



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 09:32 pm GMT

PDB ID : 5FJR  
Title : N-acyl amino acid racemase from *Amycolatopsis* sp. Ts-1-60: Q26A M50I  
G291D F323Y mutant in complex with N-acetyl naphthylalanine  
Authors : Sanchez Carron, G.; Campopiano, D.; Grogan, G.  
Deposited on : 2015-10-12  
Resolution : 2.44 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

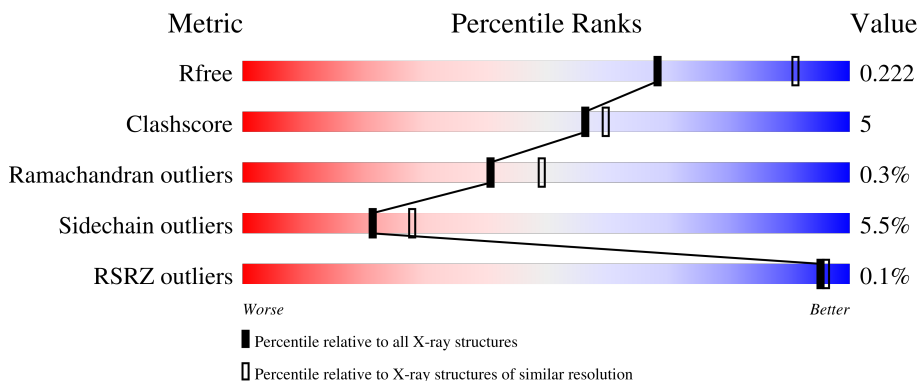
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.44 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1564 (2.46-2.42)
Clashscore	141614	1631 (2.46-2.42)
Ramachandran outliers	138981	1617 (2.46-2.42)
Sidechain outliers	138945	1617 (2.46-2.42)
RSRZ outliers	127900	1547 (2.46-2.42)

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	368	
1	B	368	
1	C	368	
1	D	368	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 11609 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.

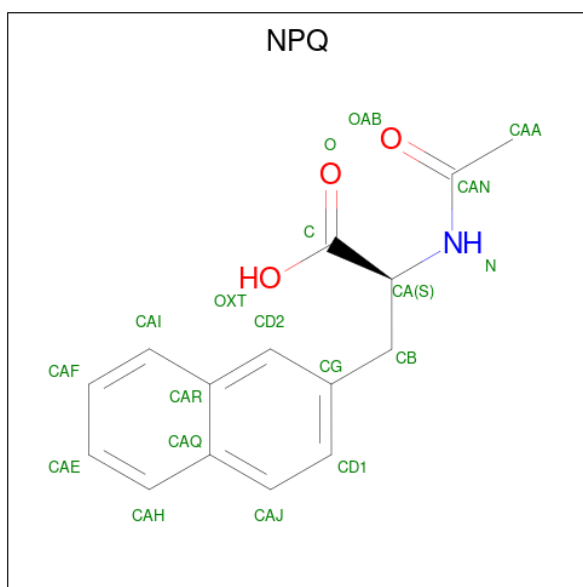
- Molecule 1 is a protein called O-SUCCINYLBENZOATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	368	2764	1758	480	515	11	0	0	0
1	B	367	2726	1742	473	501	10	0	0	0
1	C	367	2720	1735	475	500	10	0	0	0
1	D	367	2702	1726	463	503	10	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	ALA	GLN	engineered mutation	UNP Q44244
A	50	ILE	MET	engineered mutation	UNP Q44244
A	291	ASP	GLY	engineered mutation	UNP Q44244
A	323	TYR	PHE	engineered mutation	UNP Q44244
B	26	ALA	GLN	engineered mutation	UNP Q44244
B	50	ILE	MET	engineered mutation	UNP Q44244
B	291	ASP	GLY	engineered mutation	UNP Q44244
B	323	TYR	PHE	engineered mutation	UNP Q44244
C	26	ALA	GLN	engineered mutation	UNP Q44244
C	50	ILE	MET	engineered mutation	UNP Q44244
C	291	ASP	GLY	engineered mutation	UNP Q44244
C	323	TYR	PHE	engineered mutation	UNP Q44244
D	26	ALA	GLN	engineered mutation	UNP Q44244
D	50	ILE	MET	engineered mutation	UNP Q44244
D	291	ASP	GLY	engineered mutation	UNP Q44244
D	323	TYR	PHE	engineered mutation	UNP Q44244

- Molecule 2 is N-acetyl naphthylalanine (three-letter code: NPQ) (formula: C<sub>15</sub>H<sub>15</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	15	1	3		
2	B	1	Total	C	N	O	0	0
			19	15	1	3		
2	C	1	Total	C	N	O	0	0
			19	15	1	3		
2	D	1	Total	C	N	O	0	0
			19	15	1	3		

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

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total	O	0	0
			246	246		

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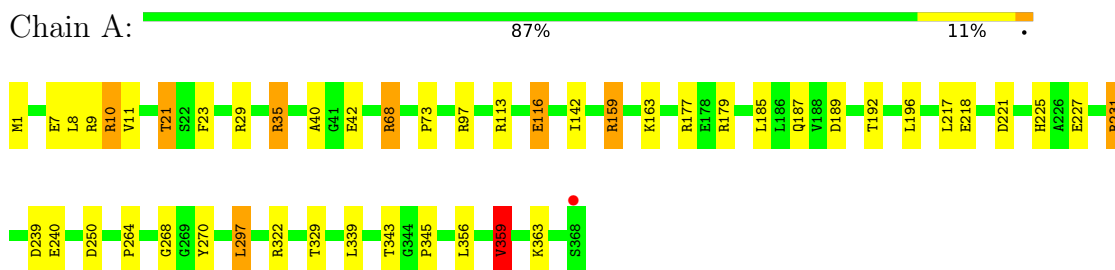
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	B	145	Total 145	O 145	0	0
4	C	118	Total 118	O 118	0	0
4	D	108	Total 108	O 108	0	0

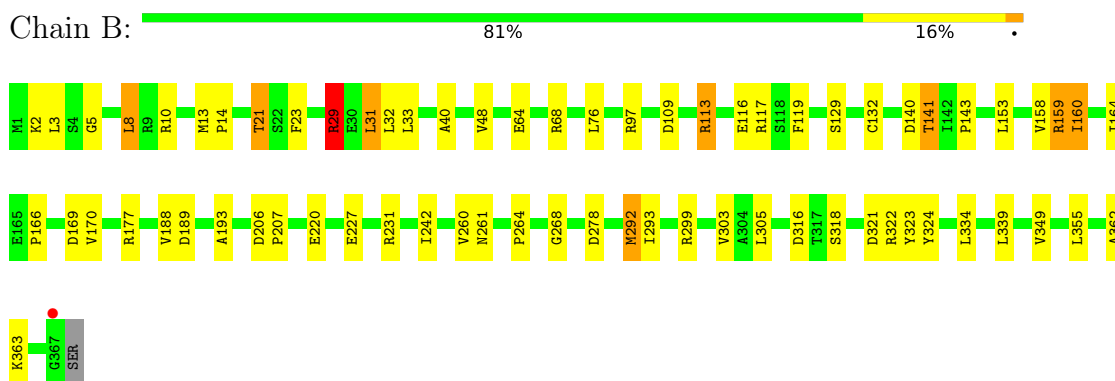
### 3 Residue-property plots

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

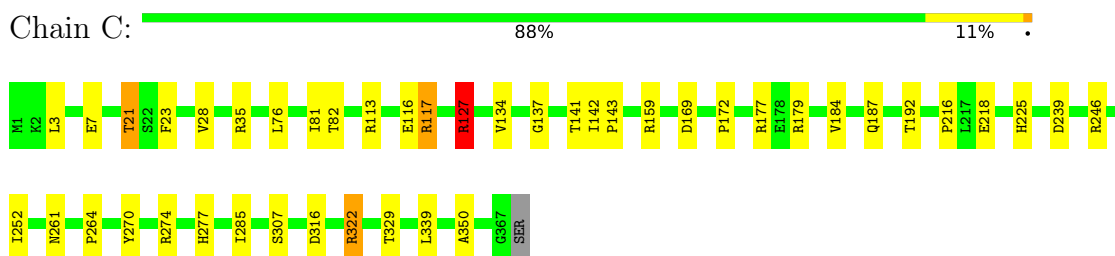
- Molecule 1: O-SUCCINYLBENZOATE SYNTHASE



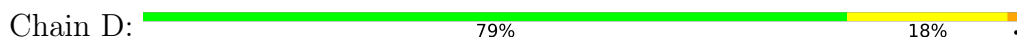
- Molecule 1: O-SUCCINYLBENZOATE SYNTHASE

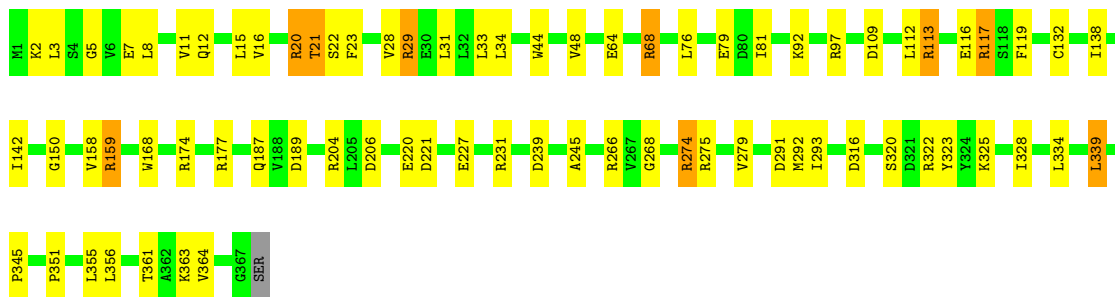


- Molecule 1: O-SUCCINYLBENZOATE SYNTHASE



- Molecule 1: O-SUCCINYLBENZOATE SYNTHASE





## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	217.67Å 217.67Å 263.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	107.89 – 2.44 107.89 – 2.44	Depositor EDS
% Data completeness (in resolution range)	100.0 (107.89-2.44) 100.0 (107.89-2.44)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.172 , 0.221 0.173 , 0.222	Depositor DCC
$R_{free}$ test set	4220 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 34.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.022 for $-2/3^*h-1/3^*k+2/3^*l,-1/3^*h-2/3^*k-2/3^*l,2/3^*h-2/3^*k+1/3^*l$ 0.016 for $-h,1/3^*h-1/3^*k+2/3^*l,2/3^*h+4/3^*k+1/3^*l$ 0.012 for $-1/3^*h+1/3^*k-2/3^*l,-k,-4/3^*h-2/3^*k+1/3^*l$	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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: MG, NPQ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.02	2/2820 (0.1%)	1.18	22/3844 (0.6%)
1	B	1.00	1/2782 (0.0%)	1.11	13/3796 (0.3%)
1	C	0.93	0/2776	1.07	7/3791 (0.2%)
1	D	1.01	3/2758 (0.1%)	1.18	21/3769 (0.6%)
All	All	0.99	6/11136 (0.1%)	1.14	63/15200 (0.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	220	GLU	CD-OE1	5.68	1.31	1.25
1	A	240	GLU	CD-OE2	5.36	1.31	1.25
1	D	239	ASP	CB-CG	5.31	1.62	1.51
1	D	361	THR	CB-CG2	5.23	1.69	1.52
1	A	250	ASP	CB-CG	5.21	1.62	1.51
1	D	220	GLU	CD-OE1	5.09	1.31	1.25

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ARG	NE-CZ-NH2	-17.84	111.38	120.30
1	A	113	ARG	NE-CZ-NH1	13.04	126.82	120.30
1	D	356	LEU	CB-CG-CD2	11.66	130.82	111.00
1	C	127	ARG	NE-CZ-NH1	10.79	125.70	120.30
1	D	159	ARG	NE-CZ-NH1	10.14	125.37	120.30
1	D	159	ARG	NE-CZ-NH2	-9.78	115.41	120.30
1	B	113	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	A	35	ARG	NE-CZ-NH2	-8.81	115.89	120.30
1	C	127	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	B	113	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	D	266	ARG	NE-CZ-NH2	-8.32	116.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	117	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	9	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	D	204	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	D	206	ASP	CB-CG-OD1	7.53	125.08	118.30
1	D	266	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	2	LYS	N-CA-C	-7.47	90.83	111.00
1	B	231	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	B	189	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	B	278	ASP	CB-CG-OD1	7.18	124.77	118.30
1	C	239	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	113	ARG	CG-CD-NE	-7.16	96.76	111.80
1	A	231	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	A	35	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	113	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	D	117	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	B	292	MET	CG-SD-CE	-6.68	89.51	100.20
1	D	189	ASP	CB-CG-OD1	6.61	124.25	118.30
1	D	109	ASP	CB-CG-OD1	6.60	124.24	118.30
1	D	204	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	343	THR	C-N-CA	-6.54	108.56	122.30
1	A	159	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	359	VAL	CG1-CB-CG2	6.49	121.28	110.90
1	D	113	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	189	ASP	CB-CG-OD1	6.44	124.09	118.30
1	A	231	ARG	CG-CD-NE	-6.37	98.42	111.80
1	A	221	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	A	185	LEU	CB-CG-CD2	6.16	121.48	111.00
1	D	221	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	D	20	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	D	275	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	D	174	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	29	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	113	ARG	CD-NE-CZ	5.97	131.96	123.60
1	A	239	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	29	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	113	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	D	189	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	160	ILE	CG1-CB-CG2	-5.55	99.18	111.40
1	D	109	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	C	113	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	10	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	D	2	LYS	N-CA-C	-5.30	96.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	LEU	CB-CG-CD2	-5.29	102.00	111.00
1	A	359	VAL	CB-CA-C	5.20	121.28	111.40
1	A	189	ASP	CB-CG-OD1	5.18	122.96	118.30
1	A	159	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	D	174	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	117	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	127	ARG	CD-NE-CZ	5.13	130.78	123.60
1	B	3	LEU	CA-CB-CG	5.10	127.04	115.30
1	A	68	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	159	ARG	CG-CD-NE	-5.05	101.19	111.80

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	2764	0	2802	20	0
1	B	2726	0	2758	32	0
1	C	2720	0	2737	24	0
1	D	2702	0	2699	34	0
2	A	19	0	0	0	0
2	B	19	0	0	0	0
2	C	19	0	0	0	0
2	D	19	0	0	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	246	0	0	4	0
4	B	145	0	0	0	0
4	C	118	0	0	2	0
4	D	108	0	0	6	0
All	All	11609	0	10996	109	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 5.

All (109) 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:B:48:VAL:HB	1:B:292:MET:HG2	1.68	0.74
1:D:21:THR:HG23	1:D:23:PHE:H	1.55	0.72
1:C:127:ARG:HH11	1:C:127:ARG:HG3	1.53	0.71
1:A:11:VAL:HG13	1:A:359:VAL:HG13	1.74	0.70
1:B:10:ARG:HD3	1:B:64:GLU:OE1	1.94	0.68
1:D:68:ARG:HH21	1:D:364:VAL:HG21	1.60	0.66
1:D:21:THR:CG2	1:D:23:PHE:H	2.12	0.63
1:A:21:THR:CG2	1:A:23:PHE:H	2.12	0.62
1:B:21:THR:HG21	1:B:23:PHE:CZ	2.34	0.61
1:C:159:ARG:NH2	1:C:316:ASP:OD1	2.28	0.60
1:B:21:THR:HG21	1:B:23:PHE:CE2	2.35	0.60
1:C:141:THR:HB	1:C:143:PRO:HD2	1.84	0.60
1:C:7:GLU:OE1	1:C:35:ARG:NH1	2.36	0.59
1:D:5:GLY:HA2	1:D:76:LEU:HD21	1.85	0.59
1:C:21:THR:CG2	1:C:23:PHE:H	2.17	0.58
1:D:159:ARG:NH2	1:D:316:ASP:OD1	2.29	0.57
4:A:2195:HOH:O	1:D:231:ARG:CD	2.52	0.57
1:D:15:LEU:HD21	1:D:29:ARG:HB2	1.86	0.57
1:C:252:ILE:HG12	1:C:285:ILE:HG13	1.87	0.57
1:B:141:THR:OG1	1:B:143:PRO:HD2	2.05	0.56
1:B:169:ASP:OD1	1:B:170:VAL:HG23	2.05	0.56
1:A:10:ARG:HD2	4:A:2059:HOH:O	2.04	0.56
4:A:2195:HOH:O	1:D:231:ARG:HD3	2.05	0.56
1:A:21:THR:HG22	1:A:23:PHE:H	1.71	0.55
1:C:216:PRO:HD2	1:C:225:HIS:CD2	2.42	0.54
1:D:325:LYS:N	4:D:2103:HOH:O	2.40	0.54
1:A:231:ARG:NH2	4:A:2183:HOH:O	2.40	0.54
1:B:21:THR:HG23	1:B:23:PHE:H	1.73	0.54
1:B:10:ARG:HG3	1:B:362:ALA:HB3	1.89	0.54
1:C:216:PRO:HD2	1:C:225:HIS:NE2	2.23	0.53
1:B:29:ARG:HD2	1:B:31:LEU:HD23	1.92	0.52
1:D:334:LEU:HD12	1:D:339:LEU:HD13	1.92	0.52
1:C:169:ASP:O	1:C:172:PRO:HD2	2.10	0.52
1:B:299:ARG:O	1:B:303:VAL:HG23	2.09	0.51
1:A:21:THR:HG21	1:A:23:PHE:CE2	2.46	0.51
1:C:192:THR:HB	1:C:218:GLU:HA	1.91	0.51
1:A:21:THR:HG21	1:A:23:PHE:CZ	2.45	0.51
1:B:159:ARG:NH2	1:B:316:ASP:OD1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:ARG:O	1:C:277:HIS:HB3	2.11	0.50
1:D:48:VAL:HB	1:D:292:MET:HG3	1.93	0.50
1:C:21:THR:HG22	1:C:23:PHE:H	1.75	0.50
1:C:264:PRO:HG2	1:C:270:TYR:CE1	2.46	0.50
1:D:112:LEU:HB3	1:D:117:ARG:O	2.12	0.49
1:B:164:ILE:HD13	1:B:188:VAL:HB	1.96	0.48
1:C:3:LEU:HD23	1:C:76:LEU:HD23	1.94	0.48
1:A:116:GLU:HA	1:A:345:PRO:HB3	1.95	0.47
1:B:48:VAL:HB	1:B:292:MET:CG	2.42	0.47
1:B:132:CYS:O	1:B:158:VAL:HG22	2.14	0.47
1:B:166:PRO:HD3	1:B:193:ALA:HB1	1.97	0.47
1:D:293:ILE:HG23	1:D:323:TYR:CG	2.51	0.46
1:D:3:LEU:O	4:D:2001:HOH:O	2.21	0.46
1:B:8:LEU:HD21	1:B:32:LEU:HD13	1.98	0.46
1:B:334:LEU:HD12	1:B:339:LEU:CD1	2.46	0.46
1:D:97:ARG:O	1:D:268:GLY:HA2	2.16	0.46
1:C:329:THR:HG22	1:C:350:ALA:O	2.15	0.46
1:D:44:TRP:CZ2	1:D:351:PRO:HG2	2.51	0.46
1:D:159:ARG:HD2	1:D:187:GLN:OE1	2.16	0.45
1:A:264:PRO:HG2	1:A:270:TYR:CE2	2.51	0.45
1:B:321:ASP:HA	1:B:324:TYR:O	2.16	0.45
1:C:21:THR:HG21	1:C:23:PHE:CZ	2.51	0.45
1:B:5:GLY:HA2	1:B:76:LEU:HD21	1.98	0.45
1:D:8:LEU:HD21	1:D:64:GLU:HG3	1.99	0.45
1:C:127:ARG:HB2	1:C:307:SER:HB2	1.99	0.45
1:A:35:ARG:NE	1:A:42:GLU:OE2	2.44	0.45
1:A:192:THR:HB	1:A:218:GLU:HA	1.98	0.45
1:B:97:ARG:O	1:B:268:GLY:HA2	2.16	0.45
1:B:242:ILE:HG13	1:B:260:VAL:HG13	1.99	0.45
1:D:33:LEU:HD23	1:D:33:LEU:HA	1.76	0.44
1:C:137:GLY:HA3	4:C:2003:HOH:O	2.16	0.44
1:D:33:LEU:O	1:D:34:LEU:HD23	2.18	0.44
1:A:1:MET:HE1	1:A:40:ALA:HB2	1.99	0.44
1:B:299:ARG:NH1	1:B:318:SER:O	2.50	0.43
1:D:132:CYS:O	1:D:158:VAL:HG22	2.17	0.43
1:D:291:ASP:O	2:D:1368:NPQ:CAA	2.66	0.43
1:A:7:GLU:CD	1:A:35:ARG:HH11	2.21	0.43
1:B:21:THR:CG2	1:B:23:PHE:CD2	3.01	0.43
1:B:129:SER:HB2	1:B:339:LEU:O	2.18	0.43
1:C:82:THR:CG2	4:C:2032:HOH:O	2.66	0.43
1:A:297:LEU:HD13	1:A:329:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ARG:NH2	4:D:2038:HOH:O	2.52	0.43
1:B:109:ASP:OD2	1:B:113:ARG:NH1	2.51	0.42
1:D:20:ARG:HD2	4:D:2006:HOH:O	2.18	0.42
1:B:21:THR:CG2	1:B:23:PHE:H	2.31	0.42
1:A:159:ARG:HD2	1:A:187:GLN:OE1	2.19	0.42
1:D:328:ILE:O	1:D:351:PRO:HA	2.20	0.42
1:D:355:LEU:HD23	1:D:355:LEU:HA	1.92	0.42
1:A:163:LYS:HA	1:A:163:LYS:HD3	1.93	0.41
1:A:217:LEU:HB2	1:A:225:HIS:CE1	2.55	0.41
1:B:264:PRO:HG3	1:B:305:LEU:HD22	2.01	0.41
1:B:293:ILE:HG12	1:B:323:TYR:CE1	2.55	0.41
1:C:134:VAL:CG2	1:C:322:ARG:HD3	2.50	0.41
1:A:21:THR:HG23	1:A:23:PHE:H	1.84	0.41
1:D:116:GLU:HA	1:D:345:PRO:HB3	2.01	0.41
1:D:138:ILE:HG23	1:D:168:TRP:CD1	2.55	0.41
1:A:97:ARG:O	1:A:268:GLY:HA2	2.20	0.41
1:D:7:GLU:OE2	1:D:363:LYS:HD2	2.20	0.41
1:C:21:THR:HG21	1:C:23:PHE:CE1	2.56	0.41
1:D:11:VAL:HG12	1:D:12:GLN:N	2.35	0.41
1:A:218:GLU:OE2	1:C:246:ARG:NH1	2.54	0.41
1:D:274:ARG:NH1	4:D:2091:HOH:O	2.53	0.41
1:D:245:ALA:HB1	1:D:279:VAL:HG21	2.02	0.40
1:B:33:LEU:HA	1:B:33:LEU:HD23	1.73	0.40
1:B:159:ARG:HG2	1:B:160:ILE:N	2.35	0.40
1:D:22:SER:HB3	4:D:2009:HOH:O	2.21	0.40
1:B:206:ASP:N	1:B:207:PRO:CD	2.84	0.40
1:D:44:TRP:CE2	1:D:351:PRO:HG2	2.55	0.40
1:C:117:ARG:HG3	1:C:117:ARG:HH11	1.86	0.40
1:B:13:MET:HA	1:B:14:PRO:HD2	1.87	0.40
1:C:159:ARG:HD2	1:C:187:GLN:OE1	2.21	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	366/368 (100%)	356 (97%)	10 (3%)	0	100	100
1	B	365/368 (99%)	347 (95%)	17 (5%)	1 (0%)	41	49
1	C	365/368 (99%)	346 (95%)	19 (5%)	0	100	100
1	D	365/368 (99%)	340 (93%)	22 (6%)	3 (1%)	19	22
All	All	1461/1472 (99%)	1389 (95%)	68 (5%)	4 (0%)	41	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	ALA
1	D	16	VAL
1	D	79	GLU
1	D	150	GLY

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	289/291 (99%)	273 (94%)	16 (6%)	21	28
1	B	279/291 (96%)	261 (94%)	18 (6%)	17	21
1	C	277/291 (95%)	265 (96%)	12 (4%)	29	38
1	D	274/291 (94%)	259 (94%)	15 (6%)	21	28
All	All	1119/1164 (96%)	1058 (94%)	61 (6%)	21	28

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	LEU
1	A	21	THR
1	A	29	ARG
1	A	68	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	73	PRO
1	A	116	GLU
1	A	142	ILE
1	A	177	ARG
1	A	179	ARG
1	A	227	GLU
1	A	297	LEU
1	A	322	ARG
1	A	339	LEU
1	A	356	LEU
1	A	359	VAL
1	A	363	LYS
1	B	8	LEU
1	B	21	THR
1	B	29	ARG
1	B	31	LEU
1	B	68	ARG
1	B	116	GLU
1	B	119	PHE
1	B	140	ASP
1	B	141	THR
1	B	153	LEU
1	B	159	ARG
1	B	177	ARG
1	B	227	GLU
1	B	261	ASN
1	B	322	ARG
1	B	349	VAL
1	B	355	LEU
1	B	363	LYS
1	C	21	THR
1	C	28	VAL
1	C	81	ILE
1	C	116	GLU
1	C	127	ARG
1	C	142	ILE
1	C	177	ARG
1	C	179	ARG
1	C	184	VAL
1	C	261	ASN
1	C	322	ARG
1	C	339	LEU

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Mol	Chain	Res	Type
1	D	21	THR
1	D	28	VAL
1	D	29	ARG
1	D	31	LEU
1	D	68	ARG
1	D	81	ILE
1	D	92	LYS
1	D	119	PHE
1	D	142	ILE
1	D	177	ARG
1	D	227	GLU
1	D	274	ARG
1	D	320	SER
1	D	322	ARG
1	D	339	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	12	GLN
1	D	338	HIS

### 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 8 ligands modelled in this entry, 4 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$
2	NPQ	B	1368	3	20,20,20	1.87	5 (25%)	27,27,27	2.21	9 (33%)
2	NPQ	C	1368	3	20,20,20	1.70	4 (20%)	27,27,27	1.96	4 (14%)
2	NPQ	A	1369	3	20,20,20	1.63	4 (20%)	27,27,27	2.34	8 (29%)
2	NPQ	D	1368	3	20,20,20	2.07	3 (15%)	27,27,27	2.12	9 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NPQ	B	1368	3	-	6/12/12/12	0/2/2/2
2	NPQ	C	1368	3	-	8/12/12/12	0/2/2/2
2	NPQ	A	1369	3	-	8/12/12/12	0/2/2/2
2	NPQ	D	1368	3	-	6/12/12/12	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1368	NPQ	CB-CG	-6.73	1.35	1.51
2	C	1368	NPQ	CB-CG	-4.69	1.40	1.51
2	B	1368	NPQ	CA-C	4.52	1.64	1.52
2	D	1368	NPQ	CA-C	4.40	1.64	1.52
2	B	1368	NPQ	CB-CG	-4.27	1.41	1.51
2	A	1369	NPQ	CB-CG	-3.67	1.42	1.51
2	C	1368	NPQ	CAJ-CD1	2.95	1.42	1.36
2	A	1369	NPQ	CA-N	-2.66	1.40	1.45
2	B	1368	NPQ	CA-N	-2.65	1.40	1.45
2	C	1368	NPQ	CAE-CAH	2.39	1.42	1.36
2	C	1368	NPQ	O-C	2.31	1.29	1.22
2	A	1369	NPQ	CAF-CAI	2.27	1.41	1.36
2	B	1368	NPQ	CD2-CG	2.19	1.42	1.37
2	A	1369	NPQ	CAJ-CD1	2.15	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1368	NPQ	CAF-CAI	2.14	1.41	1.36
2	B	1368	NPQ	CAF-CAI	2.13	1.41	1.36

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1368	NPQ	CA-N-CAN	5.94	139.13	121.48
2	C	1368	NPQ	C-CA-N	-5.79	96.84	110.55
2	A	1369	NPQ	CA-N-CAN	5.18	136.88	121.48
2	C	1368	NPQ	CG-CB-CA	5.16	127.61	113.39
2	A	1369	NPQ	CB-CA-N	4.92	121.16	110.79
2	B	1368	NPQ	CG-CB-CA	4.64	126.19	113.39
2	D	1368	NPQ	CA-N-CAN	4.62	135.19	121.48
2	D	1368	NPQ	C-CA-N	-4.59	99.68	110.55
2	A	1369	NPQ	C-CA-N	-4.50	99.90	110.55
2	A	1369	NPQ	CAA-CAN-N	4.37	123.49	116.10
2	B	1368	NPQ	C-CA-N	-3.81	101.52	110.55
2	A	1369	NPQ	CG-CB-CA	3.61	123.34	113.39
2	D	1368	NPQ	CB-CG-CD1	-3.37	114.22	120.91
2	B	1368	NPQ	OAB-CAN-N	-3.26	115.95	121.95
2	D	1368	NPQ	CAH-CAQ-CAR	3.21	124.67	118.92
2	C	1368	NPQ	CB-CA-N	3.12	117.37	110.79
2	D	1368	NPQ	CAJ-CAQ-CAH	-3.11	115.93	123.19
2	B	1368	NPQ	CB-CG-CD1	-2.98	114.99	120.91
2	A	1369	NPQ	OAB-CAN-N	-2.79	116.81	121.95
2	B	1368	NPQ	CB-CA-N	2.77	116.62	110.79
2	D	1368	NPQ	CG-CD2-CAR	-2.69	115.93	121.22
2	A	1369	NPQ	OAB-CAN-CAA	-2.62	117.19	122.06
2	B	1368	NPQ	CAA-CAN-N	2.40	120.15	116.10
2	A	1369	NPQ	CB-CA-C	-2.30	104.89	110.42
2	D	1368	NPQ	CD2-CAR-CAQ	2.22	122.13	118.96
2	D	1368	NPQ	CAE-CAF-CAI	2.19	123.51	120.44
2	D	1368	NPQ	OXT-C-CA	2.19	120.67	113.40
2	B	1368	NPQ	CB-CG-CD2	2.17	125.35	120.57
2	C	1368	NPQ	O-C-CA	-2.09	115.40	122.26
2	B	1368	NPQ	CAJ-CAQ-CAH	-2.01	118.49	123.19

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1369	NPQ	CAA-CAN-N-CA

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Mol	Chain	Res	Type	Atoms
2	A	1369	NPQ	OAB-CAN-N-CA
2	B	1368	NPQ	CAA-CAN-N-CA
2	B	1368	NPQ	OAB-CAN-N-CA
2	C	1368	NPQ	CAA-CAN-N-CA
2	D	1368	NPQ	CAA-CAN-N-CA
2	D	1368	NPQ	OAB-CAN-N-CA
2	A	1369	NPQ	C-CA-CB-CG
2	A	1369	NPQ	N-CA-CB-CG
2	C	1368	NPQ	OAB-CAN-N-CA
2	A	1369	NPQ	OXT-C-CA-N
2	C	1368	NPQ	O-C-CA-N
2	C	1368	NPQ	OXT-C-CA-N
2	A	1369	NPQ	O-C-CA-N
2	B	1368	NPQ	O-C-CA-N
2	D	1368	NPQ	O-C-CA-N
2	D	1368	NPQ	OXT-C-CA-N
2	C	1368	NPQ	OXT-C-CA-CB
2	C	1368	NPQ	C-CA-CB-CG
2	A	1369	NPQ	OXT-C-CA-CB
2	B	1368	NPQ	OXT-C-CA-N
2	C	1368	NPQ	O-C-CA-CB
2	A	1369	NPQ	O-C-CA-CB
2	D	1368	NPQ	O-C-CA-CB
2	B	1368	NPQ	O-C-CA-CB
2	B	1368	NPQ	OXT-C-CA-CB
2	D	1368	NPQ	OXT-C-CA-CB
2	C	1368	NPQ	N-CA-CB-CG

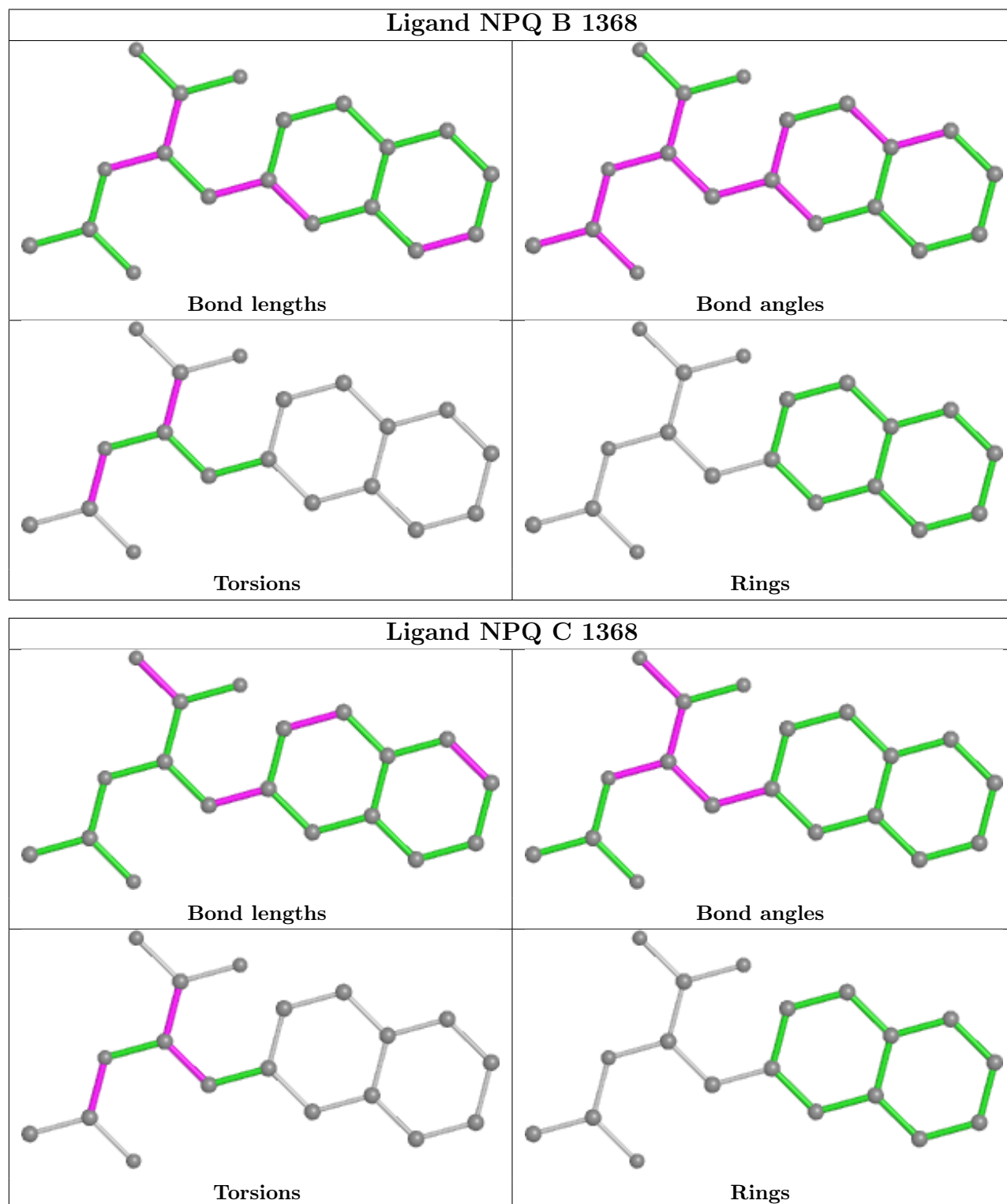
There are no ring outliers.

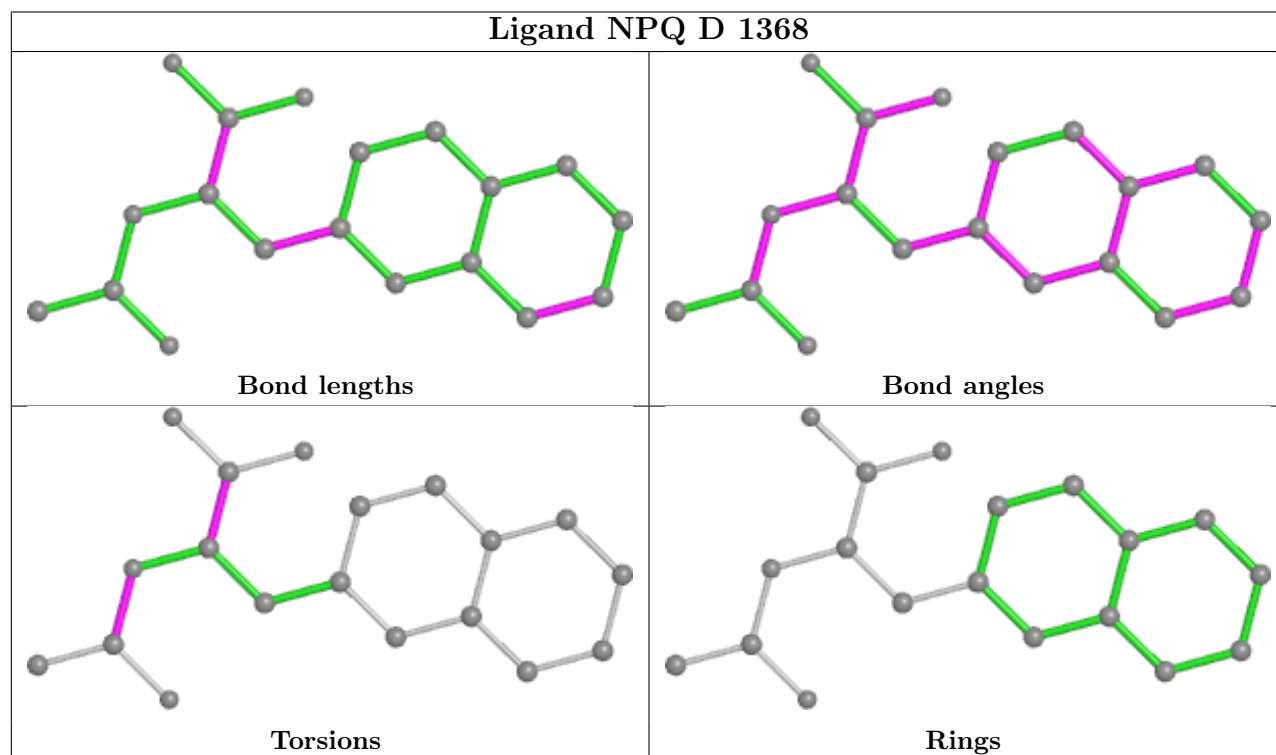
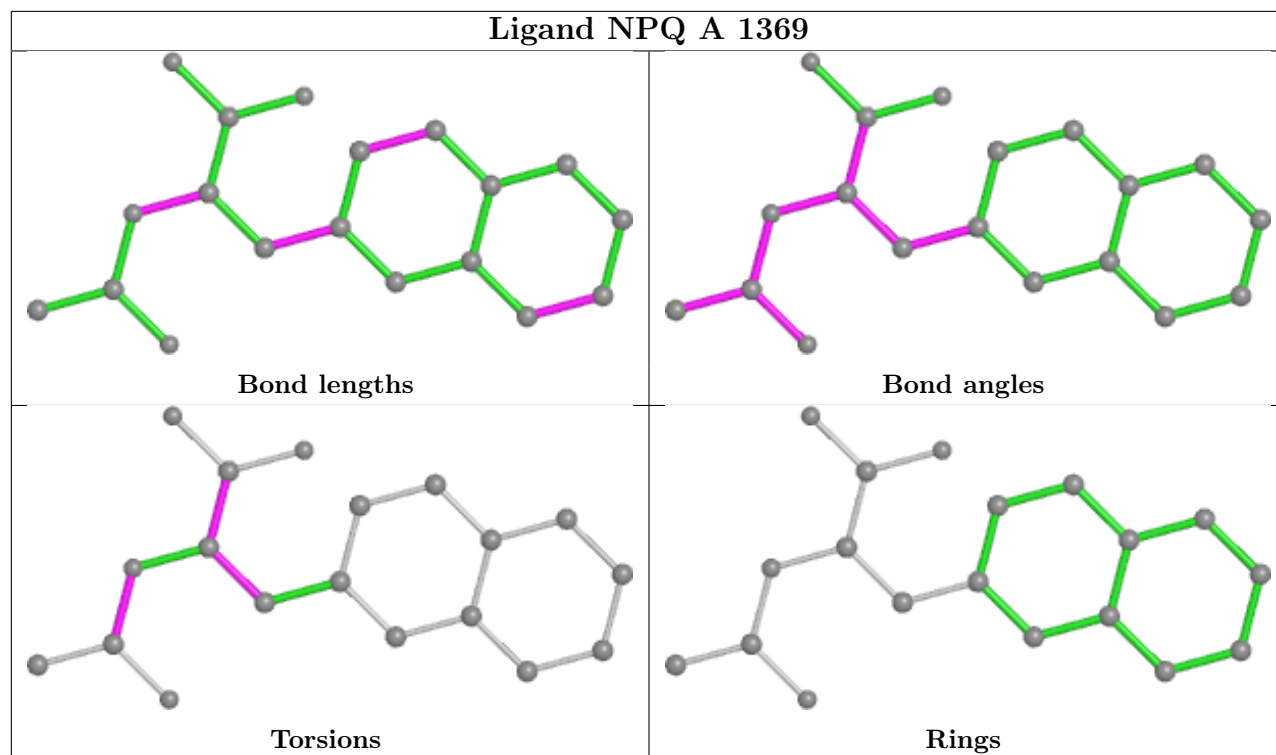
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1368	NPQ	1	0

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

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





## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	368/368 (100%)	-0.42	1 (0%) 94   94	28, 38, 59, 83	0
1	B	367/368 (99%)	-0.32	1 (0%) 94   94	30, 49, 72, 99	0
1	C	367/368 (99%)	-0.38	0 100   100	29, 50, 72, 112	0
1	D	367/368 (99%)	-0.25	0 100   100	29, 52, 78, 94	0
All	All	1469/1472 (99%)	-0.34	2 (0%) 95   96	28, 47, 72, 112	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	SER	2.4
1	B	367	GLY	2.1

### 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.

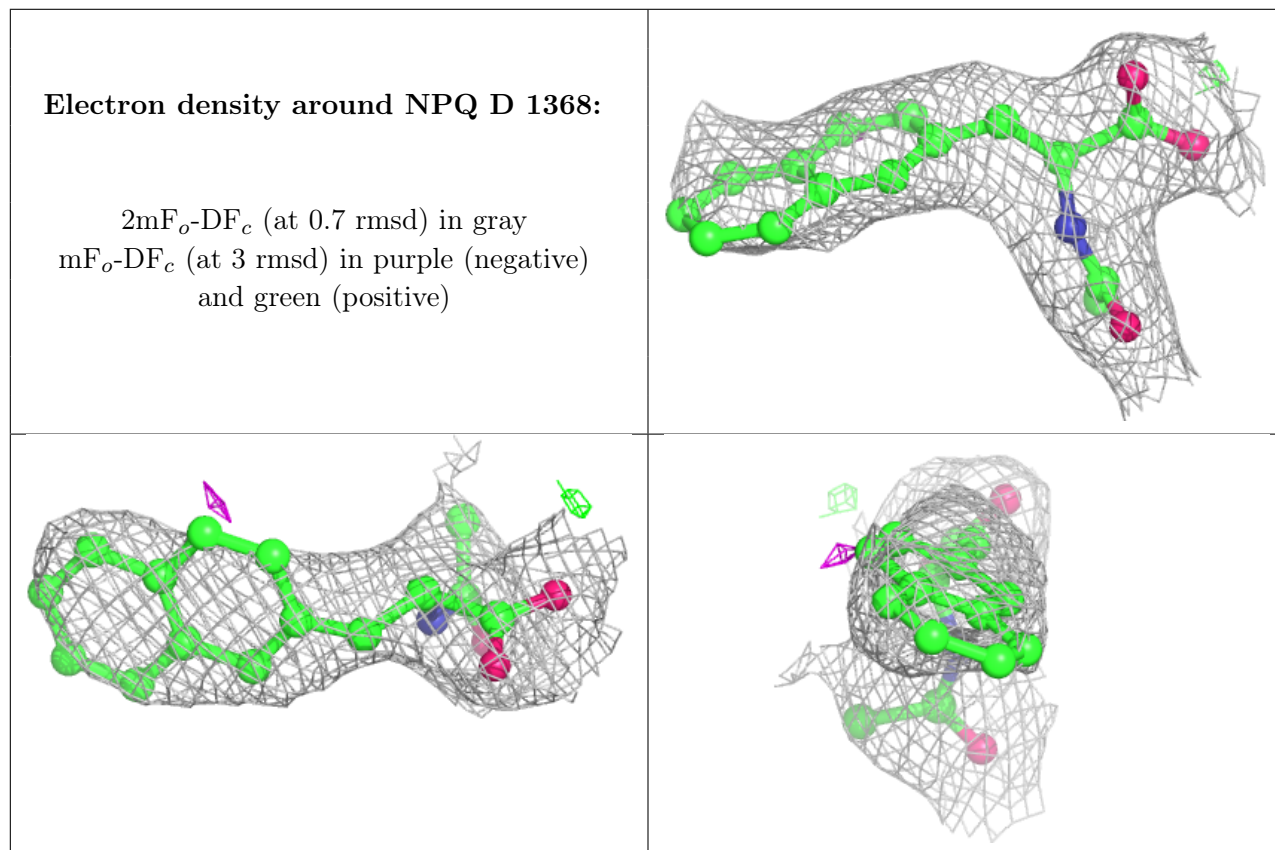
### 6.4 Ligands [i](#)

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.



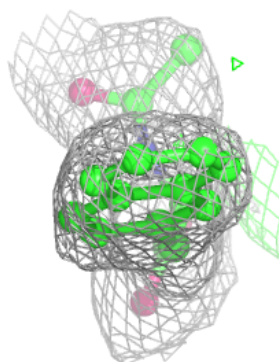
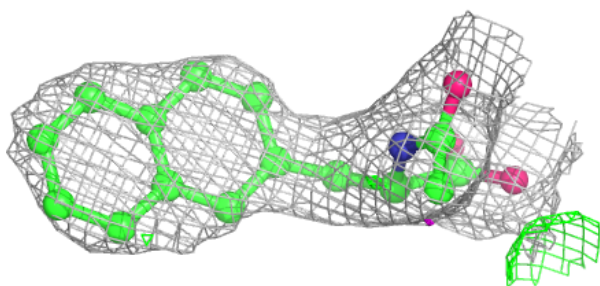
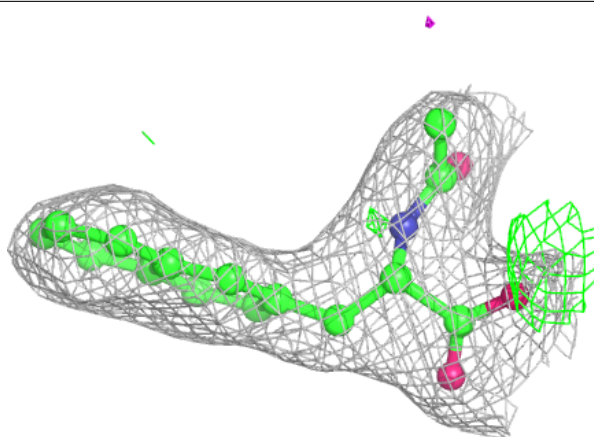
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	1369	1/1	0.91	0.09	58,58,58,58	0
2	NPQ	D	1368	19/19	0.95	0.18	44,59,95,97	0
3	MG	A	1370	1/1	0.96	0.11	42,42,42,42	0
2	NPQ	B	1368	19/19	0.96	0.16	41,61,80,80	0
2	NPQ	C	1368	19/19	0.97	0.13	40,50,66,68	0
2	NPQ	A	1369	19/19	0.98	0.16	31,40,46,61	0
3	MG	C	1369	1/1	0.98	0.04	52,52,52,52	0
3	MG	D	1369	1/1	0.98	0.12	54,54,54,54	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.

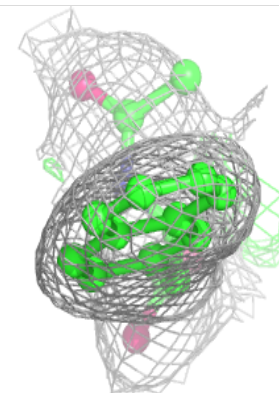
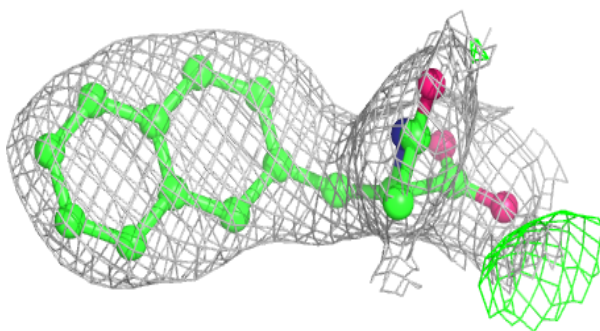
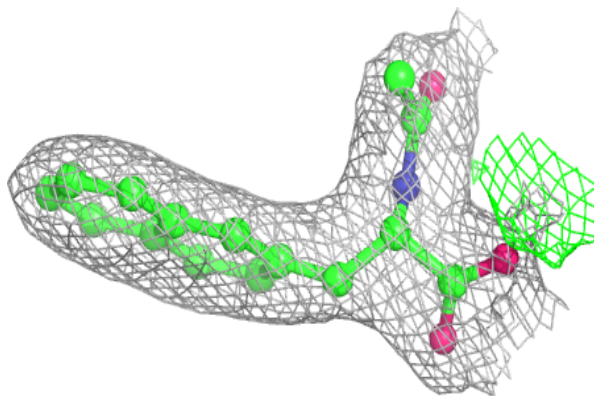


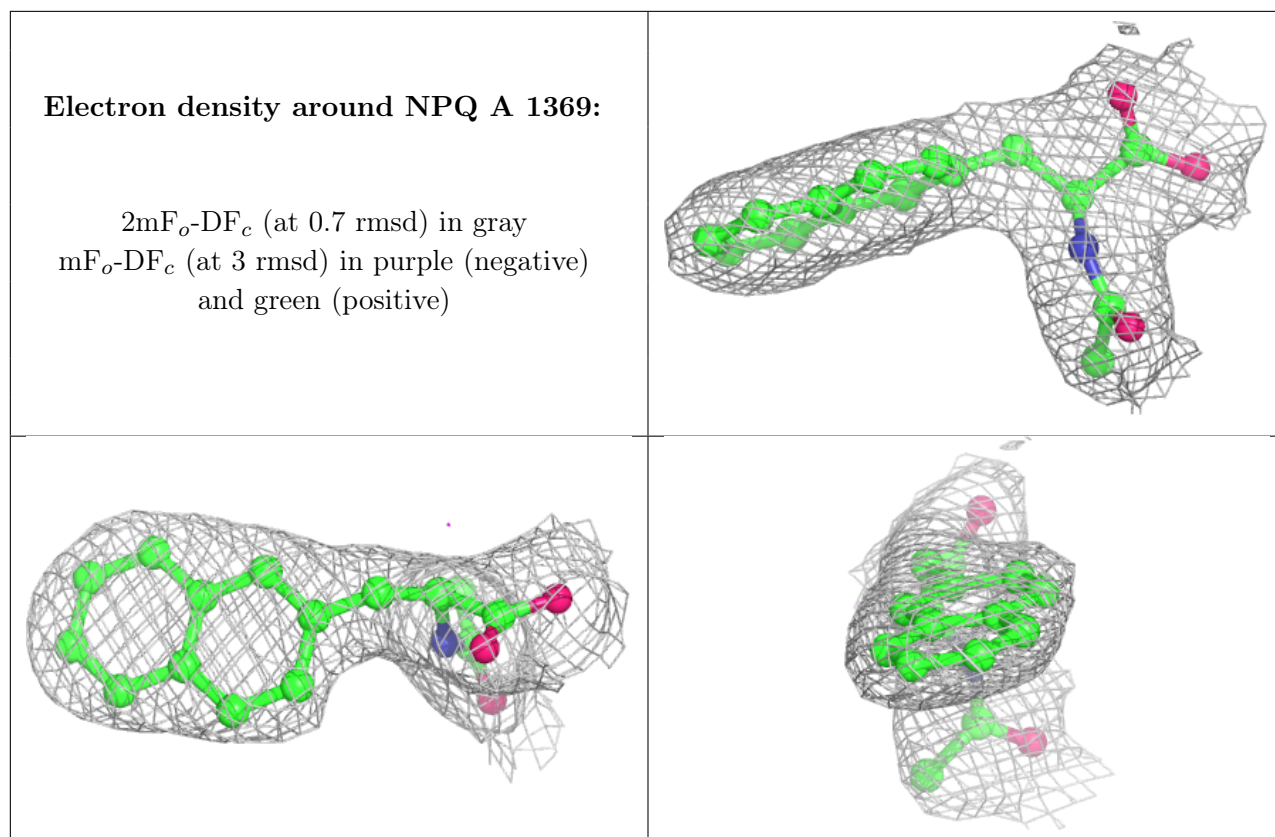
**Electron density around NPQ B 1368:**

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

**Electron density around NPQ C 1368:**

$2mF_o-DF_c$  (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.