



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:48 PM UTC

PDB ID : 2RC5 / pdb_00002rc5
Title : Refined structure of FNR from *Leptospira interrogans*
Authors : Nascimento, A.S.; Catalano-Dupuy, D.L.; Polikarpov, I.; Ceccarelli, E.A.
Deposited on : 2007-09-19
Resolution : 2.43 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

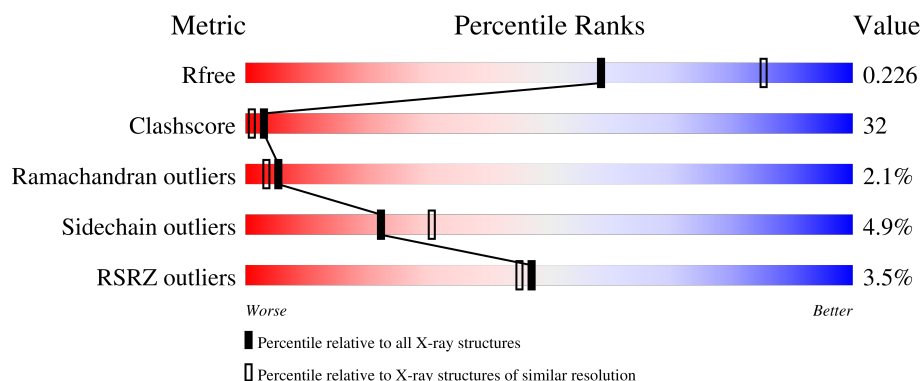
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

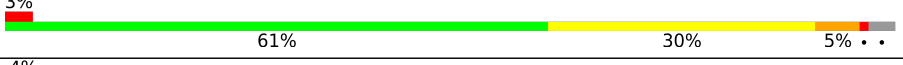
The reported resolution of this entry is 2.43 Å.

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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (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 ≥ 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	314	
1	B	314	
1	C	314	
1	D	314	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	315	-	-	X	-
2	SO4	A	316	-	-	X	-
2	SO4	B	315	-	-	X	-
2	SO4	C	315	-	-	X	-
2	SO4	C	316	-	-	X	-
2	SO4	C	317	-	-	X	-
2	SO4	D	315	-	-	X	-

2 Entry composition [i](#)

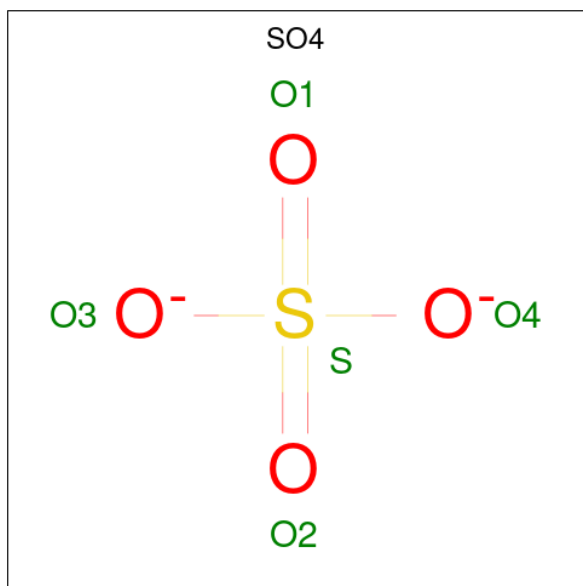
There are 5 unique types of molecules in this entry. The entry contains 10963 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ferredoxin-NADP reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2374	1516	397	449	12			
1	B	301	Total	C	N	O	S	0	0	0
			2348	1496	393	447	12			
1	C	304	Total	C	N	O	S	0	0	0
			2373	1513	397	451	12			
1	D	306	Total	C	N	O	S	0	0	0
			2382	1520	399	451	12			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

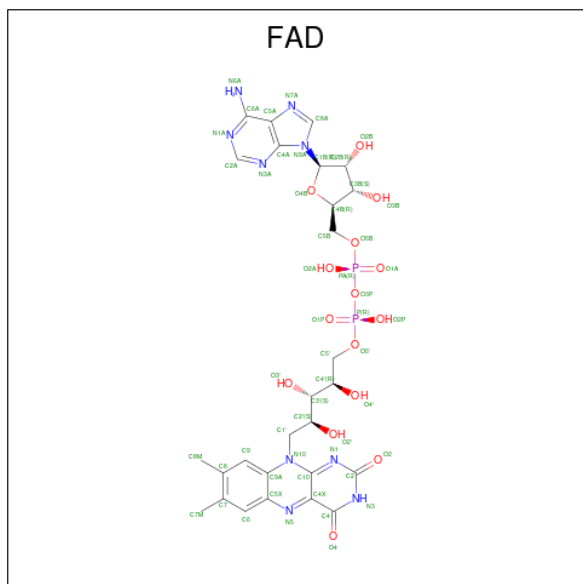
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- 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 FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

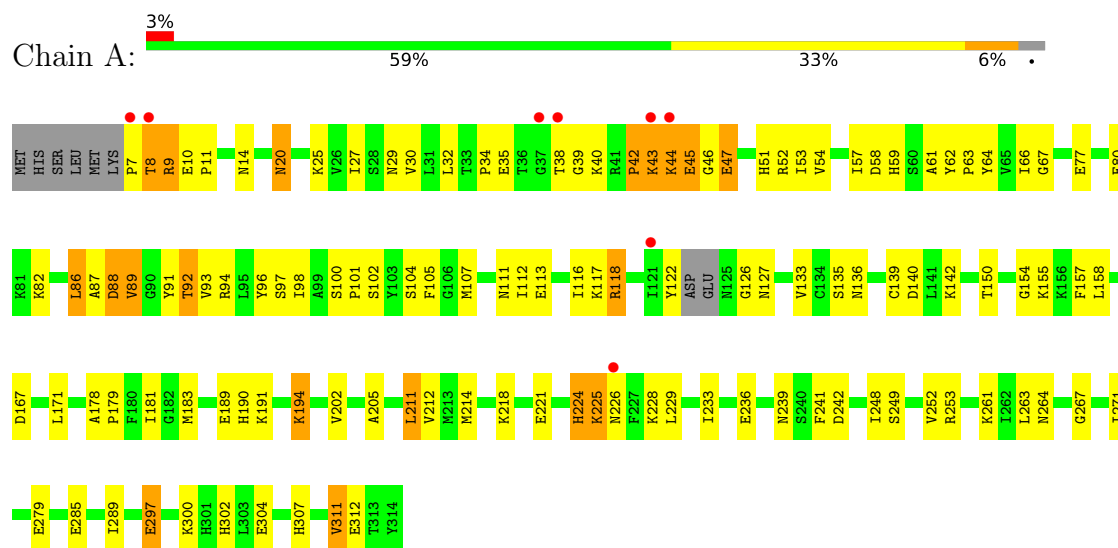
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	297	Total	O	0	0
			297	297		
5	B	307	Total	O	0	0
			307	307		
5	C	329	Total	O	0	0
			329	329		
5	D	305	Total	O	0	0
			305	305		

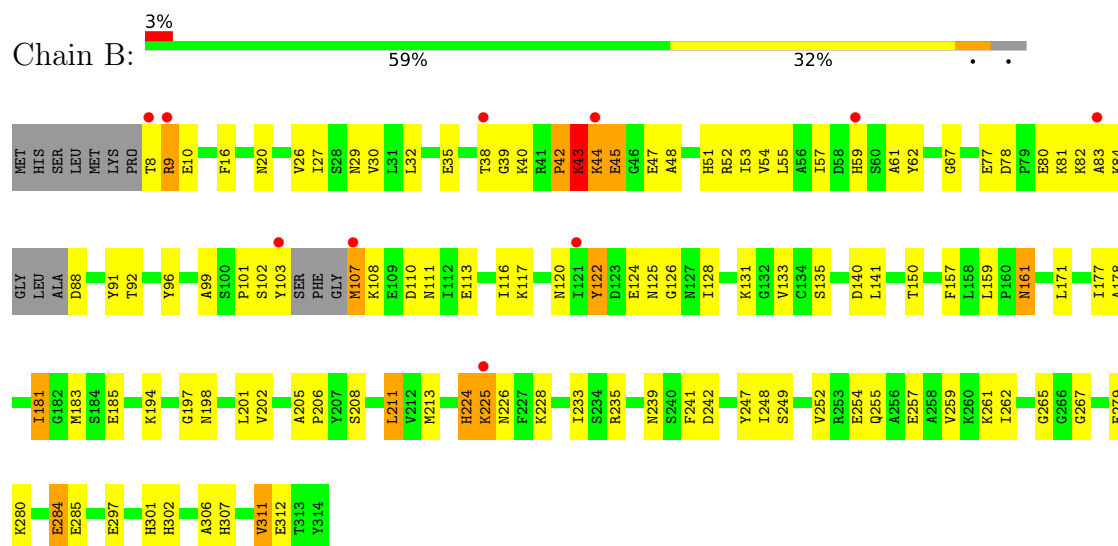
3 Residue-property plots [i](#)

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: Ferredoxin-NADP reductase

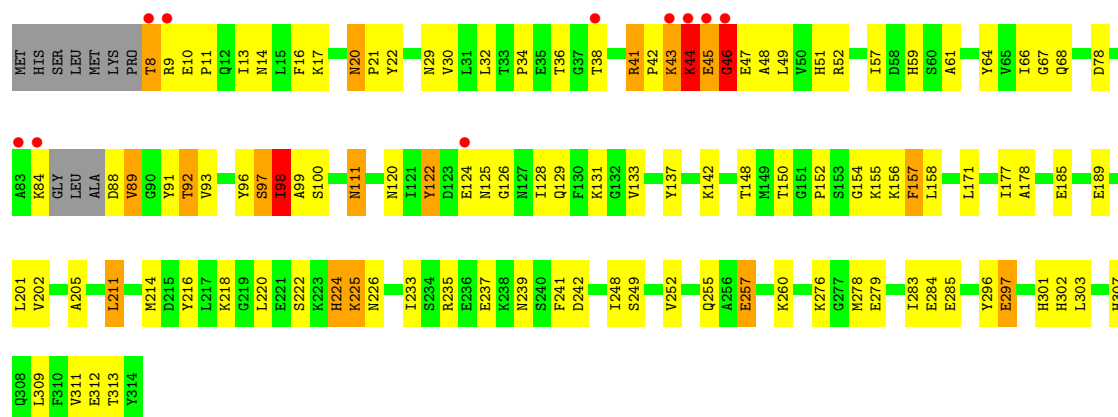


• Molecule 1: Ferredoxin-NADP reductase

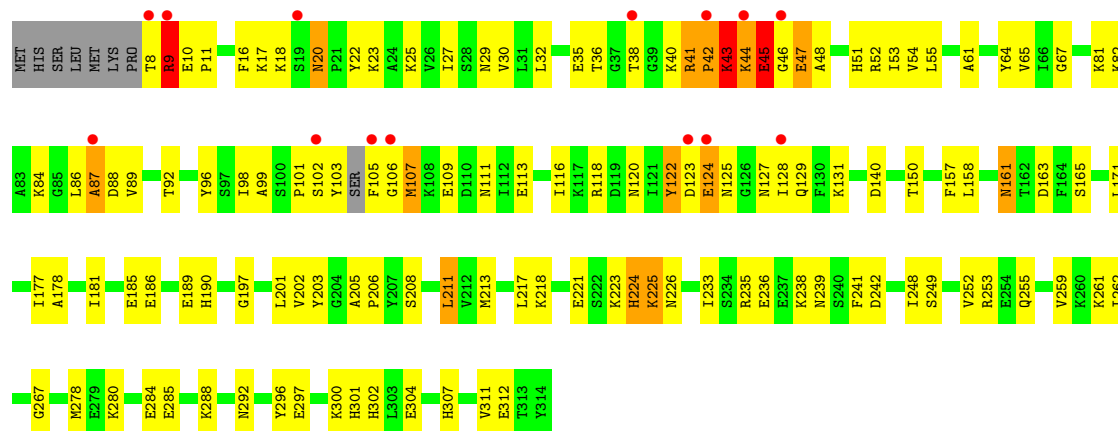


• Molecule 1: Ferredoxin-NADP reductase





● Molecule 1: Ferredoxin-NADP reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.11Å 111.83Å 89.91Å 90.00° 92.76° 90.00°	Depositor
Resolution (Å)	44.90 – 2.43 44.90 – 2.43	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.90-2.43) 98.4 (44.90-2.43)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.42Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.225 , 0.255 0.197 , 0.226	Depositor DCC
R_{free} test set	2413 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.065 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10963	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.78% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, FAD, SO4

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	0.65	2/2425 (0.1%)	0.90	2/3265 (0.1%)
1	B	0.64	2/2396 (0.1%)	1.04	6/3224 (0.2%)
1	C	0.72	4/2423 (0.2%)	0.91	4/3260 (0.1%)
1	D	0.67	2/2432 (0.1%)	0.93	3/3272 (0.1%)
All	All	0.67	10/9676 (0.1%)	0.95	15/13021 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
1	C	0	3
1	D	0	2
All	All	0	10

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	97	SER	C-O	-9.30	1.13	1.24
1	D	48	ALA	C-O	-7.06	1.15	1.23
1	B	108	LYS	C-O	6.80	1.32	1.24
1	A	97	SER	C-O	-6.79	1.15	1.23
1	C	48	ALA	CA-CB	-6.50	1.43	1.52
1	B	48	ALA	C-O	-6.15	1.16	1.23
1	C	41	ARG	C-O	-5.40	1.17	1.24
1	C	48	ALA	C-O	-5.34	1.16	1.23
1	A	47	GLU	CA-C	-5.04	1.46	1.52
1	D	43	LYS	CA-C	-5.00	1.46	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	43	LYS	N-CA-CB	-26.48	68.83	110.14
1	B	43	LYS	N-CA-C	-8.95	97.86	111.56
1	D	47	GLU	N-CA-C	7.48	120.60	108.41
1	B	107	MET	CA-C-N	6.99	134.89	121.54
1	B	107	MET	C-N-CA	6.99	134.89	121.54
1	C	224	HIS	N-CA-C	6.42	120.73	112.12
1	A	224	HIS	N-CA-C	6.24	120.48	112.12
1	B	48	ALA	N-CA-C	6.18	120.84	107.49
1	D	224	HIS	N-CA-C	5.76	120.33	113.12
1	B	224	HIS	N-CA-C	5.72	120.26	113.12
1	C	98	ILE	N-CA-CB	5.63	120.51	111.23
1	D	41	ARG	O-C-N	5.41	126.02	121.31
1	C	49	LEU	N-CA-C	5.27	117.31	107.99
1	A	27	ILE	N-CA-C	-5.17	106.64	111.45
1	C	111	ASN	N-CA-C	5.15	116.12	108.60

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	42	PRO	Peptide
1	A	43	LYS	Peptide
1	A	45	GLU	Peptide
1	B	42	PRO	Peptide
1	B	43	LYS	Peptide
1	C	43	LYS	Peptide
1	C	44	LYS	Peptide
1	C	46	GLY	Peptide
1	D	43	LYS	Peptide
1	D	45	GLU	Peptide

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	2374	0	2356	142	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2348	0	2328	135	4
1	C	2373	0	2357	161	1
1	D	2382	0	2365	170	3
2	A	10	0	0	8	4
2	B	5	0	0	4	1
2	C	15	0	0	17	3
2	D	5	0	0	5	1
3	A	1	0	0	0	0
4	A	53	0	31	1	0
4	B	53	0	31	1	0
4	C	53	0	29	4	0
4	D	53	0	31	2	0
5	A	297	0	0	62	0
5	B	307	0	0	65	1
5	C	329	0	0	78	1
5	D	305	0	0	82	2
All	All	10963	0	9528	611	11

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 32.

All (611) 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:D:292:ASN:HA	5:D:622:HOH:O	1.18	1.35
1:A:261:LYS:HD3	5:A:678:HOH:O	1.17	1.31
1:B:194:LYS:HE2	5:B:611:HOH:O	1.15	1.30
1:A:8:THR:HB	5:A:551:HOH:O	1.35	1.26
1:C:235:ARG:HD3	5:C:867:HOH:O	1.32	1.26
1:C:142:LYS:HE3	5:C:1012:HOH:O	1.30	1.26
1:D:111:ASN:HB3	5:D:479:HOH:O	1.34	1.25
1:D:124:GLU:HB3	5:D:584:HOH:O	1.08	1.24
1:B:82:LYS:CE	5:B:556:HOH:O	1.83	1.23
1:C:142:LYS:HE2	5:C:822:HOH:O	1.30	1.23
1:A:92:THR:HG21	5:A:542:HOH:O	1.35	1.23
1:C:42:PRO:O	1:C:45:GLU:HB2	1.09	1.22
1:B:82:LYS:HE3	5:B:556:HOH:O	1.31	1.22
1:C:9:ARG:HB2	5:C:1032:HOH:O	1.04	1.22
1:C:224:HIS:NE2	2:C:317:SO4:O3	1.72	1.21
1:C:17:LYS:HD2	5:C:1011:HOH:O	1.04	1.20
1:B:9:ARG:HA	5:B:495:HOH:O	1.03	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ARG:HA	5:D:561:HOH:O	1.40	1.19
1:B:107:MET:HB3	5:B:547:HOH:O	1.41	1.17
1:C:42:PRO:O	1:C:45:GLU:CB	1.90	1.17
1:D:261:LYS:HD3	5:D:566:HOH:O	1.40	1.17
1:C:155:LYS:HD3	5:C:1025:HOH:O	1.42	1.16
1:B:235:ARG:HG2	5:B:627:HOH:O	1.46	1.15
1:C:42:PRO:HG2	1:C:45:GLU:CG	1.78	1.14
1:C:224:HIS:CE1	2:C:317:SO4:O3	2.02	1.13
1:C:44:LYS:CB	1:C:125:ASN:O	1.97	1.12
1:D:25:LYS:HG2	5:D:675:HOH:O	1.50	1.12
1:C:9:ARG:HD2	5:C:818:HOH:O	1.50	1.11
1:D:261:LYS:CD	5:D:566:HOH:O	1.96	1.11
1:B:257:GLU:HG3	5:B:639:HOH:O	1.50	1.10
1:D:109:GLU:HB2	5:D:536:HOH:O	1.51	1.08
1:A:42:PRO:HD2	1:A:45:GLU:OE1	1.53	1.08
1:D:253:ARG:HG2	5:D:606:HOH:O	1.52	1.08
1:B:107:MET:N	5:B:551:HOH:O	1.86	1.07
1:C:142:LYS:HG2	5:C:993:HOH:O	1.55	1.06
1:C:142:LYS:CE	5:C:1012:HOH:O	1.90	1.05
1:B:88:ASP:C	5:B:479:HOH:O	1.97	1.05
1:C:84:LYS:C	5:C:807:HOH:O	1.98	1.05
1:A:8:THR:CB	5:A:551:HOH:O	1.96	1.05
1:B:82:LYS:NZ	5:B:556:HOH:O	1.89	1.04
1:D:42:PRO:HG2	1:D:45:GLU:OE1	1.56	1.03
1:B:10:GLU:HB2	5:B:508:HOH:O	1.57	1.02
1:B:235:ARG:CG	5:B:627:HOH:O	2.06	1.00
1:C:42:PRO:HA	5:C:828:HOH:O	1.59	1.00
1:C:44:LYS:HA	1:C:126:GLY:HA3	1.43	1.00
1:C:92:THR:HG23	5:C:836:HOH:O	1.59	0.99
1:C:42:PRO:HG2	1:C:45:GLU:HG3	1.45	0.98
1:B:224:HIS:CD2	5:B:497:HOH:O	2.16	0.98
1:D:261:LYS:CG	5:D:566:HOH:O	2.09	0.98
1:D:307:HIS:NE2	2:D:315:SO4:O4	1.96	0.98
1:D:42:PRO:HB2	1:D:44:LYS:O	1.63	0.98
1:B:88:ASP:HB2	5:B:479:HOH:O	1.62	0.97
1:A:302:HIS:NE2	2:A:315:SO4:O2	1.96	0.97
1:B:38:THR:O	5:B:487:HOH:O	1.80	0.97
1:B:83:ALA:HB3	5:B:473:HOH:O	1.65	0.96
1:D:288:LYS:HE2	5:D:617:HOH:O	1.64	0.96
1:A:118:ARG:NH2	1:A:140:ASP:OD1	1.98	0.96
1:B:35:GLU:HG2	5:B:511:HOH:O	1.66	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:GLU:CB	5:D:536:HOH:O	2.08	0.95
1:C:42:PRO:CG	1:C:45:GLU:HG3	1.97	0.94
1:A:80:GLU:OE1	5:A:679:HOH:O	1.82	0.94
1:A:58:ASP:OD1	5:A:653:HOH:O	1.86	0.94
1:D:9:ARG:CA	5:D:561:HOH:O	2.04	0.94
1:D:9:ARG:C	5:D:561:HOH:O	2.09	0.94
1:D:106:GLY:O	5:D:506:HOH:O	1.84	0.94
1:A:44:LYS:O	1:A:45:GLU:HB2	1.67	0.93
1:B:239:ASN:HD21	1:B:242:ASP:H	1.14	0.92
1:C:38:THR:O	5:C:794:HOH:O	1.85	0.92
1:D:288:LYS:CE	5:D:617:HOH:O	2.15	0.92
1:D:118:ARG:O	5:D:504:HOH:O	1.86	0.92
1:C:260:LYS:HE2	5:C:796:HOH:O	1.67	0.92
1:D:42:PRO:HD2	1:D:45:GLU:OE1	1.67	0.92
1:D:105:PHE:CE1	5:D:697:HOH:O	2.22	0.92
1:A:51:HIS:HE1	5:A:652:HOH:O	1.53	0.91
1:B:235:ARG:HD3	5:B:627:HOH:O	1.70	0.91
1:C:42:PRO:HG2	1:C:45:GLU:HG2	1.51	0.91
1:D:42:PRO:CG	1:D:45:GLU:OE1	2.19	0.91
1:D:46:GLY:O	5:D:508:HOH:O	1.89	0.91
1:B:10:GLU:CB	5:B:508:HOH:O	2.13	0.90
1:D:109:GLU:N	5:D:536:HOH:O	2.05	0.90
1:C:9:ARG:CD	5:C:818:HOH:O	2.07	0.90
1:A:38:THR:O	5:A:492:HOH:O	1.88	0.90
1:C:241:PHE:O	5:C:850:HOH:O	1.87	0.90
1:D:296:TYR:HB2	5:D:608:HOH:O	1.71	0.90
1:A:7:PRO:HD3	1:A:59:HIS:CD2	2.07	0.90
1:B:88:ASP:CB	5:B:479:HOH:O	2.16	0.89
1:A:205:ALA:HB3	1:A:211:LEU:HD13	1.53	0.88
1:D:23:LYS:O	5:D:587:HOH:O	1.91	0.88
1:A:43:LYS:CB	5:A:565:HOH:O	2.21	0.88
1:D:288:LYS:NZ	5:D:617:HOH:O	2.03	0.87
1:B:83:ALA:CB	5:B:473:HOH:O	2.21	0.87
1:B:235:ARG:CD	5:B:627:HOH:O	2.21	0.87
1:D:225:LYS:HD2	5:D:502:HOH:O	1.73	0.87
1:C:224:HIS:NE2	2:C:317:SO4:S	2.43	0.87
1:D:189:GLU:HG3	5:D:526:HOH:O	1.74	0.86
1:A:9:ARG:HG3	5:A:501:HOH:O	1.74	0.86
1:A:261:LYS:NZ	5:A:511:HOH:O	2.08	0.86
1:B:205:ALA:HB3	1:B:211:LEU:HD13	1.58	0.86
1:D:42:PRO:CD	1:D:45:GLU:OE1	2.24	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:PRO:C	1:B:44:LYS:O	2.19	0.86
1:C:257:GLU:CD	5:C:823:HOH:O	2.19	0.86
1:C:142:LYS:NZ	5:C:1012:HOH:O	2.01	0.86
1:A:8:THR:N	5:A:551:HOH:O	2.09	0.85
1:C:92:THR:HG21	5:C:938:HOH:O	1.76	0.85
1:A:126:GLY:O	5:A:499:HOH:O	1.95	0.85
1:C:36:THR:HG22	5:C:861:HOH:O	1.76	0.84
1:C:9:ARG:HG2	5:C:818:HOH:O	1.78	0.84
1:B:43:LYS:CB	5:B:721:HOH:O	2.25	0.84
1:C:42:PRO:CD	1:C:45:GLU:HG3	2.06	0.84
1:C:42:PRO:HD2	1:C:45:GLU:HG3	1.58	0.84
1:D:307:HIS:NE2	2:D:315:SO4:S	2.50	0.83
1:B:224:HIS:C	1:B:226:ASN:H	1.85	0.83
1:B:228:LYS:NZ	5:B:636:HOH:O	2.10	0.83
1:A:312:GLU:OE2	5:A:498:HOH:O	1.97	0.83
1:A:7:PRO:HG2	1:A:63:PRO:HA	1.61	0.83
1:B:44:LYS:O	1:B:45:GLU:HB2	1.78	0.83
1:C:302:HIS:NE2	2:C:315:SO4:S	2.51	0.83
1:C:260:LYS:CD	5:C:1024:HOH:O	2.26	0.82
1:B:47:GLU:HB2	1:B:122:TYR:OH	1.80	0.82
1:B:88:ASP:CB	5:B:471:HOH:O	2.27	0.82
1:D:280:LYS:HE3	5:D:538:HOH:O	1.79	0.82
1:C:78:ASP:OD2	5:C:987:HOH:O	1.96	0.82
1:C:44:LYS:CA	1:C:126:GLY:HA3	2.09	0.82
1:C:44:LYS:HA	1:C:126:GLY:CA	2.10	0.81
1:D:239:ASN:HD21	1:D:242:ASP:H	1.26	0.81
1:A:9:ARG:CG	5:A:501:HOH:O	2.25	0.81
1:B:88:ASP:CA	5:B:479:HOH:O	2.27	0.81
1:D:261:LYS:HG2	5:D:566:HOH:O	1.76	0.81
1:C:307:HIS:NE2	2:C:316:SO4:O4	2.14	0.81
1:B:88:ASP:OD2	5:B:471:HOH:O	1.97	0.81
1:C:307:HIS:NE2	2:C:316:SO4:S	2.53	0.80
1:A:263:LEU:O	5:A:579:HOH:O	2.00	0.80
1:D:307:HIS:NE2	2:D:315:SO4:O1	2.13	0.80
1:A:189:GLU:OE1	5:A:488:HOH:O	1.99	0.80
1:A:264:ASN:ND2	5:A:563:HOH:O	1.98	0.80
1:C:189:GLU:CD	2:C:317:SO4:O1	2.25	0.80
1:B:51:HIS:HE1	5:B:573:HOH:O	1.65	0.80
1:B:224:HIS:HD2	5:B:497:HOH:O	1.54	0.80
1:C:9:ARG:CG	5:C:818:HOH:O	2.25	0.79
4:C:415:FAD:N3A	5:C:809:HOH:O	2.15	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:GLU:CD	5:D:536:HOH:O	2.26	0.79
1:C:129:GLN:NE2	5:C:800:HOH:O	2.15	0.79
1:D:225:LYS:CG	5:D:628:HOH:O	2.31	0.79
1:B:239:ASN:HD22	1:B:241:PHE:H	1.31	0.79
1:D:43:LYS:CB	5:D:674:HOH:O	2.31	0.78
1:D:238:LYS:HE3	5:D:563:HOH:O	1.82	0.78
1:D:225:LYS:HG3	5:D:628:HOH:O	1.83	0.78
1:A:94:ARG:HA	5:A:518:HOH:O	1.83	0.78
1:C:129:GLN:CG	5:C:800:HOH:O	2.31	0.78
1:D:42:PRO:O	1:D:43:LYS:CB	2.30	0.78
1:A:224:HIS:O	1:A:225:LYS:HB2	1.84	0.77
1:D:280:LYS:CE	5:D:538:HOH:O	2.31	0.77
1:B:126:GLY:O	5:B:484:HOH:O	1.99	0.77
1:C:155:LYS:CD	5:C:1025:HOH:O	2.15	0.77
1:B:83:ALA:C	5:B:473:HOH:O	2.27	0.76
1:C:307:HIS:ND1	5:C:960:HOH:O	2.17	0.76
1:D:105:PHE:CD1	5:D:697:HOH:O	2.37	0.76
1:A:42:PRO:CD	1:A:45:GLU:OE1	2.32	0.76
1:A:52:ARG:HD3	5:A:491:HOH:O	1.85	0.76
1:C:156:LYS:HD3	5:C:827:HOH:O	1.85	0.76
1:D:292:ASN:CA	5:D:622:HOH:O	1.96	0.76
1:B:280:LYS:O	1:B:284:GLU:HG2	1.86	0.76
1:C:257:GLU:HB2	5:C:821:HOH:O	1.84	0.75
1:D:224:HIS:C	1:D:226:ASN:H	1.93	0.75
2:C:315:SO4:O4	5:C:785:HOH:O	2.01	0.75
1:C:38:THR:HG21	5:C:921:HOH:O	1.85	0.75
1:C:224:HIS:O	1:C:225:LYS:HB2	1.85	0.75
1:A:307:HIS:NE2	2:A:316:SO4:O4	2.20	0.75
1:B:35:GLU:CG	5:B:511:HOH:O	2.29	0.75
1:B:42:PRO:O	1:B:44:LYS:O	2.05	0.75
1:B:47:GLU:HB2	1:B:122:TYR:CZ	2.22	0.75
1:A:302:HIS:NE2	2:A:315:SO4:S	2.57	0.74
1:A:9:ARG:HD3	5:A:501:HOH:O	1.87	0.74
1:C:260:LYS:CE	5:C:796:HOH:O	2.30	0.74
1:D:238:LYS:CE	5:D:563:HOH:O	2.36	0.74
5:A:488:HOH:O	1:B:124:GLU:OE1	2.05	0.74
1:B:225:LYS:HA	5:B:661:HOH:O	1.86	0.73
1:D:165:SER:OG	5:D:717:HOH:O	2.05	0.73
1:A:9:ARG:CD	5:A:501:HOH:O	2.37	0.73
1:A:14:ASN:HA	5:A:624:HOH:O	1.87	0.73
1:A:236:GLU:OE1	5:A:553:HOH:O	2.04	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:ALA:HB3	1:C:211:LEU:HD13	1.70	0.73
1:B:307:HIS:CD2	5:B:510:HOH:O	2.42	0.73
1:C:51:HIS:HE1	5:C:793:HOH:O	1.72	0.72
1:C:307:HIS:NE2	2:C:316:SO4:O3	2.18	0.72
1:B:307:HIS:HD2	5:B:510:HOH:O	1.71	0.72
1:C:92:THR:CG2	5:C:938:HOH:O	2.37	0.72
1:D:205:ALA:HB3	1:D:211:LEU:HD13	1.71	0.71
1:C:142:LYS:CG	5:C:993:HOH:O	2.23	0.71
1:C:8:THR:N	5:C:880:HOH:O	2.22	0.71
1:D:280:LYS:HD2	5:D:542:HOH:O	1.90	0.71
1:C:42:PRO:CG	1:C:45:GLU:CG	2.60	0.70
1:A:239:ASN:HD21	1:A:242:ASP:H	1.36	0.70
1:A:300:LYS:NZ	5:A:615:HOH:O	2.18	0.70
1:A:194:LYS:CD	5:A:645:HOH:O	2.39	0.70
1:C:84:LYS:O	5:C:807:HOH:O	2.04	0.70
1:D:124:GLU:CB	5:D:584:HOH:O	1.84	0.70
1:D:124:GLU:CG	5:D:584:HOH:O	2.24	0.70
1:C:189:GLU:OE2	2:C:317:SO4:O1	2.09	0.70
1:C:239:ASN:HD22	1:C:241:PHE:H	1.39	0.69
1:C:156:LYS:CD	5:C:827:HOH:O	2.40	0.69
1:D:127:ASN:ND2	5:D:498:HOH:O	2.23	0.69
1:A:92:THR:HG22	5:A:493:HOH:O	1.92	0.69
4:C:415:FAD:O1A	5:C:925:HOH:O	2.10	0.69
1:B:254:GLU:OE2	5:B:614:HOH:O	2.11	0.69
1:C:260:LYS:HD3	5:C:1024:HOH:O	1.88	0.69
1:A:171:LEU:HD23	1:A:202:VAL:HB	1.74	0.69
1:A:194:LYS:HD3	5:A:645:HOH:O	1.92	0.69
1:A:54:VAL:HG22	1:A:113:GLU:HG2	1.75	0.68
1:D:239:ASN:ND2	1:D:242:ASP:H	1.91	0.68
1:A:239:ASN:ND2	1:A:242:ASP:H	1.91	0.68
1:A:302:HIS:CD2	2:A:315:SO4:O2	2.47	0.68
1:D:105:PHE:CD1	5:D:592:HOH:O	2.45	0.68
1:A:14:ASN:OD1	5:A:624:HOH:O	2.11	0.68
1:B:102:SER:O	5:B:670:HOH:O	2.12	0.67
1:D:9:ARG:N	5:D:505:HOH:O	2.26	0.67
1:D:47:GLU:HB2	1:D:122:TYR:CZ	2.30	0.67
1:A:7:PRO:HG3	1:A:59:HIS:HB3	1.76	0.67
1:B:111:ASN:ND2	5:B:621:HOH:O	2.19	0.67
1:D:123:ASP:HB3	1:D:129:GLN:HG3	1.76	0.67
1:D:42:PRO:CB	1:D:44:LYS:O	2.28	0.67
1:D:307:HIS:CD2	2:D:315:SO4:O4	2.48	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:PRO:HG3	1:A:158:LEU:HD11	1.76	0.66
1:D:38:THR:O	5:D:639:HOH:O	2.14	0.66
1:D:221:GLU:OE1	5:D:619:HOH:O	2.13	0.66
1:A:7:PRO:CG	1:A:63:PRO:HA	2.26	0.66
1:C:129:GLN:HG2	5:C:800:HOH:O	1.90	0.66
1:B:8:THR:HB	5:B:441:HOH:O	1.95	0.65
1:D:8:THR:CB	5:D:505:HOH:O	2.44	0.65
1:D:106:GLY:O	5:D:589:HOH:O	2.14	0.65
1:C:307:HIS:CD2	2:C:316:SO4:O4	2.50	0.65
1:C:307:HIS:CD2	5:C:835:HOH:O	2.49	0.65
1:C:239:ASN:HD21	1:C:242:ASP:H	1.45	0.65
1:D:177:ILE:HD11	1:D:201:LEU:HD21	1.79	0.65
1:D:225:LYS:CE	5:D:502:HOH:O	2.45	0.65
1:B:140:ASP:OD2	5:B:620:HOH:O	2.14	0.65
1:D:280:LYS:O	1:D:284:GLU:HG2	1.98	0.64
1:C:17:LYS:CD	5:C:1011:HOH:O	1.84	0.64
1:B:53:ILE:HD12	1:B:116:ILE:HD12	1.79	0.64
1:C:9:ARG:NE	5:C:992:HOH:O	2.25	0.64
1:B:312:GLU:OE1	5:B:616:HOH:O	2.15	0.64
1:C:302:HIS:CE1	2:C:315:SO4:O3	2.51	0.64
1:D:105:PHE:HE1	5:D:697:HOH:O	1.69	0.63
1:D:27:ILE:HD11	5:D:714:HOH:O	1.98	0.63
1:D:101:PRO:HG3	1:D:185:GLU:HG2	1.79	0.63
1:D:47:GLU:HB2	1:D:122:TYR:CE2	2.34	0.63
1:D:131:LYS:HD3	5:D:432:HOH:O	1.97	0.63
1:A:47:GLU:HB2	1:A:122:TYR:OH	1.98	0.63
1:C:44:LYS:CB	1:C:125:ASN:C	2.70	0.63
1:D:9:ARG:NE	5:D:545:HOH:O	2.32	0.63
1:C:122:TYR:CE2	1:C:128:ILE:HG12	2.34	0.62
1:B:8:THR:HG21	5:B:645:HOH:O	1.98	0.62
1:B:239:ASN:ND2	1:B:242:ASP:H	1.92	0.62
1:D:102:SER:O	5:D:476:HOH:O	2.16	0.62
1:A:7:PRO:HG3	1:A:59:HIS:CB	2.30	0.62
1:B:44:LYS:CB	5:B:692:HOH:O	2.46	0.62
1:A:7:PRO:CD	1:A:59:HIS:CD2	2.81	0.62
1:C:11:PRO:HG3	1:C:158:LEU:HD11	1.81	0.62
1:D:105:PHE:HD1	5:D:592:HOH:O	1.82	0.62
1:D:123:ASP:O	1:D:125:ASN:N	2.32	0.62
1:A:9:ARG:HD3	5:A:521:HOH:O	2.00	0.62
1:A:43:LYS:N	1:A:44:LYS:O	2.32	0.62
1:B:101:PRO:HG3	1:B:185:GLU:HG2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:HIS:NE2	5:D:543:HOH:O	1.93	0.61
1:A:189:GLU:OE2	5:A:570:HOH:O	2.16	0.61
1:B:54:VAL:HG22	1:B:113:GLU:HG2	1.82	0.61
1:D:27:ILE:HD12	5:D:479:HOH:O	1.99	0.61
1:A:214:MET:HE3	1:A:218:LYS:HE3	1.80	0.61
1:B:307:HIS:CE1	2:B:315:SO4:O4	2.54	0.61
1:B:44:LYS:O	1:B:45:GLU:CB	2.47	0.61
1:D:8:THR:CB	5:D:537:HOH:O	2.49	0.61
1:B:198:ASN:HB3	5:B:474:HOH:O	2.01	0.61
1:A:307:HIS:CE1	5:A:627:HOH:O	2.53	0.61
1:D:280:LYS:HB2	5:D:542:HOH:O	2.00	0.61
1:C:42:PRO:CA	5:C:828:HOH:O	2.33	0.60
1:D:43:LYS:O	1:D:46:GLY:HA3	2.02	0.60
1:A:93:VAL:HG23	5:A:424:HOH:O	2.01	0.60
1:A:249:SER:O	1:A:285:GLU:HG2	2.01	0.60
1:D:312:GLU:HG2	5:D:593:HOH:O	2.01	0.60
1:C:297:GLU:HB2	5:C:838:HOH:O	2.01	0.60
1:A:8:THR:CG2	5:A:551:HOH:O	2.42	0.60
1:B:84:LYS:HG3	5:B:473:HOH:O	2.01	0.60
1:B:307:HIS:CE1	2:B:315:SO4:S	2.95	0.60
1:C:222:SER:HB2	5:C:819:HOH:O	2.01	0.60
1:A:9:ARG:CD	5:A:521:HOH:O	2.48	0.60
1:A:7:PRO:O	1:A:8:THR:O	2.20	0.60
1:D:161:ASN:C	1:D:161:ASN:HD22	2.10	0.59
1:D:55:LEU:O	1:D:111:ASN:HB2	2.02	0.59
1:A:304:GLU:HA	5:A:519:HOH:O	2.03	0.59
1:C:97:SER:O	1:C:98:ILE:HB	2.01	0.59
1:A:307:HIS:NE2	2:A:316:SO4:S	2.75	0.59
1:B:101:PRO:HG2	1:B:107:MET:HE1	1.84	0.59
1:D:29:ASN:OD1	1:D:51:HIS:HD2	1.84	0.59
1:A:51:HIS:CE1	5:A:652:HOH:O	2.40	0.59
1:C:171:LEU:HD23	1:C:202:VAL:HB	1.85	0.59
1:A:53:ILE:HD13	1:A:116:ILE:HD12	1.84	0.58
1:C:242:ASP:HB2	1:D:29:ASN:O	2.02	0.58
1:A:42:PRO:C	1:A:44:LYS:O	2.46	0.58
1:A:239:ASN:HD22	1:A:241:PHE:H	1.51	0.58
1:C:124:GLU:HG3	1:D:223:LYS:HG3	1.86	0.58
1:A:191:LYS:HD3	5:A:689:HOH:O	2.04	0.57
1:D:225:LYS:HG2	5:D:628:HOH:O	1.99	0.57
1:A:86:LEU:O	1:A:87:ALA:HB3	2.05	0.57
1:B:84:LYS:N	5:B:473:HOH:O	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ARG:HE	1:A:139:CYS:CB	2.17	0.57
1:C:124:GLU:N	5:C:858:HOH:O	2.37	0.57
1:C:276:LYS:HG3	5:C:927:HOH:O	2.03	0.57
1:D:239:ASN:HD22	1:D:241:PHE:H	1.51	0.57
1:B:55:LEU:O	1:B:111:ASN:HB2	2.04	0.57
1:B:197:GLY:O	1:B:226:ASN:ND2	2.34	0.57
1:A:194:LYS:HD2	5:A:645:HOH:O	2.04	0.57
1:D:29:ASN:OD1	1:D:51:HIS:CD2	2.58	0.56
1:B:249:SER:O	1:B:285:GLU:HG2	2.05	0.56
1:D:86:LEU:O	1:D:87:ALA:HB3	2.04	0.56
1:B:102:SER:O	1:B:103:TYR:CB	2.54	0.56
1:A:307:HIS:CD2	2:A:316:SO4:O4	2.57	0.56
1:B:239:ASN:HD22	1:B:241:PHE:N	2.00	0.56
1:C:214:MET:HE3	1:C:218:LYS:HE2	1.86	0.56
1:A:77:GLU:OE1	1:A:82:LYS:HD3	2.06	0.56
1:A:142:LYS:HE2	5:A:574:HOH:O	2.06	0.56
1:C:260:LYS:HD2	5:C:1024:HOH:O	2.01	0.56
1:C:260:LYS:NZ	5:C:796:HOH:O	2.29	0.56
1:C:68:GLN:O	1:C:97:SER:O	2.23	0.56
1:C:88:ASP:O	1:C:89:VAL:HB	2.05	0.56
1:C:239:ASN:ND2	1:C:242:ASP:H	2.04	0.55
1:C:34:PRO:HG3	5:C:808:HOH:O	2.05	0.55
1:A:311:VAL:HG11	5:A:615:HOH:O	2.05	0.55
1:B:77:GLU:OE1	5:B:556:HOH:O	2.18	0.55
1:B:262:ILE:HG23	1:B:267:GLY:C	2.32	0.55
1:A:155:LYS:HD2	5:A:558:HOH:O	2.06	0.55
1:B:224:HIS:CB	5:B:497:HOH:O	2.55	0.55
1:D:224:HIS:C	1:D:226:ASN:N	2.65	0.55
1:B:177:ILE:HD11	1:B:201:LEU:HD21	1.89	0.54
1:B:279:GLU:HG3	1:B:311:VAL:HG21	1.89	0.54
1:C:97:SER:O	1:C:98:ILE:CB	2.53	0.54
1:A:221:GLU:O	5:A:505:HOH:O	2.19	0.54
1:C:66:ILE:HD13	1:C:100:SER:O	2.08	0.54
1:D:18:LYS:HD2	5:D:673:HOH:O	2.08	0.54
1:A:35:GLU:HA	5:A:576:HOH:O	2.08	0.54
1:B:131:LYS:HD3	5:B:501:HOH:O	2.07	0.54
1:B:47:GLU:HB2	1:B:122:TYR:CE2	2.43	0.54
1:C:93:VAL:HG23	5:C:713:HOH:O	2.08	0.54
1:D:102:SER:O	1:D:103:TYR:CB	2.55	0.54
1:B:248:ILE:O	1:B:252:VAL:HG23	2.07	0.53
1:D:42:PRO:HB2	1:D:44:LYS:C	2.33	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:HIS:C	1:B:226:ASN:N	2.59	0.53
1:A:92:THR:CG2	5:A:542:HOH:O	2.14	0.53
1:D:32:LEU:HD11	1:D:52:ARG:HB2	1.91	0.53
1:C:237:GLU:N	5:C:909:HOH:O	2.42	0.53
1:D:205:ALA:CB	1:D:211:LEU:HD13	2.36	0.53
1:D:218:LYS:HG2	5:D:692:HOH:O	2.07	0.53
1:B:205:ALA:CB	1:B:211:LEU:HD13	2.35	0.53
1:C:302:HIS:NE2	2:C:315:SO4:O3	2.42	0.53
1:D:253:ARG:CG	5:D:606:HOH:O	2.30	0.53
1:A:224:HIS:O	1:A:225:LYS:CB	2.55	0.52
1:D:43:LYS:O	5:D:710:HOH:O	2.19	0.52
1:A:105:PHE:O	5:A:669:HOH:O	2.19	0.52
1:D:213:MET:O	1:D:217:LEU:HG	2.09	0.52
1:D:249:SER:O	1:D:285:GLU:HG2	2.10	0.52
1:D:8:THR:C	5:D:505:HOH:O	2.52	0.52
1:B:67:GLY:HA3	1:B:157:PHE:O	2.10	0.52
1:C:249:SER:O	1:C:285:GLU:HG2	2.10	0.52
1:A:7:PRO:HB3	1:A:59:HIS:HD2	1.74	0.52
1:B:47:GLU:HB2	1:B:122:TYR:HH	1.75	0.52
1:B:43:LYS:N	1:B:44:LYS:O	2.43	0.51
1:B:128:ILE:HG21	1:B:131:LYS:HG3	1.91	0.51
1:A:38:THR:HG22	1:A:39:GLY:H	1.75	0.51
1:D:96:TYR:CE1	4:D:415:FAD:H2'	2.46	0.51
1:C:45:GLU:HA	1:C:45:GLU:OE1	2.10	0.51
1:C:235:ARG:HG2	5:C:995:HOH:O	2.11	0.51
1:B:27:ILE:HD13	5:B:621:HOH:O	2.09	0.51
1:B:307:HIS:NE2	2:B:315:SO4:O4	2.44	0.51
1:B:248:ILE:N	5:B:500:HOH:O	2.29	0.51
1:D:280:LYS:CD	5:D:542:HOH:O	2.51	0.51
1:B:10:GLU:HB3	5:B:508:HOH:O	1.95	0.51
1:D:53:ILE:HD12	1:D:116:ILE:HD12	1.93	0.51
1:D:255:GLN:O	1:D:259:VAL:HG23	2.11	0.51
1:A:96:TYR:CE1	4:A:415:FAD:H2'	2.45	0.51
1:B:103:TYR:HB2	5:B:470:HOH:O	2.10	0.51
1:D:197:GLY:O	1:D:226:ASN:ND2	2.35	0.51
1:B:205:ALA:O	1:B:233:ILE:HA	2.11	0.51
1:A:7:PRO:HD2	1:A:64:TYR:N	2.26	0.50
1:B:265:GLY:O	5:B:657:HOH:O	2.19	0.50
1:D:206:PRO:HB3	1:D:235:ARG:NE	2.26	0.50
1:B:125:ASN:HB2	5:B:477:HOH:O	2.10	0.50
2:C:315:SO4:O4	5:C:862:HOH:O	2.17	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ASN:HB2	1:D:122:TYR:CE1	2.46	0.50
1:D:262:ILE:HG23	1:D:267:GLY:C	2.36	0.50
1:A:7:PRO:O	1:A:8:THR:C	2.53	0.50
1:A:43:LYS:O	1:A:126:GLY:HA3	2.12	0.50
2:A:315:SO4:O4	5:A:496:HOH:O	2.17	0.50
1:A:205:ALA:CB	1:A:211:LEU:HD13	2.35	0.50
1:B:224:HIS:HB3	5:B:497:HOH:O	2.12	0.50
1:D:67:GLY:HA3	1:D:157:PHE:O	2.11	0.50
1:B:224:HIS:O	1:B:226:ASN:N	2.41	0.50
1:D:163:ASP:CG	5:D:546:HOH:O	2.55	0.50
1:D:225:LYS:HA	1:D:225:LYS:HZ3	1.75	0.50
1:C:11:PRO:HG3	1:C:158:LEU:CD1	2.42	0.49
1:C:177:ILE:HD11	1:C:201:LEU:HD21	1.93	0.49
1:B:29:ASN:OD1	1:B:51:HIS:CD2	2.64	0.49
1:B:120:ASN:HB2	1:B:122:TYR:CE1	2.47	0.49
1:B:181:ILE:CD1	1:B:213:MET:HG3	2.41	0.49
1:B:103:TYR:HA	1:B:107:MET:SD	2.52	0.49
1:B:206:PRO:HB3	1:B:235:ARG:HE	1.76	0.49
1:C:20:ASN:CG	1:C:20:ASN:O	2.56	0.49
1:C:276:LYS:CG	5:C:927:HOH:O	2.59	0.49
1:C:45:GLU:O	1:C:46:GLY:O	2.30	0.49
1:C:43:LYS:O	1:C:44:LYS:CB	2.60	0.49
1:A:64:TYR:CE1	1:A:98:ILE:HG21	2.48	0.49
1:D:238:LYS:HE2	5:D:563:HOH:O	2.08	0.49
1:A:118:ARG:HE	1:A:139:CYS:HB3	1.77	0.49
1:B:102:SER:O	1:B:103:TYR:HB2	2.12	0.49
1:A:91:TYR:CE1	1:A:133:VAL:HG21	2.48	0.49
1:A:11:PRO:HG3	1:A:158:LEU:CD1	2.39	0.49
1:C:122:TYR:HE2	1:C:128:ILE:HG12	1.76	0.49
1:A:118:ARG:HG2	1:A:136:ASN:OD1	2.12	0.48
1:C:285:GLU:OE1	5:C:973:HOH:O	2.20	0.48
1:D:9:ARG:HD3	1:D:161:ASN:HB2	1.93	0.48
1:D:16:PHE:HE2	1:D:61:ALA:O	1.95	0.48
1:C:255:GLN:OE1	5:C:966:HOH:O	2.19	0.48
1:A:214:MET:HE1	1:A:229:LEU:HD21	1.96	0.48
1:B:117:LYS:O	1:B:135:SER:HB2	2.13	0.48
1:C:137:TYR:HA	5:C:913:HOH:O	2.14	0.48
1:A:98:ILE:HG12	1:A:112:ILE:HD11	1.96	0.48
1:B:29:ASN:OD1	1:B:51:HIS:HD2	1.97	0.48
1:D:208:SER:O	1:D:211:LEU:HB2	2.14	0.48
1:B:206:PRO:HB3	1:B:235:ARG:NE	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:GLU:CD	1:C:189:GLU:HG3	2.39	0.48
1:A:59:HIS:HE1	1:A:111:ASN:O	1.97	0.47
1:A:8:THR:HG22	5:A:551:HOH:O	2.11	0.47
1:C:279:GLU:CG	1:C:311:VAL:HG21	2.44	0.47
1:D:103:TYR:CD2	1:D:106:GLY:HA2	2.49	0.47
1:C:96:TYR:CE1	4:C:415:FAD:H2'	2.50	0.47
1:C:296:TYR:OH	5:C:811:HOH:O	2.08	0.47
1:D:103:TYR:HA	1:D:107:MET:SD	2.54	0.47
1:D:106:GLY:H	1:D:107:MET:HE3	1.79	0.47
1:D:140:ASP:OD1	5:D:614:HOH:O	2.20	0.47
1:B:9:ARG:C	5:B:495:HOH:O	2.39	0.47
1:D:51:HIS:HE1	5:D:642:HOH:O	1.97	0.47
1:C:92:THR:CG2	5:C:836:HOH:O	2.36	0.47
1:D:43:LYS:C	1:D:46:GLY:HA2	2.40	0.47
1:A:101:PRO:HG2	1:A:104:SER:C	2.40	0.47
1:B:16:PHE:HE2	1:B:61:ALA:O	1.97	0.47
1:B:181:ILE:HD13	1:B:213:MET:HG3	1.97	0.47
1:B:208:SER:O	1:B:211:LEU:HB2	2.14	0.47
1:D:86:LEU:O	1:D:87:ALA:CB	2.63	0.47
1:A:279:GLU:CB	1:A:311:VAL:HG21	2.45	0.47
1:A:7:PRO:CG	1:A:59:HIS:CD2	2.98	0.47
1:B:96:TYR:CE1	4:B:415:FAD:H2'	2.50	0.47
1:B:224:HIS:CG	5:B:497:HOH:O	2.54	0.47
1:C:13:ILE:HA	1:C:152:PRO:O	2.15	0.46
1:C:99:ALA:HA	1:C:178:ALA:O	2.15	0.46
1:D:225:LYS:HE2	5:D:502:HOH:O	2.13	0.46
1:A:9:ARG:NH1	5:A:435:HOH:O	2.48	0.46
1:A:66:ILE:HD13	1:A:100:SER:O	2.15	0.46
1:A:107:MET:HE1	5:A:633:HOH:O	2.15	0.46
1:A:205:ALA:HB3	1:A:211:LEU:CD1	2.36	0.46
1:C:45:GLU:C	1:C:46:GLY:O	2.58	0.46
1:A:34:PRO:HD3	5:A:531:HOH:O	2.15	0.46
1:A:117:LYS:O	1:A:135:SER:HB2	2.16	0.46
1:A:179:PRO:HB3	5:A:523:HOH:O	2.15	0.46
1:A:307:HIS:ND1	5:A:627:HOH:O	2.35	0.46
1:B:255:GLN:O	1:B:259:VAL:HG23	2.15	0.46
1:C:21:PRO:HB2	1:C:148:THR:HG23	1.98	0.46
1:C:224:HIS:C	1:C:226:ASN:H	2.23	0.46
1:C:302:HIS:NE2	2:C:315:SO4:O1	2.42	0.46
1:D:54:VAL:HG22	1:D:113:GLU:HG2	1.97	0.46
1:D:225:LYS:HA	1:D:225:LYS:NZ	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLY:HA3	1:A:157:PHE:O	2.15	0.46
1:C:59:HIS:HE1	1:C:111:ASN:O	1.98	0.46
1:A:40:LYS:HG2	5:A:625:HOH:O	2.15	0.46
1:C:41:ARG:HD3	1:C:46:GLY:O	2.14	0.46
1:D:106:GLY:CA	5:D:589:HOH:O	2.63	0.46
1:D:205:ALA:O	1:D:233:ILE:HA	2.14	0.46
1:A:194:LYS:NZ	5:A:522:HOH:O	2.49	0.46
1:D:300:LYS:O	1:D:304:GLU:HG3	2.15	0.46
1:C:14:ASN:HB2	5:C:908:HOH:O	2.16	0.46
1:C:44:LYS:N	1:C:126:GLY:HA3	2.30	0.46
1:C:220:LEU:O	1:C:224:HIS:ND1	2.48	0.46
1:D:36:THR:HA	5:D:567:HOH:O	2.16	0.46
1:D:181:ILE:HD13	1:D:213:MET:HG3	1.97	0.46
1:A:38:THR:HG22	1:A:39:GLY:N	2.30	0.46
1:D:16:PHE:CG	1:D:22:TYR:HB2	2.51	0.46
1:D:181:ILE:CD1	1:D:213:MET:HG3	2.46	0.46
1:A:279:GLU:CG	1:A:311:VAL:HG21	2.47	0.45
1:B:307:HIS:CE1	2:B:315:SO4:O3	2.68	0.45
1:D:99:ALA:HA	1:D:178:ALA:O	2.15	0.45
1:C:120:ASN:HB2	1:C:122:TYR:CZ	2.51	0.45
1:C:307:HIS:HD2	5:C:835:HOH:O	1.89	0.45
1:D:81:LYS:NZ	1:D:92:THR:HG22	2.31	0.45
1:B:42:PRO:HD2	1:B:45:GLU:OE1	2.17	0.45
1:C:313:THR:OG1	5:C:927:HOH:O	2.05	0.45
1:D:186:GLU:HA	1:D:190:HIS:HB2	1.97	0.45
1:A:20:ASN:CG	1:A:20:ASN:O	2.59	0.45
1:B:88:ASP:HB3	5:B:471:HOH:O	2.01	0.45
1:D:43:LYS:O	1:D:46:GLY:CA	2.65	0.45
1:A:42:PRO:CG	1:A:45:GLU:OE1	2.64	0.45
1:A:224:HIS:C	1:A:226:ASN:H	2.25	0.45
1:A:271:ILE:HB	1:A:311:VAL:HG23	1.99	0.45
1:D:171:LEU:HD23	1:D:202:VAL:HB	1.99	0.45
1:D:248:ILE:O	1:D:252:VAL:HG23	2.17	0.45
1:C:257:GLU:CG	5:C:823:HOH:O	2.61	0.45
1:D:44:LYS:HA	1:D:45:GLU:HA	1.48	0.45
1:D:300:LYS:HE3	5:D:624:HOH:O	2.17	0.45
1:A:57:ILE:HD12	1:A:62:TYR:HB3	1.98	0.44
1:B:171:LEU:HD23	1:B:202:VAL:HB	1.98	0.44
1:D:202:VAL:HG12	1:D:248:ILE:HG22	1.99	0.44
1:C:222:SER:CB	5:C:819:HOH:O	2.62	0.44
1:D:16:PHE:CE2	1:D:61:ALA:O	2.70	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:HIS:HD2	5:D:463:HOH:O	1.99	0.44
1:D:103:TYR:CE2	1:D:106:GLY:HA2	2.52	0.44
1:B:280:LYS:HB3	5:B:600:HOH:O	2.17	0.44
1:B:9:ARG:HD2	1:B:9:ARG:N	2.32	0.44
1:C:22:TYR:HE2	1:C:57:ILE:HG22	1.83	0.44
1:B:59:HIS:HB3	1:B:110:ASP:OD1	2.16	0.44
1:C:67:GLY:HA3	1:C:157:PHE:O	2.17	0.44
1:B:39:GLY:HA2	5:B:540:HOH:O	2.17	0.44
1:C:257:GLU:HG3	5:C:823:HOH:O	2.18	0.44
1:A:205:ALA:O	1:A:233:ILE:HA	2.17	0.43
1:D:38:THR:N	5:D:516:HOH:O	2.50	0.43
1:D:64:TYR:CE1	1:D:98:ILE:HG21	2.53	0.43
1:B:261:LYS:HD3	5:B:478:HOH:O	2.18	0.43
1:D:185:GLU:OE2	1:D:190:HIS:NE2	2.51	0.43
1:B:161:ASN:C	1:B:161:ASN:HD22	2.26	0.43
1:D:177:ILE:HB	1:D:203:TYR:CE1	2.53	0.43
1:A:32:LEU:HD13	1:A:212:VAL:HB	1.99	0.43
1:C:237:GLU:C	5:C:909:HOH:O	2.60	0.43
1:D:307:HIS:CE1	2:D:315:SO4:O1	2.69	0.43
1:A:307:HIS:NE2	2:A:316:SO4:O1	2.51	0.43
4:C:415:FAD:H1'1	4:C:415:FAD:H9	1.58	0.43
1:D:106:GLY:HA3	5:D:663:HOH:O	2.17	0.43
1:B:40:LYS:O	1:B:42:PRO:HD3	2.18	0.43
1:C:68:GLN:HG2	1:C:154:GLY:O	2.18	0.43
1:D:8:THR:C	1:D:10:GLU:H	2.26	0.43
1:D:27:ILE:CD1	5:D:714:HOH:O	2.59	0.43
1:B:9:ARG:CA	5:B:495:HOH:O	1.90	0.43
1:D:41:ARG:HA	1:D:42:PRO:HD3	1.73	0.43
1:D:102:SER:O	1:D:103:TYR:HB2	2.19	0.43
1:D:124:GLU:HG2	5:D:584:HOH:O	2.06	0.43
1:A:307:HIS:CD2	5:A:575:HOH:O	2.72	0.43
1:C:156:LYS:HD2	5:C:827:HOH:O	2.16	0.43
1:B:57:ILE:HD12	1:B:62:TYR:HB3	2.01	0.42
1:C:185:GLU:HB2	1:C:216:TYR:OH	2.19	0.42
1:C:279:GLU:CB	1:C:311:VAL:HG21	2.49	0.42
1:A:45:GLU:O	1:A:46:GLY:O	2.38	0.42
1:A:248:ILE:O	1:A:252:VAL:HG23	2.18	0.42
1:C:278:MET:HA	5:C:885:HOH:O	2.18	0.42
1:A:61:ALA:C	1:A:63:PRO:HD3	2.44	0.42
1:A:86:LEU:O	1:A:87:ALA:CB	2.67	0.42
1:C:47:GLU:HB2	1:C:122:TYR:OH	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ASN:HB2	1:C:122:TYR:CE1	2.54	0.42
1:A:101:PRO:O	1:A:102:SER:C	2.60	0.42
1:C:32:LEU:HD11	1:C:52:ARG:HB2	2.02	0.42
4:D:415:FAD:H9	4:D:415:FAD:H1'1	1.83	0.42
1:C:189:GLU:OE1	2:C:317:SO4:O1	2.37	0.42
1:C:312:GLU:HA	1:C:312:GLU:OE2	2.19	0.42
1:B:35:GLU:O	1:B:38:THR:HB	2.19	0.42
1:B:99:ALA:HA	1:B:178:ALA:O	2.19	0.42
1:B:159:LEU:HG	1:B:183:MET:HG2	2.01	0.42
1:C:45:GLU:O	1:C:46:GLY:C	2.62	0.42
1:C:91:TYR:CE1	1:C:133:VAL:HG21	2.54	0.42
1:A:32:LEU:HD11	1:A:52:ARG:HB2	2.02	0.42
1:A:167:ASP:O	1:A:267:GLY:HA3	2.20	0.42
1:B:27:ILE:CD1	5:B:621:HOH:O	2.66	0.42
1:B:32:LEU:HD21	1:B:52:ARG:HB2	2.01	0.42
1:D:40:LYS:HD3	1:D:236:GLU:OE2	2.19	0.42
1:A:118:ARG:HE	1:A:139:CYS:HB2	1.83	0.42
1:A:107:MET:HG3	1:A:190:HIS:CE1	2.54	0.42
1:D:17:LYS:H	1:D:20:ASN:ND2	2.17	0.42
1:A:35:GLU:HG2	5:A:576:HOH:O	2.20	0.42
1:A:154:GLY:HA3	5:A:597:HOH:O	2.19	0.42
1:B:247:TYR:HA	5:B:500:HOH:O	2.18	0.42
1:B:306:ALA:O	1:B:307:HIS:HB2	2.19	0.41
1:A:178:ALA:HA	1:A:181:ILE:HD12	2.02	0.41
1:A:179:PRO:O	1:A:183:MET:HG3	2.21	0.41
1:B:91:TYR:CE1	1:B:133:VAL:HG21	2.55	0.41
1:A:29:ASN:O	1:B:242:ASP:HB2	2.20	0.41
1:A:228:LYS:HE2	5:A:642:HOH:O	2.21	0.41
1:B:26:VAL:HG21	1:B:141:LEU:HB3	2.02	0.41
1:C:248:ILE:O	1:C:252:VAL:HG23	2.20	0.41
1:D:84:LYS:HE3	1:D:86:LEU:HD11	2.02	0.41
1:A:253:ARG:HA	1:A:289:ILE:HD11	2.01	0.41
1:C:124:GLU:HB2	1:D:223:LYS:HD2	2.03	0.41
1:C:284:GLU:HB2	5:C:930:HOH:O	2.20	0.41
1:C:52:ARG:HD3	5:C:810:HOH:O	2.19	0.41
1:C:224:HIS:NE2	2:C:317:SO4:O2	2.52	0.41
1:C:283:ILE:CD1	1:C:309:LEU:HD21	2.51	0.41
1:A:88:ASP:HB3	1:A:89:VAL:H	1.75	0.41
1:D:171:LEU:HD21	1:D:252:VAL:HG22	2.03	0.41
1:B:78:ASP:HB3	1:B:81:LYS:HB2	2.02	0.41
1:C:57:ILE:HD11	1:C:64:TYR:HE2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:LYS:NZ	5:D:538:HOH:O	2.45	0.41
1:D:225:LYS:CD	5:D:502:HOH:O	2.42	0.41
1:A:7:PRO:CB	1:A:59:HIS:HD2	2.34	0.41
1:B:32:LEU:HD11	1:B:52:ARG:HB2	2.02	0.41
1:C:16:PHE:HE2	1:C:61:ALA:O	2.03	0.41
1:C:131:LYS:HE3	5:C:1026:HOH:O	2.21	0.41
1:C:225:LYS:N	1:C:225:LYS:HE2	2.35	0.41
1:D:45:GLU:N	1:D:46:GLY:HA2	2.35	0.41
1:D:111:ASN:ND2	5:D:479:HOH:O	2.45	0.41
1:D:47:GLU:CB	1:D:122:TYR:CZ	3.02	0.41
1:A:25:LYS:NZ	5:A:632:HOH:O	2.53	0.40
1:C:185:GLU:O	1:C:189:GLU:HB2	2.21	0.40
1:C:205:ALA:O	1:C:233:ILE:HA	2.21	0.40
1:A:14:ASN:CB	5:A:624:HOH:O	2.69	0.40
1:C:9:ARG:HG3	5:C:761:HOH:O	2.20	0.40
1:C:38:THR:CG2	5:C:1035:HOH:O	2.70	0.40
1:D:224:HIS:O	1:D:226:ASN:N	2.48	0.40
1:C:29:ASN:OD1	1:C:51:HIS:CD2	2.74	0.40
1:C:311:VAL:HG22	1:C:313:THR:HG23	2.03	0.40
1:D:11:PRO:HG3	1:D:158:LEU:CD1	2.51	0.40

All (11) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:GLU:OE2	2:B:315:SO4:O3[2_555]	1.49	0.71
1:B:297:GLU:OE1	2:A:316:SO4:O1[2_545]	1.80	0.40
1:B:301:HIS:ND1	2:A:316:SO4:O2[2_545]	1.86	0.34
2:C:317:SO4:O4	5:D:584:HOH:O[1_655]	1.87	0.33
1:D:297:GLU:OE1	2:C:316:SO4:O3[2_454]	1.97	0.23
1:D:17:LYS:NZ	5:B:479:HOH:O[2_454]	2.00	0.20
1:D:297:GLU:OE2	2:C:316:SO4:O1[2_454]	2.04	0.16
1:C:301:HIS:ND1	2:D:315:SO4:O4[2_444]	2.11	0.09
1:B:297:GLU:OE2	2:A:316:SO4:O1[2_545]	2.12	0.08
5:C:942:HOH:O	5:D:663:HOH:O[2_544]	2.15	0.05
1:B:302:HIS:NE2	2:A:315:SO4:O3[2_545]	2.16	0.04

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	302/314 (96%)	281 (93%)	14 (5%)	7 (2%)	5	2
1	B	295/314 (94%)	284 (96%)	9 (3%)	2 (1%)	18	21
1	C	300/314 (96%)	284 (95%)	8 (3%)	8 (3%)	4	2
1	D	302/314 (96%)	280 (93%)	14 (5%)	8 (3%)	4	2
All	All	1199/1256 (96%)	1129 (94%)	45 (4%)	25 (2%)	5	3

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	C	46	GLY
1	C	89	VAL
1	D	124	GLU
1	A	9	ARG
1	A	44	LYS
1	A	89	VAL
1	B	122	TYR
1	C	44	LYS
1	C	122	TYR
1	D	43	LYS
1	D	44	LYS
1	D	87	ALA
1	A	88	ASP
1	B	44	LYS
1	C	98	ILE
1	D	9	ARG
1	D	122	TYR
1	A	10	GLU
1	C	10	GLU
1	C	45	GLU
1	C	157	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	225	LYS
1	D	89	VAL
1	D	42	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	254/266 (96%)	243 (96%)	11 (4%)	26	36
1	B	253/266 (95%)	240 (95%)	13 (5%)	21	29
1	C	256/266 (96%)	246 (96%)	10 (4%)	28	40
1	D	255/266 (96%)	239 (94%)	16 (6%)	16	21
All	All	1018/1064 (96%)	968 (95%)	50 (5%)	22	31

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	30	VAL
1	A	86	LEU
1	A	92	THR
1	A	118	ARG
1	A	127	ASN
1	A	150	THR
1	A	194	LYS
1	A	211	LEU
1	A	297	GLU
1	A	311	VAL
1	B	9	ARG
1	B	20	ASN
1	B	30	VAL
1	B	45	GLU
1	B	80	GLU
1	B	92	THR
1	B	150	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	161	ASN
1	B	181	ILE
1	B	211	LEU
1	B	225	LYS
1	B	284	GLU
1	B	311	VAL
1	C	8	THR
1	C	20	ASN
1	C	30	VAL
1	C	92	THR
1	C	150	THR
1	C	211	LEU
1	C	225	LYS
1	C	257	GLU
1	C	297	GLU
1	C	303	LEU
1	D	9	ARG
1	D	20	ASN
1	D	30	VAL
1	D	35	GLU
1	D	45	GLU
1	D	65	VAL
1	D	82	LYS
1	D	88	ASP
1	D	107	MET
1	D	128	ILE
1	D	150	THR
1	D	161	ASN
1	D	211	LEU
1	D	225	LYS
1	D	278	MET
1	D	311	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	59	HIS
1	A	129	GLN
1	A	239	ASN
1	B	12	GLN
1	B	20	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	51	HIS
1	B	161	ASN
1	B	224	HIS
1	B	239	ASN
1	B	307	HIS
1	C	20	ASN
1	C	51	HIS
1	C	59	HIS
1	C	239	ASN
1	C	301	HIS
1	D	20	ASN
1	D	51	HIS
1	D	59	HIS
1	D	129	GLN
1	D	161	ASN
1	D	224	HIS
1	D	239	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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	SO4	C	317	-	4,4,4	0.33	0	6,6,6	0.83	0
4	FAD	C	415	-	58,58,58	2.36	29 (50%)	85,89,89	1.83	21 (24%)
2	SO4	A	316	-	4,4,4	0.58	0	6,6,6	0.57	0
2	SO4	A	315	-	4,4,4	0.45	0	6,6,6	0.67	0
2	SO4	B	315	-	4,4,4	0.46	0	6,6,6	0.58	0
4	FAD	D	415	-	58,58,58	1.19	4 (6%)	85,89,89	1.56	16 (18%)
4	FAD	A	415	-	58,58,58	1.14	4 (6%)	85,89,89	1.55	15 (17%)
4	FAD	B	415	-	58,58,58	1.10	5 (8%)	85,89,89	1.57	14 (16%)
2	SO4	C	315	-	4,4,4	0.43	0	6,6,6	0.76	0
2	SO4	C	316	-	4,4,4	0.64	0	6,6,6	0.65	0
2	SO4	D	315	-	4,4,4	0.48	0	6,6,6	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FAD	B	415	-	-	3/34/50/50	0/6/6/6
4	FAD	A	415	-	-	4/34/50/50	0/6/6/6
4	FAD	C	415	-	-	14/34/50/50	0/6/6/6
4	FAD	D	415	-	-	3/34/50/50	0/6/6/6

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	415	FAD	P-O3P	-4.41	1.54	1.59
4	C	415	FAD	C9A-N10	-4.21	1.33	1.41
4	C	415	FAD	C5A-N7A	-4.18	1.31	1.39
4	A	415	FAD	C4X-N5	3.74	1.38	1.30
4	D	415	FAD	C4X-N5	3.72	1.38	1.30
4	C	415	FAD	O2'-C2'	-3.65	1.35	1.43
4	C	415	FAD	O4B-C4B	-3.62	1.36	1.45
4	B	415	FAD	C4X-N5	3.59	1.38	1.30
4	C	415	FAD	C4'-C3'	-3.43	1.47	1.53
4	C	415	FAD	C2-N3	-3.35	1.31	1.39
4	C	415	FAD	O2-C2	-3.34	1.17	1.24
4	C	415	FAD	PA-O2A	-3.32	1.40	1.55
4	C	415	FAD	O4-C4	-3.16	1.17	1.23
4	C	415	FAD	P-O2P	-3.15	1.40	1.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	415	FAD	P-O1P	-3.07	1.40	1.50
4	A	415	FAD	C2A-N1A	2.98	1.39	1.33
4	B	415	FAD	C2A-N1A	2.97	1.39	1.33
4	C	415	FAD	C5X-N5	-2.95	1.34	1.39
4	C	415	FAD	PA-O1A	-2.95	1.40	1.50
4	C	415	FAD	C6-C5X	-2.93	1.35	1.40
4	C	415	FAD	C5A-C4A	-2.93	1.33	1.39
4	D	415	FAD	C2A-N1A	2.85	1.39	1.33
4	C	415	FAD	C4X-C10	-2.84	1.35	1.44
4	C	415	FAD	PA-O3P	-2.82	1.56	1.59
4	C	415	FAD	C4X-C4	-2.75	1.34	1.44
4	C	415	FAD	C8A-N9A	-2.75	1.32	1.37
4	C	415	FAD	C4-N3	-2.71	1.33	1.38
4	A	415	FAD	C10-N1	2.71	1.38	1.33
4	C	415	FAD	O2B-C2B	-2.68	1.36	1.43
4	A	415	FAD	C2A-N3A	2.65	1.38	1.33
4	D	415	FAD	C10-N1	2.63	1.38	1.33
4	D	415	FAD	C2A-N3A	2.61	1.38	1.33
4	C	415	FAD	C2'-C3'	-2.59	1.48	1.53
4	C	415	FAD	C9-C8	-2.53	1.36	1.39
4	C	415	FAD	C4A-N9A	-2.50	1.32	1.37
4	B	415	FAD	C2A-N3A	2.48	1.38	1.33
4	C	415	FAD	O3B-C3B	-2.43	1.36	1.43
4	C	415	FAD	C9A-C5X	-2.37	1.37	1.41
4	C	415	FAD	C9-C9A	-2.14	1.36	1.39
4	B	415	FAD	C10-N1	2.11	1.37	1.33
4	B	415	FAD	C8A-N7A	2.06	1.35	1.31
4	C	415	FAD	C6-C7	-2.05	1.36	1.39

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	415	FAD	N3A-C2A-N1A	-6.43	118.85	128.58
4	C	415	FAD	C5'-C4'-C3'	-6.37	100.20	112.22
4	D	415	FAD	N3A-C2A-N1A	-5.77	119.86	128.58
4	A	415	FAD	N3A-C2A-N1A	-5.72	119.92	128.58
4	C	415	FAD	C5A-C4A-N3A	-5.00	119.83	126.72
4	C	415	FAD	N3A-C2A-N1A	-4.65	121.54	128.58
4	C	415	FAD	N9A-C8A-N7A	-4.33	107.80	113.94
4	A	415	FAD	C5A-C4A-N3A	-4.24	120.88	126.72
4	D	415	FAD	C5A-C4A-N3A	-4.20	120.93	126.72
4	B	415	FAD	N9A-C8A-N7A	-4.14	108.06	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	415	FAD	N9A-C8A-N7A	-4.01	108.25	113.94
4	A	415	FAD	N9A-C8A-N7A	-4.00	108.27	113.94
4	C	415	FAD	C5A-N7A-C8A	3.75	109.34	103.45
4	D	415	FAD	C5A-N7A-C8A	3.52	108.99	103.45
4	C	415	FAD	O3'-C3'-C2'	3.48	116.83	108.93
4	D	415	FAD	O4B-C1B-N9A	3.40	114.62	108.09
4	D	415	FAD	C2A-N3A-C4A	3.39	120.10	111.83
4	C	415	FAD	C2A-N3A-C4A	3.30	119.90	111.83
4	A	415	FAD	C2A-N3A-C4A	3.28	119.84	111.83
4	C	415	FAD	N3A-C4A-N9A	3.27	132.73	127.17
4	B	415	FAD	C5A-N7A-C8A	3.22	108.51	103.45
4	A	415	FAD	C5A-N7A-C8A	3.22	108.51	103.45
4	B	415	FAD	C5A-C4A-N3A	-3.19	122.33	126.72
4	A	415	FAD	N3A-C4A-N9A	3.18	132.57	127.17
4	C	415	FAD	O2A-PA-O3P	3.16	115.81	107.27
4	A	415	FAD	C4-N3-C2	-3.10	120.14	125.64
4	B	415	FAD	C2A-N3A-C4A	3.09	119.37	111.83
4	D	415	FAD	N3A-C4A-N9A	3.03	132.31	127.17
4	D	415	FAD	C4-N3-C2	-3.03	120.27	125.64
4	C	415	FAD	C4X-C4-N3	2.97	120.81	113.25
4	A	415	FAD	C4X-C4-N3	2.94	120.75	113.25
4	B	415	FAD	C4X-C10-N10	2.91	120.64	116.48
4	C	415	FAD	C4A-C5A-N7A	-2.80	107.38	110.58
4	B	415	FAD	C4-N3-C2	-2.75	120.76	125.64
4	D	415	FAD	C4X-C4-N3	2.75	120.25	113.25
4	B	415	FAD	C10-C4X-N5	-2.74	119.22	124.81
4	B	415	FAD	C4A-N9A-C8A	2.67	108.54	105.74
4	A	415	FAD	C9A-C5X-N5	-2.56	119.74	122.45
4	D	415	FAD	C10-C4X-N5	-2.53	119.65	124.81
4	C	415	FAD	O5'-C5'-C4'	-2.52	102.63	109.36
4	C	415	FAD	C6A-C5A-C4A	2.52	120.62	117.18
4	C	415	FAD	O4'-C4'-C5'	2.52	115.54	109.99
4	A	415	FAD	C4A-N9A-C8A	2.48	108.34	105.74
4	A	415	FAD	C10-C4X-N5	-2.48	119.74	124.81
4	A	415	FAD	C4-C4X-N5	2.47	121.62	118.21
4	C	415	FAD	C4X-C10-N10	2.45	119.99	116.48
4	C	415	FAD	C4-N3-C2	-2.45	121.29	125.64
4	B	415	FAD	N3A-C4A-N9A	2.36	131.18	127.17
4	B	415	FAD	C4X-C4-N3	2.34	119.20	113.25
4	A	415	FAD	C4X-C10-N10	2.30	119.77	116.48
4	D	415	FAD	C4A-C5A-N7A	-2.29	107.96	110.58
4	A	415	FAD	C5A-C6A-N6A	-2.26	117.69	123.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	415	FAD	C9A-C5X-N5	-2.25	120.06	122.45
4	C	415	FAD	C4X-C10-N1	-2.23	119.11	124.59
4	B	415	FAD	C4A-N9A-C1B	-2.22	121.44	126.63
4	C	415	FAD	C10-N1-C2	2.20	121.61	116.85
4	D	415	FAD	C4A-N9A-C8A	2.20	108.04	105.74
4	C	415	FAD	C4A-N9A-C8A	2.19	108.04	105.74
4	B	415	FAD	C2A-N1A-C6A	2.15	122.26	118.73
4	B	415	FAD	C4-C4X-N5	2.14	121.17	118.21
4	A	415	FAD	O4-C4-C4X	-2.14	120.89	126.53
4	D	415	FAD	C4X-C10-N10	2.12	119.52	116.48
4	D	415	FAD	C4-C4X-N5	2.12	121.13	118.21
4	D	415	FAD	O4-C4-C4X	-2.12	120.94	126.53
4	C	415	FAD	C9A-C5X-N5	-2.09	120.24	122.45
4	C	415	FAD	C5X-C9A-N10	2.08	119.85	117.97

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	415	FAD	C5B-O5B-PA-O1A
4	C	415	FAD	C5B-O5B-PA-O1A
4	C	415	FAD	N10-C1'-C2'-O2'
4	C	415	FAD	N10-C1'-C2'-C3'
4	C	415	FAD	C1'-C2'-C3'-O3'
4	C	415	FAD	C1'-C2'-C3'-C4'
4	C	415	FAD	O2'-C2'-C3'-O3'
4	C	415	FAD	O2'-C2'-C3'-C4'
4	C	415	FAD	C3'-C4'-C5'-O5'
4	C	415	FAD	C5'-O5'-P-O1P
4	C	415	FAD	C5'-O5'-P-O2P
4	C	415	FAD	C5'-O5'-P-O3P
4	A	415	FAD	C2B-C1B-N9A-C8A
4	C	415	FAD	PA-O3P-P-O1P
4	C	415	FAD	O4'-C4'-C5'-O5'
4	B	415	FAD	C2B-C1B-N9A-C8A
4	D	415	FAD	C2B-C1B-N9A-C8A
4	A	415	FAD	O4B-C1B-N9A-C8A
4	B	415	FAD	O4B-C1B-N9A-C8A
4	D	415	FAD	O4B-C1B-N9A-C8A
4	A	415	FAD	PA-O3P-P-O2P
4	B	415	FAD	PA-O3P-P-O2P
4	C	415	FAD	PA-O3P-P-O2P

Continued on next page...

Continued from previous page...

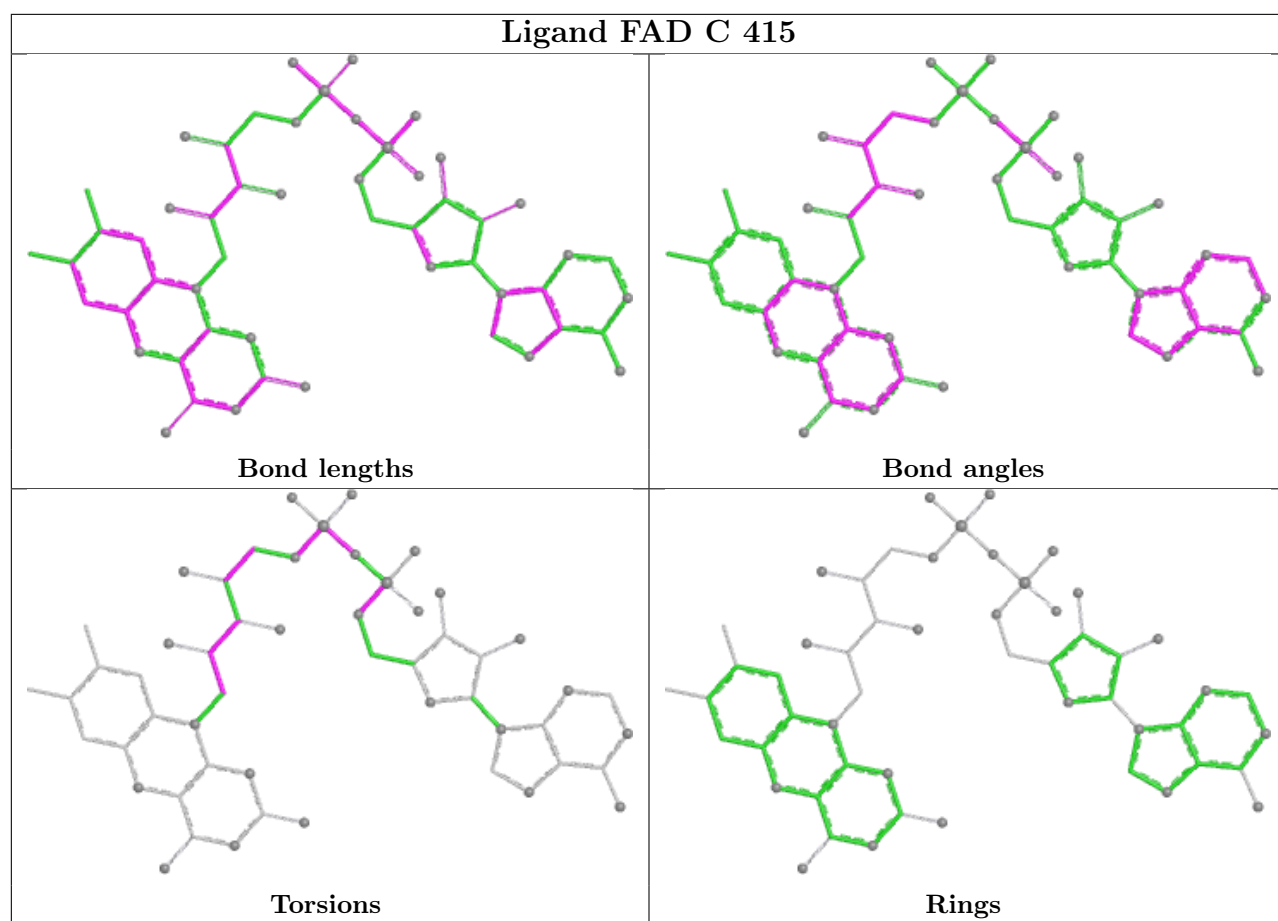
Mol	Chain	Res	Type	Atoms
4	D	415	FAD	PA-O3P-P-O2P

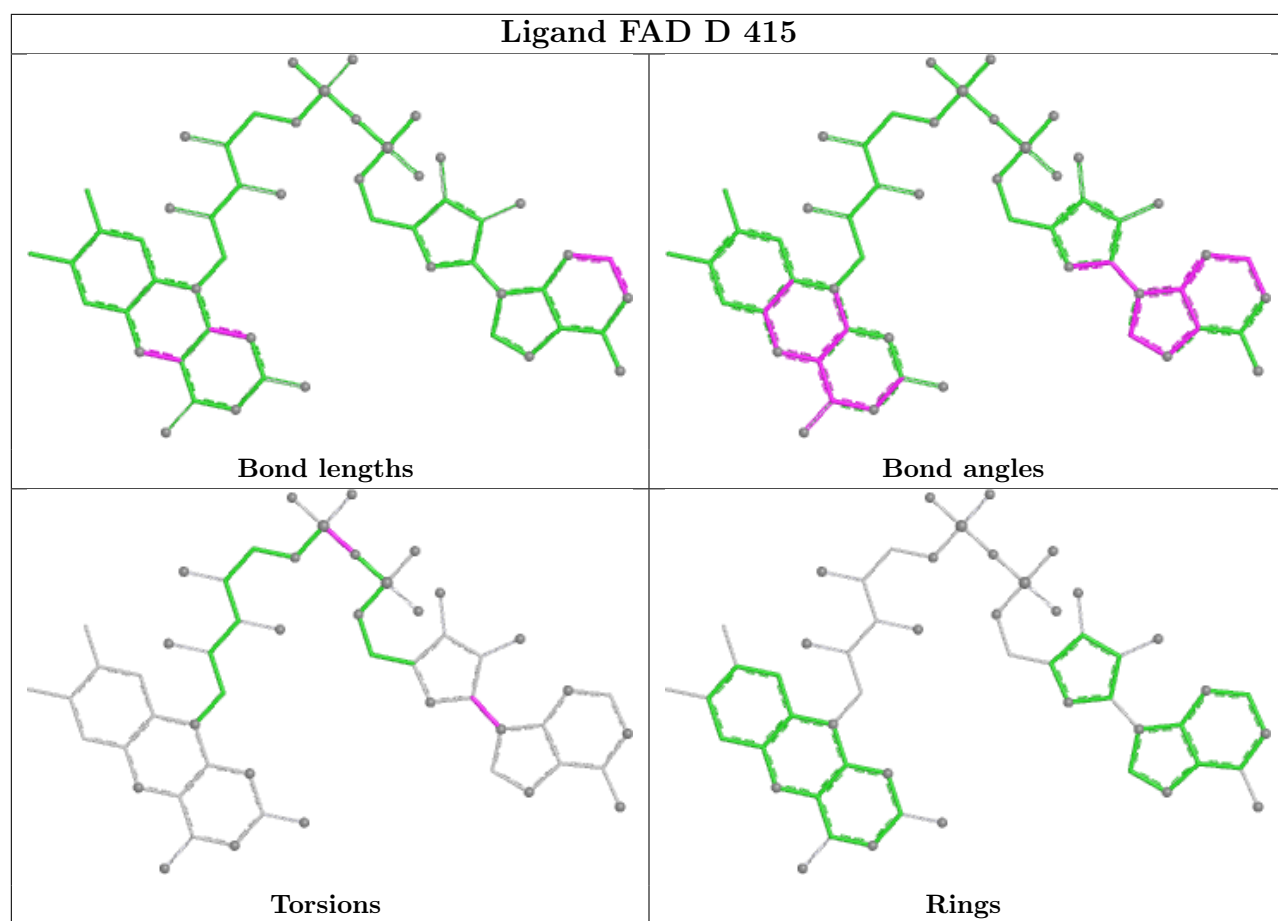
There are no ring outliers.

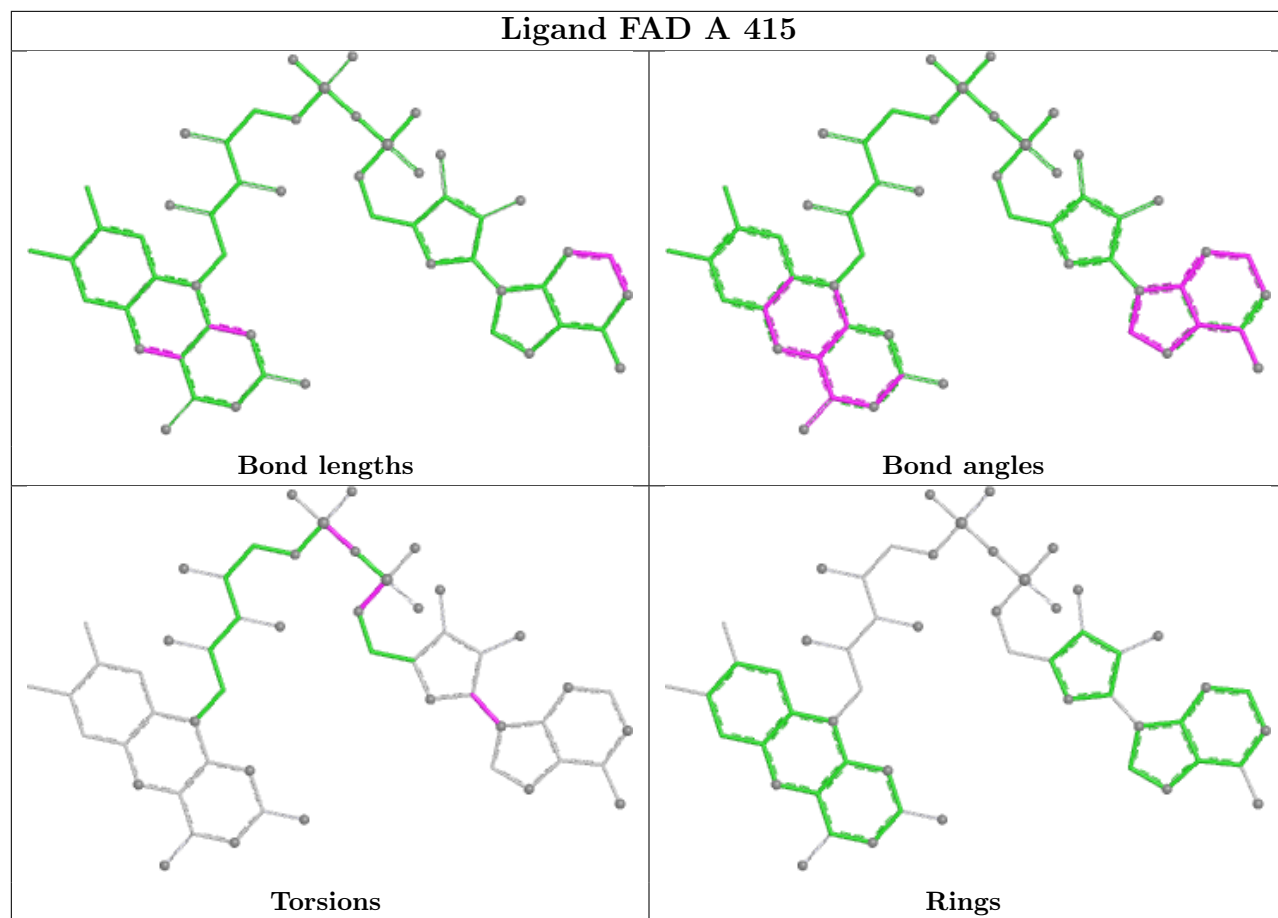
11 monomers are involved in 51 short contacts:

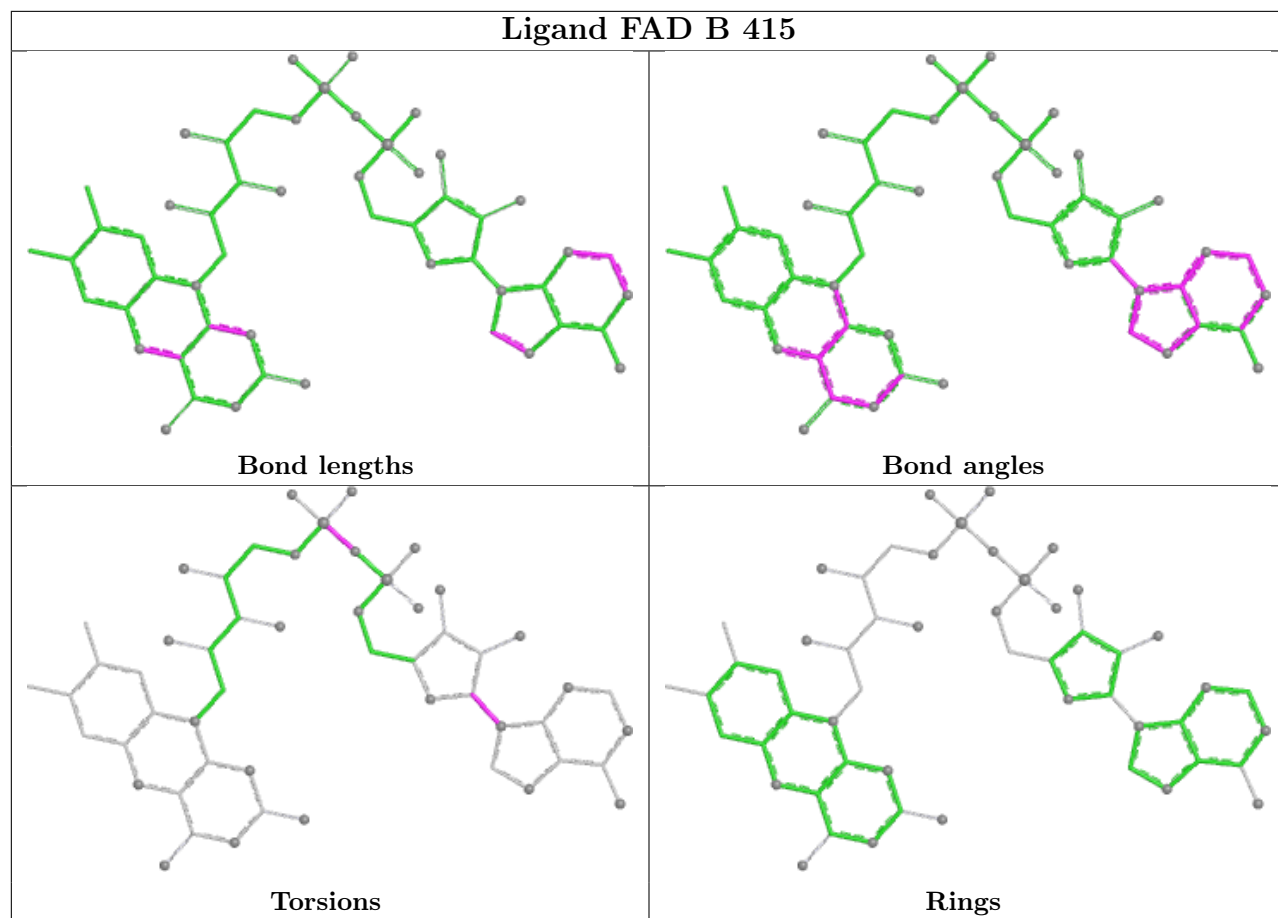
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	317	SO4	7	1
4	C	415	FAD	4	0
2	A	316	SO4	4	3
2	A	315	SO4	4	1
2	B	315	SO4	4	1
4	D	415	FAD	2	0
4	A	415	FAD	1	0
4	B	415	FAD	1	0
2	C	315	SO4	6	0
2	C	316	SO4	4	2
2	D	315	SO4	5	1

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	306/314 (97%)	0.02	8 (2%) 57 57	12, 24, 47, 61	1 (0%)
1	B	301/314 (95%)	0.01	10 (3%) 49 48	12, 23, 50, 74	2 (0%)
1	C	304/314 (96%)	0.01	10 (3%) 49 48	7, 22, 42, 75	5 (1%)
1	D	306/314 (97%)	0.10	14 (4%) 37 34	10, 23, 56, 72	3 (0%)
All	All	1217/1256 (96%)	0.03	42 (3%) 47 45	7, 23, 49, 75	11 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	105	PHE	6.7
1	A	8	THR	6.5
1	C	46	GLY	5.2
1	C	9	ARG	4.9
1	B	8	THR	4.4
1	D	106	GLY	4.1
1	C	83	ALA	4.0
1	C	84	LYS	3.9
1	D	46	GLY	3.8
1	C	8	THR	3.8
1	D	9	ARG	3.7
1	C	44	LYS	3.5
1	A	226	ASN	3.3
1	A	43	LYS	3.3
1	B	59	HIS	3.2
1	D	44	LYS	3.2
1	D	8	THR	3.1
1	D	124	GLU	3.0
1	D	123	ASP	2.9
1	C	45	GLU	2.9
1	B	225	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	38	THR	2.6
1	B	38	THR	2.6
1	A	7	PRO	2.5
1	A	38	THR	2.5
1	B	83	ALA	2.4
1	D	87	ALA	2.4
1	D	19	SER	2.3
1	C	38	THR	2.3
1	D	102	SER	2.3
1	B	107	MET	2.3
1	D	42	PRO	2.3
1	B	103	TYR	2.2
1	C	124	GLU	2.2
1	A	37	GLY	2.2
1	A	121	ILE	2.2
1	D	128	ILE	2.1
1	B	9	ARG	2.1
1	B	44	LYS	2.1
1	A	44	LYS	2.1
1	B	121	ILE	2.0
1	C	43	LYS	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($\text{\AA}^2$)	Q<0.9
2	SO4	A	316	5/5	0.94	0.10	18,18,25,25	0
2	SO4	C	315	5/5	0.94	0.12	20,20,20,20	0

Continued on next page...

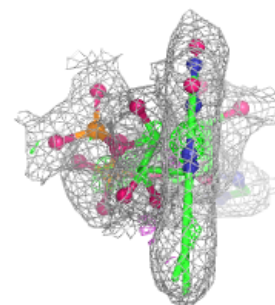
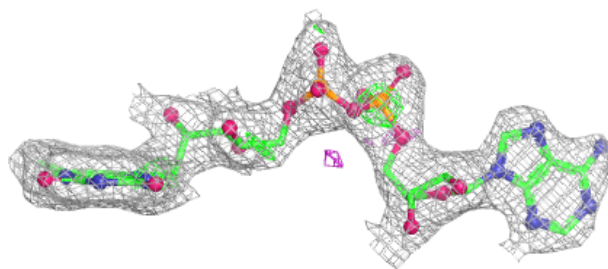
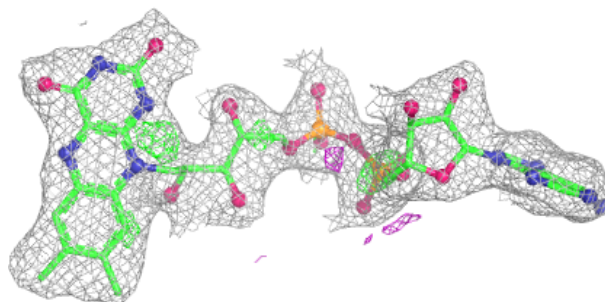
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	315	5/5	0.94	0.13	22,23,23,23	0
4	FAD	B	415	53/53	0.94	0.11	27,32,33,34	0
4	FAD	C	415	53/53	0.94	0.14	44,45,46,46	0
4	FAD	D	415	53/53	0.94	0.10	24,25,26,26	0
2	SO4	C	316	5/5	0.95	0.10	19,19,19,19	0
2	SO4	C	317	5/5	0.95	0.08	28,29,29,29	0
4	FAD	A	415	53/53	0.96	0.08	24,26,27,29	0
2	SO4	B	315	5/5	0.96	0.08	24,24,25,25	0
2	SO4	A	315	5/5	0.97	0.10	21,21,21,22	0
3	ZN	A	317	1/1	0.98	0.04	43,43,43,43	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.

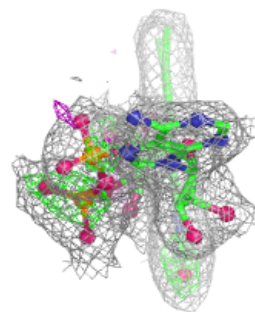
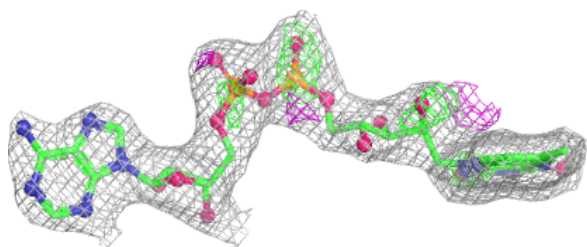
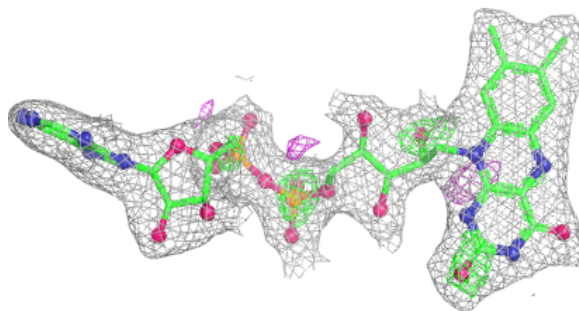
Electron density around FAD B 415:

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

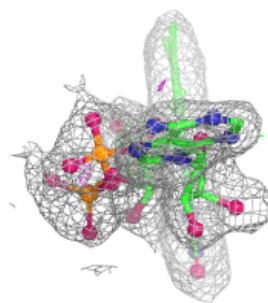
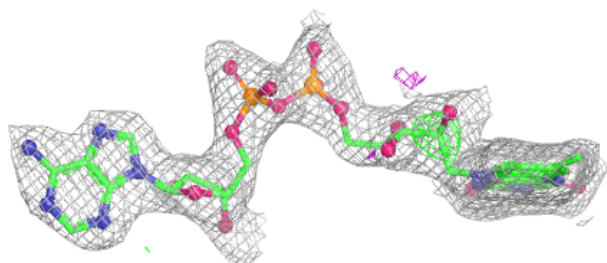
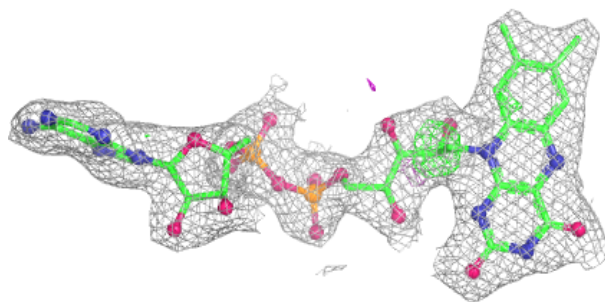


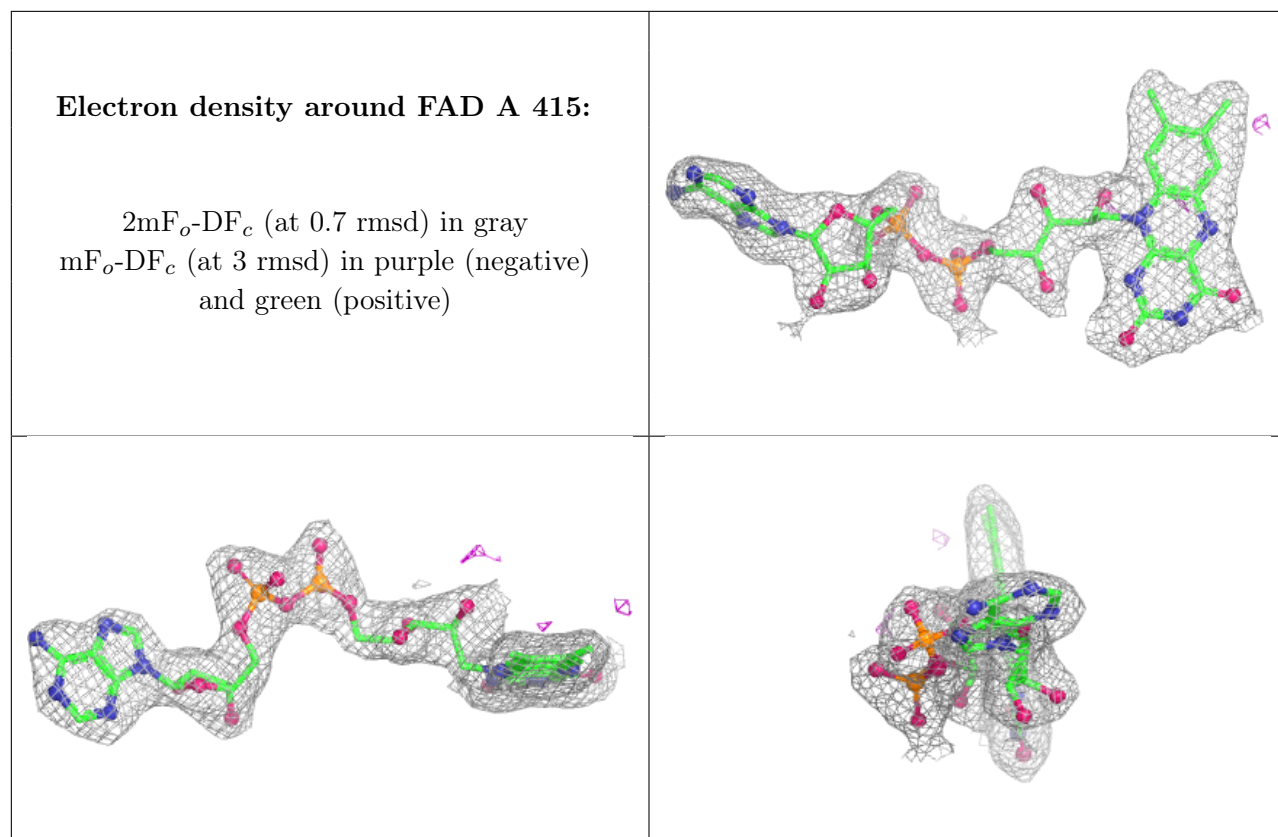
Electron density around FAD C 415:

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

**Electron density around FAD D 415:**

$2mF_o-DF_c$ (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.