



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:13 PM UTC

PDB ID : 1WDK / pdb_00001wdk
Title : fatty acid beta-oxidation multienzyme complex from *Pseudomonas fragi*, form I (native2)
Authors : Ishikawa, M.; Tsuchiya, D.; Oyama, T.; Tsunaka, Y.; Morikawa, K.
Deposited on : 2004-05-17
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

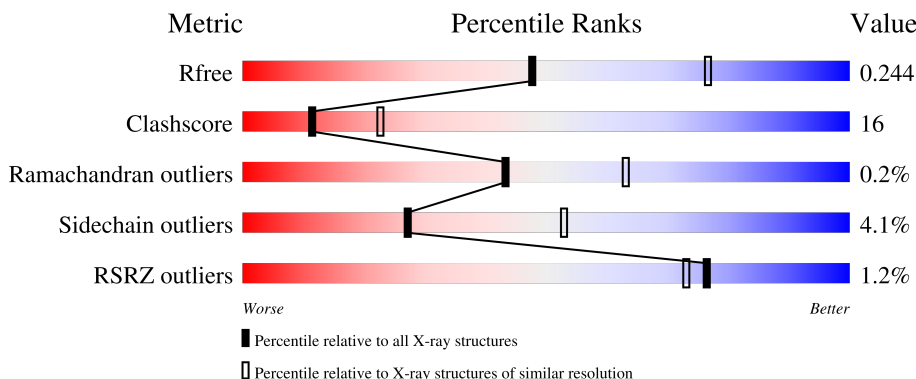
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	715	
1	B	715	
2	C	390	
2	D	390	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17701 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 Fatty oxidation complex alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	0	0
			5324	3400	894	1003	27			
1	B	711	Total	C	N	O	S	0	0	0
			5333	3404	898	1004	27			

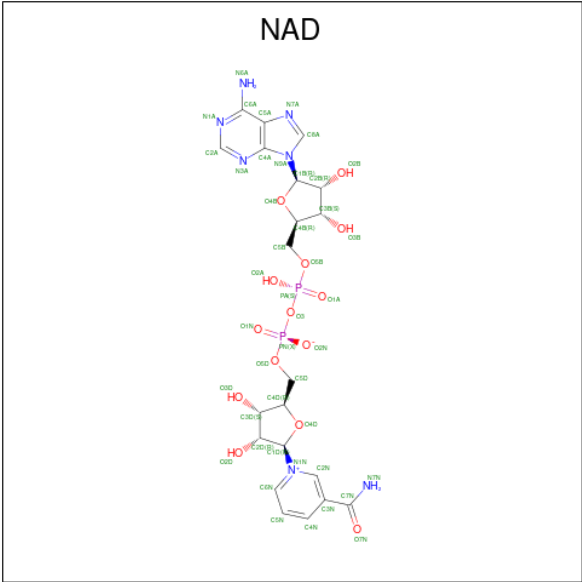
- Molecule 2 is a protein called 3-ketoacyl-CoA thiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	390	Total	C	N	O	S	0	0	0
			2893	1801	515	548	29			
2	D	390	Total	C	N	O	S	0	0	0
			2889	1798	514	548	29			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

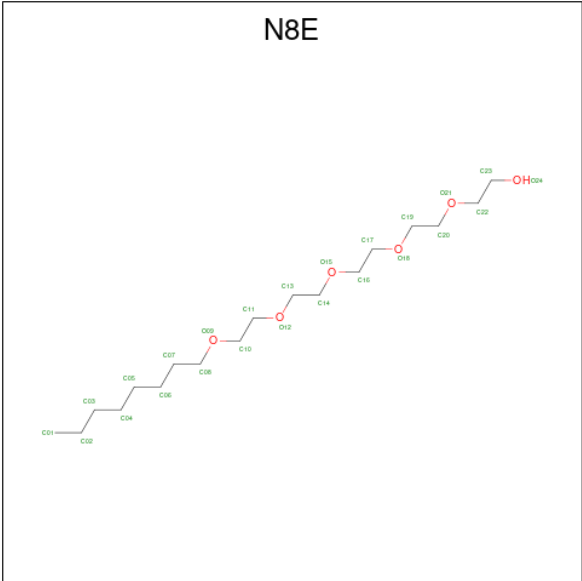
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (CCD ID: NAD) (formula: C₂₁H₂₇N₇O₁₄P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 44	C 21	N 7	O 14	P 2	0	0
4	B	1	Total 44	C 21	N 7	O 14	P 2	0	0

- Molecule 5 is 3,6,9,12,15-PENTAOXATRICOSAN-1-OL (CCD ID: N8E) (formula: C₁₈H₃₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			24	18	6		

Continued on next page...

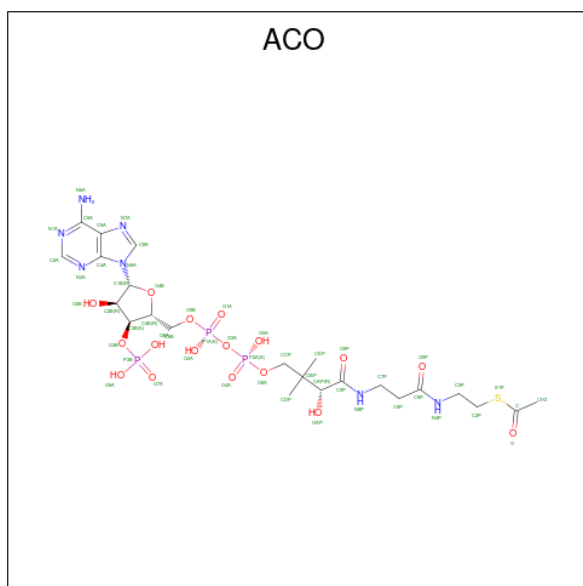
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			24	18	6		
5	B	1	Total	C	O	0	0
			24	18	6		
5	B	1	Total	C	O	0	0
			24	18	6		

- Molecule 6 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	1	Total	Hg	0	0
			1	1		
6	D	1	Total	Hg	0	0
			1	1		

- Molecule 7 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
7	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

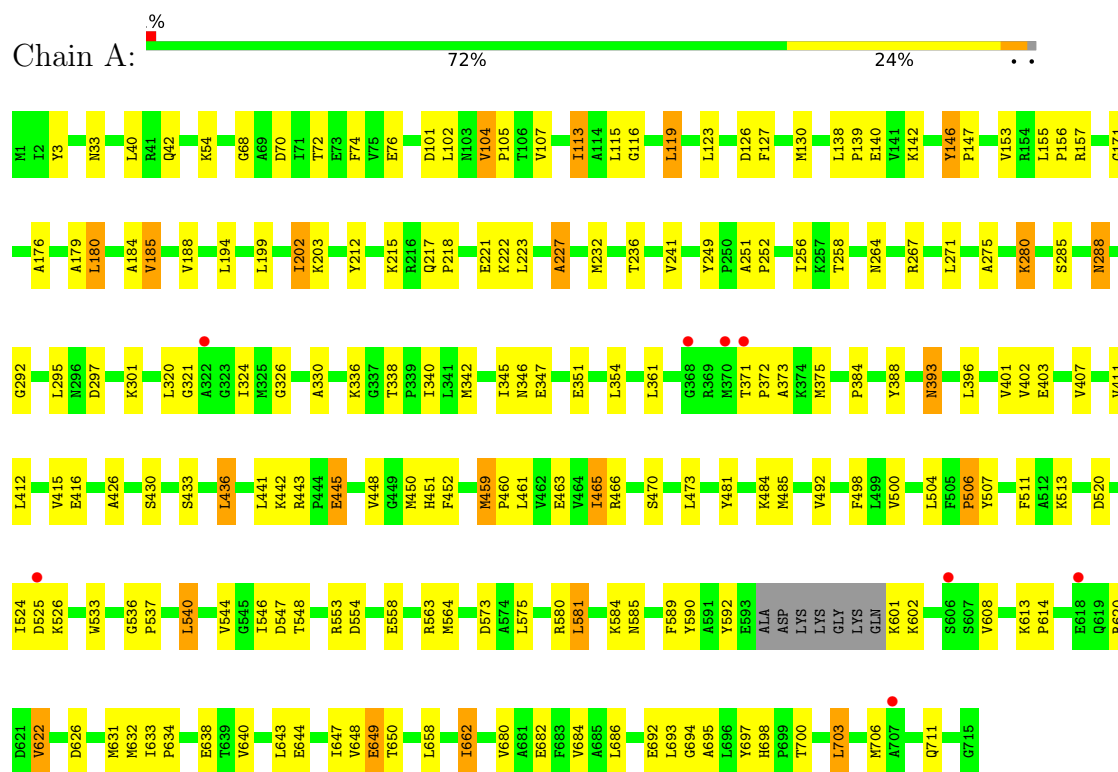
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	286	Total 286	O 286	0	0
8	B	309	Total 309	O 309	0	0
8	C	205	Total 205	O 205	0	0
8	D	173	Total 173	O 173	0	0

3 Residue-property plots

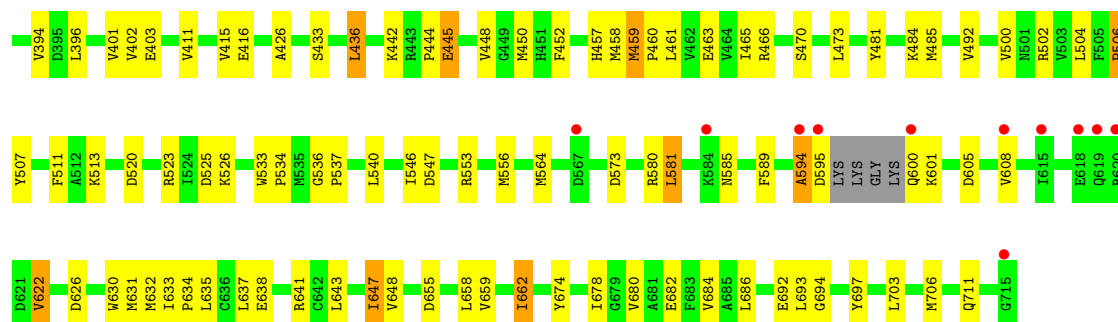
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



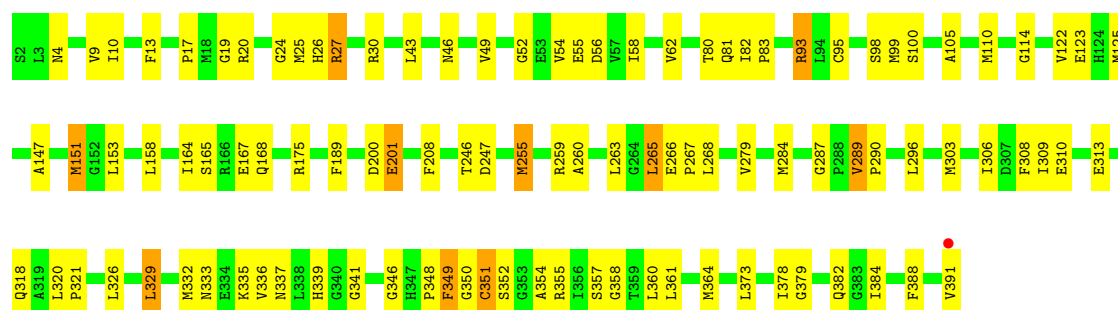
• Molecule 1: Fatty oxidation complex alpha subunit





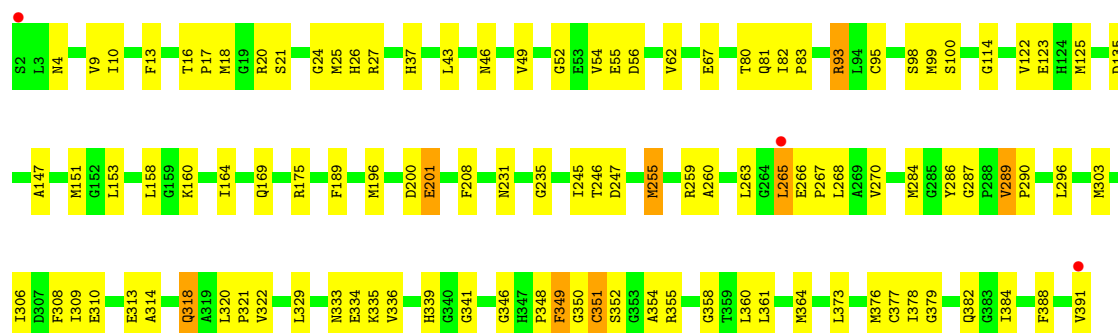
• Molecule 2: 3-ketoacyl-CoA thiolase

Chain C: 74% 24%



• Molecule 2: 3-ketoacyl-CoA thiolase

Chain D: 72% 26%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.71Å 94.58Å 160.00Å 90.00° 111.45° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.50) 95.1 (20.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.203 , 0.244 0.202 , 0.244	Depositor DCC
R_{free} test set	5875 reflections (7.09%)	wwPDB-VP
Wilson B-factor (Å ²)	28.5	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17701	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAD, ACO, N8E, HG

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	0.41	0/5410	0.92	16/7310 (0.2%)
1	B	0.42	0/5419	0.92	20/7325 (0.3%)
2	C	0.49	2/2941 (0.1%)	0.97	6/3967 (0.2%)
2	D	0.48	1/2937 (0.0%)	0.94	5/3963 (0.1%)
All	All	0.44	3/16707 (0.0%)	0.93	47/22565 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	255	MET	SD-CE	-7.59	1.60	1.79
2	C	151	MET	SD-CE	-6.16	1.64	1.79
2	D	255	MET	SD-CE	-5.12	1.66	1.79

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	TYR	CA-C-N	8.33	127.63	118.97
1	A	249	TYR	C-N-CA	8.33	127.63	118.97
2	C	93	ARG	N-CA-C	-8.19	100.74	110.41
2	C	352	SER	N-CA-C	8.08	120.80	111.11
1	B	249	TYR	CA-C-N	8.00	127.94	119.05
1	B	249	TYR	C-N-CA	8.00	127.94	119.05
1	B	184	ALA	N-CA-C	-7.95	102.60	111.82
2	D	352	SER	N-CA-C	7.89	120.57	111.11
1	B	227	ALA	N-CA-C	-7.73	102.93	111.36
1	A	184	ALA	N-CA-C	-7.45	103.18	111.82
1	A	227	ALA	N-CA-C	-7.12	103.52	111.28
1	B	500	VAL	N-CA-C	7.08	117.17	110.30
1	A	632	MET	N-CA-C	6.98	118.96	111.36
1	A	500	VAL	N-CA-C	6.68	116.78	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	268	LEU	N-CA-C	-6.62	103.88	112.23
1	B	632	MET	N-CA-C	6.62	118.58	111.36
2	D	17	PRO	N-CA-C	-6.61	100.81	111.19
1	B	267	ARG	N-CA-C	6.57	118.13	110.97
1	A	459	MET	CA-C-N	6.55	126.13	119.19
1	A	459	MET	C-N-CA	6.55	126.13	119.19
2	C	17	PRO	N-CA-C	-6.51	100.97	111.19
1	B	461	LEU	N-CA-C	6.13	119.89	110.20
1	A	581	LEU	N-CA-C	6.03	120.25	113.01
1	B	694	GLY	N-CA-C	5.97	118.49	111.63
2	D	93	ARG	N-CA-C	-5.90	100.68	109.83
1	B	581	LEU	N-CA-C	5.86	120.04	113.01
2	D	268	LEU	N-CA-C	-5.83	104.88	112.23
1	A	589	PHE	N-CA-C	-5.72	104.65	111.69
1	B	459	MET	CA-C-N	5.72	125.25	119.19
1	B	459	MET	C-N-CA	5.72	125.25	119.19
2	C	326	LEU	N-CA-C	-5.61	106.40	113.18
1	A	526	LYS	N-CA-C	-5.51	105.42	111.82
1	A	506	PRO	N-CA-C	-5.43	106.32	113.65
1	A	694	GLY	N-CA-C	5.40	118.64	110.97
1	B	526	LYS	N-CA-C	-5.39	105.57	111.82
1	B	161	VAL	N-CA-C	5.36	115.80	110.23
1	A	461	LEU	N-CA-C	5.33	118.36	110.48
1	B	594	ALA	N-CA-C	5.32	115.06	108.19
1	B	589	PHE	N-CA-C	-5.20	105.30	111.69
1	B	383	ARG	CA-C-N	5.15	125.09	119.78
1	B	383	ARG	C-N-CA	5.15	125.09	119.78
2	D	351	CYS	N-CA-C	5.15	118.72	112.23
1	A	649	GLU	N-CA-C	5.15	116.97	111.36
1	B	506	PRO	N-CA-C	-5.06	106.81	113.65
1	A	465	ILE	N-CA-C	5.05	115.95	108.23
1	B	154	ARG	N-CA-C	5.04	117.55	111.40
2	C	351	CYS	N-CA-C	5.04	118.58	112.23

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	5324	0	5391	165	0
1	B	5333	0	5385	159	0
2	C	2893	0	2903	112	0
2	D	2889	0	2892	118	0
3	A	1	0	0	0	0
4	A	44	0	26	2	0
4	B	44	0	26	2	0
5	A	48	0	76	8	0
5	B	48	0	76	8	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
7	C	51	0	34	3	0
7	D	51	0	34	4	0
8	A	286	0	0	8	0
8	B	309	0	0	13	0
8	C	205	0	0	4	0
8	D	173	0	0	9	0
All	All	17701	0	16843	540	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 16.

All (540) 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:525:ASP:HB2	1:B:536:GLY:HA3	1.23	1.17
1:A:525:ASP:HB2	1:A:536:GLY:HA3	1.21	1.13
1:A:695:ALA:HA	1:A:698:HIS:HD2	1.19	1.04
1:A:695:ALA:HA	1:A:698:HIS:CD2	1.93	1.02
1:B:595:ASP:HA	1:B:600:GLN:HA	1.41	1.00
2:C:360:LEU:HG	2:C:364:MET:HE2	1.43	0.98
1:B:320:LEU:HD11	1:B:415:VAL:HG21	1.46	0.97
2:C:125:MET:HE3	2:C:246:THR:H	1.28	0.97
1:A:320:LEU:HD11	1:A:415:VAL:HG21	1.50	0.93
2:D:125:MET:HE3	2:D:246:THR:H	1.34	0.91
1:B:130:MET:HE1	1:B:179:ALA:HB3	1.52	0.91
1:A:525:ASP:CB	1:A:536:GLY:HA3	2.01	0.91
1:A:130:MET:HE1	1:A:179:ALA:HB3	1.56	0.87
1:A:622:VAL:HG22	1:A:626:ASP:HB2	1.55	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:255:MET:HE1	2:D:263:LEU:HD12	1.57	0.84
1:B:525:ASP:CB	1:B:536:GLY:HA3	2.05	0.84
2:C:98:SER:HB3	2:C:354:ALA:H	1.43	0.84
2:D:98:SER:HB3	2:D:354:ALA:H	1.43	0.83
2:D:360:LEU:HG	2:D:364:MET:HE2	1.58	0.83
1:B:537:PRO:HG2	1:B:631:MET:HE3	1.61	0.82
1:B:706:MET:HB2	1:B:711:GLN:HB2	1.62	0.82
1:B:622:VAL:HG22	1:B:626:ASP:HB2	1.61	0.82
2:C:125:MET:HE2	2:C:348:PRO:HA	1.62	0.82
2:C:43:LEU:HD11	2:C:82:ILE:HD11	1.63	0.80
2:C:46:ASN:O	2:C:49:VAL:HG22	1.82	0.80
2:D:151:MET:HE3	2:D:284:MET:HE2	1.63	0.80
1:A:371:THR:HG22	1:A:373:ALA:H	1.47	0.79
2:D:151:MET:HE1	2:D:379:GLY:HA2	1.63	0.79
1:A:706:MET:HB2	1:A:711:GLN:HB2	1.65	0.79
1:B:371:THR:HG22	1:B:373:ALA:H	1.47	0.78
1:B:658:LEU:O	1:B:662:ILE:HG22	1.82	0.77
1:A:347:GLU:O	1:A:351:GLU:HG2	1.84	0.77
2:D:125:MET:HE3	2:D:246:THR:N	1.99	0.77
2:C:25:MET:HE2	2:C:26:HIS:CE1	2.21	0.76
2:C:125:MET:HE3	2:C:246:THR:N	2.00	0.76
2:C:55:GLU:HG3	2:C:114:GLY:HA2	1.68	0.76
1:B:401:VAL:HG12	1:B:402:VAL:N	2.01	0.75
2:C:265:LEU:HD23	2:C:265:LEU:H	1.52	0.75
2:D:265:LEU:H	2:D:265:LEU:HD23	1.51	0.74
1:B:502:ARG:HA	1:B:556:MET:HE2	1.70	0.74
2:C:255:MET:HE3	2:C:259:ARG:HB3	1.70	0.73
2:C:287:GLY:O	2:C:290:PRO:HD2	1.88	0.73
2:D:125:MET:HE2	2:D:348:PRO:HA	1.70	0.73
2:C:255:MET:HE1	2:C:263:LEU:HD12	1.69	0.73
1:A:232:MET:HE2	2:C:147:ALA:HB1	1.68	0.72
1:B:166:GLU:HG2	8:B:2272:HOH:O	1.89	0.72
2:D:80:THR:HG22	2:D:81:GLN:N	2.04	0.72
2:D:306:ILE:HD13	2:D:373:LEU:HB2	1.72	0.72
2:C:80:THR:HG22	2:C:81:GLN:N	2.05	0.72
1:A:537:PRO:HG2	1:A:631:MET:HE3	1.70	0.71
2:C:306:ILE:HD13	2:C:373:LEU:HB2	1.72	0.71
1:A:130:MET:HE1	1:A:179:ALA:CB	2.20	0.71
2:C:201:GLU:CD	2:C:201:GLU:H	1.99	0.71
2:D:313:GLU:CD	2:D:341:GLY:HA3	2.16	0.71
1:A:375:MET:HE2	1:B:375:MET:HE2	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ALA:HB3	1:B:252:PRO:HD3	1.73	0.70
2:D:46:ASN:O	2:D:49:VAL:HG22	1.90	0.70
1:A:506:PRO:HG2	1:A:638:GLU:HG2	1.73	0.70
2:C:255:MET:HE2	2:C:260:ALA:CA	2.21	0.70
1:B:34:ARG:HH22	5:B:2003:N8E:H221	1.57	0.69
1:A:554:ASP:O	1:A:558:GLU:HG3	1.92	0.69
1:B:232:MET:HE3	1:B:236:THR:CG2	2.22	0.69
1:A:401:VAL:HG12	1:A:402:VAL:N	2.05	0.69
2:C:99:MET:HB3	2:C:384:ILE:HD13	1.74	0.69
2:C:313:GLU:CD	2:C:341:GLY:HA3	2.18	0.69
1:A:525:ASP:HB3	1:A:537:PRO:HD2	1.75	0.69
1:B:347:GLU:O	1:B:351:GLU:HG2	1.92	0.69
2:C:151:MET:HE1	2:C:379:GLY:HA2	1.75	0.69
1:A:280:LYS:HB2	1:A:280:LYS:NZ	2.08	0.69
1:A:116:GLY:HA3	5:A:1003:N8E:H021	1.74	0.68
2:C:52:GLY:HA2	2:C:83:PRO:HG2	1.75	0.68
2:D:43:LEU:HD11	2:D:82:ILE:HD11	1.77	0.67
1:A:504:LEU:O	1:A:507:TYR:HB3	1.94	0.67
2:C:284:MET:HE1	7:C:3001:ACO:HH33	1.76	0.67
1:A:354:LEU:HD21	1:A:384:PRO:HG3	1.77	0.67
2:C:151:MET:HE2	7:C:3001:ACO:HH32	1.74	0.67
2:D:99:MET:HB3	2:D:384:ILE:HD13	1.76	0.67
1:B:157:ARG:HG3	1:B:223:LEU:HD23	1.76	0.67
2:D:263:LEU:HB2	2:D:265:LEU:CD2	2.25	0.67
2:D:263:LEU:HB2	2:D:265:LEU:HD22	1.77	0.67
1:A:251:ALA:HB3	1:A:252:PRO:HD3	1.76	0.66
2:D:55:GLU:HG3	2:D:114:GLY:HA2	1.77	0.66
2:D:95:CYS:SG	7:D:4001:ACO:HH32	2.35	0.66
1:A:361:LEU:HB3	1:A:375:MET:HG3	1.76	0.66
1:B:280:LYS:HB2	1:B:280:LYS:NZ	2.09	0.66
1:A:232:MET:HE3	1:A:236:THR:CG2	2.26	0.66
1:B:130:MET:HE1	1:B:179:ALA:CB	2.26	0.66
1:B:354:LEU:HD21	1:B:384:PRO:HG3	1.76	0.66
1:B:504:LEU:O	1:B:507:TYR:HB3	1.96	0.66
2:D:201:GLU:H	2:D:201:GLU:CD	2.02	0.66
2:C:55:GLU:HG3	2:C:114:GLY:CA	2.26	0.65
2:C:255:MET:HE2	2:C:260:ALA:HA	1.77	0.65
1:A:592:TYR:HA	1:A:601:LYS:O	1.96	0.65
2:D:255:MET:HE2	2:D:260:ALA:HA	1.79	0.65
1:A:113:ILE:HG23	1:A:115:LEU:HG	1.79	0.64
1:A:232:MET:HE1	2:C:153:LEU:HB3	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:MET:HE2	2:D:26:HIS:CE1	2.32	0.64
2:D:52:GLY:HA2	2:D:83:PRO:HG2	1.79	0.64
2:D:255:MET:HE2	2:D:260:ALA:CA	2.27	0.64
1:A:285:SER:HA	1:A:288:ASN:HD21	1.62	0.64
2:D:289:VAL:HG22	2:D:290:PRO:HD3	1.79	0.64
1:A:338:THR:OG1	1:A:484:LYS:HE3	1.97	0.64
1:B:537:PRO:HG2	1:B:631:MET:CE	2.25	0.64
2:D:98:SER:HB3	2:D:354:ALA:N	2.13	0.64
1:A:275:ALA:HB3	8:A:1095:HOH:O	1.98	0.64
1:B:506:PRO:HG3	1:B:564:MET:HE2	1.78	0.64
2:C:378:ILE:HB	2:C:382:GLN:HB2	1.79	0.64
2:D:125:MET:CE	2:D:246:THR:H	2.09	0.64
1:B:361:LEU:HB3	1:B:375:MET:HG3	1.80	0.64
1:B:140:GLU:HB2	1:B:146:TYR:HA	1.80	0.63
1:B:232:MET:HE2	2:D:147:ALA:HB1	1.80	0.63
1:B:288:ASN:N	1:B:288:ASN:HD22	1.95	0.63
2:C:98:SER:HB3	2:C:354:ALA:N	2.13	0.63
2:D:378:ILE:HB	2:D:382:GLN:HB2	1.80	0.63
1:A:130:MET:HE3	1:A:176:ALA:HA	1.81	0.62
1:B:213:LYS:HE3	8:B:2269:HOH:O	1.99	0.62
2:C:98:SER:CB	2:C:354:ALA:H	2.12	0.62
2:C:93:ARG:HH22	2:D:56:ASP:CG	2.07	0.62
2:C:255:MET:HE2	2:C:260:ALA:N	2.15	0.62
2:C:361:LEU:HA	2:C:364:MET:HE3	1.82	0.61
1:B:371:THR:HG22	1:B:373:ALA:N	2.15	0.61
2:D:265:LEU:HD23	2:D:265:LEU:N	2.15	0.61
1:A:537:PRO:HG2	1:A:631:MET:CE	2.29	0.61
1:B:506:PRO:HG2	1:B:638:GLU:HG2	1.82	0.61
2:C:263:LEU:HB2	2:C:265:LEU:HD22	1.81	0.61
2:D:55:GLU:HG3	2:D:114:GLY:CA	2.31	0.61
1:A:127:PHE:CE2	1:A:215:LYS:HD2	2.36	0.61
1:B:622:VAL:HG22	1:B:626:ASP:CB	2.30	0.61
1:A:140:GLU:HB2	1:A:146:TYR:HA	1.83	0.61
1:B:285:SER:HA	1:B:288:ASN:HD21	1.64	0.60
1:A:563:ARG:HH11	1:A:564:MET:HE3	1.66	0.60
1:B:232:MET:HE3	1:B:236:THR:HG21	1.82	0.60
1:A:288:ASN:N	1:A:288:ASN:HD22	1.98	0.60
2:C:260:ALA:O	2:C:265:LEU:HD23	2.00	0.60
1:B:338:THR:OG1	1:B:484:LYS:HE3	2.02	0.60
2:D:296:LEU:HD21	2:D:306:ILE:HD11	1.83	0.60
1:A:547:ASP:HB3	1:A:581:LEU:HD22	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:MET:HE2	2:C:147:ALA:CB	2.30	0.60
1:B:401:VAL:CG1	1:B:402:VAL:N	2.64	0.60
2:C:56:ASP:CG	2:D:93:ARG:HH22	2.08	0.60
2:C:255:MET:HE3	2:C:259:ARG:CB	2.32	0.59
1:A:371:THR:HG22	1:A:373:ALA:N	2.16	0.59
1:B:525:ASP:HB3	1:B:537:PRO:HD2	1.83	0.59
2:D:98:SER:CB	2:D:354:ALA:H	2.12	0.59
2:D:284:MET:SD	7:D:4001:ACO:HH33	2.42	0.59
1:A:372:PRO:O	1:B:375:MET:HE1	2.02	0.59
1:A:581:LEU:HB2	1:A:585:ASN:HB2	1.83	0.59
2:C:93:ARG:HG2	2:C:378:ILE:HD13	1.85	0.59
2:D:303:MET:HE2	2:D:309:ILE:HD11	1.85	0.59
1:B:130:MET:CE	1:B:176:ALA:HA	2.32	0.59
1:B:34:ARG:NH2	5:B:2003:N8E:H201	2.18	0.58
2:C:246:THR:HB	2:C:348:PRO:HG3	1.85	0.58
2:C:360:LEU:CG	2:C:364:MET:HE2	2.28	0.58
1:B:457:HIS:CE1	1:B:458:MET:HG2	2.39	0.58
2:C:125:MET:CE	2:C:246:THR:H	2.10	0.58
2:D:151:MET:HE3	2:D:284:MET:CE	2.33	0.58
2:D:260:ALA:O	2:D:265:LEU:HD23	2.04	0.58
2:D:160:LYS:HE2	8:D:4140:HOH:O	2.03	0.58
1:A:232:MET:HE3	1:A:236:THR:HG21	1.85	0.58
2:C:200:ASP:HB2	2:C:201:GLU:OE2	2.04	0.58
1:A:533:TRP:HZ3	1:A:662:ILE:HG23	1.68	0.58
1:A:620:ARG:HH12	1:A:692:GLU:CD	2.11	0.58
1:B:401:VAL:HG12	1:B:402:VAL:H	1.67	0.58
1:A:563:ARG:NH1	1:A:564:MET:HE3	2.18	0.58
1:B:450:MET:HG2	1:B:452:PHE:CE1	2.38	0.58
1:A:288:ASN:H	1:A:288:ASN:ND2	2.02	0.57
2:C:80:THR:HG22	2:C:82:ILE:H	1.70	0.57
2:C:164:ILE:CD1	2:C:321:PRO:HG3	2.35	0.57
1:B:71:ILE:HD11	1:B:291:ILE:HG23	1.86	0.57
1:B:459:MET:HB3	8:B:2252:HOH:O	2.04	0.57
1:B:157:ARG:HD3	1:B:221:GLU:O	2.04	0.57
2:C:175:ARG:NH2	2:C:336:VAL:O	2.37	0.57
1:A:649:GLU:HG2	1:A:650:THR:HG23	1.87	0.57
2:C:56:ASP:OD1	2:D:93:ARG:NH2	2.38	0.57
1:A:105:PRO:HG3	1:A:212:TYR:CD2	2.40	0.57
1:A:101:ASP:CG	1:A:267:ARG:HH22	2.12	0.57
1:A:388:TYR:CE2	1:A:415:VAL:HG22	2.40	0.57
1:A:401:VAL:CG1	1:A:402:VAL:N	2.68	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:ARG:NH2	1:A:692:GLU:OE1	2.37	0.56
1:B:581:LEU:HB2	1:B:585:ASN:HB2	1.86	0.56
1:B:130:MET:HE3	1:B:176:ALA:HA	1.88	0.56
1:B:388:TYR:CE2	1:B:415:VAL:HG22	2.40	0.56
2:C:246:THR:HG22	2:C:247:ASP:N	2.20	0.56
2:D:164:ILE:CD1	2:D:321:PRO:HG3	2.35	0.56
1:B:88:GLY:HA3	5:B:2003:N8E:H162	1.87	0.56
1:B:232:MET:CE	1:B:236:THR:HG21	2.35	0.56
1:B:288:ASN:N	1:B:288:ASN:ND2	2.53	0.56
2:C:263:LEU:HB2	2:C:265:LEU:CD2	2.35	0.56
2:C:391:VAL:HG13	2:C:391:VAL:O	2.05	0.56
2:D:246:THR:HG22	2:D:247:ASP:N	2.20	0.56
1:A:375:MET:HE1	1:B:372:PRO:O	2.06	0.56
1:B:401:VAL:CG1	1:B:402:VAL:H	2.18	0.56
2:C:284:MET:CE	7:C:3001:ACO:HH33	2.35	0.56
2:D:80:THR:HG22	2:D:81:GLN:H	1.71	0.56
2:D:122:VAL:HG22	2:D:123:GLU:N	2.20	0.56
2:D:361:LEU:HD23	2:D:364:MET:HE3	1.88	0.56
1:A:459:MET:HE1	5:A:1002:N8E:H112	1.87	0.56
1:A:622:VAL:HG22	1:A:626:ASP:CB	2.33	0.56
2:C:80:THR:CG2	2:C:81:GLN:N	2.68	0.56
2:C:122:VAL:HG22	2:C:123:GLU:N	2.19	0.56
2:D:151:MET:HE1	2:D:379:GLY:CA	2.35	0.56
1:B:285:SER:O	1:B:288:ASN:ND2	2.39	0.56
1:B:523:ARG:HH22	1:B:622:VAL:HG12	1.71	0.56
2:D:80:THR:CG2	2:D:81:GLN:N	2.68	0.56
1:A:492:VAL:HG13	1:A:647:ILE:HG23	1.87	0.55
1:B:523:ARG:NH2	1:B:622:VAL:HG12	2.21	0.55
2:C:361:LEU:HD23	2:C:364:MET:CE	2.37	0.55
1:A:74:PHE:HZ	5:A:1003:N8E:H031	1.71	0.55
2:C:296:LEU:HD21	2:C:306:ILE:HD11	1.88	0.55
1:B:157:ARG:NH2	8:B:2033:HOH:O	2.39	0.55
2:D:287:GLY:O	2:D:290:PRO:HD2	2.06	0.55
1:B:101:ASP:CG	1:B:267:ARG:HH22	2.15	0.55
2:D:376:MET:HB2	8:D:4174:HOH:O	2.06	0.55
2:D:391:VAL:HG13	2:D:391:VAL:O	2.06	0.55
2:C:20:ARG:O	2:C:24:GLY:HA3	2.06	0.55
2:C:265:LEU:HD23	2:C:265:LEU:N	2.19	0.55
1:A:113:ILE:CG2	1:A:115:LEU:HG	2.36	0.55
1:A:105:PRO:HG3	1:A:212:TYR:CE2	2.41	0.55
1:B:403:GLU:HG2	4:B:2001:NAD:H3D	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:VAL:HG13	1:B:647:ILE:HG23	1.89	0.55
1:A:232:MET:CE	1:A:236:THR:HG21	2.36	0.54
2:D:255:MET:HE3	2:D:259:ARG:HB3	1.89	0.54
1:A:320:LEU:CD1	1:A:415:VAL:HG21	2.32	0.54
1:B:594:ALA:H	1:B:601:LYS:CB	2.20	0.54
2:D:175:ARG:NH1	2:D:333:ASN:OD1	2.40	0.54
1:A:288:ASN:N	1:A:288:ASN:ND2	2.52	0.54
1:A:416:GLU:OE1	1:A:442:LYS:HG2	2.08	0.54
2:D:9:VAL:HG13	2:D:267:PRO:HB3	1.89	0.54
1:A:138:LEU:O	1:A:171:GLY:HA2	2.07	0.54
1:B:34:ARG:HH22	5:B:2003:N8E:H201	1.72	0.54
1:B:232:MET:HE2	2:D:147:ALA:CB	2.37	0.54
2:C:27:ARG:HD2	8:C:3099:HOH:O	2.08	0.54
1:B:280:LYS:HB2	1:B:280:LYS:HZ3	1.71	0.54
1:B:336:LYS:HB2	8:B:2289:HOH:O	2.08	0.54
2:C:80:THR:CG2	2:C:82:ILE:HG12	2.38	0.54
1:B:113:ILE:HG22	1:B:115:LEU:HG	1.89	0.53
2:C:289:VAL:HG22	2:C:290:PRO:HD3	1.89	0.53
1:A:466:ARG:HG3	1:A:470:SER:HB2	1.89	0.53
1:A:393:ASN:C	1:A:393:ASN:HD22	2.16	0.53
2:C:339:HIS:HD2	8:C:3193:HOH:O	1.90	0.53
1:A:553:ARG:HH12	1:A:573:ASP:CG	2.17	0.53
1:B:113:ILE:CG2	1:B:115:LEU:HG	2.39	0.53
1:B:250:PRO:HD2	8:B:2065:HOH:O	2.09	0.53
1:B:288:ASN:ND2	1:B:288:ASN:H	2.07	0.53
2:C:93:ARG:NH2	2:D:56:ASP:OD1	2.42	0.53
2:D:175:ARG:NH2	2:D:336:VAL:O	2.41	0.53
1:A:199:LEU:HD11	1:A:203:LYS:NZ	2.24	0.52
1:A:481:TYR:CE2	1:A:485:MET:HE2	2.44	0.52
1:B:232:MET:HE3	1:B:236:THR:HG23	1.90	0.52
1:A:180:LEU:HG	1:A:188:VAL:HG23	1.90	0.52
1:A:321:GLY:O	1:A:326:GLY:HA3	2.09	0.52
1:B:325:MET:O	1:B:329:ILE:HG13	2.08	0.52
1:B:682:GLU:OE1	1:B:682:GLU:N	2.39	0.52
2:C:260:ALA:HA	2:C:265:LEU:HD21	1.90	0.52
2:C:175:ARG:NH1	2:C:333:ASN:OD1	2.42	0.52
1:B:466:ARG:HG3	1:B:470:SER:HB2	1.91	0.52
2:C:93:ARG:HD2	2:C:100:SER:OG	2.09	0.52
1:B:553:ARG:HH12	1:B:573:ASP:CG	2.18	0.52
2:D:25:MET:HE1	2:D:208:PHE:HB2	1.92	0.52
2:D:334:GLU:HB2	8:D:4020:HOH:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:167:GLU:HG3	8:C:3107:HOH:O	2.08	0.52
1:A:157:ARG:NH2	8:A:1216:HOH:O	2.41	0.52
1:A:590:TYR:CE2	1:A:602:LYS:HE2	2.45	0.52
1:A:640:VAL:O	1:A:644:GLU:HG3	2.10	0.52
1:B:232:MET:HE1	2:D:153:LEU:HB3	1.91	0.52
1:B:321:GLY:O	1:B:326:GLY:HA3	2.09	0.52
2:D:93:ARG:HG2	2:D:378:ILE:HD13	1.91	0.52
2:D:20:ARG:O	2:D:24:GLY:HA3	2.10	0.52
2:D:151:MET:HG2	8:D:4172:HOH:O	2.09	0.52
2:D:255:MET:HE2	2:D:260:ALA:N	2.25	0.52
2:D:263:LEU:CB	2:D:265:LEU:HD22	2.40	0.52
2:C:19:GLY:O	2:C:246:THR:HG23	2.10	0.52
1:A:241:VAL:HG21	1:A:256:ILE:HD11	1.91	0.51
1:A:72:THR:O	1:A:76:GLU:HG3	2.10	0.51
1:B:155:LEU:HB3	1:B:156:PRO:HD3	1.92	0.51
1:B:140:GLU:HG3	1:B:147:PRO:N	2.25	0.51
1:B:595:ASP:HA	1:B:600:GLN:CA	2.27	0.51
1:A:157:ARG:HG3	1:A:223:LEU:HD23	1.91	0.51
2:C:9:VAL:HG13	2:C:267:PRO:HB3	1.93	0.51
2:C:361:LEU:HD23	2:C:364:MET:HE3	1.92	0.51
1:B:3:TYR:OH	1:B:42:GLN:NE2	2.44	0.51
2:D:314:ALA:HB2	7:D:4001:ACO:O	2.10	0.51
2:D:289:VAL:HG22	2:D:290:PRO:CD	2.40	0.51
2:C:165:SER:OG	2:C:168:GLN:HG3	2.11	0.51
1:A:74:PHE:CZ	5:A:1003:N8E:H031	2.46	0.50
1:A:403:GLU:HG2	4:A:1001:NAD:H3D	1.92	0.50
1:B:116:GLY:HA2	1:B:140:GLU:OE1	2.11	0.50
1:B:445:GLU:CD	1:B:445:GLU:H	2.18	0.50
1:A:393:ASN:C	1:A:393:ASN:ND2	2.69	0.50
1:A:68:GLY:HA3	5:A:1003:N8E:H032	1.93	0.50
2:D:296:LEU:HD21	2:D:306:ILE:CD1	2.42	0.50
1:A:153:VAL:HG21	1:A:271:LEU:HD23	1.94	0.50
2:C:49:VAL:HG23	2:C:49:VAL:O	2.10	0.50
2:D:260:ALA:HA	2:D:265:LEU:HD21	1.94	0.50
2:D:364:MET:HE1	2:D:388:PHE:HB2	1.94	0.50
1:B:199:LEU:HD11	1:B:203:LYS:NZ	2.26	0.50
1:A:155:LEU:HB3	1:A:156:PRO:HD3	1.93	0.49
1:A:430:SER:HB3	1:A:451:HIS:NE2	2.26	0.49
1:A:401:VAL:CG1	1:A:402:VAL:H	2.24	0.49
1:B:460:PRO:HG2	5:B:2002:N8E:H142	1.94	0.49
2:C:80:THR:HG22	2:C:81:GLN:H	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:310:GLU:HG3	2:C:360:LEU:HB2	1.94	0.49
2:D:98:SER:OG	2:D:350:GLY:O	2.23	0.49
2:D:265:LEU:CD2	2:D:265:LEU:N	2.75	0.49
1:A:511:PHE:CD1	1:A:631:MET:HE1	2.48	0.49
1:B:312:LYS:HD3	8:B:2127:HOH:O	2.12	0.49
2:C:80:THR:HG21	2:C:82:ILE:HG12	1.95	0.49
1:A:227:ALA:HB3	8:A:1244:HOH:O	2.13	0.49
2:C:4:ASN:HB3	8:C:3116:HOH:O	2.13	0.49
1:B:416:GLU:OE1	1:B:442:LYS:HG2	2.12	0.49
1:B:20:LEU:HD23	1:B:20:LEU:C	2.38	0.49
1:A:411:VAL:O	1:A:415:VAL:HG23	2.13	0.49
2:C:255:MET:HE3	2:C:259:ARG:CG	2.43	0.49
2:C:296:LEU:HD21	2:C:306:ILE:CD1	2.42	0.49
2:D:54:VAL:HG21	2:D:82:ILE:CD1	2.41	0.49
1:A:684:VAL:HG22	1:A:703:LEU:HD22	1.94	0.49
2:D:164:ILE:HG22	2:D:169:GLN:HE21	1.77	0.49
1:A:68:GLY:HA2	5:A:1003:N8E:H012	1.95	0.48
2:C:98:SER:OG	2:C:350:GLY:O	2.27	0.48
2:D:13:PHE:CZ	2:D:358:GLY:HA3	2.48	0.48
1:A:547:ASP:OD1	1:A:548:THR:N	2.46	0.48
2:D:13:PHE:CE2	2:D:358:GLY:HA3	2.48	0.48
1:B:330:ALA:HA	1:B:340:ILE:HD13	1.95	0.48
1:B:138:LEU:O	1:B:171:GLY:HA2	2.13	0.48
1:A:199:LEU:C	1:A:199:LEU:HD13	2.39	0.48
2:D:80:THR:CG2	2:D:81:GLN:H	2.26	0.48
1:A:157:ARG:HD3	1:A:221:GLU:O	2.13	0.48
1:B:80:LEU:O	1:B:283:LYS:NZ	2.47	0.48
2:D:67:GLU:HG3	8:D:4069:HOH:O	2.13	0.48
1:A:388:TYR:HE2	1:A:415:VAL:HG22	1.79	0.48
1:A:511:PHE:HD1	1:A:631:MET:HE1	1.78	0.48
2:C:265:LEU:CD2	2:C:265:LEU:N	2.77	0.48
2:D:80:THR:HG22	2:D:82:ILE:H	1.78	0.48
1:A:140:GLU:HG3	1:A:147:PRO:N	2.29	0.48
2:C:329:LEU:HD23	2:C:332:MET:HE3	1.96	0.48
1:B:511:PHE:HD1	1:B:631:MET:HE1	1.79	0.48
5:B:2003:N8E:H081	8:B:2309:HOH:O	2.13	0.48
2:C:110:MET:HE1	8:D:4049:HOH:O	2.13	0.48
2:D:4:ASN:HB3	8:D:4127:HOH:O	2.13	0.48
1:B:130:MET:HE2	1:B:185:VAL:HG21	1.96	0.47
1:A:330:ALA:HA	1:A:340:ILE:HD13	1.96	0.47
1:A:580:ARG:CZ	1:A:608:VAL:HG22	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:MET:HE2	1:B:382:ILE:HG21	1.95	0.47
2:C:10:ILE:HD12	2:C:10:ILE:N	2.29	0.47
2:D:310:GLU:HG3	2:D:360:LEU:HB2	1.96	0.47
1:A:684:VAL:CG2	1:A:703:LEU:HD22	2.44	0.47
1:B:361:LEU:HD21	1:B:378:VAL:HG11	1.97	0.47
1:B:511:PHE:CD1	1:B:631:MET:HE1	2.49	0.47
2:D:93:ARG:HD2	2:D:100:SER:OG	2.14	0.47
1:A:658:LEU:O	1:A:662:ILE:HG22	2.14	0.47
1:B:674:TYR:CZ	1:B:678:ILE:HD11	2.50	0.47
1:B:127:PHE:CE2	1:B:215:LYS:HD2	2.49	0.47
1:A:54:LYS:C	1:A:104:VAL:HG22	2.40	0.47
1:A:280:LYS:HB2	1:A:280:LYS:HZ3	1.77	0.47
1:A:232:MET:HE3	1:A:236:THR:HG23	1.96	0.47
1:A:347:GLU:HA	1:A:347:GLU:OE2	2.15	0.47
1:A:584:LYS:HG3	1:A:585:ASN:N	2.30	0.47
2:D:303:MET:CE	2:D:309:ILE:HD11	2.45	0.47
1:A:33:ASN:HB3	8:A:1230:HOH:O	2.15	0.46
1:B:180:LEU:HG	1:B:188:VAL:HG23	1.96	0.46
1:A:130:MET:CE	1:A:176:ALA:HA	2.43	0.46
2:C:122:VAL:CG2	2:C:123:GLU:N	2.78	0.46
1:A:401:VAL:HG12	1:A:402:VAL:H	1.75	0.46
2:D:361:LEU:HD23	2:D:364:MET:CE	2.45	0.46
1:B:320:LEU:CD1	1:B:415:VAL:HG21	2.31	0.46
2:C:151:MET:HE3	2:C:284:MET:HE2	1.98	0.46
2:D:10:ILE:N	2:D:10:ILE:HD12	2.30	0.46
1:A:445:GLU:CD	1:A:445:GLU:H	2.24	0.46
1:B:635:LEU:C	1:B:635:LEU:HD23	2.40	0.46
1:B:433:SER:HB3	1:B:436:LEU:HB2	1.96	0.46
1:B:77:ASN:HD21	5:B:2003:N8E:H112	1.80	0.46
2:C:189:PHE:CZ	2:C:339:HIS:HB3	2.50	0.46
1:A:692:GLU:HG3	1:A:693:LEU:N	2.31	0.46
1:B:72:THR:O	1:B:76:GLU:HG3	2.16	0.46
1:A:217:GLN:HB3	1:A:218:PRO:HD3	1.97	0.46
1:A:292:GLY:HA2	1:A:295:LEU:HD12	1.98	0.46
1:A:682:GLU:OE1	1:A:682:GLU:N	2.42	0.46
1:A:119:LEU:HD22	1:A:123:LEU:HG	1.97	0.46
1:A:373:ALA:HA	1:B:362:VAL:HG21	1.98	0.46
1:A:533:TRP:CZ3	1:A:662:ILE:HG23	2.49	0.45
1:A:285:SER:O	1:A:288:ASN:ND2	2.48	0.45
1:B:105:PRO:HG3	1:B:212:TYR:CD2	2.52	0.45
1:B:426:ALA:HA	1:B:448:VAL:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ALA:O	1:B:290:LEU:HG	2.16	0.45
1:A:680:VAL:O	1:A:684:VAL:HG23	2.15	0.45
1:B:54:LYS:C	1:B:104:VAL:CG2	2.90	0.45
2:C:201:GLU:CD	2:C:201:GLU:N	2.72	0.45
2:D:37:HIS:HD2	2:D:196:MET:HE3	1.81	0.45
2:D:200:ASP:HB2	2:D:201:GLU:OE2	2.16	0.45
1:B:146:TYR:CD1	1:B:146:TYR:C	2.95	0.45
1:B:547:ASP:HB3	1:B:581:LEU:HD22	1.98	0.45
2:D:9:VAL:HG22	2:D:270:VAL:HG22	1.99	0.45
2:D:164:ILE:HD11	2:D:321:PRO:HG3	1.99	0.45
1:B:403:GLU:HG2	4:B:2001:NAD:C3D	2.46	0.45
2:C:246:THR:HG22	2:C:247:ASP:H	1.81	0.45
1:A:222:LYS:HB2	1:A:264:ASN:HA	1.99	0.45
2:D:255:MET:HE3	2:D:259:ARG:CB	2.47	0.45
2:D:360:LEU:CG	2:D:364:MET:HE2	2.37	0.45
2:D:308:PHE:HA	2:D:335:LYS:HB2	1.99	0.45
1:B:222:LYS:HB2	1:B:264:ASN:HA	1.97	0.45
1:B:241:VAL:HG21	1:B:256:ILE:HD11	1.99	0.45
2:C:246:THR:OG1	2:C:346:GLY:HA3	2.16	0.45
1:A:280:LYS:HB2	1:A:280:LYS:HZ2	1.82	0.44
1:A:575:LEU:HD22	1:A:580:ARG:HD3	1.99	0.44
1:B:54:LYS:C	1:B:104:VAL:HG22	2.42	0.44
1:B:213:LYS:HG3	8:B:2269:HOH:O	2.17	0.44
2:C:164:ILE:HD11	2:C:321:PRO:HG3	1.99	0.44
2:C:255:MET:CE	2:C:259:ARG:C	2.90	0.44
1:A:336:LYS:HE2	8:A:1189:HOH:O	2.16	0.44
1:A:466:ARG:NH2	8:A:1179:HOH:O	2.49	0.44
1:B:463:GLU:O	1:B:465:ILE:HD12	2.17	0.44
1:A:139:PRO:O	1:A:142:LYS:HB2	2.17	0.44
1:A:433:SER:HB3	1:A:436:LEU:HB2	1.99	0.44
1:B:139:PRO:O	1:B:142:LYS:HB2	2.18	0.44
1:B:580:ARG:CZ	1:B:608:VAL:HG22	2.47	0.44
2:C:80:THR:CG2	2:C:81:GLN:H	2.29	0.44
1:B:466:ARG:HD3	8:B:2234:HOH:O	2.17	0.44
1:B:120:GLU:OE1	5:B:2003:N8E:H011	2.18	0.43
1:B:388:TYR:HE2	1:B:415:VAL:HG22	1.82	0.43
1:B:680:VAL:O	1:B:684:VAL:HG23	2.18	0.43
1:A:465:ILE:HG12	1:A:498:PHE:CD2	2.53	0.43
1:B:481:TYR:CE2	1:B:485:MET:HE2	2.52	0.43
1:B:637:LEU:O	1:B:641:ARG:HG3	2.18	0.43
2:D:246:THR:OG1	2:D:346:GLY:HA3	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:MET:HE2	1:A:185:VAL:HG21	1.99	0.43
1:A:199:LEU:HD11	1:A:203:LYS:CE	2.48	0.43
1:A:407:VAL:O	1:A:411:VAL:HG23	2.18	0.43
1:B:320:LEU:HD13	1:B:411:VAL:CG1	2.49	0.43
2:C:25:MET:HE1	2:C:208:PHE:HB2	2.00	0.43
1:B:630:TRP:CE2	1:B:693:LEU:HD11	2.53	0.43
2:C:364:MET:HE1	2:C:388:PHE:HB2	2.01	0.43
2:D:80:THR:CG2	2:D:82:ILE:HG12	2.48	0.43
1:B:114:ALA:HB3	1:B:136:ILE:HG22	1.99	0.43
1:B:655:ASP:O	1:B:659:VAL:HG23	2.18	0.43
2:D:360:LEU:HG	2:D:364:MET:CE	2.40	0.43
1:A:199:LEU:HD11	1:A:203:LYS:HE3	2.00	0.43
1:A:426:ALA:HA	1:A:448:VAL:O	2.18	0.43
1:B:120:GLU:CD	1:B:149:PHE:HB2	2.44	0.43
2:C:13:PHE:CE2	2:C:358:GLY:HA3	2.54	0.43
2:C:30:ARG:HH22	2:D:135:ASP:CG	2.26	0.43
2:C:289:VAL:HG22	2:C:290:PRO:CD	2.49	0.43
1:A:54:LYS:O	1:A:104:VAL:HG22	2.19	0.43
1:A:459:MET:HA	1:A:460:PRO:HD3	1.70	0.43
1:B:146:TYR:HB2	1:B:147:PRO:HD2	2.00	0.43
2:D:49:VAL:O	2:D:49:VAL:HG23	2.17	0.43
2:D:361:LEU:HA	2:D:364:MET:HE3	2.01	0.43
1:A:540:LEU:O	1:A:544:VAL:HG23	2.19	0.43
1:B:697:TYR:CD1	1:B:697:TYR:N	2.86	0.43
1:B:513:LYS:HE3	1:B:693:LEU:O	2.19	0.43
2:C:287:GLY:C	2:C:290:PRO:HD2	2.43	0.43
1:B:102:LEU:C	1:B:104:VAL:H	2.27	0.42
1:B:605:ASP:O	1:B:608:VAL:HG23	2.19	0.42
1:B:633:ILE:HB	1:B:634:PRO:HD3	2.00	0.42
2:D:164:ILE:HG22	2:D:169:GLN:HG3	2.01	0.42
1:A:463:GLU:O	1:A:465:ILE:HD12	2.19	0.42
2:D:255:MET:HE3	2:D:259:ARG:CG	2.49	0.42
1:A:3:TYR:OH	1:A:42:GLN:NE2	2.52	0.42
1:B:157:ARG:HG2	8:B:2283:HOH:O	2.19	0.42
1:A:403:GLU:HG2	4:A:1001:NAD:C3D	2.49	0.42
1:A:692:GLU:HG2	8:A:1225:HOH:O	2.18	0.42
2:C:54:VAL:HG21	2:C:82:ILE:HD12	2.02	0.42
1:A:146:TYR:HB2	1:A:147:PRO:CD	2.49	0.42
2:D:266:GLU:HA	2:D:267:PRO:HD3	1.89	0.42
1:A:126:ASP:O	1:A:215:LYS:HD3	2.20	0.42
1:B:411:VAL:O	1:B:415:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:377:CYS:SG	7:D:4001:ACO:HH31	2.59	0.42
1:A:320:LEU:HD13	1:A:411:VAL:CG1	2.50	0.42
1:A:546:ILE:HB	1:A:581:LEU:HA	2.02	0.42
2:C:266:GLU:HA	2:C:267:PRO:HD3	1.89	0.42
1:A:622:VAL:CG2	1:A:626:ASP:HB2	2.39	0.42
1:B:442:LYS:C	1:B:444:PRO:HD3	2.45	0.42
1:B:520:ASP:HB2	8:B:2298:HOH:O	2.20	0.42
2:C:336:VAL:O	2:C:337:ASN:C	2.62	0.42
2:D:55:GLU:HG2	8:D:4022:HOH:O	2.20	0.42
1:B:146:TYR:O	1:B:147:PRO:C	2.63	0.42
1:A:146:TYR:CD1	1:A:146:TYR:C	2.97	0.41
1:B:199:LEU:HD13	1:B:199:LEU:C	2.45	0.41
2:C:263:LEU:CB	2:C:265:LEU:HD22	2.49	0.41
2:D:21:SER:HB2	2:D:245:ILE:HG22	2.03	0.41
1:B:147:PRO:HB3	1:B:151:GLY:HA3	2.01	0.41
2:D:25:MET:CE	2:D:208:PHE:HB2	2.49	0.41
1:A:396:LEU:C	1:A:396:LEU:HD23	2.45	0.41
1:A:513:LYS:HE3	1:A:693:LEU:O	2.19	0.41
1:B:194:LEU:HD23	1:B:194:LEU:HA	1.87	0.41
1:B:391:PHE:HA	1:B:394:VAL:HG23	2.02	0.41
2:C:279:VAL:CG1	2:C:290:PRO:HG2	2.50	0.41
2:C:357:SER:O	2:C:361:LEU:HG	2.20	0.41
1:A:460:PRO:HG2	5:A:1002:N8E:H162	2.02	0.41
1:A:633:ILE:HB	1:A:634:PRO:HD3	2.01	0.41
1:B:465:ILE:HA	1:B:492:VAL:O	2.20	0.41
1:A:412:LEU:HB3	1:A:441:LEU:HD21	2.03	0.41
1:A:546:ILE:N	1:A:581:LEU:O	2.50	0.41
1:B:140:GLU:HG3	1:B:147:PRO:CD	2.51	0.41
2:C:13:PHE:CZ	2:C:358:GLY:HA3	2.55	0.41
2:C:303:MET:HE2	2:C:309:ILE:HD11	2.02	0.41
2:D:318:GLN:O	2:D:322:VAL:HG23	2.20	0.41
1:A:297:ASP:OD1	1:A:301:LYS:HE3	2.21	0.41
1:A:613:LYS:CB	1:A:614:PRO:HD3	2.49	0.41
2:D:62:VAL:HG21	2:D:349:PHE:HB3	2.01	0.41
2:D:231:ASN:HB3	2:D:235:GLY:HA3	2.03	0.41
1:A:700:THR:OG1	1:A:703:LEU:HB2	2.21	0.41
1:B:396:LEU:C	1:B:396:LEU:HD23	2.46	0.41
2:D:16:THR:O	2:D:18:MET:HE2	2.20	0.41
2:D:164:ILE:CG2	2:D:169:GLN:HG3	2.50	0.41
1:A:70:ASP:HA	5:A:1003:N8E:H132	2.02	0.41
1:A:116:GLY:HA2	1:A:140:GLU:OE1	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:TYR:HB2	1:A:147:PRO:HD2	2.02	0.41
1:A:520:ASP:O	1:A:524:ILE:HG13	2.21	0.41
1:B:533:TRP:HA	1:B:534:PRO:HD3	1.97	0.41
1:B:546:ILE:N	1:B:581:LEU:O	2.49	0.41
2:C:24:GLY:O	2:C:27:ARG:HB3	2.21	0.41
2:C:320:LEU:HB2	2:C:321:PRO:HD3	2.01	0.41
2:C:348:PRO:O	2:C:349:PHE:C	2.64	0.41
2:D:164:ILE:N	2:D:164:ILE:HD12	2.35	0.41
2:D:320:LEU:HB2	2:D:321:PRO:HD3	2.01	0.41
2:D:391:VAL:HG21	8:D:4132:HOH:O	2.19	0.41
1:A:107:VAL:CG2	1:A:202:ILE:HG12	2.51	0.41
1:A:146:TYR:C	1:A:146:TYR:HD1	2.29	0.41
1:A:345:ILE:HG13	1:A:346:ASN:ND2	2.36	0.41
1:B:199:LEU:HD11	1:B:203:LYS:HE3	2.03	0.41
1:B:546:ILE:HB	1:B:581:LEU:HA	2.03	0.41
2:C:308:PHE:HA	2:C:335:LYS:HB2	2.03	0.41
2:D:189:PHE:CZ	2:D:339:HIS:HB3	2.56	0.41
2:D:201:GLU:CD	2:D:201:GLU:N	2.76	0.41
2:D:310:GLU:CG	2:D:360:LEU:HB2	2.51	0.41
1:B:146:TYR:C	1:B:146:TYR:HD1	2.30	0.40
2:D:348:PRO:O	2:D:349:PHE:C	2.62	0.40
1:A:157:ARG:HG2	8:A:1072:HOH:O	2.22	0.40
1:B:9:THR:HG23	8:B:2143:HOH:O	2.20	0.40
1:B:107:VAL:HG22	1:B:127:PHE:HB2	2.02	0.40
1:B:199:LEU:HD11	1:B:203:LYS:CE	2.51	0.40
2:C:58:ILE:HD12	2:C:105:ALA:HB2	2.03	0.40
2:C:62:VAL:HG21	2:C:349:PHE:HB3	2.02	0.40
1:A:450:MET:HG2	1:A:452:PHE:CE1	2.56	0.40
1:A:697:TYR:CD1	1:A:697:TYR:N	2.89	0.40
1:B:261:LYS:HB3	1:B:261:LYS:HE2	1.81	0.40
2:C:310:GLU:CG	2:C:360:LEU:HB2	2.51	0.40
1:A:443:ARG:HA	1:A:445:GLU:OE2	2.22	0.40
1:B:98:ASP:O	1:B:102:LEU:HD13	2.22	0.40
2:D:286:TYR:O	2:D:289:VAL:HG13	2.20	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	704/715 (98%)	668 (95%)	35 (5%)	1 (0%)	48	68
1	B	707/715 (99%)	672 (95%)	34 (5%)	1 (0%)	48	68
2	C	388/390 (100%)	370 (95%)	17 (4%)	1 (0%)	36	55
2	D	388/390 (100%)	367 (95%)	20 (5%)	1 (0%)	36	55
All	All	2187/2210 (99%)	2077 (95%)	106 (5%)	4 (0%)	43	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	324	ILE
1	B	324	ILE
2	C	349	PHE
2	D	349	PHE

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	547/562 (97%)	522 (95%)	25 (5%)	24	48
1	B	545/562 (97%)	519 (95%)	26 (5%)	23	46
2	C	307/307 (100%)	297 (97%)	10 (3%)	33	61
2	D	306/307 (100%)	297 (97%)	9 (3%)	37	65
All	All	1705/1738 (98%)	1635 (96%)	70 (4%)	27	53

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	102	LEU
1	A	104	VAL
1	A	113	ILE
1	A	119	LEU
1	A	146	TYR
1	A	180	LEU
1	A	185	VAL
1	A	194	LEU
1	A	202	ILE
1	A	258	THR
1	A	280	LYS
1	A	288	ASN
1	A	342	MET
1	A	393	ASN
1	A	436	LEU
1	A	445	GLU
1	A	473	LEU
1	A	540	LEU
1	A	622	VAL
1	A	643	LEU
1	A	648	VAL
1	A	662	ILE
1	A	686	LEU
1	A	703	LEU
1	B	40	LEU
1	B	102	LEU
1	B	104	VAL
1	B	119	LEU
1	B	140	GLU
1	B	146	TYR
1	B	157	ARG
1	B	180	LEU
1	B	185	VAL
1	B	194	LEU
1	B	202	ILE
1	B	280	LYS
1	B	288	ASN
1	B	342	MET
1	B	436	LEU
1	B	445	GLU
1	B	473	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	540	LEU
1	B	622	VAL
1	B	643	LEU
1	B	647	ILE
1	B	648	VAL
1	B	662	ILE
1	B	686	LEU
1	B	692	GLU
1	B	703	LEU
2	C	27	ARG
2	C	95	CYS
2	C	158	LEU
2	C	201	GLU
2	C	265	LEU
2	C	289	VAL
2	C	318	GLN
2	C	329	LEU
2	C	351	CYS
2	C	355	ARG
2	D	27	ARG
2	D	158	LEU
2	D	201	GLU
2	D	265	LEU
2	D	289	VAL
2	D	318	GLN
2	D	329	LEU
2	D	351	CYS
2	D	355	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	42	GLN
1	A	77	ASN
1	A	244	GLN
1	A	288	ASN
1	A	296	ASN
1	A	298	GLN
1	A	393	ASN
1	A	409	GLN
1	A	501	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	619	GLN
1	A	698	HIS
1	A	709	ASN
1	B	38	ASN
1	B	42	GLN
1	B	77	ASN
1	B	288	ASN
1	B	296	ASN
1	B	298	GLN
1	B	409	GLN
1	B	457	HIS
1	B	551	HIS
1	B	583	GLN
1	B	698	HIS
1	B	709	ASN
2	C	4	ASN
2	C	89	GLN
2	C	113	ASN
2	C	162	HIS
2	C	169	GLN
2	C	197	GLN
2	C	231	ASN
2	D	4	ASN
2	D	37	HIS
2	D	89	GLN
2	D	107	GLN
2	D	113	ASN
2	D	169	GLN
2	D	197	GLN
2	D	362	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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
5	N8E	A	1002	-	23,23,23	0.46	0	22,22,22	0.44	0
5	N8E	B	2003	-	23,23,23	0.49	0	22,22,22	0.41	0
5	N8E	A	1003	-	23,23,23	0.46	0	22,22,22	0.44	0
7	ACO	C	3001	6	51,53,53	0.75	0	73,79,79	0.75	1 (1%)
4	NAD	A	1001	-	46,48,48	1.56	6 (13%)	64,73,73	1.34	4 (6%)
7	ACO	D	4001	6	51,53,53	0.69	0	73,79,79	0.67	1 (1%)
4	NAD	B	2001	-	46,48,48	1.59	6 (13%)	64,73,73	1.34	4 (6%)
5	N8E	B	2002	-	23,23,23	0.46	0	22,22,22	0.41	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
5	N8E	A	1002	-	-	15/21/21/21	-
5	N8E	B	2003	-	-	13/21/21/21	-
5	N8E	A	1003	-	-	15/21/21/21	-
7	ACO	C	3001	6	-	8/51/67/67	0/3/3/3
4	NAD	A	1001	-	-	12/30/62/62	0/5/5/5
7	ACO	D	4001	6	-	12/51/67/67	0/3/3/3
4	NAD	B	2001	-	-	11/30/62/62	0/5/5/5
5	N8E	B	2002	-	-	13/21/21/21	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1001	NAD	C3N-C7N	5.91	1.59	1.50
4	B	2001	NAD	C3N-C7N	5.58	1.58	1.50
4	B	2001	NAD	C2N-N1N	4.79	1.40	1.35
4	A	1001	NAD	C2N-N1N	4.26	1.39	1.35
4	A	1001	NAD	C4N-C3N	3.80	1.45	1.39
4	B	2001	NAD	C6N-N1N	3.71	1.43	1.35
4	B	2001	NAD	C4N-C3N	3.65	1.45	1.39
4	A	1001	NAD	C6N-N1N	3.58	1.43	1.35
4	B	2001	NAD	PN-O3	2.63	1.62	1.59
4	B	2001	NAD	C5N-C4N	2.30	1.42	1.38
4	A	1001	NAD	C5N-C4N	2.25	1.42	1.38
4	A	1001	NAD	C4A-N3A	2.02	1.38	1.34

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1001	NAD	C5N-C4N-C3N	-6.77	113.70	120.36
4	B	2001	NAD	C5N-C4N-C3N	-6.62	113.86	120.36
4	A	1001	NAD	C6N-C5N-C4N	5.58	127.49	119.45
4	B	2001	NAD	C6N-C5N-C4N	5.53	127.42	119.45
7	C	3001	ACO	C2P-S1P-C	4.58	123.44	101.42
4	A	1001	NAD	C5N-C6N-N1N	-4.08	114.81	120.38
4	B	2001	NAD	C5N-C6N-N1N	-4.03	114.89	120.38
7	D	4001	ACO	C2P-S1P-C	3.90	120.17	101.42
4	B	2001	NAD	C2N-C3N-C4N	2.85	121.58	118.26
4	A	1001	NAD	C2N-C3N-C4N	2.75	121.46	118.26

There are no chirality outliers.

All (99) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	NAD	O4D-C1D-N1N-C2N
4	A	1001	NAD	C2N-C3N-C7N-O7N
4	A	1001	NAD	C2N-C3N-C7N-N7N
4	B	2001	NAD	O4D-C1D-N1N-C2N
4	B	2001	NAD	C2N-C3N-C7N-O7N
4	B	2001	NAD	C2N-C3N-C7N-N7N
4	B	2001	NAD	C4N-C3N-C7N-N7N
7	C	3001	ACO	C5B-O5B-P1A-O1A
7	C	3001	ACO	C5B-O5B-P1A-O3A
7	C	3001	ACO	S1P-C2P-C3P-N4P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	C	3001	ACO	C3P-C2P-S1P-C
7	C	3001	ACO	O-C-S1P-C2P
7	C	3001	ACO	CH3-C-S1P-C2P
7	D	4001	ACO	C3B-C4B-C5B-O5B
7	D	4001	ACO	S1P-C2P-C3P-N4P
7	D	4001	ACO	O-C-S1P-C2P
7	D	4001	ACO	CH3-C-S1P-C2P
4	B	2001	NAD	C4N-C3N-C7N-O7N
7	D	4001	ACO	O4B-C4B-C5B-O5B
5	B	2002	N8E	O15-C16-C17-O18
5	B	2003	N8E	O09-C10-C11-O12
4	A	1001	NAD	C4N-C3N-C7N-N7N
5	A	1002	N8E	O18-C19-C20-O21
5	A	1003	N8E	O12-C13-C14-O15
5	A	1003	N8E	O15-C16-C17-O18
5	A	1002	N8E	O15-C16-C17-O18
4	A	1001	NAD	C4N-C3N-C7N-O7N
5	A	1002	N8E	O09-C10-C11-O12
5	A	1003	N8E	O09-C10-C11-O12
5	A	1002	N8E	C06-C07-C08-O09
5	A	1002	N8E	O12-C13-C14-O15
5	B	2003	N8E	C06-C07-C08-O09
5	A	1003	N8E	O18-C19-C20-O21
5	B	2002	N8E	C03-C04-C05-C06
5	B	2002	N8E	O12-C13-C14-O15
4	A	1001	NAD	C3D-C4D-C5D-O5D
4	B	2001	NAD	O4B-C4B-C5B-O5B
5	A	1003	N8E	C05-C06-C07-C08
5	A	1002	N8E	C04-C05-C06-C07
5	A	1002	N8E	C05-C06-C07-C08
5	B	2003	N8E	C05-C06-C07-C08
5	A	1003	N8E	C03-C04-C05-C06
5	A	1003	N8E	C04-C05-C06-C07
5	B	2002	N8E	C02-C03-C04-C05
4	B	2001	NAD	C3B-C4B-C5B-O5B
5	B	2003	N8E	C04-C05-C06-C07
5	B	2002	N8E	C01-C02-C03-C04
5	B	2003	N8E	C03-C04-C05-C06
4	A	1001	NAD	O4B-C4B-C5B-O5B
4	A	1001	NAD	C3B-C4B-C5B-O5B
5	A	1002	N8E	C01-C02-C03-C04
5	B	2002	N8E	O18-C19-C20-O21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
7	C	3001	ACO	C5P-C6P-C7P-N8P
5	B	2003	N8E	C23-C22-O21-C20
5	A	1003	N8E	C06-C07-C08-O09
5	A	1002	N8E	C16-C17-O18-C19
5	B	2002	N8E	C10-C11-O12-C13
5	A	1002	N8E	C20-C19-O18-C17
5	A	1003	N8E	C17-C16-O15-C14
5	B	2002	N8E	C23-C22-O21-C20
5	A	1002	N8E	C17-C16-O15-C14
5	A	1002	N8E	C10-C11-O12-C13
5	B	2003	N8E	C11-C10-O09-C08
5	A	1002	N8E	C23-C22-O21-C20
5	A	1002	N8E	C11-C10-O09-C08
4	A	1001	NAD	O4D-C4D-C5D-O5D
7	D	4001	ACO	P2A-O3A-P1A-O2A
5	B	2002	N8E	C04-C05-C06-C07
5	B	2003	N8E	C14-C13-O12-C11
5	A	1003	N8E	C07-C08-O09-C10
5	B	2003	N8E	C07-C08-O09-C10
5	A	1003	N8E	C20-C19-O18-C17
5	A	1003	N8E	C02-C03-C04-C05
7	D	4001	ACO	C3P-C2P-S1P-C
4	A	1001	NAD	C2B-C1B-N9A-C8A
7	D	4001	ACO	C5B-O5B-P1A-O1A
7	D	4001	ACO	CCP-O6A-P2A-O4A
5	B	2002	N8E	C06-C07-C08-O09
7	D	4001	ACO	C5P-C6P-C7P-N8P
5	B	2003	N8E	C13-C14-O15-C16
5	A	1003	N8E	C16-C17-O18-C19
5	B	2002	N8E	C07-C08-O09-C10
5	B	2002	N8E	C20-C19-O18-C17
5	A	1002	N8E	C13-C14-O15-C16
7	D	4001	ACO	C4B-C5B-O5B-P1A
4	A	1001	NAD	O4D-C1D-N1N-C6N
4	B	2001	NAD	O4D-C1D-N1N-C6N
5	A	1003	N8E	C23-C22-O21-C20
4	B	2001	NAD	PA-O3-PN-O1N
5	B	2003	N8E	C20-C19-O18-C17
4	B	2001	NAD	C2B-C1B-N9A-C8A
5	B	2003	N8E	C19-C20-O21-C22
5	B	2003	N8E	C17-C16-O15-C14
7	D	4001	ACO	P2A-O3A-P1A-O1A

Continued on next page...

Continued from previous page...

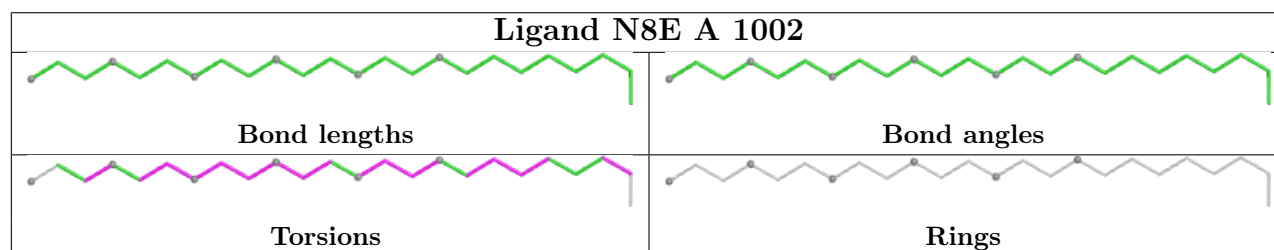
Mol	Chain	Res	Type	Atoms
5	B	2002	N8E	C11-C10-O09-C08
5	A	1003	N8E	C19-C20-O21-C22
7	C	3001	ACO	C3B-C4B-C5B-O5B
4	A	1001	NAD	O4B-C1B-N9A-C8A
4	B	2001	NAD	PA-O3-PN-O2N

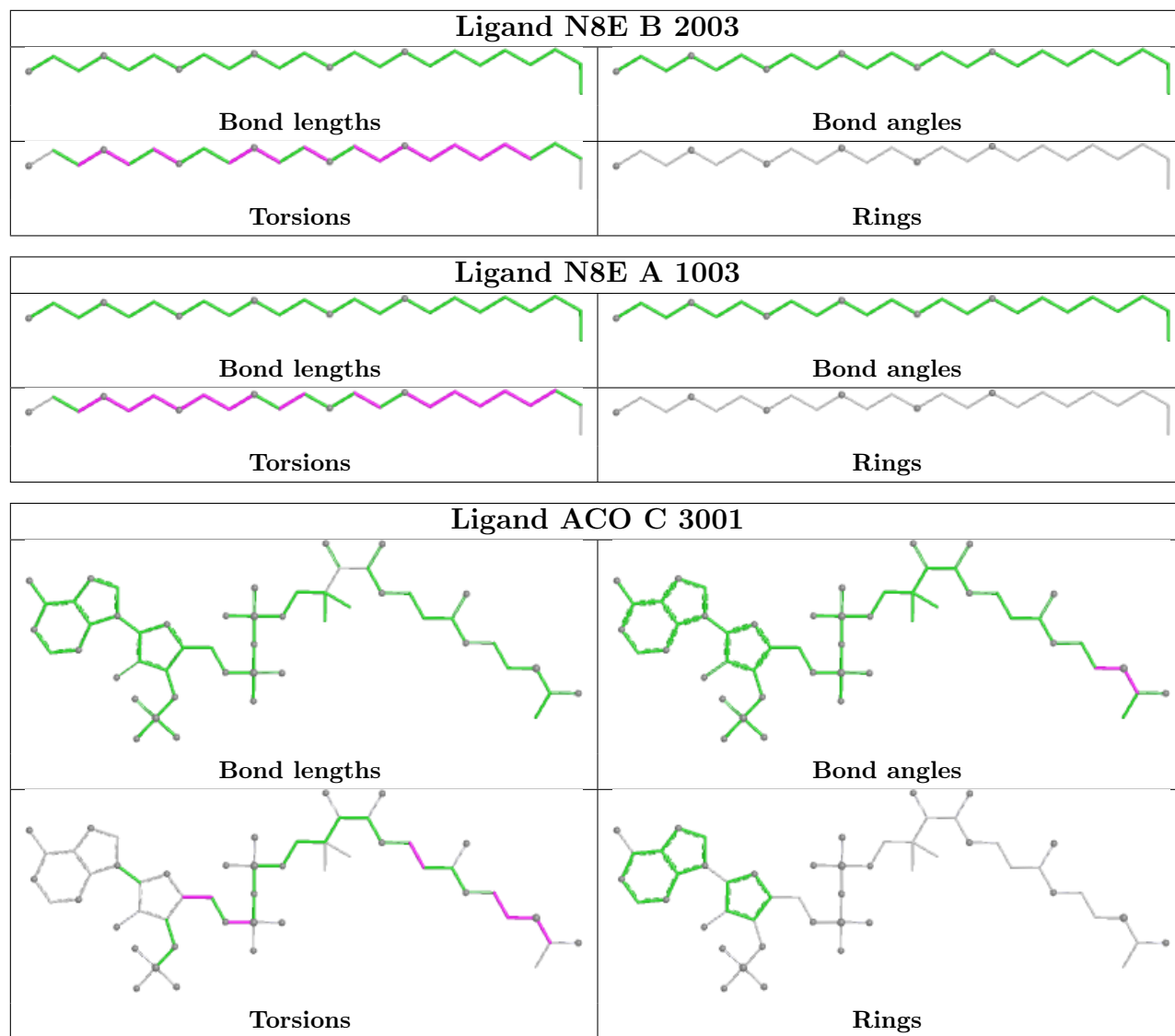
There are no ring outliers.

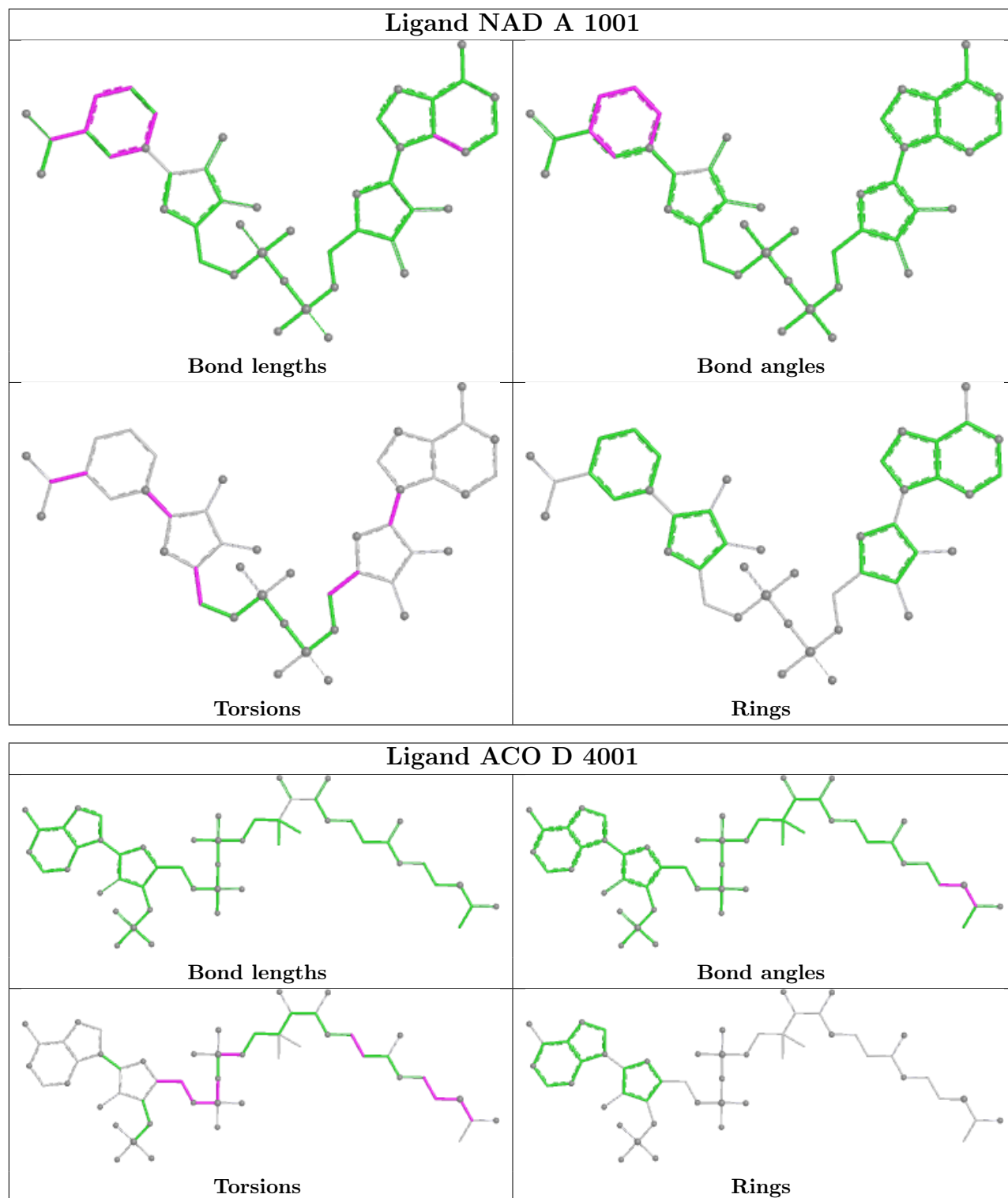
8 monomers are involved in 27 short contacts:

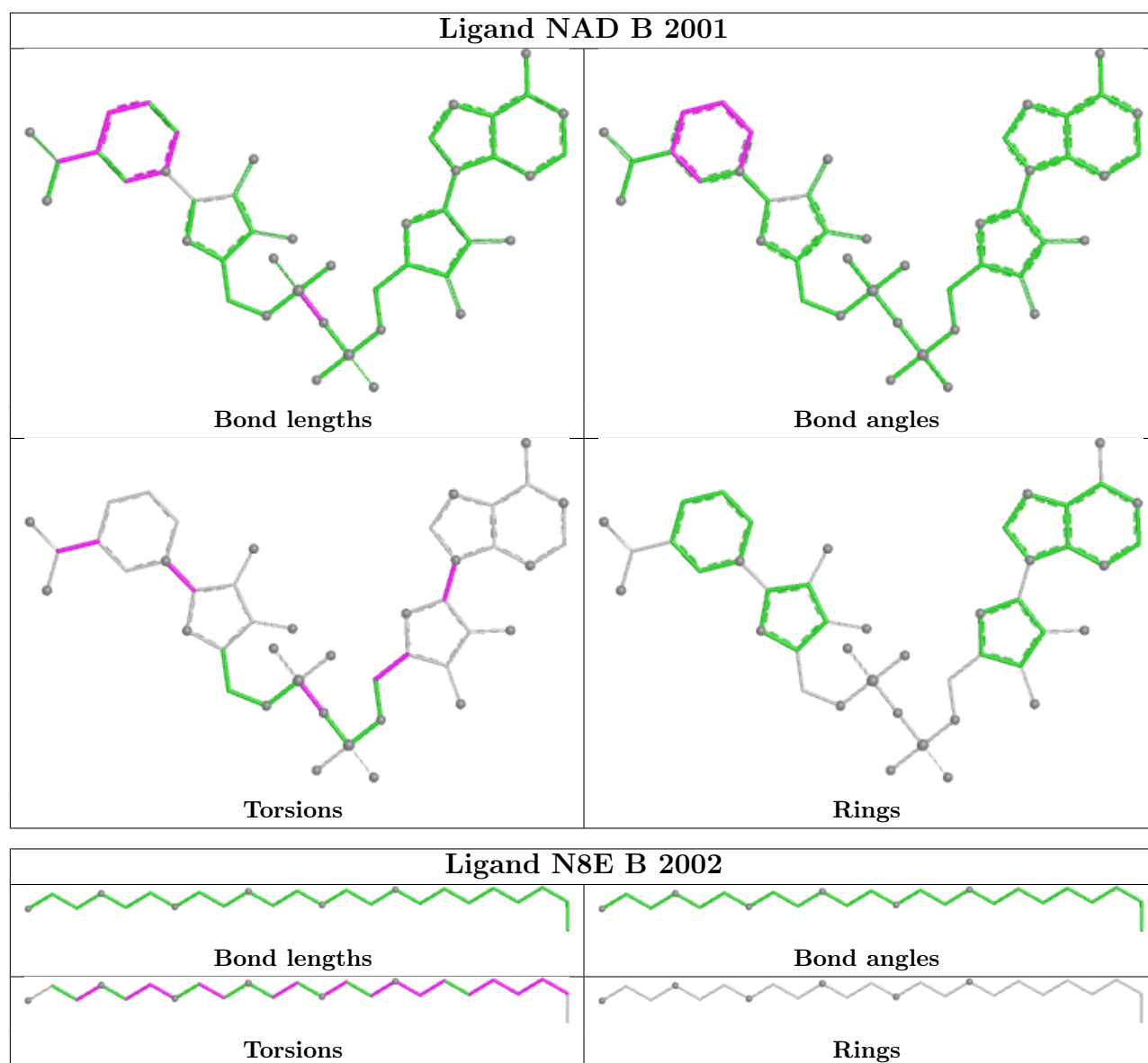
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1002	N8E	2	0
5	B	2003	N8E	7	0
5	A	1003	N8E	6	0
7	C	3001	ACO	3	0
4	A	1001	NAD	2	0
7	D	4001	ACO	4	0
4	B	2001	NAD	2	0
5	B	2002	N8E	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	708/715 (99%)	-0.08	8 (1%) 78 75	14, 29, 51, 72	0
1	B	711/715 (99%)	-0.07	15 (2%) 63 59	13, 29, 52, 71	0
2	C	390/390 (100%)	-0.44	1 (0%) 90 87	11, 21, 35, 52	0
2	D	390/390 (100%)	-0.43	3 (0%) 82 80	10, 21, 35, 52	0
All	All	2199/2210 (99%)	-0.20	27 (1%) 76 73	10, 26, 48, 72	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	2	SER	4.8
1	B	594	ALA	4.3
1	B	567	ASP	3.9
1	B	294	PHE	3.5
1	B	620	ARG	3.3
1	B	618	GLU	3.2
1	B	584	LYS	3.2
2	C	391	VAL	3.0
1	A	371	THR	2.9
1	B	619	GLN	2.9
1	A	525	ASP	2.9
1	B	715	GLY	2.7
2	D	391	VAL	2.6
1	B	323	GLY	2.6
1	A	322	ALA	2.5
1	B	600	GLN	2.5
1	A	618	GLU	2.4
1	A	368	GLY	2.3
1	B	615	ILE	2.3
2	D	265	LEU	2.2
1	B	362	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	606	SER	2.2
1	B	595	ASP	2.2
1	B	371	THR	2.1
1	B	608	VAL	2.1
1	A	707	ALA	2.0
1	A	370	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

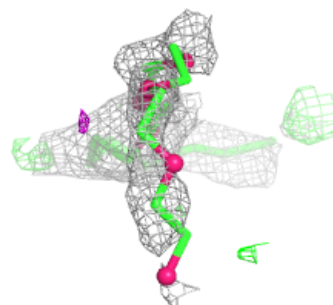
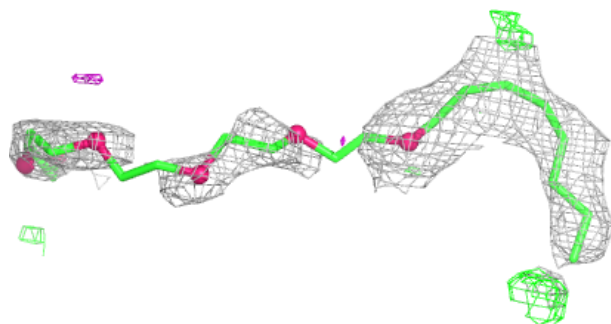
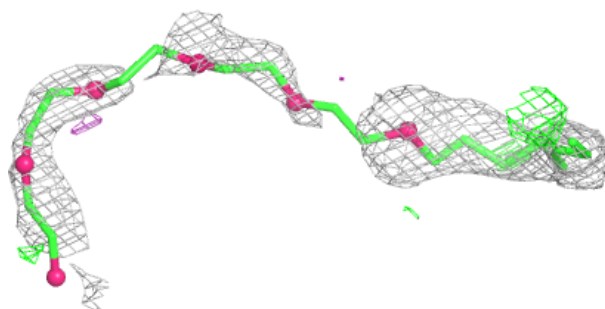
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	N8E	A	1003	24/24	0.71	0.22	62,83,88,89	0
5	N8E	B	2003	24/24	0.74	0.19	29,61,81,81	0
7	ACO	C	3001	51/51	0.77	0.20	69,102,115,116	0
5	N8E	B	2002	24/24	0.79	0.16	42,55,59,60	0
7	ACO	D	4001	51/51	0.80	0.20	72,90,97,98	0
5	N8E	A	1002	24/24	0.81	0.18	50,67,70,71	0
4	NAD	B	2001	44/44	0.90	0.11	41,51,73,73	0
4	NAD	A	1001	44/44	0.92	0.10	46,50,60,61	0
3	ZN	A	716	1/1	0.97	0.06	43,43,43,43	0
6	HG	C	392	1/1	0.98	0.08	87,87,87,87	0
6	HG	D	1	1/1	0.99	0.05	75,75,75,75	0

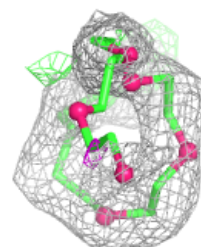
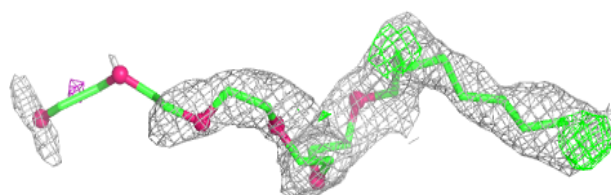
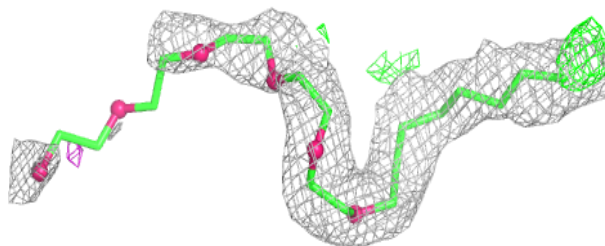
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around N8E A 1003:

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

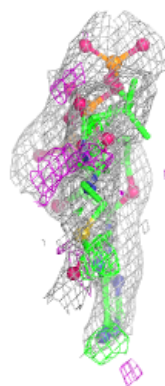
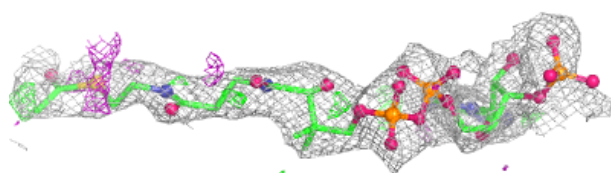
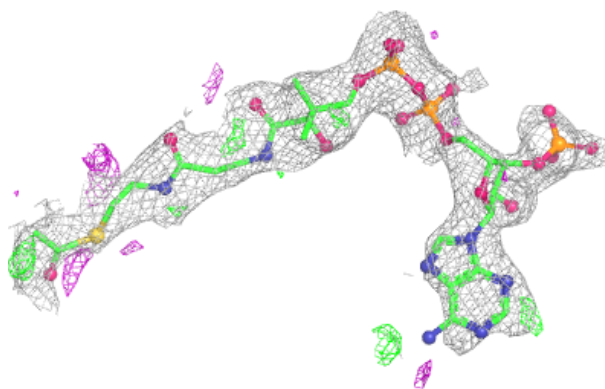
**Electron density around N8E B 2003:**

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

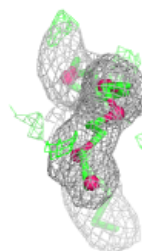
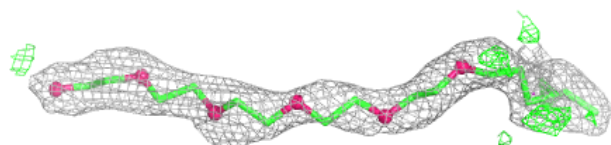
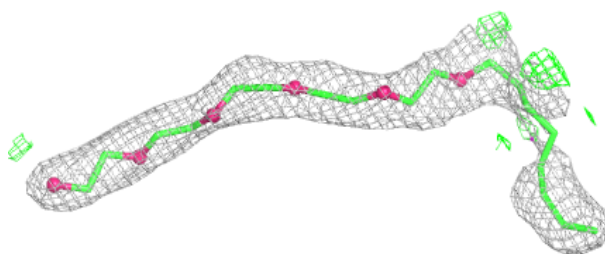


Electron density around ACO C 3001:

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

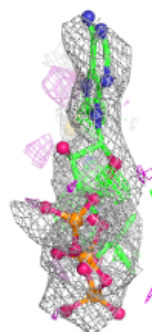
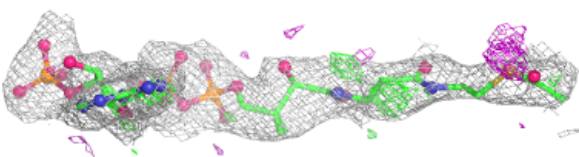
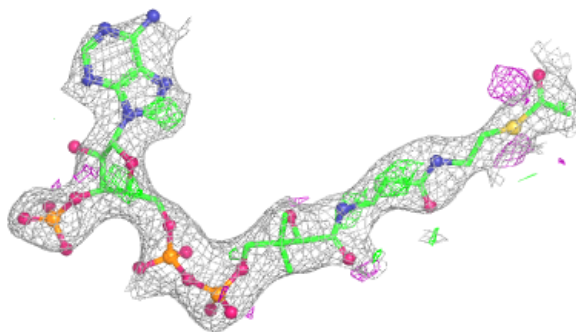
**Electron density around N8E B 2002:**

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

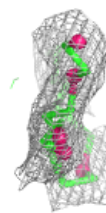
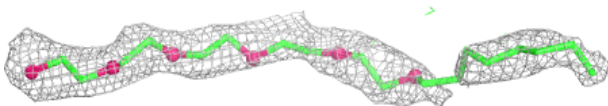
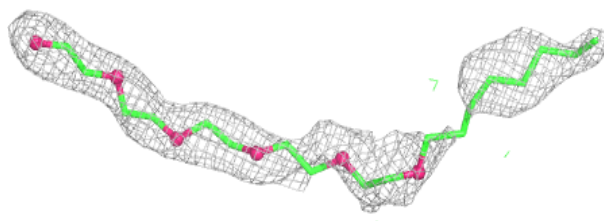


Electron density around ACO D 4001:

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

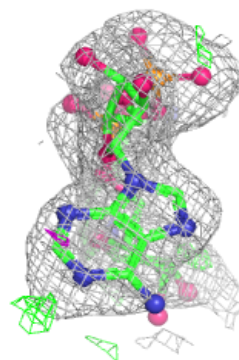
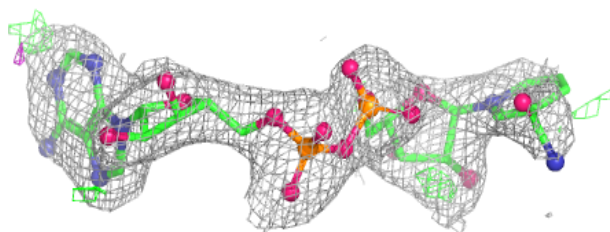
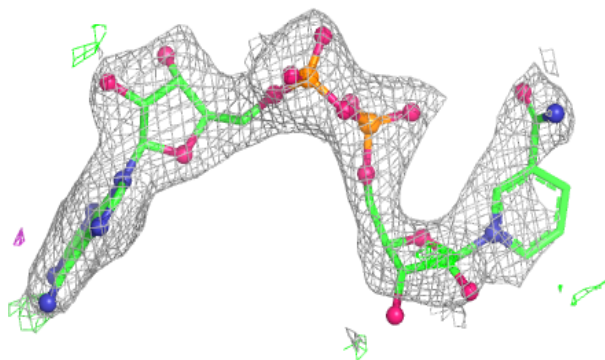
**Electron density around N8E A 1002:**

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

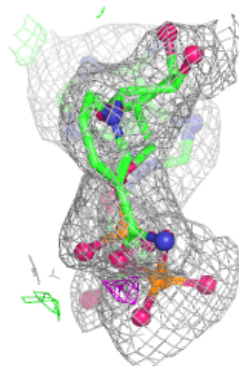
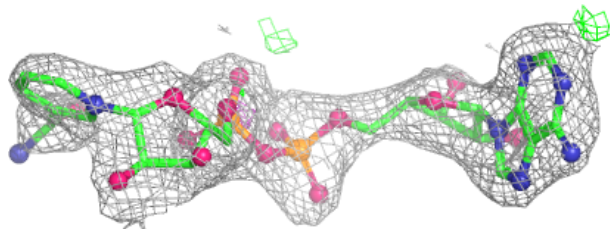
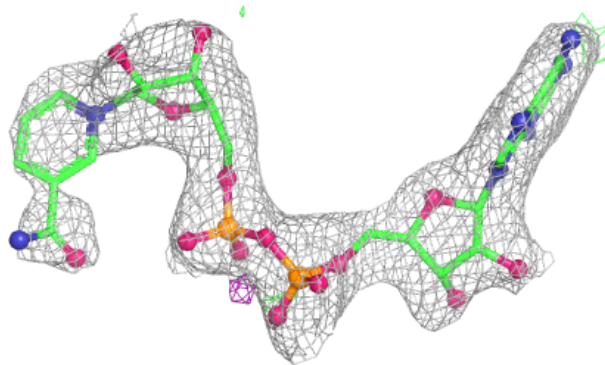


Electron density around NAD B 2001:

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

**Electron density around NAD A 1001:**

$2mF_o-DF_c$ (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.