	18 (5%) 30 27	43, 76, 133, 153	0
All	All	2330/2700 (86%)	0.31	125 (5%) 32 28	25, 74, 150, 178	2 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	613	LEU	4.3
2	F	223	PHE	4.2
1	C	480	LEU	4.0
2	D	317	ILE	3.7
2	B	30	LEU	3.6
2	D	197	LEU	3.5
2	D	242	VAL	3.3
2	F	369	VAL	3.2
2	D	353	LYS	3.2
2	H	240	TYR	3.1
1	G	355	ILE	3.1
2	F	33	LEU	3.1
2	F	130	TYR	3.1
2	F	30	LEU	3.0
2	H	223	PHE	3.0
1	A	506	THR	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	79	GLY	2.9
2	D	224	VAL	2.9
2	D	143	MET	2.9
1	E	360	PHE	2.8
2	D	311	PHE	2.8
1	E	489	LEU	2.8
2	B	263	ILE	2.8
2	D	352	LEU	2.8
1	G	415	ASP	2.8
2	H	200	SER	2.7
1	C	565	TYR	2.7
2	D	33	LEU	2.7
2	F	37	LEU	2.7
2	D	247	TRP	2.7
2	D	125	TYR	2.7
2	D	235	LEU	2.7
2	H	138	GLU	2.6
2	B	138	GLU	2.6
2	H	380	GLY	2.6
2	D	142	CYS	2.6
1	C	506	THR	2.6
1	C	555	ASP	2.6
2	D	95	ALA	2.6
1	E	507	GLY	2.5
2	F	222	ALA	2.5
2	D	355	LEU	2.5
1	G	505	PRO	2.5
2	F	167	GLY	2.5
2	D	171	ILE	2.5
1	C	566	ALA	2.5
2	D	332	LEU	2.4
1	C	558	ILE	2.4
1	C	518	ARG	2.4
2	F	380	GLY	2.4
1	C	380	VAL	2.4
2	D	174	ILE	2.4
2	H	378	THR	2.4
2	D	371	PHE	2.4
2	D	221	ASN	2.4
2	D	130	TYR	2.4
2	B	264	PRO	2.4
2	D	369	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	138	GLU	2.4
1	C	360	PHE	2.4
2	H	207	CYS	2.4
2	F	50	LEU	2.3
2	F	53	PHE	2.3
2	D	180	LEU	2.3
2	H	36	LYS	2.3
2	H	224	VAL	2.3
2	D	204	ILE	2.3
2	H	370	ASP	2.3
2	D	63	LEU	2.3
2	D	198	VAL	2.3
2	D	186	ILE	2.3
2	F	263	ILE	2.3
2	D	346	PRO	2.3
2	D	380	GLY	2.3
2	F	166	LEU	2.3
1	E	413	THR	2.3
2	D	323	PRO	2.3
2	B	199	ASN	2.2
2	B	380	GLY	2.2
2	D	52	ALA	2.2
2	F	366	ALA	2.2
2	D	230	MET	2.2
1	G	357	SER	2.2
2	D	329	VAL	2.2
2	H	199	ASN	2.2
2	F	42	LEU	2.2
2	D	196	ILE	2.2
2	D	357	VAL	2.2
2	D	271	LEU	2.2
2	B	136	ASP	2.2
2	D	60	VAL	2.2
2	D	117	VAL	2.2
1	C	522	ASN	2.1
2	F	73	GLU	2.1
2	D	361	ILE	2.1
2	F	224	VAL	2.1
2	D	200	SER	2.1
1	C	559	PHE	2.1
1	G	545	GLU	2.1
2	H	62	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	139	ILE	2.1
1	C	512	MET	2.1
1	A	427	SER	2.1
1	E	610	GLN	2.1
2	D	251	LEU	2.1
2	D	342	LEU	2.1
2	F	268	ALA	2.1
2	H	37	LEU	2.0
2	H	239	HIS	2.1
2	H	273	LEU	2.0
2	H	32	ALA	2.0
2	B	51	GLU	2.0
2	D	173	VAL	2.0
2	D	254	VAL	2.0
2	H	160	ARG	2.0
2	D	121	CYS	2.0
1	G	387	PHE	2.0
2	H	33	LEU	2.0
2	D	164	GLN	2.0
1	A	492	VAL	2.0
1	C	379	VAL	2.0
1	C	509	VAL	2.0
1	C	525	PHE	2.0
1	E	488	GLY	2.0
2	D	37	LEU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

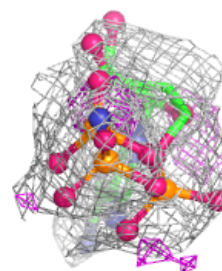
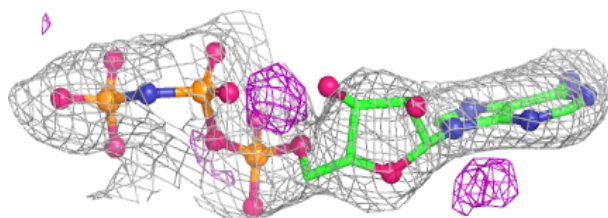
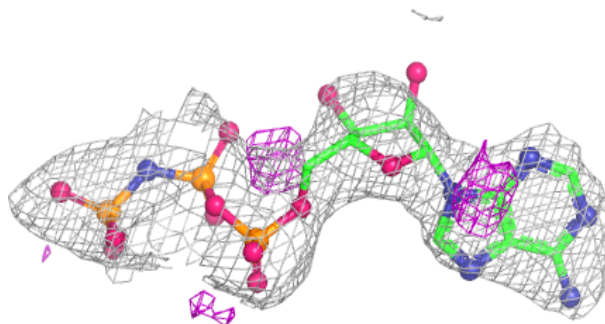


Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	ANP	H	402	31/31	0.82	0.12	94,106,131,167	0
4	CHU	D	401	33/33	0.85	0.14	89,116,129,131	0
3	324	C	701	27/27	0.93	0.10	47,65,77,91	0
3	324	G	701	27/27	0.93	0.09	33,57,74,89	0
4	CHU	F	401	33/33	0.94	0.11	63,70,87,93	0
3	324	E	701	27/27	0.96	0.08	38,45,56,62	0
4	CHU	B	401	33/33	0.97	0.06	32,43,55,62	0
4	CHU	H	401	33/33	0.97	0.08	37,50,68,76	0
3	324	A	701	27/27	0.97	0.07	34,41,48,59	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.

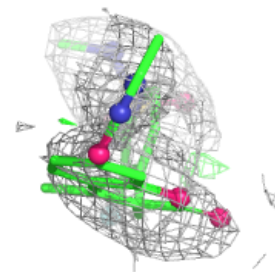
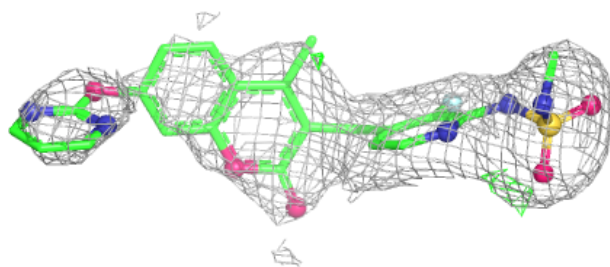
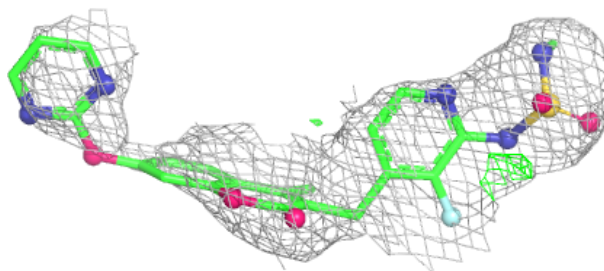
#### Electron density around ANP H 402:

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



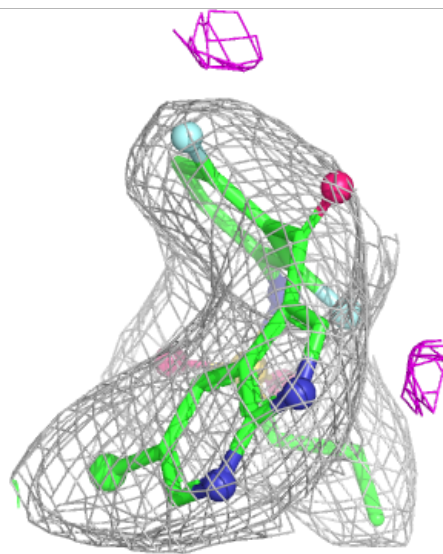
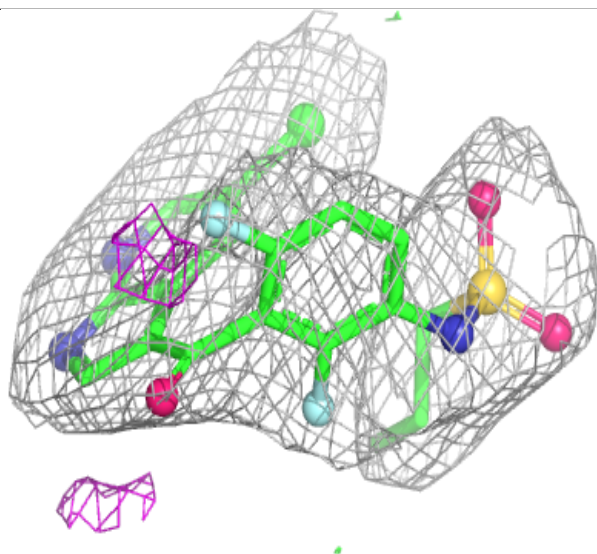
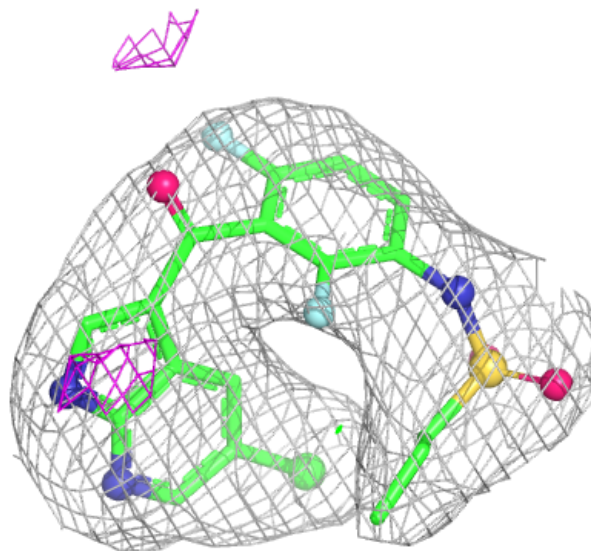
**Electron density around CHU D 401:**

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



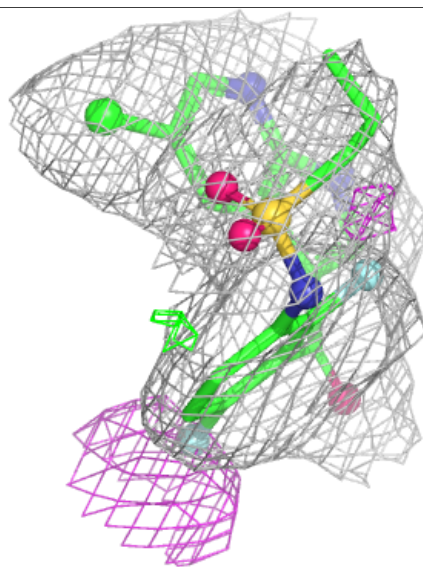
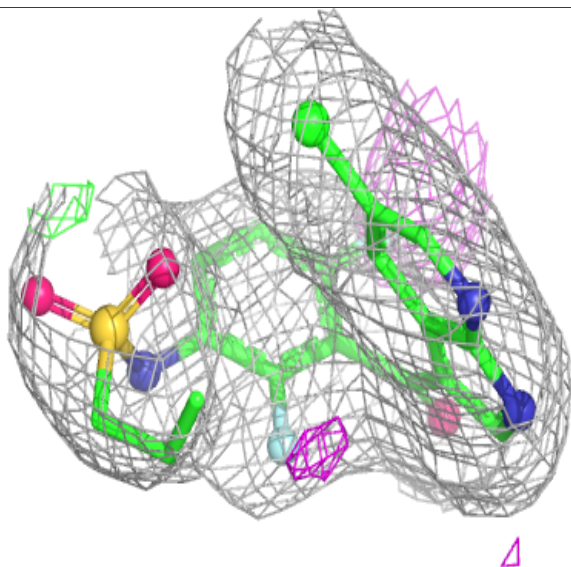
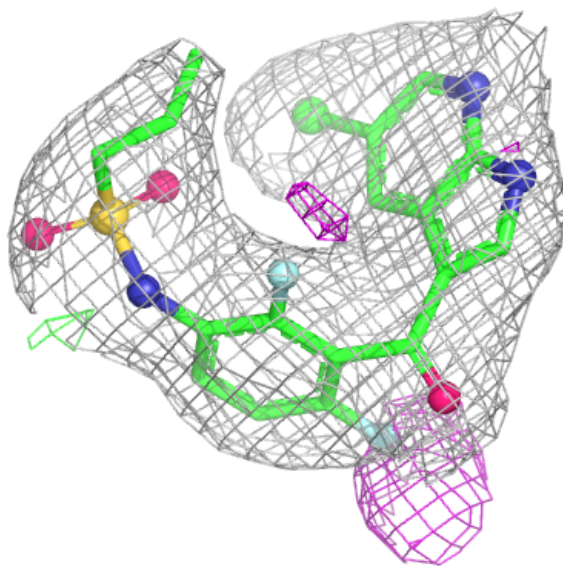
**Electron density around 324 C 701:**

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



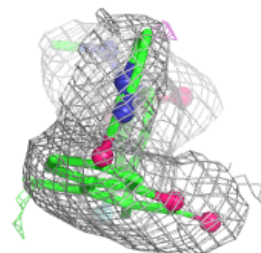
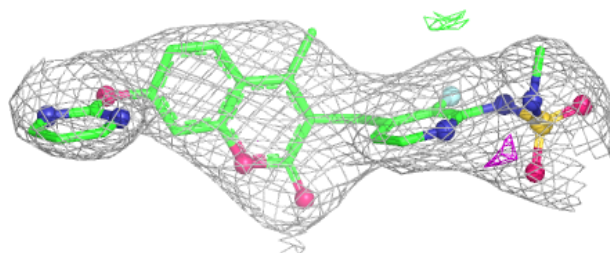
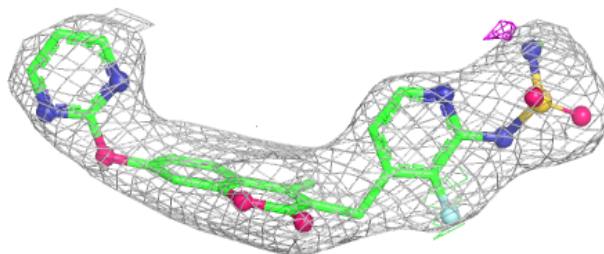
**Electron density around 324 G 701:**

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

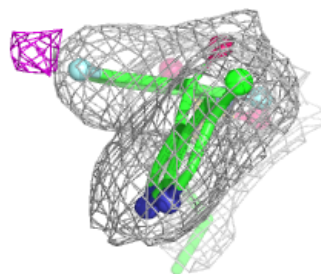
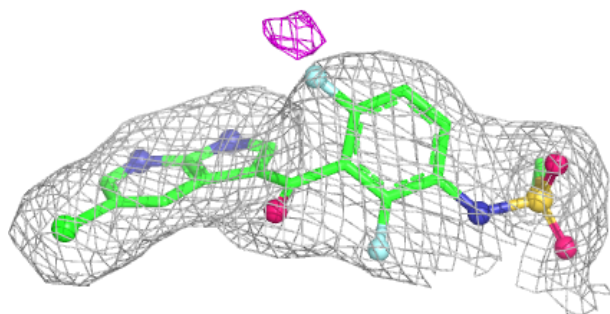
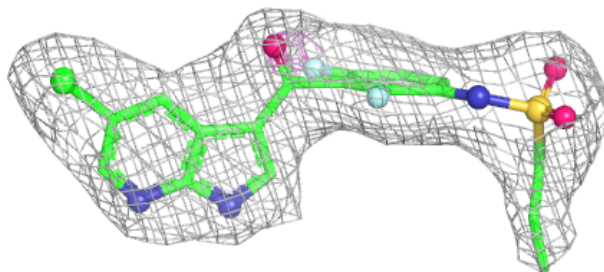


**Electron density around CHU F 401:**

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

**Electron density around 324 E 701:**

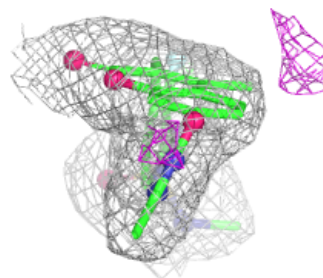
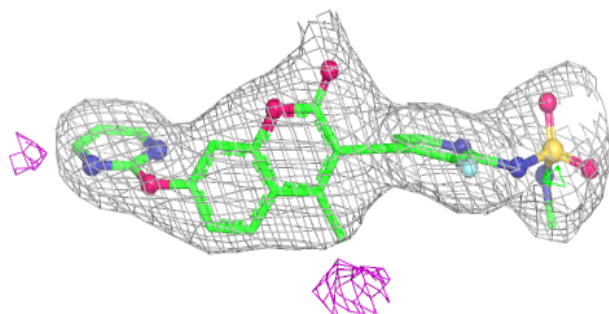
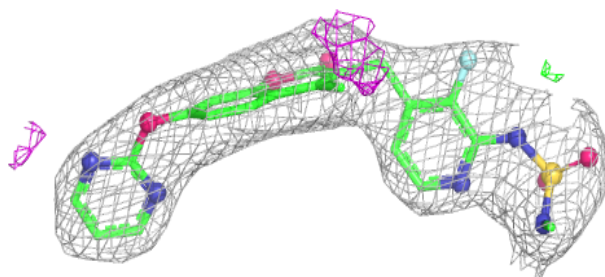
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



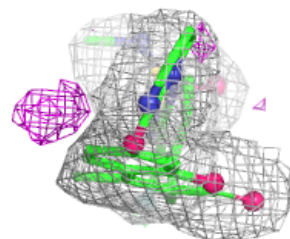
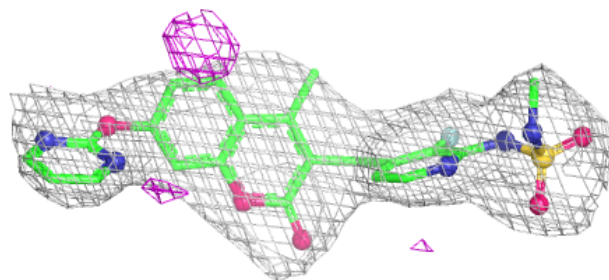
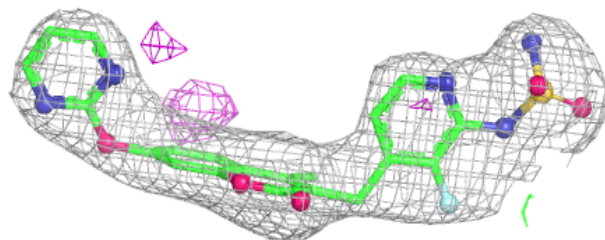


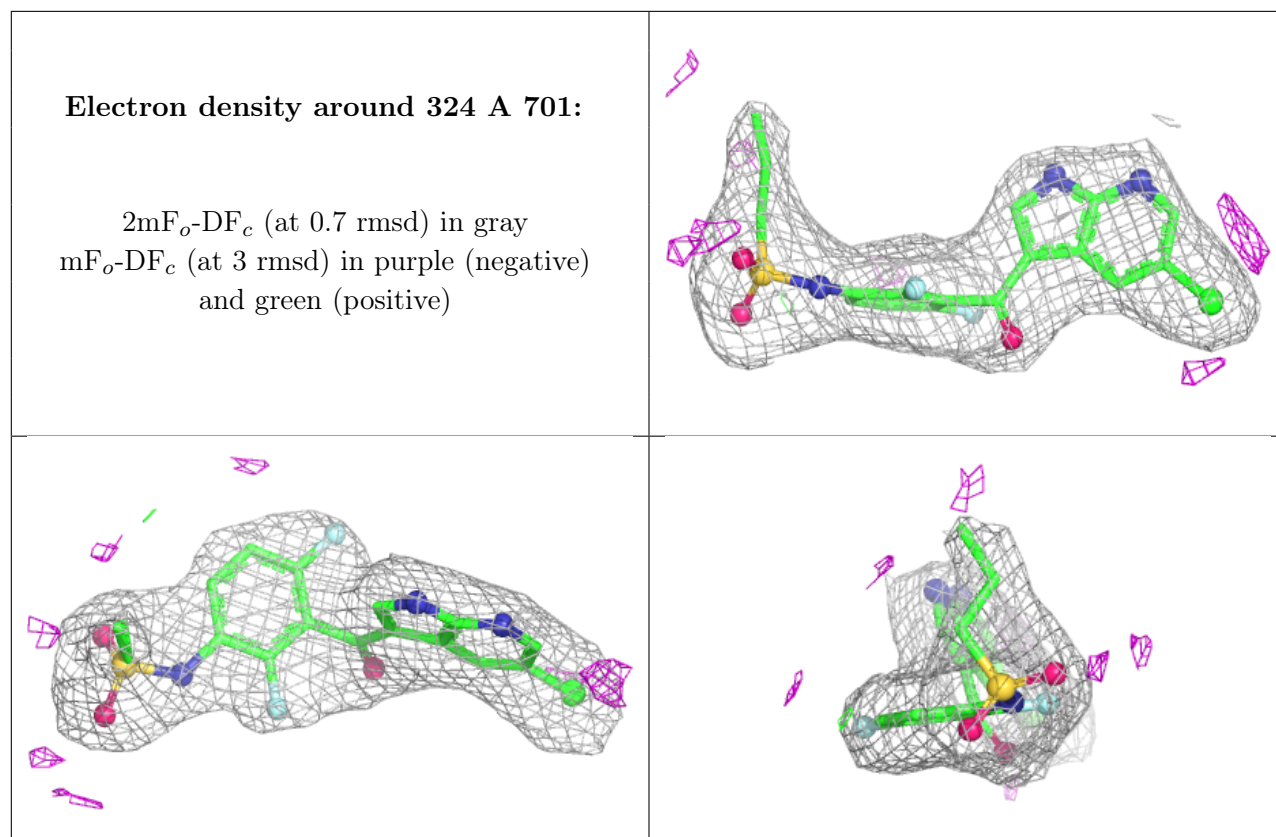
**Electron density around CHU B 401:**

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

**Electron density around CHU 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.