



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2020 – 10:55 AM EST

PDB ID : 6P8T  
Title : Acinetobacter baumannii tRNA synthetase in complex with compound 1  
Authors : Kahne, D.; Baidin, V.; Owens, T.W.  
Deposited on : 2019-06-07  
Resolution : 3.15 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.

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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 : 2.14.6  
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) : 2.14.6

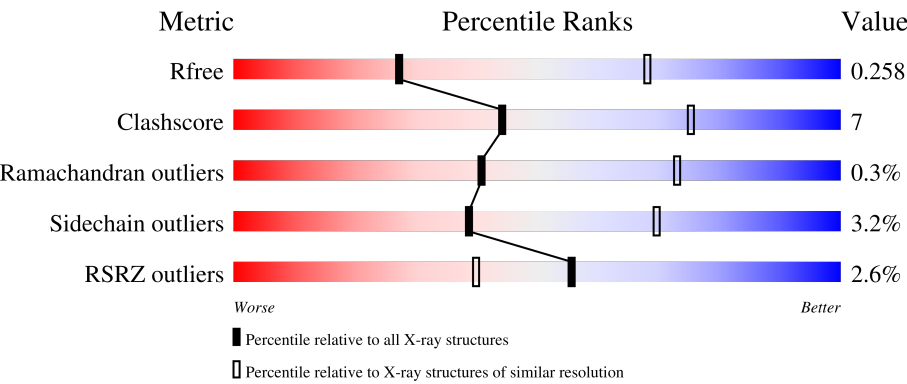
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 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 <sub>free</sub>	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 on 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	793	<div><div>4%</div><div>82%</div><div>17%</div><div>.</div></div>
1	B	793	<div><div>3%</div><div>80%</div><div>18%</div><div>..</div></div>
1	E	793	<div><div>%</div><div>82%</div><div>17%</div><div>.</div></div>
1	F	793	<div><div>%</div><div>48%</div><div>10%</div><div>42%</div><div>.</div></div>
2	C	330	<div><div>2%</div><div>75%</div><div>22%</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
2	D	330	<div><div><div>%</div><div><div></div><div>55%</div><div>14%</div><div>30%</div></div><div></div></div></div>
2	G	330	<div><div><div>4%</div><div><div></div><div>73%</div><div>14%</div><div>12%</div></div><div></div></div></div>
2	H	330	<div><div><div>4%</div><div><div></div><div>81%</div><div>18%</div></div><div></div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30223 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 Phenylalanine-tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	792	Total	C	N	O	S	0	0	0
			5938	3735	1020	1165	18			
1	B	777	Total	C	N	O	S	0	0	0
			5857	3683	1011	1143	20			
1	E	793	Total	C	N	O	S	0	0	0
			6031	3800	1028	1181	22			
1	F	463	Total	C	N	O	S	0	0	0
			3476	2196	592	678	10			

- Molecule 2 is a protein called Phenylalanine-tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	320	Total	C	N	O	S	0	0	0
			2442	1547	429	455	11			
2	D	231	Total	C	N	O	S	0	0	0
			1825	1172	317	326	10			
2	G	292	Total	C	N	O	S	0	0	0
			2200	1390	389	411	10			
2	H	326	Total	C	N	O	S	0	0	0
			2384	1499	426	448	11			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	MET	-	initiating methionine	UNP D0CA72
C	2	ARG	-	expression tag	UNP D0CA72
C	3	VAL	-	expression tag	UNP D0CA72
C	4	THR	-	expression tag	UNP D0CA72
D	1	MET	-	initiating methionine	UNP D0CA72
D	2	ARG	-	expression tag	UNP D0CA72
D	3	VAL	-	expression tag	UNP D0CA72
D	4	THR	-	expression tag	UNP D0CA72

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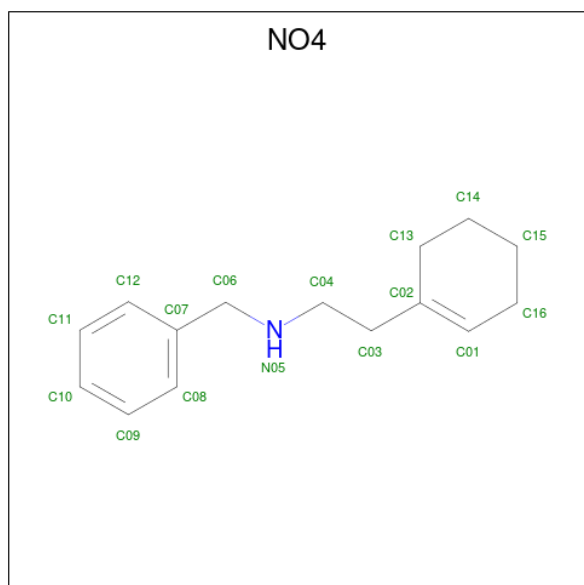
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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP D0CA72
G	2	ARG	-	expression tag	UNP D0CA72
G	3	VAL	-	expression tag	UNP D0CA72
G	4	THR	-	expression tag	UNP D0CA72
H	1	MET	-	initiating methionine	UNP D0CA72
H	2	ARG	-	expression tag	UNP D0CA72
H	3	VAL	-	expression tag	UNP D0CA72
H	4	THR	-	expression tag	UNP D0CA72

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0

- Molecule 4 is N-benzyl-2-(cyclohex-1-en-1-yl)ethan-1-amine (three-letter code: NO4) (formula: C<sub>15</sub>H<sub>21</sub>N) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C N 16 15 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	N	0	0
			16	15	1		
4	G	1	Total	C	N	0	0
			16	15	1		
4	H	1	Total	C	N	0	0
			16	15	1		

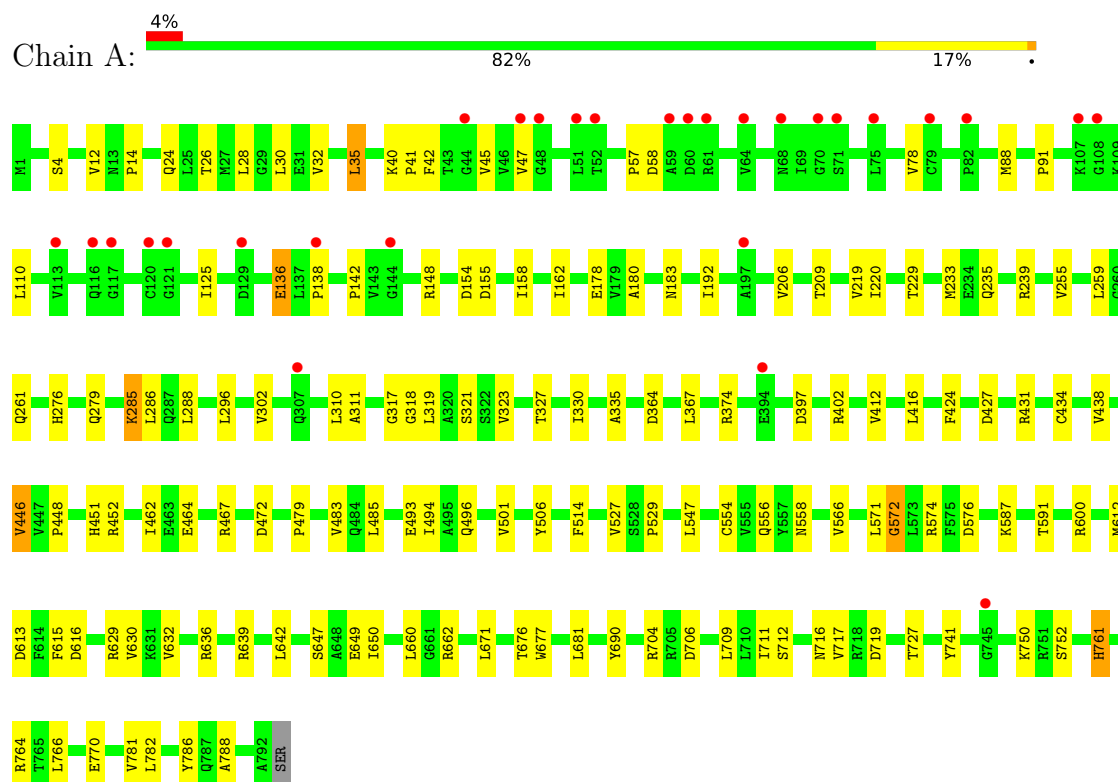
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	2	Total	O	0	0
			2	2		
5	G	1	Total	O	0	0
			1	1		

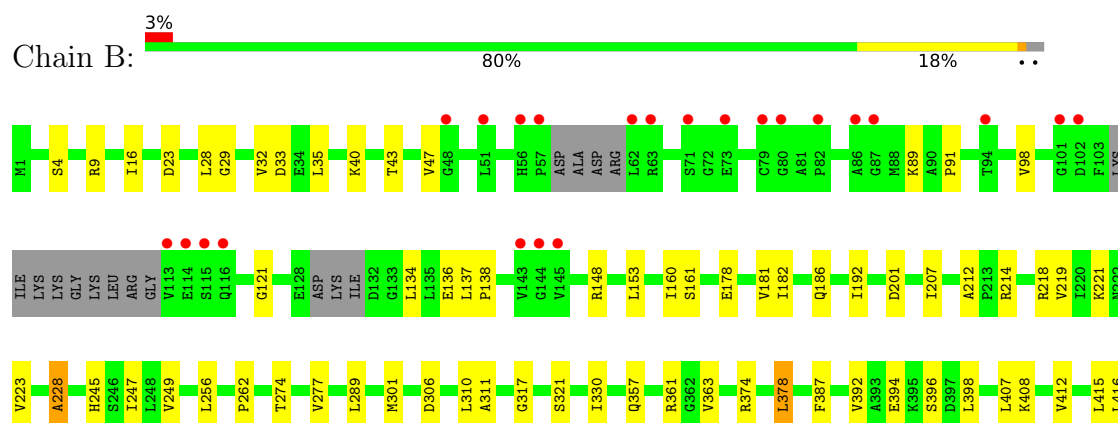
### 3 Residue-property plots [i](#)

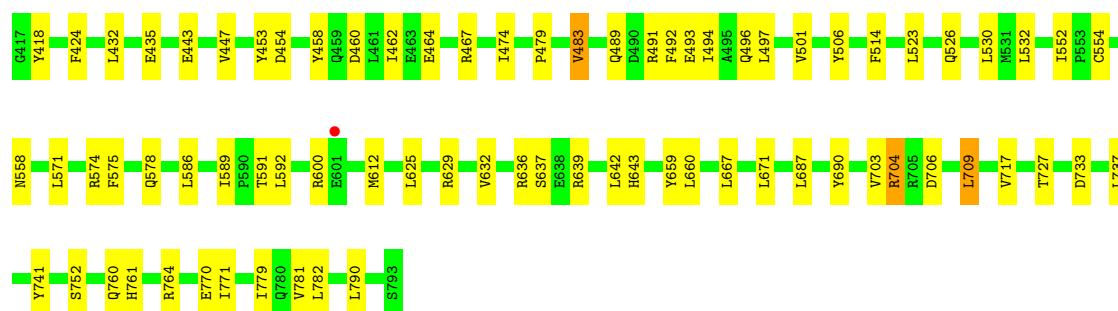
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phenylalanine-tRNA ligase beta subunit

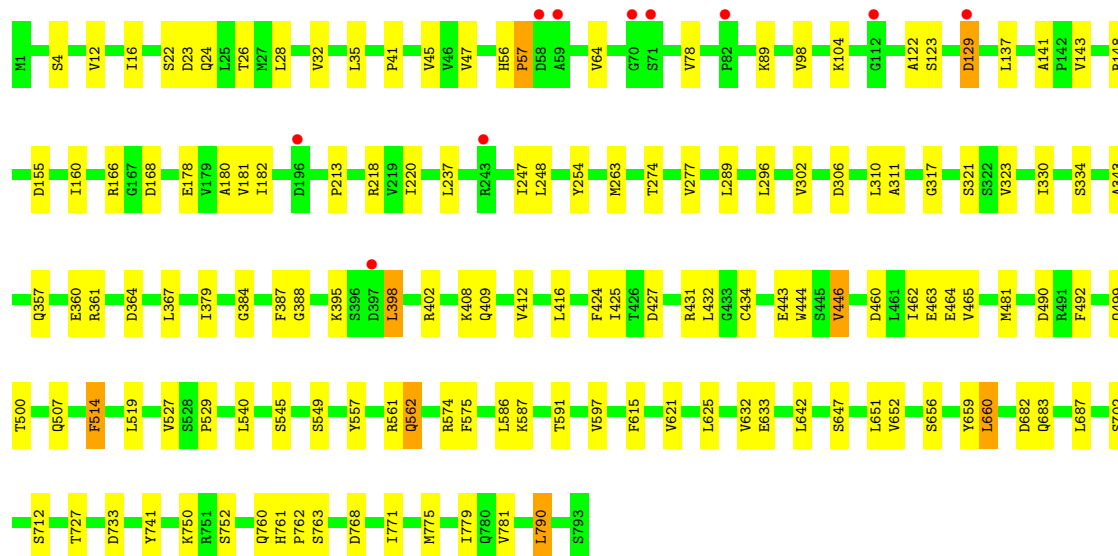
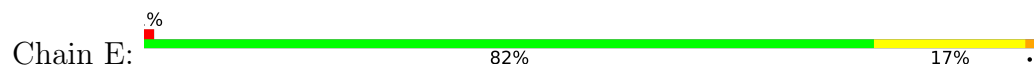


#### • Molecule 1: Phenylalanine-tRNA ligase beta subunit

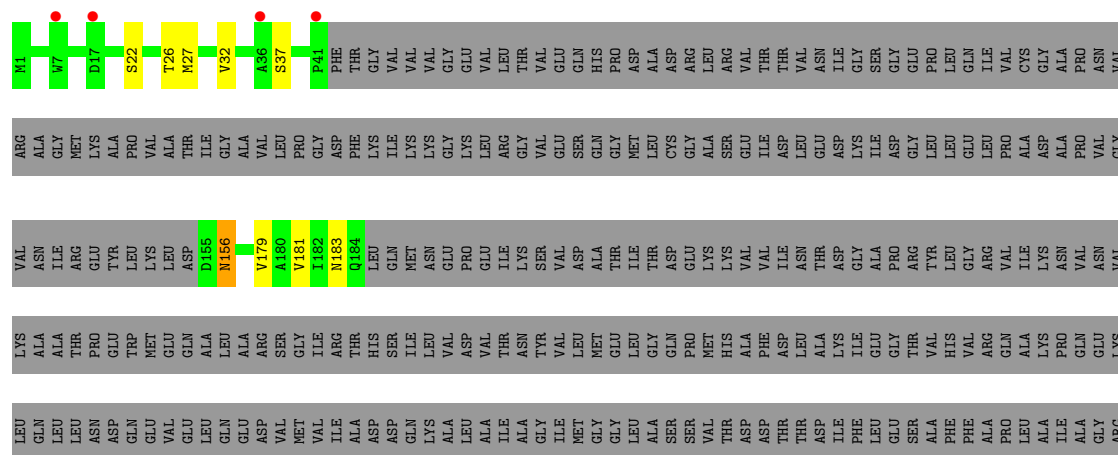




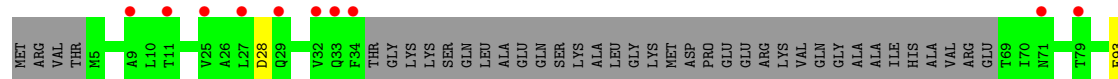
● Molecule 1: Phenylalanine-tRNA ligase beta subunit

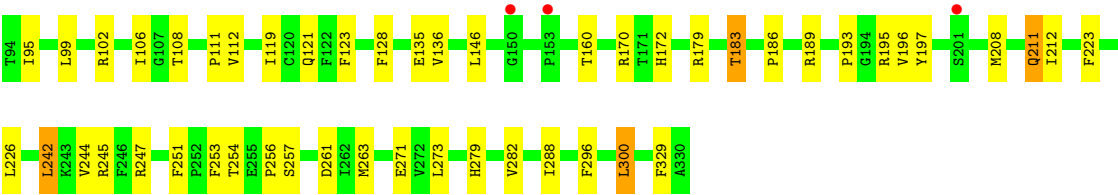


● Molecule 1: Phenylalanine-tRNA ligase beta subunit

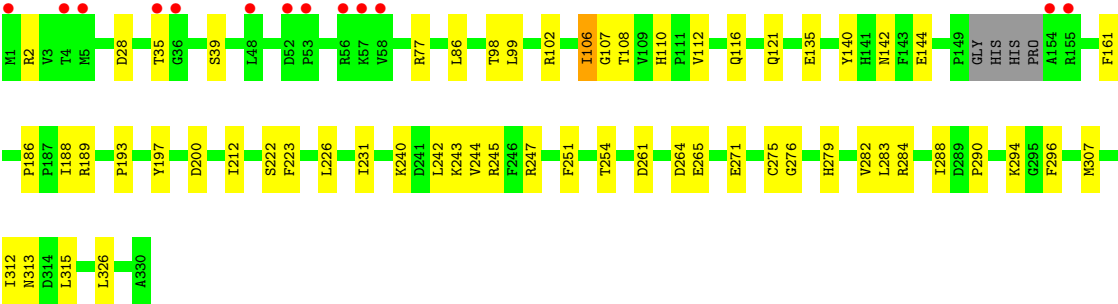
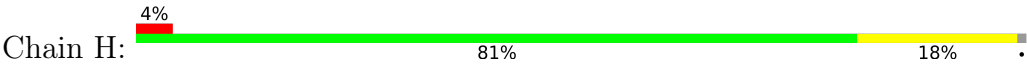








● Molecule 2: Phenylalanine-tRNA ligase alpha subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.27Å 172.47Å 191.89Å 90.00° 103.11° 90.00°	Depositor
Resolution (Å)	19.92 – 3.15 19.92 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.92-3.15) 98.6 (19.92-3.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.26 (at 3.15Å)	Xtriage
Refinement program	PHENIX 1.18_3845	Depositor
R, $R_{free}$	0.236 , 0.258 0.236 , 0.258	Depositor DCC
$R_{free}$ test set	1617 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	95.7	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 54.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	30223	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NO4, MG

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	0.23	0/6039	0.42	0/8228
1	B	0.24	0/5954	0.42	0/8099
1	E	0.24	0/6132	0.42	0/8336
1	F	0.23	0/3540	0.42	0/4827
2	C	0.24	0/2491	0.42	0/3382
2	D	0.24	0/1873	0.43	0/2538
2	G	0.24	0/2248	0.41	0/3056
2	H	0.24	0/2430	0.41	0/3304
All	All	0.24	0/30707	0.42	0/41770

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5938	0	5687	85	0
1	B	5857	0	5622	78	0
1	E	6031	0	5891	78	0
1	F	3476	0	3236	51	0
2	C	2442	0	2323	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	1825	0	1748	33	0
2	G	2200	0	2037	27	0
2	H	2384	0	2176	30	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
4	C	16	0	0	0	0
4	D	16	0	0	0	0
4	G	16	0	0	0	0
4	H	16	0	0	0	0
5	E	2	0	0	0	0
5	G	1	0	0	0	0
All	All	30223	0	28720	386	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (386) 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:47:VAL:HA	1:A:91:PRO:HA	1.67	0.74
1:A:310:LEU:HD12	1:A:321:SER:HB3	1.72	0.71
1:A:178:GLU:OE2	1:A:467:ARG:NH1	2.26	0.69
1:B:704:ARG:NH1	1:B:706:ASP:OD1	2.26	0.69
1:A:709:LEU:HD21	1:A:782:LEU:HD13	1.74	0.69
1:A:704:ARG:NH1	1:A:706:ASP:OD1	2.25	0.68
1:B:228:ALA:HB3	1:B:247:ILE:HG12	1.75	0.68
2:C:140:TYR:HA	2:C:144:GLU:HB2	1.76	0.68
1:A:26:THR:HG22	1:A:32:VAL:H	1.59	0.67
1:B:493:GLU:HB2	1:B:496:GLN:HG2	1.76	0.67
1:E:481:MET:SD	2:G:189:ARG:NH1	2.66	0.67
1:B:310:LEU:HD12	1:B:321:SER:HB3	1.75	0.67
2:C:271:GLU:O	2:C:304:ARG:NH1	2.27	0.67
2:G:242:LEU:HD13	2:G:244:VAL:HG23	1.76	0.66
1:A:716:ASN:HB3	2:D:98:THR:HG21	1.76	0.66
2:C:68:GLU:OE1	2:C:72:ASN:ND2	2.29	0.65
2:C:116:GLN:HG3	2:C:212:ILE:HD11	1.78	0.65
1:A:717:VAL:HG22	2:D:98:THR:HG23	1.78	0.65
1:B:764:ARG:NH1	1:B:770:GLU:OE2	2.27	0.64
1:B:415:LEU:HD11	2:D:256:PRO:HD3	1.80	0.64
1:A:452:ARG:NH1	1:A:464:GLU:OE2	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:414:GLN:HE22	2:H:294:LYS:HE2	1.63	0.63
1:A:206:VAL:HG21	1:A:276:HIS:HA	1.81	0.63
2:D:159:ASP:HA	2:D:199:CYS:HB2	1.81	0.63
1:A:209:THR:HG22	1:A:279:GLN:HG2	1.80	0.62
1:E:24:GLN:HG2	1:E:182:ILE:HD13	1.81	0.62
1:A:494:ILE:HD11	1:A:571:LEU:HD13	1.81	0.62
1:A:711:ILE:HD13	1:A:788:ALA:HB2	1.81	0.62
1:A:547:LEU:HD21	1:A:572:GLY:HA2	1.81	0.61
1:A:600:ARG:O	2:C:104:GLN:NE2	2.33	0.61
2:H:247:ARG:NH2	2:H:271:GLU:OE2	2.31	0.61
2:H:186:PRO:HD3	2:H:288:ILE:HD12	1.82	0.61
1:B:43:THR:H	1:B:98:VAL:HG21	1.66	0.61
1:A:47:VAL:HG22	1:A:91:PRO:HG3	1.83	0.60
2:H:231:ILE:HG12	2:H:244:VAL:HG11	1.83	0.60
1:A:636:ARG:HG2	2:D:97:ILE:HD12	1.83	0.60
2:G:193:PRO:HB3	2:G:212:ILE:HG12	1.83	0.60
1:B:741:TYR:HB3	1:B:752:SER:HB3	1.83	0.60
1:B:47:VAL:HA	1:B:91:PRO:HA	1.84	0.59
2:D:273:LEU:HB3	2:D:300:LEU:HB3	1.83	0.59
1:F:546:THR:HG22	1:F:548:LEU:H	1.68	0.59
1:E:768:ASP:HA	1:E:771:ILE:HB	1.83	0.59
1:B:717:VAL:HG11	1:B:737:LEU:HD22	1.85	0.59
2:D:303:GLU:OE2	2:D:319:TYR:OH	2.20	0.59
1:B:274:THR:N	1:B:306:ASP:OD1	2.36	0.59
1:F:22:SER:HB2	1:F:32:VAL:HG11	1.85	0.59
1:B:483:VAL:HG23	2:C:126:ALA:HB1	1.85	0.58
1:E:412:VAL:HG12	1:E:462:ILE:HG12	1.85	0.58
1:F:402:ARG:NH1	1:F:449:PRO:O	2.33	0.58
1:F:181:VAL:HG21	1:F:432:LEU:HD13	1.84	0.58
2:C:186:PRO:HD3	2:C:288:ILE:HD12	1.84	0.58
2:H:264:ASP:OD1	2:H:265:GLU:N	2.37	0.58
1:E:98:VAL:HG12	1:E:104:LYS:HG2	1.86	0.58
1:B:407:LEU:HD23	1:B:458:TYR:HB2	1.86	0.57
1:F:539:ASP:OD1	1:F:539:ASP:N	2.36	0.57
1:B:497:LEU:HD21	1:B:592:LEU:HD22	1.87	0.57
1:A:364:ASP:HB3	1:A:367:LEU:HB2	1.85	0.57
2:D:247:ARG:NH1	2:D:261:ASP:OD2	2.38	0.57
2:D:108:THR:HG21	2:D:326:LEU:HB3	1.86	0.57
1:F:524:ASN:ND2	1:F:527:VAL:O	2.38	0.57
1:A:288:LEU:HA	1:A:318:GLY:HA2	1.86	0.57
1:A:35:LEU:HD12	1:A:158:ILE:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:CYS:O	1:B:558:ASN:ND2	2.38	0.57
1:F:613:ASP:OD2	2:G:102:ARG:NH2	2.38	0.57
1:F:639:ARG:HB2	1:F:642:LEU:HD23	1.86	0.57
1:E:425:ILE:HG12	1:E:465:VAL:HG21	1.86	0.57
1:F:709:LEU:HD21	1:F:782:LEU:HD13	1.87	0.57
1:F:715:ILE:O	1:F:751:ARG:NH2	2.38	0.56
1:A:4:SER:OG	1:A:155:ASP:OD2	2.23	0.56
1:B:523:LEU:HD23	1:B:667:LEU:HD21	1.86	0.56
1:E:26:THR:HG22	1:E:32:VAL:H	1.70	0.56
1:A:576:ASP:HB3	1:A:587:LYS:HB2	1.86	0.56
2:H:108:THR:HG21	2:H:326:LEU:HB3	1.86	0.56
1:B:412:VAL:HG23	1:B:462:ILE:HG23	1.87	0.56
1:B:89:LYS:O	1:B:137:LEU:N	2.37	0.56
1:E:247:ILE:HG23	1:E:248:LEU:HD22	1.88	0.56
1:E:562:GLN:HE22	1:F:701:PRO:HB3	1.71	0.56
1:E:89:LYS:HE3	1:E:143:VAL:HG13	1.88	0.56
1:B:526:GLN:O	1:B:578:GLN:NE2	2.39	0.56
2:H:140:TYR:HA	2:H:144:GLU:HB2	1.87	0.56
1:B:223:VAL:HG21	1:B:330:ILE:HD12	1.89	0.55
2:D:135:GLU:OE2	2:D:197:TYR:OH	2.23	0.55
2:H:251:PHE:HB2	2:H:254:THR:HB	1.88	0.55
2:G:251:PHE:HD2	2:G:257:SER:HB3	1.72	0.55
1:E:4:SER:OG	1:E:155:ASP:OD2	2.25	0.55
2:C:125:LYS:HA	2:D:125:LYS:HA	1.89	0.55
1:B:494:ILE:HD11	1:B:571:LEU:HD13	1.89	0.54
2:H:193:PRO:HB3	2:H:212:ILE:HG12	1.89	0.54
1:A:613:ASP:OD2	2:D:102:ARG:NH2	2.40	0.54
1:E:166:ARG:NH1	1:E:168:ASP:OD1	2.41	0.54
1:A:88:MET:HB3	1:A:138:PRO:HB3	1.90	0.54
1:B:709:LEU:HD11	1:B:782:LEU:HD13	1.90	0.54
1:E:499:GLN:NE2	1:F:500:THR:OG1	2.37	0.54
1:F:633:GLU:OE1	1:F:718:ARG:NE	2.41	0.54
2:C:314:ASP:HB3	2:C:317:MET:HG3	1.90	0.54
1:E:575:PHE:HB3	1:E:586:LEU:HD11	1.90	0.54
2:H:240:LYS:HE3	2:H:242:LEU:HD21	1.90	0.54
1:B:201:ASP:OD2	1:B:221:LYS:NZ	2.34	0.53
1:E:741:TYR:HB3	1:E:752:SER:HB3	1.88	0.53
2:C:135:GLU:OE1	2:C:197:TYR:OH	2.22	0.53
2:C:4:THR:O	2:C:40:GLN:NE2	2.39	0.53
1:A:727:THR:HG21	1:A:781:VAL:HG11	1.91	0.53
1:B:43:THR:HB	1:B:98:VAL:HG11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ARG:NH2	1:B:16:ILE:O	2.41	0.53
1:B:28:LEU:HD11	1:B:182:ILE:HB	1.91	0.53
1:F:412:VAL:HG22	1:F:462:ILE:HG12	1.90	0.53
1:A:501:VAL:HG12	1:A:506:TYR:HB2	1.90	0.53
2:C:264:ASP:OD1	2:C:265:GLU:N	2.36	0.52
1:A:259:LEU:HD23	1:A:367:LEU:HD11	1.91	0.52
1:F:766:LEU:HB3	1:F:771:ILE:HD11	1.90	0.52
1:A:600:ARG:HB2	1:A:612:MET:HG2	1.91	0.52
1:A:30:LEU:HD22	1:A:162:ILE:HG22	1.92	0.52
1:B:212:ALA:HB2	1:B:301:MET:HE1	1.91	0.52
1:B:214:ARG:NH1	1:B:394:GLU:OE2	2.43	0.51
2:D:123:PHE:HB3	2:D:128:PHE:HB2	1.93	0.51
1:B:408:LYS:HD2	1:B:443:GLU:HG2	1.91	0.51
2:G:119:ILE:HD13	2:G:300:LEU:HD11	1.92	0.51
2:H:35:THR:O	2:H:39:SER:OG	2.27	0.51
1:E:727:THR:HG21	1:E:781:VAL:HG21	1.92	0.51
1:E:733:ASP:HB2	1:E:760:GLN:HB2	1.92	0.51
1:F:717:VAL:HG21	2:G:99:LEU:HD23	1.90	0.51
1:B:256:LEU:HD12	1:B:262:PRO:HB3	1.92	0.51
1:E:22:SER:HB3	1:E:32:VAL:HG21	1.92	0.51
1:A:650:ILE:HD11	1:A:660:LEU:HD23	1.91	0.51
1:F:37:SER:HA	1:F:156:ASN:HA	1.93	0.51
1:A:192:ILE:HD13	1:A:374:ARG:HD2	1.93	0.51
1:A:764:ARG:NH2	1:A:770:GLU:OE1	2.43	0.51
1:F:179:VAL:O	1:F:183:ASN:ND2	2.30	0.51
1:F:724:ILE:HG12	1:F:778:ILE:HD11	1.92	0.51
1:B:207:ILE:HA	1:B:277:VAL:HG13	1.93	0.50
1:B:703:VAL:HG11	1:B:771:ILE:HD13	1.92	0.50
1:E:527:VAL:HG13	1:E:529:PRO:HD3	1.91	0.50
1:A:761:HIS:CD2	1:A:766:LEU:HG	2.46	0.50
1:B:357:GLN:O	1:B:361:ARG:HG2	2.12	0.50
2:C:303:GLU:OE2	2:C:319:TYR:OH	2.29	0.50
1:E:296:LEU:HD13	1:E:302:VAL:HG11	1.92	0.50
1:A:40:LYS:HE2	1:A:41:PRO:HD2	1.92	0.50
1:B:363:VAL:O	1:B:453:TYR:OH	2.21	0.50
2:C:162:TYR:HA	2:C:168:LEU:HA	1.93	0.50
2:C:230:LEU:HD13	2:C:273:LEU:HD11	1.94	0.50
1:E:408:LYS:HG2	1:E:443:GLU:HG2	1.93	0.50
1:E:12:VAL:HG21	1:E:180:ALA:HB2	1.94	0.50
1:E:463:GLU:HG3	2:G:256:PRO:HB3	1.94	0.50
2:C:123:PHE:HE2	2:C:229:LEU:HD11	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:GLN:HE21	1:B:491:ARG:HH21	1.60	0.49
1:E:574:ARG:NH2	1:E:682:ASP:OD1	2.45	0.49
1:F:532:LEU:HD22	2:H:161:PHE:HB3	1.93	0.49
2:G:251:PHE:HB2	2:G:254:THR:HB	1.93	0.49
1:E:779:ILE:HG23	1:E:790:LEU:HD11	1.93	0.49
2:G:196:VAL:HG21	2:G:211:GLN:HG3	1.95	0.49
2:D:270:LEU:HD12	2:D:304:ARG:HH22	1.77	0.49
1:E:519:LEU:HD22	1:E:549:SER:HA	1.95	0.49
1:F:727:THR:HG21	1:F:781:VAL:HG11	1.95	0.49
1:B:575:PHE:HB3	1:B:586:LEU:HD11	1.94	0.49
1:F:420:VAL:HG13	1:F:425:ILE:HD11	1.93	0.49
1:B:642:LEU:HD11	1:B:659:TYR:CD1	2.47	0.49
2:H:283:LEU:HG	2:H:288:ILE:HB	1.95	0.49
1:A:434:CYS:HB3	1:A:446:VAL:HG23	1.93	0.49
1:B:121:GLY:HA2	1:B:134:LEU:HA	1.94	0.49
1:E:274:THR:N	1:E:306:ASP:OD1	2.46	0.49
1:E:220:ILE:HD12	1:E:330:ILE:HD11	1.95	0.49
1:A:402:ARG:HG2	1:A:448:PRO:HG2	1.95	0.49
1:E:364:ASP:HB3	1:E:367:LEU:HB2	1.95	0.49
1:E:379:ILE:O	1:E:384:GLY:N	2.39	0.49
1:E:642:LEU:HD13	1:E:647:SER:HB2	1.94	0.49
1:F:739:ASP:HB3	1:F:754:ALA:HB3	1.94	0.49
1:E:213:PRO:HB3	1:E:398:LEU:HD12	1.95	0.48
1:B:733:ASP:HB2	1:B:760:GLN:HB2	1.95	0.48
2:D:231:ILE:HG12	2:D:244:VAL:HG21	1.96	0.48
1:A:220:ILE:HD12	1:A:330:ILE:HD11	1.95	0.48
1:E:712:SER:HA	1:E:750:LYS:HA	1.95	0.48
1:F:612:MET:O	1:F:677:TRP:NE1	2.47	0.48
1:A:323:VAL:HG12	1:A:327:THR:HG21	1.96	0.48
1:E:642:LEU:HD11	1:E:659:TYR:CD1	2.49	0.48
2:G:170:ARG:NH2	2:G:195:ARG:O	2.45	0.48
1:B:574:ARG:HE	1:B:591:THR:HG21	1.78	0.48
2:D:244:VAL:HG12	2:D:262:ILE:HG22	1.96	0.48
2:C:251:PHE:HD2	2:C:257:SER:HB3	1.78	0.48
2:H:106:ILE:HD13	2:H:107:GLY:H	1.78	0.48
2:H:284:ARG:HB2	2:H:290:PRO:HD3	1.95	0.48
1:A:630:VAL:HG12	1:A:632:VAL:HG23	1.96	0.48
1:A:255:VAL:HG13	1:A:259:LEU:HD13	1.96	0.48
1:A:574:ARG:HE	1:A:591:THR:HG21	1.79	0.48
1:B:727:THR:HG21	1:B:781:VAL:HG11	1.96	0.48
1:E:434:CYS:HB3	1:E:446:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:574:ARG:NE	1:E:591:THR:HG21	2.29	0.48
1:F:600:ARG:HB3	1:F:612:MET:HB3	1.94	0.47
2:H:279:HIS:HB3	2:H:282:VAL:HG12	1.96	0.47
1:E:395:LYS:HE3	1:E:398:LEU:HD21	1.96	0.47
1:A:42:PHE:CZ	1:A:148:ARG:HD3	2.48	0.47
1:B:600:ARG:HB2	1:B:612:MET:HG2	1.96	0.47
1:A:485:LEU:H	2:D:232:ASN:HD21	1.63	0.47
2:C:177:GLN:HB3	2:C:215:LEU:HD22	1.96	0.47
1:E:28:LEU:HD13	1:E:182:ILE:HD12	1.95	0.47
1:A:574:ARG:NE	1:A:591:THR:HG21	2.29	0.47
2:C:110:HIS:ND1	2:C:112:VAL:HG22	2.30	0.47
2:C:123:PHE:HB3	2:C:128:PHE:HB2	1.97	0.47
1:F:711:ILE:HD11	1:F:786:TYR:HB3	1.97	0.47
2:H:315:LEU:H	2:H:315:LEU:HD23	1.79	0.47
1:A:483:VAL:HB	1:B:479:PRO:HG2	1.96	0.47
1:B:625:LEU:HD13	1:B:632:VAL:HG11	1.95	0.47
1:B:643:HIS:HE2	2:C:93:GLU:HG3	1.80	0.47
1:E:343:ALA:HA	1:E:360:GLU:HG2	1.96	0.47
1:F:548:LEU:HD21	1:F:678:VAL:HG21	1.97	0.47
1:A:662:ARG:HB3	1:A:677:TRP:CZ3	2.50	0.47
1:F:600:ARG:HD3	1:F:600:ARG:H	1.78	0.47
1:A:12:VAL:HG21	1:A:180:ALA:HB2	1.97	0.47
1:A:412:VAL:HG22	1:A:462:ILE:HG12	1.97	0.46
2:C:118:ARG:O	2:C:121:GLN:HG3	2.15	0.46
1:F:576:ASP:HB3	1:F:587:LYS:HB2	1.96	0.46
2:C:35:THR:O	2:C:39:SER:OG	2.30	0.46
2:C:231:ILE:HG12	2:C:244:VAL:HG11	1.98	0.46
1:B:636:ARG:NH2	2:C:95:ILE:O	2.44	0.46
2:D:251:PHE:HB2	2:D:254:THR:OG1	2.15	0.46
2:H:116:GLN:HA	2:H:212:ILE:HD11	1.97	0.46
1:B:454:ASP:N	1:B:454:ASP:OD1	2.48	0.46
2:C:193:PRO:HB3	2:C:212:ILE:HG12	1.97	0.46
2:H:226:LEU:HD21	2:H:275:CYS:SG	2.55	0.46
1:B:245:HIS:HB3	1:B:249:VAL:HG11	1.97	0.46
1:A:261:GLN:NE2	1:A:335:ALA:O	2.46	0.46
1:E:561:ARG:O	1:E:562:GLN:HG2	2.16	0.46
1:F:643:HIS:NE2	2:G:93:GLU:OE1	2.49	0.46
1:B:218:ARG:HD3	1:B:387:PHE:HD1	1.81	0.46
1:B:435:GLU:HB2	1:B:447:VAL:HB	1.98	0.46
1:E:625:LEU:HD13	1:E:632:VAL:HG11	1.97	0.46
1:F:662:ARG:HB2	1:F:677:TRP:CZ3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:ARG:O	2:D:121:GLN:HG3	2.16	0.46
1:A:47:VAL:HG21	1:A:142:PRO:HG2	1.98	0.45
1:E:89:LYS:HB3	1:E:137:LEU:HB2	1.98	0.45
1:E:500:THR:OG1	1:F:499:GLN:NE2	2.43	0.45
1:A:472:ASP:N	1:A:472:ASP:OD1	2.40	0.45
1:E:218:ARG:NH1	1:E:388:GLY:O	2.50	0.45
1:E:357:GLN:O	1:E:361:ARG:HG2	2.15	0.45
1:A:91:PRO:HD2	1:A:136:GLU:CB	2.46	0.45
1:E:64:VAL:HG13	1:E:78:VAL:HG22	1.99	0.45
1:F:26:THR:OG1	1:F:32:VAL:HG12	2.16	0.45
1:F:606:HIS:CE1	2:H:102:ARG:HB2	2.52	0.45
1:A:286:LEU:HD22	1:A:288:LEU:HD23	1.98	0.45
1:E:632:VAL:HG12	1:E:652:VAL:HG22	1.98	0.45
1:B:552:ILE:HG21	1:B:671:LEU:HD13	1.98	0.45
1:E:218:ARG:NH1	1:E:387:PHE:HB3	2.32	0.45
2:C:6:SER:HB3	2:C:9:ALA:HB3	1.99	0.45
1:A:527:VAL:HG13	1:A:529:PRO:HD3	1.98	0.45
1:B:761:HIS:CE1	1:B:764:ARG:HG2	2.52	0.45
1:E:41:PRO:HA	1:E:148:ARG:HH12	1.82	0.45
1:A:761:HIS:HD2	1:A:766:LEU:HG	1.82	0.44
1:B:192:ILE:HD13	1:B:374:ARG:HD2	1.99	0.44
1:A:28:LEU:HD23	1:A:178:GLU:HB3	1.98	0.44
1:A:479:PRO:HG2	1:B:483:VAL:HG13	1.98	0.44
1:A:571:LEU:HA	1:A:572:GLY:HA3	1.66	0.44
1:B:501:VAL:HG12	1:B:506:TYR:HB2	1.98	0.44
2:H:200:ASP:N	2:H:200:ASP:OD1	2.49	0.44
2:H:226:LEU:HD12	2:H:296:PHE:CD1	2.53	0.44
2:C:129:THR:HG23	2:C:190:ILE:HG22	2.00	0.44
1:E:28:LEU:HD23	1:E:178:GLU:HG3	1.99	0.44
1:E:402:ARG:HD3	1:E:402:ARG:HA	1.84	0.44
1:F:575:PHE:HB3	1:F:586:LEU:HD21	1.99	0.44
2:H:307:MET:HA	2:H:312:ILE:HG12	2.00	0.44
1:B:33:ASP:OD1	1:B:161:SER:HB2	2.17	0.44
1:F:469:ASP:O	1:F:473:ASN:ND2	2.47	0.44
1:F:498:ARG:HA	1:F:501:VAL:HG22	2.00	0.44
2:G:186:PRO:HD3	2:G:288:ILE:HD12	2.00	0.44
2:H:135:GLU:OE1	2:H:197:TYR:OH	2.35	0.44
1:B:574:ARG:NE	1:B:591:THR:HG21	2.33	0.43
2:G:245:ARG:NH2	2:G:261:ASP:OD2	2.51	0.43
1:A:364:ASP:OD1	1:A:451:HIS:HB3	2.18	0.43
2:D:173:THR:O	2:D:177:GLN:NE2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:SER:C	1:B:398:LEU:H	2.21	0.43
1:E:47:VAL:HG11	1:E:141:ALA:HB1	2.00	0.43
1:E:621:VAL:HG21	1:E:660:LEU:HD13	2.00	0.43
1:A:148:ARG:NH1	1:A:154:ASP:OD1	2.51	0.43
1:A:493:GLU:HB2	1:A:496:GLN:HG2	2.01	0.43
1:B:497:LEU:HD22	1:B:687:LEU:HD21	2.00	0.43
2:D:254:THR:OG1	2:D:257:SER:HB3	2.18	0.43
1:E:181:VAL:HG11	1:E:432:LEU:HD12	2.01	0.43
1:F:629:ARG:HD3	1:F:690:TYR:CG	2.54	0.43
1:A:14:PRO:HB3	1:A:183:ASN:HD22	1.84	0.43
1:A:296:LEU:HD13	1:A:302:VAL:HG11	2.00	0.43
1:A:616:ASP:OD1	2:D:102:ARG:NH1	2.51	0.43
2:G:279:HIS:HB3	2:G:282:VAL:HG23	2.01	0.43
1:A:78:VAL:HG12	1:A:110:LEU:HG	1.99	0.43
1:B:311:ALA:HB1	1:B:317:GLY:HA2	2.01	0.43
1:E:702:SER:N	1:F:562:GLN:OE1	2.35	0.43
2:C:108:THR:HG21	2:C:327:ARG:HA	2.00	0.43
2:D:121:GLN:O	2:D:125:LYS:HG2	2.18	0.43
1:F:531:MET:HA	1:F:542:ALA:HA	2.00	0.43
2:G:245:ARG:HH12	2:G:247:ARG:HD3	1.84	0.43
2:G:245:ARG:NH1	2:G:247:ARG:HD3	2.34	0.43
1:E:409:GLN:HG2	1:E:444:TRP:HH2	1.83	0.43
2:G:226:LEU:HD13	2:G:296:PHE:CD1	2.53	0.43
1:A:650:ILE:HD12	1:A:681:LEU:HD21	2.00	0.43
2:H:245:ARG:NH2	2:H:261:ASP:OD2	2.52	0.43
1:A:554:CYS:O	1:A:558:ASN:ND2	2.51	0.42
2:D:279:HIS:HB3	2:D:282:VAL:HG23	2.00	0.42
1:A:615:PHE:CE1	2:D:99:LEU:HB2	2.54	0.42
1:E:460:ASP:O	1:E:464:GLU:HG2	2.19	0.42
1:F:711:ILE:HG21	1:F:720:ILE:HD11	2.01	0.42
2:C:198:ARG:HE	2:C:209:PHE:HZ	1.67	0.42
2:D:211:GLN:HA	2:D:302:VAL:HG23	2.01	0.42
2:G:135:GLU:OE1	2:G:197:TYR:OH	2.25	0.42
2:H:186:PRO:HA	2:H:188:ILE:HG13	2.01	0.42
1:B:148:ARG:HA	1:B:153:LEU:HB2	2.01	0.42
1:B:637:SER:OG	1:B:639:ARG:HG2	2.18	0.42
1:A:716:ASN:HB2	1:A:719:ASP:OD1	2.20	0.42
1:E:32:VAL:HG12	1:E:160:ILE:HD13	2.01	0.42
1:E:683:GLN:HB3	1:E:687:LEU:HD12	2.01	0.42
1:A:285:LYS:HD2	1:A:285:LYS:H	1.84	0.42
1:B:779:ILE:HA	1:B:790:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:226:LEU:HD13	2:C:296:PHE:CD1	2.55	0.42
1:A:639:ARG:NH2	1:A:649:GLU:OE2	2.51	0.42
2:D:227:LYS:HG3	2:D:246:PHE:CE1	2.55	0.42
1:E:651:LEU:HA	1:E:656:SER:HA	2.01	0.42
2:C:31:ARG:HD3	2:C:74:LEU:HD13	2.02	0.42
1:E:122:ALA:HB3	1:E:129:ASP:HA	2.02	0.42
1:E:771:ILE:O	1:E:775:MET:HG2	2.19	0.42
2:G:111:PRO:HG3	2:G:329:PHE:CD2	2.54	0.42
1:A:24:GLN:O	1:A:28:LEU:HB2	2.19	0.42
2:D:275:CYS:HA	2:D:298:PHE:HA	2.02	0.42
1:E:574:ARG:HE	1:E:591:THR:HG21	1.85	0.42
1:F:460:ASP:O	1:F:464:GLU:HG2	2.20	0.42
1:A:712:SER:HA	1:A:750:LYS:HA	2.02	0.42
1:E:427:ASP:O	1:E:431:ARG:HG3	2.20	0.42
1:E:761:HIS:ND1	1:E:762:PRO:HD2	2.35	0.42
2:C:111:PRO:HG3	2:C:329:PHE:CD2	2.55	0.42
1:F:156:ASN:OD1	1:F:156:ASN:N	2.53	0.42
1:F:404:ALA:HB2	1:F:447:VAL:HG22	2.02	0.42
2:G:146:LEU:HD23	2:G:253:PHE:CD2	2.54	0.42
2:G:179:ARG:O	2:G:183:THR:HG22	2.20	0.42
2:G:247:ARG:NH2	2:G:271:GLU:OE1	2.53	0.42
1:A:288:LEU:O	1:A:319:LEU:HB2	2.20	0.41
2:C:251:PHE:HB2	2:C:254:THR:OG1	2.20	0.41
2:C:11:THR:HG22	2:C:66:VAL:HG13	2.02	0.41
2:C:79:THR:HA	2:C:82:GLN:HG2	2.01	0.41
1:A:229:THR:HG23	1:A:233:MET:HE2	2.02	0.41
1:B:181:VAL:HG21	1:B:432:LEU:HD23	2.02	0.41
1:B:418:TYR:CE2	1:B:474:ILE:HA	2.54	0.41
1:B:29:GLY:N	2:D:248:PRO:HG2	2.35	0.41
1:F:523:LEU:HD12	1:F:641:TRP:HB2	2.01	0.41
1:A:556:GLN:HE21	1:A:671:LEU:HB3	1.85	0.41
1:B:178:GLU:OE1	1:B:467:ARG:NH2	2.53	0.41
1:B:32:VAL:HG22	1:B:160:ILE:HD13	2.03	0.41
1:B:460:ASP:O	1:B:464:GLU:HG2	2.20	0.41
1:E:237:LEU:HD21	1:E:254:TYR:HA	2.02	0.41
1:F:740:VAL:HG12	1:F:753:LEU:HD12	2.02	0.41
1:A:311:ALA:HB1	1:A:317:GLY:HA2	2.03	0.41
1:B:43:THR:HG22	1:B:98:VAL:HG21	2.02	0.41
1:F:492:PHE:CE2	1:F:497:LEU:HD23	2.55	0.41
1:E:615:PHE:HE1	2:H:99:LEU:HB2	1.85	0.41
1:A:42:PHE:CZ	1:A:125:ILE:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:MET:HE2	1:E:334:SER:HB2	2.03	0.41
1:E:633:GLU:HB2	1:E:651:LEU:HD11	2.02	0.41
1:E:702:SER:HB3	1:E:760:GLN:HG2	2.02	0.41
2:H:110:HIS:ND1	2:H:112:VAL:HG12	2.35	0.41
1:A:235:GLN:O	1:A:239:ARG:HG2	2.20	0.41
1:A:427:ASP:O	1:A:431:ARG:HG2	2.20	0.41
1:F:528:SER:N	1:F:529:PRO:HD3	2.35	0.41
1:A:629:ARG:NH2	2:D:329:PHE:O	2.52	0.41
1:F:639:ARG:HD3	1:F:641:TRP:CZ2	2.56	0.41
2:H:226:LEU:HD11	2:H:276:GLY:H	1.86	0.41
1:E:56:HIS:N	1:E:57:PRO:HD3	2.36	0.41
1:E:507:GLN:HG2	2:G:108:THR:HG23	2.03	0.41
1:A:642:LEU:HD13	1:A:647:SER:HB2	2.03	0.41
1:B:40:LYS:HA	1:B:40:LYS:HD3	1.89	0.41
1:B:378:LEU:HA	1:B:378:LEU:HD12	1.84	0.41
1:E:557:TYR:O	1:E:561:ARG:HD3	2.20	0.41
1:E:761:HIS:CD2	1:E:763:SER:HB2	2.56	0.41
1:A:741:TYR:HB3	1:A:752:SER:OG	2.22	0.40
2:D:118:ARG:NH1	2:D:237:PHE:O	2.54	0.40
1:B:532:LEU:HD12	2:D:163:PHE:HE1	1.86	0.40
1:E:514:PHE:CE1	1:E:540:LEU:HD23	2.56	0.40
2:G:195:ARG:HD3	2:G:208:MET:HE2	2.03	0.40
1:B:192:ILE:HD11	1:B:374:ARG:HA	2.03	0.40
1:B:458:TYR:O	1:B:462:ILE:HG13	2.21	0.40
1:E:123:SER:N	1:E:129:ASP:OD2	2.50	0.40
1:E:310:LEU:HD22	1:E:321:SER:HB3	2.02	0.40
1:F:565:ARG:HH12	1:F:600:ARG:C	2.24	0.40
2:G:123:PHE:HB3	2:G:128:PHE:HB2	2.02	0.40
2:G:273:LEU:HB3	2:G:300:LEU:HB3	2.03	0.40
1:B:629:ARG:HD2	1:B:690:TYR:CG	2.56	0.40
2:D:172:HIS:HA	2:D:196:VAL:HG11	2.01	0.40
1:E:311:ALA:HB1	1:E:317:GLY:HA2	2.04	0.40
1:B:492:PHE:HB3	1:B:687:LEU:HA	2.03	0.40
1:A:761:HIS:HD2	1:A:766:LEU:N	2.19	0.40
1:A:711:ILE:HD11	1:A:786:TYR:HB3	2.03	0.40
1:B:201:ASP:O	1:B:219:VAL:HG11	2.22	0.40
2:H:243:LYS:HD3	2:H:243:LYS:HA	1.88	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	790/793 (100%)	734 (93%)	52 (7%)	4 (0%)	29	65
1	B	769/793 (97%)	714 (93%)	53 (7%)	2 (0%)	41	73
1	E	791/793 (100%)	742 (94%)	48 (6%)	1 (0%)	51	83
1	F	457/793 (58%)	419 (92%)	37 (8%)	1 (0%)	47	78
2	C	316/330 (96%)	294 (93%)	20 (6%)	2 (1%)	25	62
2	D	227/330 (69%)	209 (92%)	18 (8%)	0	100	100
2	G	288/330 (87%)	273 (95%)	15 (5%)	0	100	100
2	H	322/330 (98%)	296 (92%)	25 (8%)	1 (0%)	41	73
All	All	3960/4492 (88%)	3681 (93%)	268 (7%)	11 (0%)	41	73

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	228	ALA
2	C	201	SER
1	A	45	VAL
1	A	572	GLY
2	C	2	ARG
1	A	136	GLU
1	B	138	PRO
1	F	529	PRO
2	H	2	ARG
1	A	57	PRO
1	E	57	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	607/673 (90%)	593 (98%)	14 (2%)	50	76
1	B	598/673 (89%)	581 (97%)	17 (3%)	43	73
1	E	635/673 (94%)	614 (97%)	21 (3%)	38	69
1	F	344/673 (51%)	334 (97%)	10 (3%)	42	72
2	C	242/276 (88%)	235 (97%)	7 (3%)	42	72
2	D	188/276 (68%)	185 (98%)	3 (2%)	62	83
2	G	212/276 (77%)	198 (93%)	14 (7%)	16	47
2	H	219/276 (79%)	208 (95%)	11 (5%)	24	57
All	All	3045/3796 (80%)	2948 (97%)	97 (3%)	39	70

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	58	ASP
1	A	219	VAL
1	A	285	LYS
1	A	397	ASP
1	A	416	LEU
1	A	424	PHE
1	A	438	VAL
1	A	446	VAL
1	A	514	PHE
1	A	566	VAL
1	A	676	THR
1	A	690	TYR
1	A	761	HIS
1	B	4	SER
1	B	23	ASP
1	B	35	LEU
1	B	136	GLU
1	B	186	GLN
1	B	289	LEU
1	B	378	LEU
1	B	392	VAL
1	B	416	LEU
1	B	424	PHE

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Mol	Chain	Res	Type
1	B	483	VAL
1	B	514	PHE
1	B	530	LEU
1	B	589	ILE
1	B	660	LEU
1	B	704	ARG
1	B	709	LEU
2	C	1	MET
2	C	28	ASP
2	C	77	ARG
2	C	211	GLN
2	C	223	PHE
2	C	242	LEU
2	C	270	LEU
2	D	223	PHE
2	D	257	SER
2	D	304	ARG
1	E	16	ILE
1	E	23	ASP
1	E	35	LEU
1	E	45	VAL
1	E	129	ASP
1	E	277	VAL
1	E	289	LEU
1	E	323	VAL
1	E	398	LEU
1	E	416	LEU
1	E	424	PHE
1	E	446	VAL
1	E	490	ASP
1	E	492	PHE
1	E	514	PHE
1	E	545	SER
1	E	562	GLN
1	E	587	LYS
1	E	597	VAL
1	E	660	LEU
1	E	790	LEU
1	F	27	MET
1	F	156	ASN
1	F	415	LEU
1	F	453	TYR

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Mol	Chain	Res	Type
1	F	514	PHE
1	F	566	VAL
1	F	600	ARG
1	F	676	THR
1	F	711	ILE
1	F	752	SER
2	G	28	ASP
2	G	95	ILE
2	G	106	ILE
2	G	112	VAL
2	G	121	GLN
2	G	136	VAL
2	G	160	THR
2	G	172	HIS
2	G	183	THR
2	G	211	GLN
2	G	223	PHE
2	G	242	LEU
2	G	263	MET
2	G	300	LEU
2	H	28	ASP
2	H	77	ARG
2	H	86	LEU
2	H	98	THR
2	H	106	ILE
2	H	121	GLN
2	H	142	ASN
2	H	189	ARG
2	H	222	SER
2	H	223	PHE
2	H	313	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	556	GLN
1	B	489	GLN
1	B	780	GLN
1	B	784	ASN
2	C	83	GLN
2	C	211	GLN

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Mol	Chain	Res	Type
1	E	357	GLN
1	E	439	GLN
2	G	211	GLN
2	H	72	ASN
2	H	82	GLN

### 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](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 for Mogul analysis.

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	NO4	G	401	-	17,17,17	1.90	3 (17%)	20,20,20	1.75	3 (15%)
4	NO4	H	401	-	17,17,17	1.96	5 (29%)	20,20,20	1.67	3 (15%)
4	NO4	C	401	-	17,17,17	1.97	4 (23%)	20,20,20	1.67	3 (15%)
4	NO4	D	401	-	17,17,17	1.89	3 (17%)	20,20,20	1.65	3 (15%)

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	NO4	G	401	-	-	5/7/15/15	0/2/2/2
4	NO4	H	401	-	-	5/7/15/15	0/2/2/2
4	NO4	C	401	-	-	2/7/15/15	0/2/2/2
4	NO4	D	401	-	-	2/7/15/15	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	NO4	C03-C02	5.21	1.59	1.51
4	H	401	NO4	C03-C02	5.15	1.59	1.51
4	G	401	NO4	C03-C02	4.95	1.58	1.51
4	D	401	NO4	C03-C02	4.88	1.58	1.51
4	C	401	NO4	C06-C07	2.97	1.57	1.51
4	D	401	NO4	C06-C07	2.95	1.57	1.51
4	H	401	NO4	C06-C07	2.82	1.57	1.51
4	G	401	NO4	C06-C07	2.71	1.57	1.51
4	H	401	NO4	C04-C03	2.60	1.59	1.51
4	C	401	NO4	C04-C03	2.53	1.59	1.51
4	G	401	NO4	C04-C03	2.49	1.59	1.51
4	D	401	NO4	C04-C03	2.38	1.59	1.51
4	H	401	NO4	C13-C02	2.08	1.55	1.50
4	C	401	NO4	C04-N05	2.06	1.53	1.46
4	H	401	NO4	C04-N05	2.01	1.53	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	NO4	C13-C02-C01	-5.62	115.34	121.52
4	D	401	NO4	C13-C02-C01	-5.03	115.99	121.52
4	C	401	NO4	C13-C02-C01	-5.01	116.02	121.52
4	H	401	NO4	C13-C02-C01	-4.94	116.09	121.52
4	C	401	NO4	C03-C02-C01	3.36	129.98	122.82
4	D	401	NO4	C03-C02-C01	3.26	129.76	122.82
4	G	401	NO4	C03-C02-C01	3.04	129.31	122.82
4	H	401	NO4	C03-C02-C01	2.81	128.81	122.82
4	H	401	NO4	C04-C03-C02	2.63	119.76	114.42
4	G	401	NO4	C04-C03-C02	2.54	119.58	114.42
4	C	401	NO4	C04-C03-C02	2.50	119.48	114.42
4	D	401	NO4	C04-C03-C02	2.45	119.40	114.42

There are no chirality outliers.

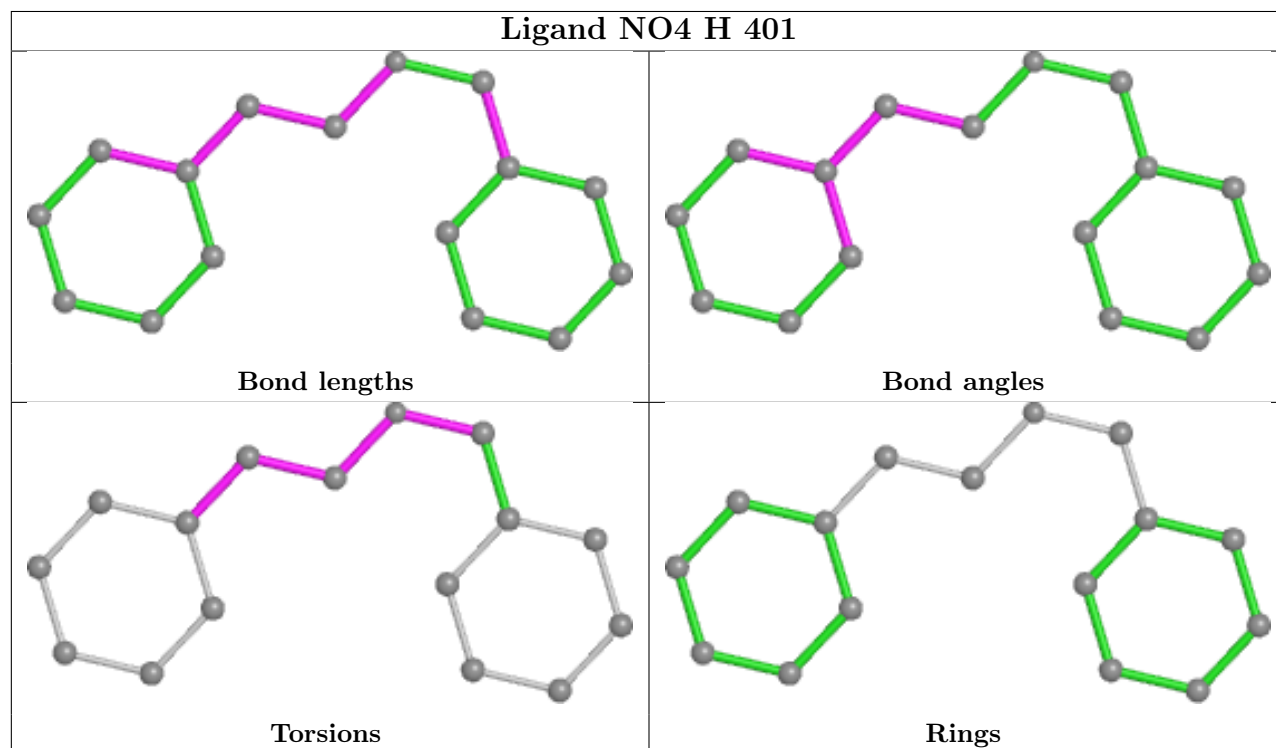
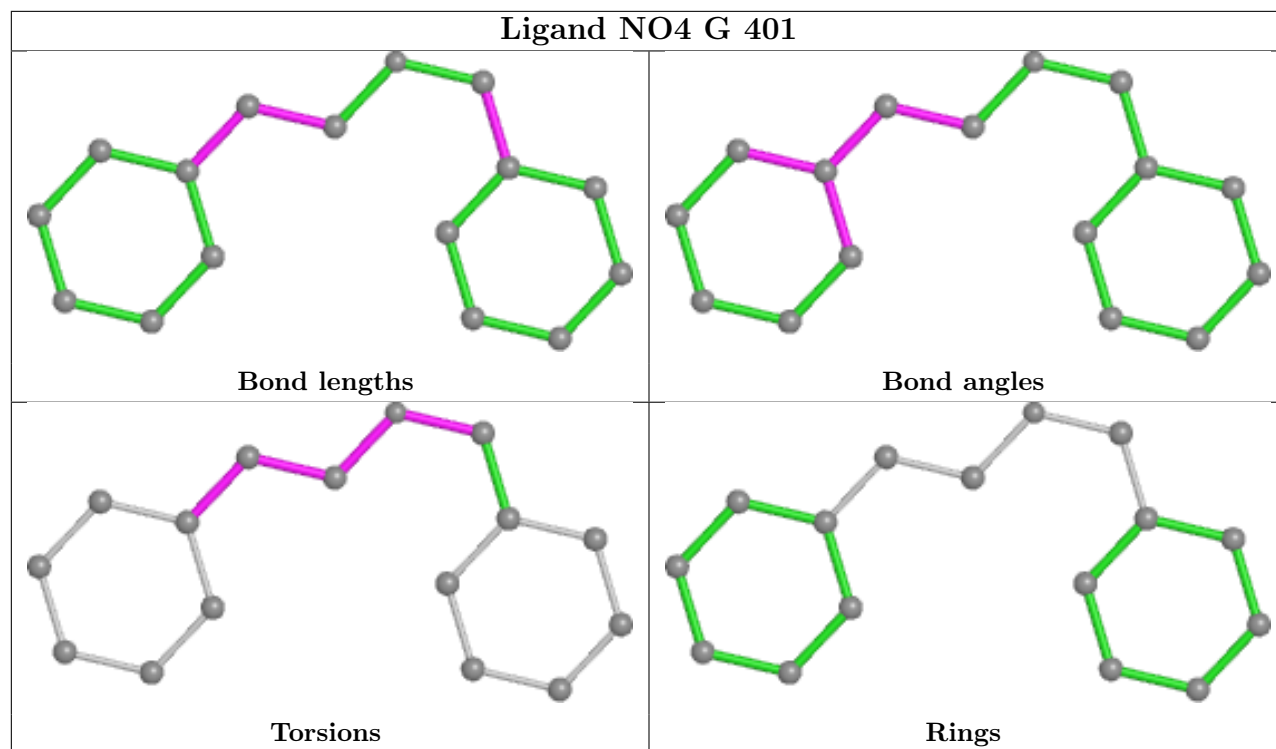
All (14) torsion outliers are listed below:

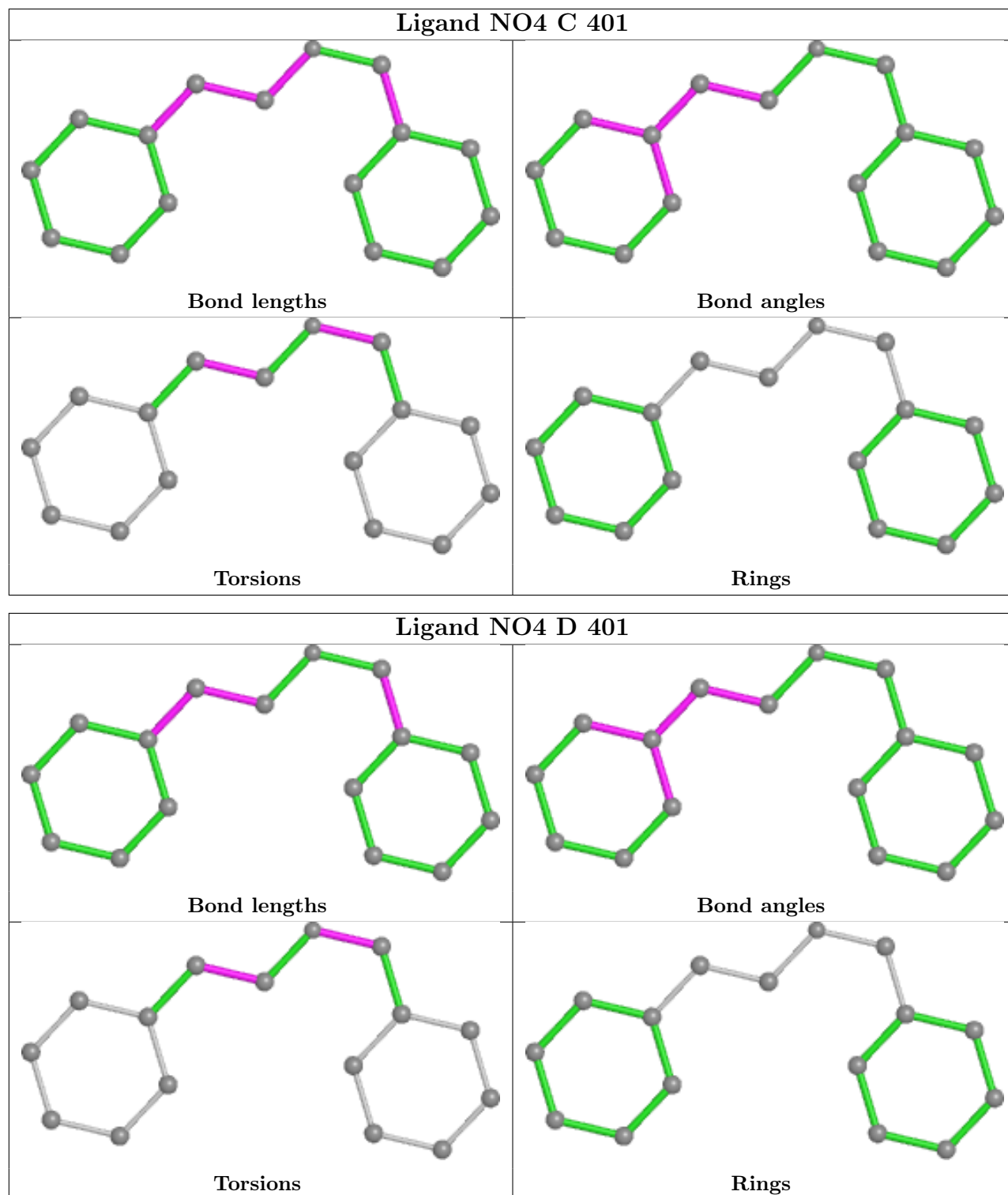
Mol	Chain	Res	Type	Atoms
4	H	401	NO4	C13-C02-C03-C04
4	H	401	NO4	C01-C02-C03-C04
4	H	401	NO4	C02-C03-C04-N05
4	H	401	NO4	C03-C04-N05-C06
4	C	401	NO4	C02-C03-C04-N05
4	D	401	NO4	C02-C03-C04-N05
4	G	401	NO4	C01-C02-C03-C04
4	G	401	NO4	C02-C03-C04-N05
4	D	401	NO4	C07-C06-N05-C04
4	H	401	NO4	C07-C06-N05-C04
4	C	401	NO4	C07-C06-N05-C04
4	G	401	NO4	C07-C06-N05-C04
4	G	401	NO4	C13-C02-C03-C04
4	G	401	NO4	C03-C04-N05-C06

There are no ring outliers.

No monomer is involved in short contacts.

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





## 5.7 Other polymers ⓘ

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	792/793 (99%)	-0.15	29 (3%)	41	25	50, 97, 200, 222	0
1	B	777/793 (97%)	-0.28	24 (3%)	49	32	46, 79, 184, 225	0
1	E	793/793 (100%)	-0.28	10 (1%)	77	66	64, 96, 137, 180	0
1	F	463/793 (58%)	-0.11	8 (1%)	70	57	71, 115, 175, 197	0
2	C	320/330 (96%)	-0.26	6 (1%)	66	53	55, 80, 155, 204	0
2	D	231/330 (70%)	-0.36	2 (0%)	84	75	53, 73, 130, 162	0
2	G	292/330 (88%)	-0.05	13 (4%)	33	19	70, 94, 212, 234	0
2	H	326/330 (98%)	0.01	13 (3%)	38	23	79, 116, 187, 246	0
All	All	3994/4492 (88%)	-0.20	105 (2%)	56	40	46, 95, 181, 246	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	48	GLY	8.4
1	B	116	GLN	7.5
1	B	144	GLY	7.0
1	B	62	LEU	6.2
1	A	60	ASP	6.1
1	B	115	SER	6.1
1	B	82	PRO	5.0
1	A	70	GLY	5.0
2	H	58	VAL	4.7
1	B	143	VAL	4.7
2	H	5	MET	4.6
1	B	101	GLY	4.5
2	C	60	GLY	4.5
1	A	61	ARG	4.5
1	F	17	ASP	4.4
2	H	1	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	59	ALA	4.2
1	F	400	PRO	3.9
1	E	397	ASP	3.8
1	B	48	GLY	3.7
2	H	154	ALA	3.6
2	G	32	VAL	3.6
2	G	27	LEU	3.5
2	G	11	THR	3.5
1	F	41	PRO	3.4
1	A	197	ALA	3.4
1	E	58	ASP	3.4
2	H	57	LYS	3.4
1	A	59	ALA	3.3
1	A	144	GLY	3.3
2	D	154	ALA	3.3
2	H	35	THR	3.3
1	E	71	SER	3.2
2	C	50	LYS	3.1
2	G	34	PHE	3.1
1	F	36	ALA	3.1
1	B	80	GLY	3.0
1	B	113	VAL	3.0
2	H	48	LEU	3.0
1	E	112	GLY	3.0
1	B	86	ALA	2.9
1	A	68	ASN	2.9
2	G	79	THR	2.9
2	H	52	ASP	2.8
1	A	51	LEU	2.8
1	F	450	SER	2.8
1	B	79	CYS	2.8
1	B	51	LEU	2.7
2	C	47	ALA	2.7
2	C	49	GLY	2.7
1	A	71	SER	2.7
2	H	53	PRO	2.7
1	E	196	ASP	2.7
1	B	71	SER	2.7
1	A	79	CYS	2.7
2	G	25	VAL	2.6
1	A	47	VAL	2.6
1	B	73	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	113	VAL	2.5
1	E	243	ARG	2.5
2	G	9	ALA	2.5
1	A	129	ASP	2.5
1	E	70	GLY	2.5
1	B	102	ASP	2.4
1	A	121	GLY	2.4
1	B	63	ARG	2.4
2	G	150	GLY	2.4
1	B	601	GLU	2.4
1	B	114	GLU	2.3
1	A	745	GLY	2.3
1	F	7	TRP	2.3
2	D	157	MET	2.3
1	A	64	VAL	2.3
1	B	87	GLY	2.2
1	B	56	HIS	2.2
1	A	52	THR	2.2
2	C	4	THR	2.2
1	B	57	PRO	2.2
2	H	4	THR	2.2
1	F	440	ALA	2.2
2	C	5	MET	2.2
2	H	36	GLY	2.2
2	G	153	PRO	2.2
1	A	117	GLY	2.2
1	E	82	PRO	2.2
1	A	394	GLU	2.2
2	G	71	ASN	2.2
1	A	138	PRO	2.1
1	B	145	VAL	2.1
1	A	108	GLY	2.1
1	A	116	GLN	2.1
1	A	120	CYS	2.1
1	E	129	ASP	2.1
1	A	107	LYS	2.1
1	B	94	THR	2.1
1	A	82	PRO	2.1
1	F	610	GLN	2.0
2	H	56	ARG	2.0
2	H	155	ARG	2.0
1	A	307	GLN	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	G	201	SER	2.0
2	G	29	GLN	2.0
2	G	33	GLN	2.0
1	A	44	GLY	2.0
1	A	75	LEU	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](#)

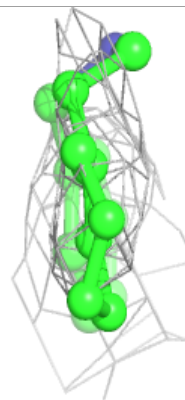
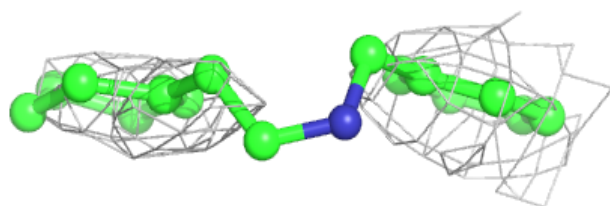
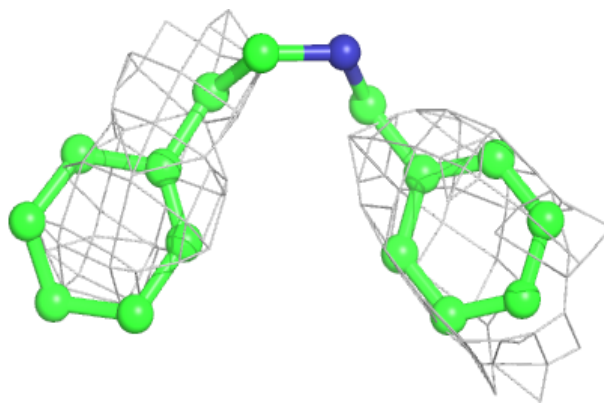
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NO4	H	401	16/16	0.83	0.31	104,113,122,126	0
4	NO4	G	401	16/16	0.91	0.25	69,76,83,84	0
4	NO4	D	401	16/16	0.92	0.21	55,65,75,75	0
4	NO4	C	401	16/16	0.94	0.22	65,69,76,77	0
3	MG	A	801	1/1	0.97	0.43	65,65,65,65	0
3	MG	B	801	1/1	0.97	0.31	54,54,54,54	0
3	MG	E	801	1/1	0.99	0.20	71,71,71,71	0

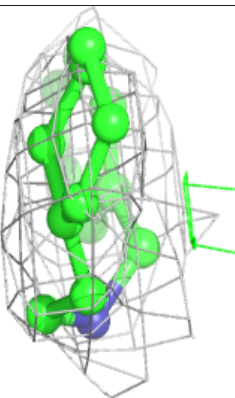
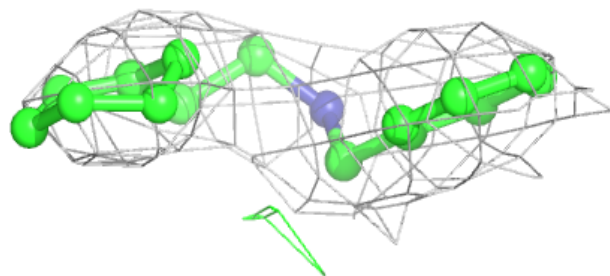
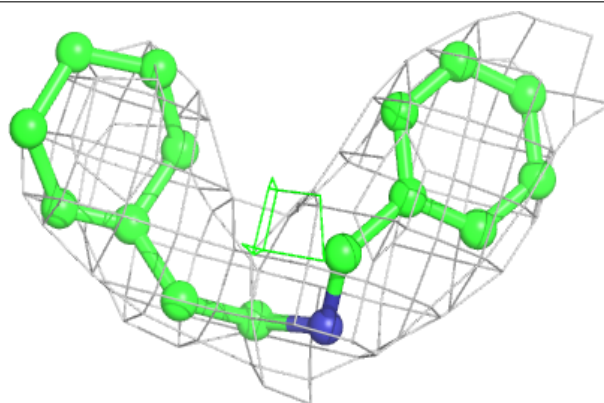
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

**Electron density around NO4 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)

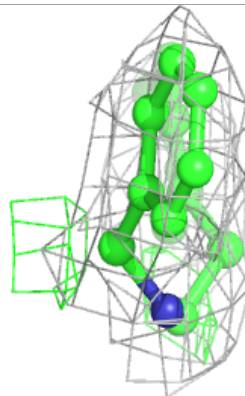
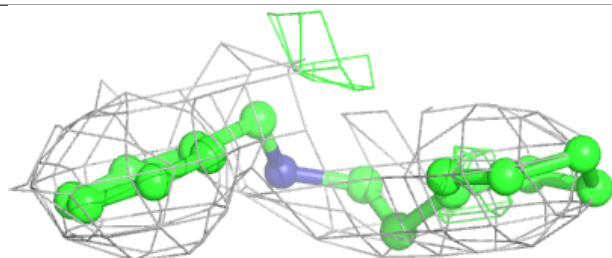
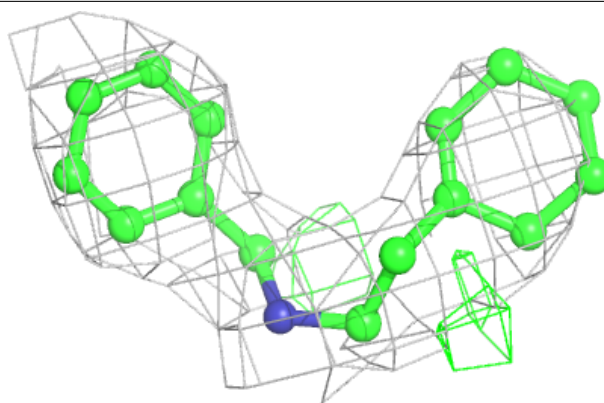
**Electron density around NO4 G 401:**

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

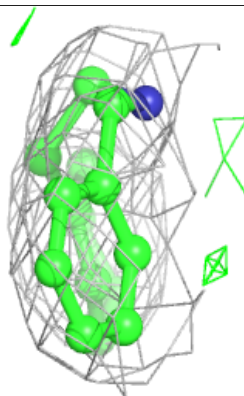
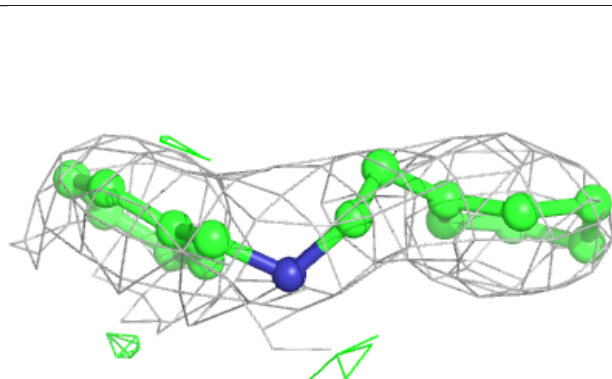
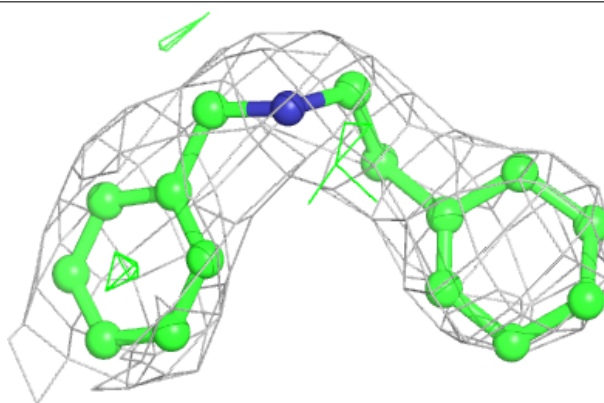


**Electron density around NO4 D 401:**

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

**Electron density around NO4 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)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.