Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:42 AM GMT

PDB ID	:	2E0I
Title	:	Crystal structure of archaeal photolyase from Sulfolobus tokodaii with two FAD molecules: Implication of a novel light-harvesting cofactor
Authors	:	Fujihashi, M.; Numoto, N.; Kobayashi, Y.; Mizushima, A.; Tsujimura, M.; Nakamura, A.; Kawarabayashi, Y.; Miki, K.
Deposited on	:	2006-10-10
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

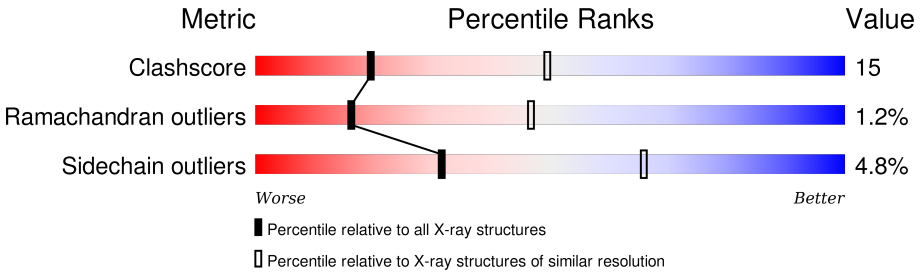
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	440	68% 26%
1	B	440	65% 30%
1	C	440	69% 25%
1	D	440	64% 30%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15166 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 432aa long hypothetical deoxyribodipyrimidine photolyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total	C	N	O	S	0	0	0
			3622	2343	613	653	13			
1	B	431	Total	C	N	O	S	0	0	0
			3643	2357	617	656	13			
1	C	428	Total	C	N	O	S	0	0	0
			3622	2343	613	653	13			
1	D	430	Total	C	N	O	S	0	0	0
			3636	2352	616	655	13			

There are 32 discrepancies between the modelled and reference sequences:

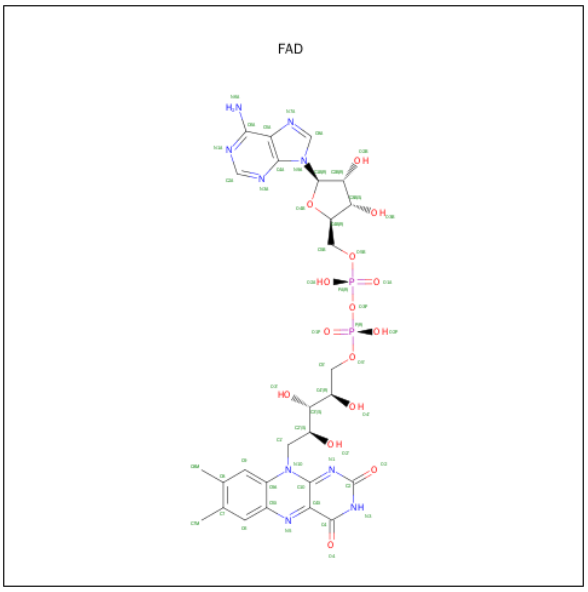
Chain	Residue	Modelled	Actual	Comment	Reference
A	433	LEU	-	EXPRESSION TAG	UNP Q973K9
A	434	GLU	-	EXPRESSION TAG	UNP Q973K9
A	435	HIS	-	EXPRESSION TAG	UNP Q973K9
A	436	HIS	-	EXPRESSION TAG	UNP Q973K9
A	437	HIS	-	EXPRESSION TAG	UNP Q973K9
A	438	HIS	-	EXPRESSION TAG	UNP Q973K9
A	439	HIS	-	EXPRESSION TAG	UNP Q973K9
A	440	HIS	-	EXPRESSION TAG	UNP Q973K9
B	433	LEU	-	EXPRESSION TAG	UNP Q973K9
B	434	GLU	-	EXPRESSION TAG	UNP Q973K9
B	435	HIS	-	EXPRESSION TAG	UNP Q973K9
B	436	HIS	-	EXPRESSION TAG	UNP Q973K9
B	437	HIS	-	EXPRESSION TAG	UNP Q973K9
B	438	HIS	-	EXPRESSION TAG	UNP Q973K9
B	439	HIS	-	EXPRESSION TAG	UNP Q973K9
B	440	HIS	-	EXPRESSION TAG	UNP Q973K9
C	433	LEU	-	EXPRESSION TAG	UNP Q973K9
C	434	GLU	-	EXPRESSION TAG	UNP Q973K9
C	435	HIS	-	EXPRESSION TAG	UNP Q973K9
C	436	HIS	-	EXPRESSION TAG	UNP Q973K9
C	437	HIS	-	EXPRESSION TAG	UNP Q973K9

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	438	HIS	-	EXPRESSION TAG	UNP Q973K9
C	439	HIS	-	EXPRESSION TAG	UNP Q973K9
C	440	HIS	-	EXPRESSION TAG	UNP Q973K9
D	433	LEU	-	EXPRESSION TAG	UNP Q973K9
D	434	GLU	-	EXPRESSION TAG	UNP Q973K9
D	435	HIS	-	EXPRESSION TAG	UNP Q973K9
D	436	HIS	-	EXPRESSION TAG	UNP Q973K9
D	437	HIS	-	EXPRESSION TAG	UNP Q973K9
D	438	HIS	-	EXPRESSION TAG	UNP Q973K9
D	439	HIS	-	EXPRESSION TAG	UNP Q973K9
D	440	HIS	-	EXPRESSION TAG	UNP Q973K9

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



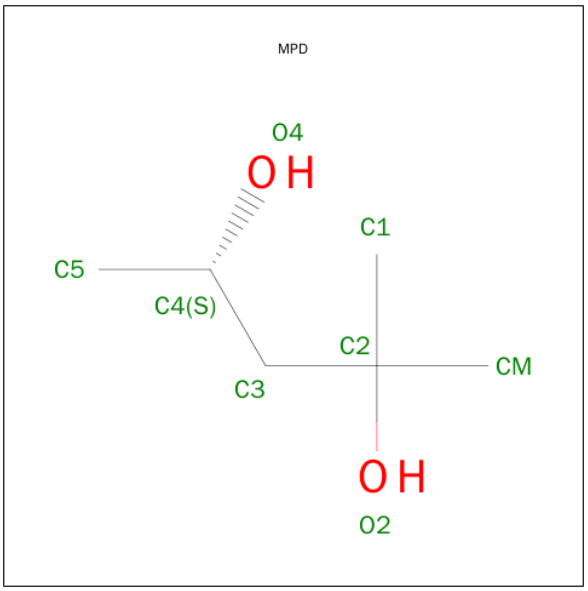
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			8	6	2			
3	B	1	Total	C	O		0	0
			8	6	2			
3	C	1	Total	C	O		0	0
			8	6	2			
3	D	1	Total	C	O		0	0
			8	6	2			
3	A	1	Total	C	O		0	0
			8	6	2			
3	C	1	Total	C	O		0	0
			8	6	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	41	Total O 41 41	0	0
4	B	38	Total O 38 38	0	0
4	C	47	Total O 47 47	0	0
4	D	45	Total O 45 45	0	0

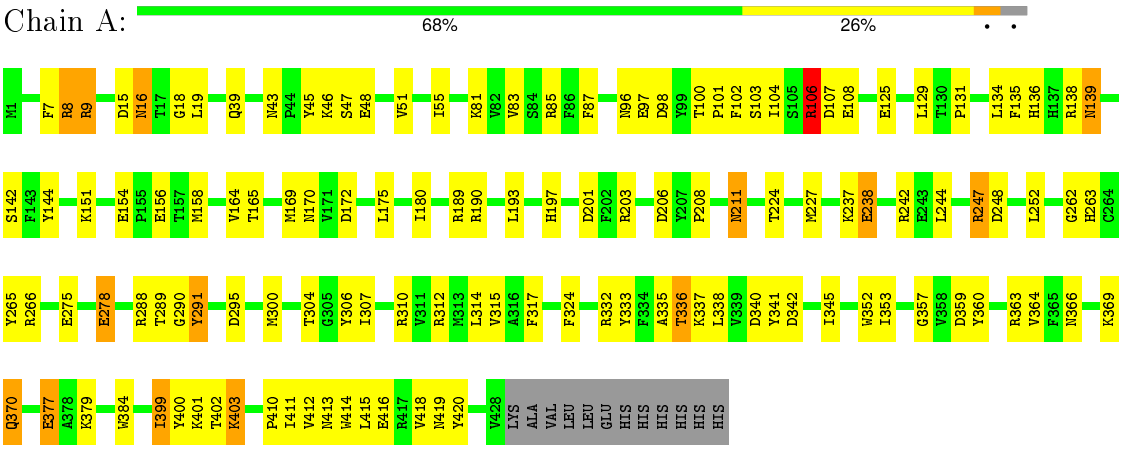
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

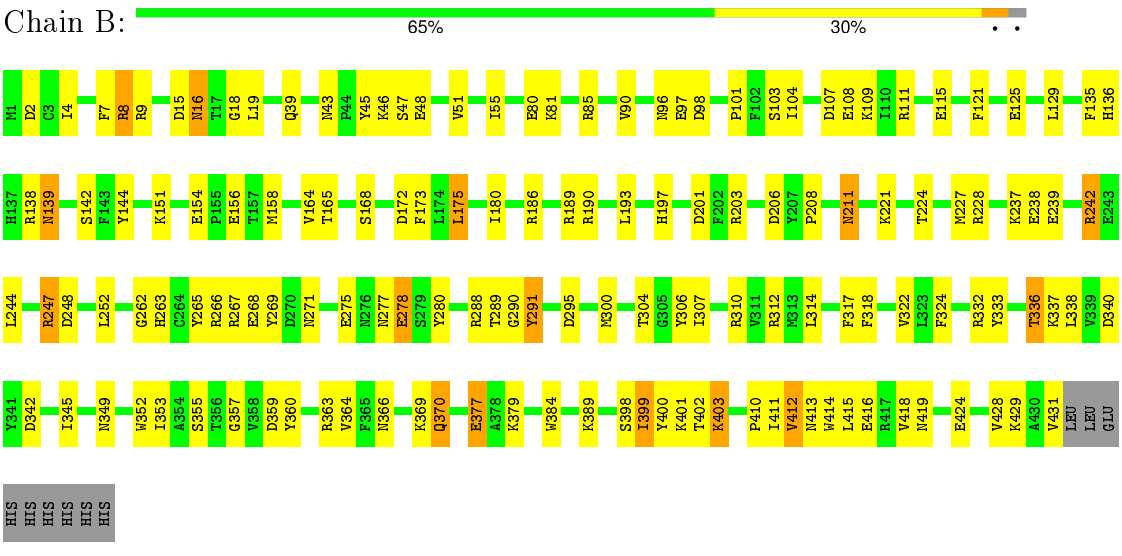
- Molecule 1: 432aa long hypothetical deoxyribodipyrimidine photolyase

Chain A:



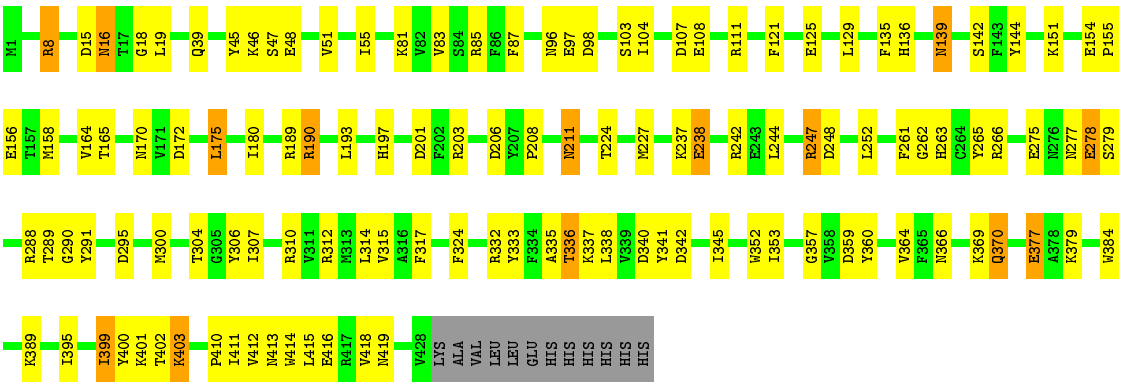
- Molecule 1: 432aa long hypothetical deoxyribodipyrimidine photolyase

Chain B:



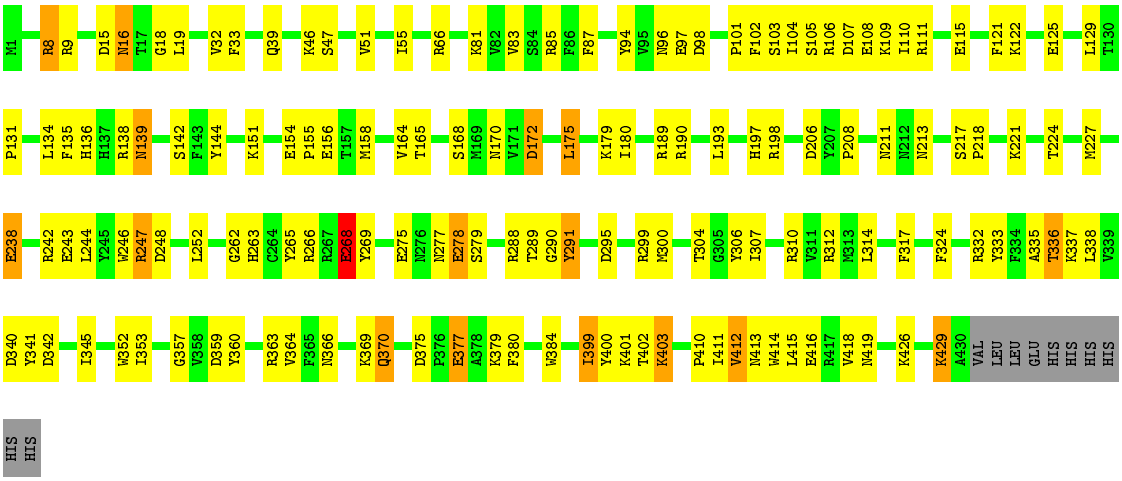
- Molecule 1: 432aa long hypothetical deoxyribodipyrimidine photolyase

Chain C:



- Molecule 1: 432aa long hypothetical deoxyribodipyrimidine photolyase

Chain D:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	79.88Å 114.72Å 167.68Å 90.00° 91.49° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80	Depositor
% Data completeness (in resolution range)	97.1 (50.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.247	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15166	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.46	0/3727	0.76	9/5040 (0.2%)
1	B	0.45	0/3748	0.69	6/5068 (0.1%)
1	C	0.46	0/3727	0.67	4/5040 (0.1%)
1	D	0.45	0/3741	0.67	5/5058 (0.1%)
All	All	0.46	0/14943	0.70	24/20206 (0.1%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	9	ARG	NE-CZ-NH1	-14.54	113.03	120.30
1	A	106	ARG	NE-CZ-NH2	13.42	127.01	120.30
1	A	9	ARG	NE-CZ-NH2	12.53	126.56	120.30
1	A	106	ARG	NE-CZ-NH1	-12.31	114.15	120.30
1	B	242	ARG	NE-CZ-NH2	-10.09	115.26	120.30
1	B	242	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	C	190	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	C	190	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	B	186	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	A	247	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	247	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	C	247	ARG	NE-CZ-NH1	-7.31	116.64	120.30
1	D	247	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	D	332	ARG	NE-CZ-NH1	-7.21	116.69	120.30
1	B	247	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	B	186	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	D	332	ARG	NE-CZ-NH2	6.85	123.73	120.30
1	A	106	ARG	CD-NE-CZ	6.67	132.94	123.60
1	C	247	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	A	9	ARG	CD-NE-CZ	6.12	132.16	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	247	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	106	ARG	CG-CD-NE	5.94	124.27	111.80
1	B	247	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	D	268	GLU	CA-CB-CG	5.02	124.44	113.40

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	3622	0	3504	104	0
1	B	3643	0	3531	119	0
1	C	3622	0	3504	96	0
1	D	3636	0	3522	120	0
2	A	106	0	62	6	0
2	B	106	0	62	6	0
2	C	106	0	62	5	0
2	D	106	0	62	7	0
3	A	16	0	28	5	0
3	B	8	0	14	3	0
3	C	16	0	28	3	0
3	D	8	0	14	2	0
4	A	41	0	0	2	0
4	B	38	0	0	3	0
4	C	47	0	0	1	0
4	D	45	0	0	3	0
All	All	15166	0	14393	442	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 15.

All (442) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:HD21	1:A:370:GLN:HG2	1.42	1.00
1:C:314:LEU:HD21	1:C:370:GLN:HG2	1.48	0.95
1:B:268:GLU:HG3	1:B:429:LYS:HE3	1.48	0.95
1:D:411:ILE:O	1:D:412:VAL:HG13	1.69	0.93
1:C:289:THR:HG22	1:C:295:ASP:OD2	1.73	0.89
1:A:289:THR:HG22	1:A:295:ASP:OD2	1.73	0.89
1:D:314:LEU:HD21	1:D:370:GLN:HG2	1.54	0.88
1:B:314:LEU:HD21	1:B:370:GLN:HG2	1.55	0.87
1:B:289:THR:HG22	1:B:295:ASP:OD2	1.76	0.86
1:D:289:THR:HG23	1:D:291:TYR:H	1.40	0.85
1:D:269:TYR:OH	1:D:429:LYS:HE2	1.77	0.84
2:D:1700:FAD:H8A	2:D:1700:FAD:H51A	1.57	0.83
1:B:411:ILE:O	1:B:412:VAL:HG13	1.78	0.83
1:A:300:MET:O	1:A:304:THR:HG22	1.79	0.83
1:D:289:THR:HG22	1:D:295:ASP:OD2	1.79	0.83
1:B:289:THR:HG23	1:B:291:TYR:H	1.44	0.82
1:D:290:GLY:HA3	1:D:410:PRO:HA	1.60	0.82
1:C:300:MET:O	1:C:304:THR:HG22	1.79	0.82
1:C:304:THR:HG23	1:C:306:TYR:H	1.45	0.82
1:D:300:MET:O	1:D:304:THR:HG22	1.80	0.81
1:B:266:ARG:HD3	1:B:360:TYR:CE1	2.15	0.80
1:C:290:GLY:HA3	1:C:410:PRO:HA	1.64	0.80
1:A:290:GLY:HA3	1:A:410:PRO:HA	1.63	0.80
1:D:304:THR:HG23	1:D:306:TYR:H	1.47	0.79
1:B:290:GLY:HA3	1:B:410:PRO:HA	1.62	0.79
1:A:304:THR:HG23	1:A:306:TYR:H	1.47	0.79
1:C:51:VAL:O	1:C:55:ILE:HG12	1.83	0.79
1:B:18:GLY:H	1:B:96:ASN:HD21	1.29	0.79
1:D:18:GLY:H	1:D:96:ASN:HD21	1.30	0.79
1:D:266:ARG:HD3	1:D:360:TYR:CE1	2.18	0.78
1:C:289:THR:HG23	1:C:291:TYR:H	1.47	0.78
1:A:266:ARG:HD3	1:A:360:TYR:CE1	2.18	0.78
1:C:266:ARG:HD3	1:C:360:TYR:CE1	2.19	0.77
1:B:300:MET:O	1:B:304:THR:HG22	1.85	0.77
1:C:18:GLY:H	1:C:96:ASN:HD21	1.33	0.76
1:A:18:GLY:H	1:A:96:ASN:HD21	1.33	0.76
1:A:289:THR:HG23	1:A:291:TYR:H	1.51	0.75
1:B:304:THR:HG23	1:B:306:TYR:H	1.50	0.75
1:A:247:ARG:NH2	2:A:1100:FAD:O2	2.20	0.75
1:A:139:ASN:HD22	1:A:139:ASN:H	1.33	0.75
1:B:104:ILE:O	1:B:108:GLU:HG3	1.88	0.74
1:D:269:TYR:CZ	1:D:429:LYS:HE2	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:247:ARG:NH2	2:D:1700:FAD:O2	2.21	0.72
1:B:51:VAL:O	1:B:55:ILE:HG12	1.89	0.72
1:A:51:VAL:O	1:A:55:ILE:HG12	1.89	0.72
1:D:377:GLU:HB2	1:D:379:LYS:HG3	1.71	0.72
1:A:411:ILE:O	1:A:412:VAL:HG13	1.90	0.71
1:D:51:VAL:O	1:D:55:ILE:HG12	1.90	0.71
1:B:377:GLU:HB2	1:B:379:LYS:HG3	1.73	0.70
1:B:247:ARG:NH2	2:B:1300:FAD:O2	2.24	0.70
1:C:139:ASN:HD22	1:C:139:ASN:H	1.37	0.70
1:A:314:LEU:CD2	1:A:370:GLN:HG2	2.18	0.70
1:D:97:GLU:OE1	1:D:125:GLU:HG2	1.92	0.70
1:A:104:ILE:O	1:A:108:GLU:HG3	1.92	0.70
1:A:307:ILE:HG13	1:A:312:ARG:HD2	1.73	0.69
1:C:307:ILE:HG13	1:C:312:ARG:HD2	1.75	0.69
1:B:8:ARG:NH2	1:B:107:ASP:OD1	2.25	0.69
1:B:266:ARG:HD3	1:B:360:TYR:HE1	1.58	0.68
1:C:104:ILE:O	1:C:108:GLU:HG3	1.91	0.68
1:D:104:ILE:O	1:D:108:GLU:HG3	1.92	0.68
1:D:307:ILE:HG13	1:D:312:ARG:HD2	1.75	0.68
2:B:1300:FAD:H8A	2:B:1300:FAD:H51A	1.75	0.67
1:D:366:ASN:HB3	1:D:369:LYS:HB2	1.76	0.67
1:A:266:ARG:HD3	1:A:360:TYR:HE1	1.58	0.67
1:D:139:ASN:HD22	1:D:139:ASN:H	1.43	0.67
1:A:377:GLU:HB2	1:A:379:LYS:HG3	1.78	0.66
1:C:377:GLU:HB2	1:C:379:LYS:HG3	1.77	0.66
1:B:97:GLU:OE1	1:B:125:GLU:HG2	1.95	0.66
1:C:266:ARG:HD3	1:C:360:TYR:HE1	1.61	0.66
1:C:314:LEU:CD2	1:C:370:GLN:HG2	2.24	0.66
1:A:366:ASN:HB3	1:A:369:LYS:HB2	1.78	0.65
1:C:46:LYS:HE3	1:C:51:VAL:HG21	1.79	0.65
1:B:366:ASN:HB3	1:B:369:LYS:HB2	1.78	0.65
2:A:1100:FAD:H51A	2:A:1100:FAD:H8A	1.78	0.65
1:C:366:ASN:HB3	1:C:369:LYS:HB2	1.78	0.65
1:B:172:ASP:HA	1:B:175:LEU:CD2	2.27	0.64
1:C:411:ILE:O	1:C:412:VAL:HG13	1.98	0.64
1:A:275:GLU:HG3	1:C:395:ILE:HG12	1.78	0.64
1:D:266:ARG:HD3	1:D:360:TYR:HE1	1.60	0.63
1:B:129:LEU:HD13	1:B:227:MET:HG3	1.80	0.63
1:C:129:LEU:HD13	1:C:227:MET:HG3	1.81	0.63
1:D:414:TRP:O	1:D:418:VAL:HG23	1.99	0.63
1:B:138:ARG:HG3	1:B:139:ASN:N	2.12	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ILE:HG13	1:B:312:ARG:HD2	1.80	0.62
1:D:8:ARG:NH2	1:D:107:ASP:OD1	2.32	0.62
1:B:2:ASP:HB2	4:B:5068:HOH:O	1.99	0.62
1:B:139:ASN:H	1:B:139:ASN:HD22	1.47	0.61
1:B:139:ASN:HD21	1:B:142:SER:HB2	1.65	0.61
1:A:415:LEU:HD13	1:A:419:ASN:ND2	2.15	0.61
1:A:129:LEU:HD13	1:A:227:MET:HG3	1.82	0.61
1:D:16:ASN:HD22	1:D:16:ASN:C	2.04	0.61
1:B:266:ARG:NH1	1:B:360:TYR:HD1	1.99	0.61
1:B:180:ILE:O	1:B:180:ILE:HG13	2.00	0.61
1:D:46:LYS:HE3	1:D:51:VAL:HG21	1.81	0.61
1:B:8:ARG:HH22	1:B:107:ASP:CG	2.04	0.60
1:D:314:LEU:CD2	1:D:370:GLN:HG2	2.29	0.60
1:C:415:LEU:HD13	1:C:419:ASN:ND2	2.16	0.60
1:B:415:LEU:HD13	1:B:419:ASN:ND2	2.17	0.60
1:B:414:TRP:O	1:B:418:VAL:HG23	2.02	0.59
1:C:266:ARG:NH1	1:C:360:TYR:HD1	2.00	0.59
1:B:46:LYS:HE3	1:B:51:VAL:HG21	1.84	0.59
1:B:206:ASP:OD1	1:B:310:ARG:HD3	2.02	0.59
1:D:266:ARG:NH1	1:D:360:TYR:HD1	2.01	0.59
1:A:193:LEU:HD22	1:B:197:HIS:CD2	2.37	0.59
1:A:46:LYS:HE3	1:A:51:VAL:HG21	1.84	0.59
1:D:129:LEU:HD13	1:D:227:MET:HG3	1.85	0.59
1:B:314:LEU:CD2	1:B:370:GLN:HG2	2.30	0.58
1:B:172:ASP:HA	1:B:175:LEU:HD23	1.84	0.58
1:C:206:ASP:OD1	1:C:310:ARG:HD3	2.04	0.58
1:A:8:ARG:NH2	1:A:107:ASP:OD1	2.37	0.58
1:A:97:GLU:OE1	1:A:125:GLU:HG2	2.04	0.58
1:D:415:LEU:HD13	1:D:419:ASN:ND2	2.19	0.58
1:D:39:GLN:HG2	2:D:1800:FAD:H52A	1.84	0.58
1:B:135:PHE:HB2	1:B:252:LEU:HD13	1.86	0.58
1:D:98:ASP:HB3	1:D:103:SER:OG	2.04	0.57
1:B:206:ASP:O	1:B:208:PRO:HD3	2.05	0.57
1:A:402:THR:OG1	1:A:403:LYS:N	2.35	0.57
1:B:413:ASN:OD1	1:B:416:GLU:HG3	2.04	0.57
1:A:266:ARG:NH1	1:A:360:TYR:HD1	2.01	0.57
1:C:135:PHE:HB2	1:C:252:LEU:HD13	1.87	0.57
1:A:39:GLN:HG2	2:A:1200:FAD:H52A	1.87	0.57
1:A:16:ASN:C	1:A:16:ASN:HD22	2.08	0.57
1:C:8:ARG:NH2	1:C:107:ASP:OD1	2.36	0.57
1:C:413:ASN:OD1	1:C:416:GLU:HG3	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:GLU:HB2	1:D:324:PHE:HD2	1.70	0.57
1:D:206:ASP:OD1	1:D:310:ARG:HD3	2.04	0.57
1:D:138:ARG:HG3	1:D:139:ASN:N	2.18	0.56
1:B:81:LYS:O	1:B:85:ARG:HG3	2.05	0.56
1:C:16:ASN:C	1:C:16:ASN:HD22	2.09	0.56
1:A:206:ASP:OD1	1:A:310:ARG:HD3	2.05	0.56
1:B:275:GLU:HB2	1:B:324:PHE:HD2	1.71	0.56
1:D:139:ASN:HD21	1:D:142:SER:HB2	1.71	0.56
1:D:8:ARG:HH22	1:D:107:ASP:CG	2.09	0.56
2:C:1500:FAD:N6A	3:C:3006:MPD:H12	2.20	0.56
1:C:352:TRP:NE1	1:C:359:ASP:HB2	2.20	0.56
1:C:139:ASN:N	1:C:139:ASN:HD22	2.01	0.56
1:B:424:GLU:O	1:B:428:VAL:HG23	2.05	0.56
1:B:16:ASN:C	1:B:16:ASN:HD22	2.09	0.55
1:A:413:ASN:OD1	1:A:416:GLU:HG3	2.07	0.55
1:C:290:GLY:HA3	1:C:410:PRO:CA	2.36	0.55
1:C:164:VAL:HG12	1:C:165:THR:N	2.22	0.55
1:D:364:VAL:HG21	1:D:418:VAL:HG11	1.88	0.55
1:B:364:VAL:HG21	1:B:418:VAL:HG11	1.89	0.55
1:A:400:TYR:CE1	1:A:401:LYS:HG3	2.42	0.55
1:D:66:ARG:HD2	4:D:5103:HOH:O	2.06	0.55
1:C:139:ASN:HD21	1:C:142:SER:HB2	1.72	0.54
1:D:413:ASN:OD1	1:D:416:GLU:HG3	2.07	0.54
1:A:151:LYS:NZ	1:A:154:GLU:OE2	2.40	0.54
1:D:336:THR:HG22	1:D:337:LYS:HG2	1.88	0.54
1:C:275:GLU:HB2	1:C:324:PHE:HD2	1.72	0.54
1:D:221:LYS:NZ	4:D:5011:HOH:O	2.40	0.54
1:A:164:VAL:HG12	1:A:165:THR:N	2.22	0.54
1:B:151:LYS:NZ	1:B:154:GLU:OE2	2.40	0.54
1:A:414:TRP:O	1:A:418:VAL:HG23	2.08	0.54
1:C:47:SER:O	1:C:51:VAL:HG23	2.08	0.54
1:A:139:ASN:HD21	1:A:142:SER:HB2	1.73	0.54
1:D:342:ASP:HB3	1:D:345:ILE:HB	1.89	0.54
1:D:135:PHE:HB2	1:D:252:LEU:HD13	1.90	0.54
1:B:98:ASP:HB3	1:B:103:SER:OG	2.07	0.54
1:D:144:TYR:CE2	1:D:242:ARG:HG3	2.43	0.54
1:D:352:TRP:NE1	1:D:359:ASP:HB2	2.23	0.54
1:A:144:TYR:CE2	1:A:242:ARG:HG3	2.43	0.54
1:A:300:MET:HG2	1:A:304:THR:HG21	1.90	0.54
1:B:227:MET:HE3	1:B:244:LEU:HG	1.90	0.54
1:A:352:TRP:NE1	1:A:359:ASP:HB2	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:THR:OG1	1:B:403:LYS:N	2.39	0.54
1:D:172:ASP:HA	1:D:175:LEU:CD2	2.38	0.54
1:C:414:TRP:O	1:C:418:VAL:HG23	2.07	0.54
1:C:300:MET:HG3	1:C:384:TRP:CZ2	2.43	0.53
1:B:300:MET:HG2	1:B:304:THR:HG21	1.89	0.53
1:B:342:ASP:HB3	1:B:345:ILE:HB	1.90	0.53
1:C:97:GLU:OE1	1:C:125:GLU:HG2	2.08	0.53
1:A:291:TYR:CD1	1:A:291:TYR:N	2.76	0.53
1:D:402:THR:OG1	1:D:403:LYS:N	2.40	0.53
1:B:291:TYR:CD1	1:B:291:TYR:N	2.77	0.53
1:B:39:GLN:HG2	2:B:1400:FAD:H52A	1.89	0.53
1:B:266:ARG:HD3	1:B:360:TYR:CD1	2.44	0.53
1:A:98:ASP:HB3	1:A:103:SER:OG	2.08	0.53
1:C:402:THR:OG1	1:C:403:LYS:N	2.41	0.53
1:D:306:TYR:O	1:D:307:ILE:HG23	2.10	0.52
2:C:1500:FAD:H51A	2:C:1500:FAD:H8A	1.89	0.52
1:C:300:MET:HG2	1:C:304:THR:HG21	1.92	0.52
1:B:48:GLU:HB3	1:B:180:ILE:HG12	1.90	0.52
1:A:201:ASP:OD1	1:A:203:ARG:HB2	2.10	0.52
1:B:139:ASN:HD21	1:B:142:SER:CB	2.22	0.52
1:D:164:VAL:HG12	1:D:165:THR:N	2.24	0.52
1:D:151:LYS:NZ	1:D:154:GLU:OE2	2.42	0.52
1:C:306:TYR:O	1:C:307:ILE:HG23	2.09	0.52
1:B:290:GLY:HA3	1:B:410:PRO:CA	2.35	0.52
1:A:420:TYR:CE1	1:C:395:ILE:CD1	2.93	0.52
1:D:172:ASP:HA	1:D:175:LEU:HD23	1.92	0.52
1:B:164:VAL:HG12	1:B:165:THR:N	2.24	0.52
1:B:352:TRP:NE1	1:B:359:ASP:HB2	2.24	0.52
1:C:304:THR:HG23	1:C:306:TYR:N	2.21	0.52
1:A:139:ASN:N	1:A:139:ASN:HD22	1.99	0.52
1:D:139:ASN:HD21	1:D:142:SER:CB	2.23	0.52
1:A:135:PHE:HB2	1:A:252:LEU:HD13	1.92	0.52
1:C:400:TYR:CE1	1:C:401:LYS:HG3	2.45	0.52
1:C:352:TRP:CE2	1:C:359:ASP:HB2	2.45	0.52
1:A:138:ARG:HG3	1:A:139:ASN:N	2.25	0.51
1:B:144:TYR:CE2	1:B:242:ARG:HG3	2.45	0.51
1:A:317:PHE:HZ	1:A:364:VAL:HG23	1.75	0.51
1:A:101:PRO:HD2	3:A:3001:MPD:HM1	1.92	0.51
1:B:269:TYR:CE1	1:B:429:LYS:HD3	2.45	0.51
1:B:172:ASP:OD2	1:B:173:PHE:N	2.43	0.51
1:C:317:PHE:HZ	1:C:364:VAL:HG23	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:VAL:HG21	1:C:418:VAL:HG11	1.93	0.51
1:B:189:ARG:HA	1:B:224:THR:HB	1.93	0.51
1:D:290:GLY:HA3	1:D:410:PRO:CA	2.34	0.51
1:A:290:GLY:HA3	1:A:410:PRO:CA	2.36	0.51
1:D:400:TYR:CE1	1:D:401:LYS:HG3	2.46	0.51
1:A:336:THR:HG22	1:A:337:LYS:HG2	1.93	0.51
1:D:300:MET:HG3	1:D:384:TRP:CZ2	2.46	0.51
1:B:317:PHE:HZ	1:B:364:VAL:HG23	1.76	0.51
1:A:352:TRP:CE2	1:A:359:ASP:HB2	2.46	0.51
1:D:317:PHE:HZ	1:D:364:VAL:HG23	1.75	0.50
1:B:415:LEU:HD13	1:B:419:ASN:HD21	1.76	0.50
1:C:291:TYR:N	1:C:291:TYR:CD1	2.78	0.50
1:A:415:LEU:HD13	1:A:419:ASN:HD21	1.77	0.50
1:A:170:ASN:OD1	1:A:172:ASP:HB2	2.12	0.50
1:A:8:ARG:HH22	1:A:107:ASP:CG	2.14	0.50
1:C:81:LYS:O	1:C:85:ARG:HG3	2.10	0.50
1:C:189:ARG:HA	1:C:224:THR:HB	1.93	0.50
1:C:227:MET:CE	1:C:244:LEU:HG	2.42	0.50
1:A:306:TYR:O	1:A:307:ILE:HG23	2.12	0.49
1:B:306:TYR:O	1:B:307:ILE:HG23	2.12	0.49
1:C:342:ASP:HB3	1:C:345:ILE:HB	1.94	0.49
1:C:48:GLU:HB3	1:C:180:ILE:CG2	2.42	0.49
1:D:291:TYR:CD1	1:D:291:TYR:N	2.79	0.49
1:B:304:THR:HG23	1:B:306:TYR:N	2.23	0.49
1:D:206:ASP:O	1:D:208:PRO:HD3	2.12	0.49
1:C:8:ARG:HH22	1:C:107:ASP:CG	2.14	0.49
1:B:399:ILE:HA	1:B:402:THR:HG22	1.94	0.49
1:C:98:ASP:HB3	1:C:103:SER:OG	2.12	0.49
1:C:336:THR:HG22	1:C:337:LYS:HG2	1.94	0.49
1:D:189:ARG:HA	1:D:224:THR:HB	1.94	0.49
1:B:411:ILE:CG2	1:B:411:ILE:O	2.59	0.49
1:D:304:THR:HG23	1:D:306:TYR:N	2.22	0.49
1:D:300:MET:HG2	1:D:304:THR:HG21	1.93	0.49
1:A:275:GLU:HB2	1:A:324:PHE:HD2	1.75	0.49
1:A:317:PHE:CZ	1:A:364:VAL:HG23	2.48	0.49
1:D:352:TRP:CE2	1:D:359:ASP:HB2	2.48	0.49
1:C:262:GLY:C	1:C:263:HIS:HD2	2.16	0.49
1:A:45:TYR:CZ	1:A:332:ARG:HG3	2.47	0.49
1:C:193:LEU:HD22	1:D:197:HIS:CD2	2.48	0.49
1:C:201:ASP:OD1	1:C:203:ARG:HB2	2.13	0.49
1:C:261:PHE:CD2	3:C:3003:MPD:HM1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:PHE:H	3:D:3004:MPD:HO2	1.61	0.48
1:D:266:ARG:HD3	1:D:360:TYR:CD1	2.47	0.48
1:D:317:PHE:CZ	1:D:364:VAL:HG23	2.48	0.48
1:A:102:PHE:H	3:A:3001:MPD:HO2	1.60	0.48
1:B:262:GLY:C	1:B:263:HIS:HD2	2.17	0.48
1:A:342:ASP:HB3	1:A:345:ILE:HB	1.95	0.48
1:C:266:ARG:HD3	1:C:360:TYR:CD1	2.47	0.48
1:D:275:GLU:HB2	1:D:324:PHE:CD2	2.48	0.48
1:B:333:TYR:O	1:B:336:THR:HB	2.14	0.48
1:A:266:ARG:HD3	1:A:360:TYR:CD1	2.49	0.48
1:A:411:ILE:HG13	1:A:412:VAL:HG22	1.95	0.48
1:D:415:LEU:HD13	1:D:419:ASN:HD21	1.78	0.48
1:A:164:VAL:CG1	1:A:165:THR:N	2.76	0.48
1:C:317:PHE:CZ	1:C:364:VAL:HG23	2.49	0.48
1:B:138:ARG:HG2	1:B:138:ARG:HH21	1.79	0.48
1:B:111:ARG:HG2	1:B:115:GLU:OE2	2.13	0.48
1:A:304:THR:HG23	1:A:306:TYR:N	2.22	0.48
1:D:399:ILE:HA	1:D:402:THR:HG22	1.96	0.48
1:A:139:ASN:H	1:A:139:ASN:ND2	2.06	0.48
1:A:227:MET:HE3	1:A:244:LEU:HG	1.95	0.48
1:C:415:LEU:HD13	1:C:419:ASN:HD21	1.77	0.48
1:B:317:PHE:CZ	1:B:364:VAL:HG23	2.49	0.48
1:C:164:VAL:CG1	1:C:165:THR:N	2.77	0.48
1:B:101:PRO:HD2	3:B:3002:MPD:HM1	1.95	0.48
1:B:228:ARG:HD3	4:B:5144:HOH:O	2.13	0.48
1:B:352:TRP:CE2	1:B:359:ASP:HB2	2.49	0.48
1:C:45:TYR:CZ	1:C:332:ARG:HG3	2.48	0.48
1:B:227:MET:CE	1:B:244:LEU:HG	2.44	0.47
1:C:247:ARG:NH2	2:C:1500:FAD:O2	2.37	0.47
1:D:105:SER:O	1:D:109:LYS:HG3	2.13	0.47
1:D:217:SER:HB3	2:D:1700:FAD:H5'2	1.95	0.47
2:A:1100:FAD:N6A	3:A:3005:MPD:H12	2.29	0.47
1:C:211:ASN:HD22	1:C:211:ASN:HA	1.58	0.47
1:D:227:MET:CE	1:D:244:LEU:HG	2.45	0.47
1:C:399:ILE:HA	1:C:402:THR:HG22	1.96	0.47
1:D:170:ASN:OD1	1:D:172:ASP:OD1	2.33	0.47
1:A:333:TYR:O	1:A:336:THR:HB	2.15	0.47
1:A:364:VAL:HG21	1:A:418:VAL:HG11	1.96	0.47
1:B:336:THR:HG22	1:B:337:LYS:HG2	1.96	0.47
1:B:265:TYR:HB3	1:B:357:GLY:HA2	1.97	0.47
1:A:262:GLY:C	1:A:263:HIS:HD2	2.18	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:TYR:CE2	1:C:242:ARG:HG3	2.50	0.47
1:A:103:SER:HA	1:A:106:ARG:HH21	1.81	0.46
1:A:300:MET:HG3	1:A:384:TRP:CZ2	2.50	0.46
1:A:139:ASN:HD21	1:A:142:SER:CB	2.27	0.46
1:D:139:ASN:HD22	1:D:139:ASN:N	2.06	0.46
1:A:39:GLN:NE2	2:A:1200:FAD:H5'2	2.30	0.46
1:B:201:ASP:OD1	1:B:203:ARG:HG2	2.15	0.46
1:A:47:SER:O	1:A:51:VAL:HG23	2.15	0.46
2:B:1400:FAD:C4A	3:B:3002:MPD:H11	2.46	0.46
1:D:139:ASN:ND2	1:D:142:SER:HB3	2.31	0.46
1:C:206:ASP:O	1:C:208:PRO:HD3	2.16	0.46
1:C:411:ILE:HG13	1:C:412:VAL:HG22	1.97	0.46
1:A:206:ASP:O	1:A:208:PRO:HD3	2.16	0.46
1:D:403:LYS:O	1:D:403:LYS:HG3	2.16	0.46
1:A:189:ARG:HA	1:A:224:THR:HB	1.98	0.46
1:B:300:MET:HG2	1:B:304:THR:CG2	2.46	0.46
1:B:239:GLU:OE1	1:B:242:ARG:NH2	2.48	0.46
1:C:151:LYS:NZ	1:C:154:GLU:OE2	2.46	0.46
1:B:9:ARG:HG2	1:B:221:LYS:O	2.16	0.46
1:D:312:ARG:HH22	1:D:340:ASP:CG	2.19	0.45
1:B:312:ARG:HH22	1:B:340:ASP:CG	2.20	0.45
1:B:164:VAL:CG1	1:B:165:THR:N	2.79	0.45
1:A:15:ASP:HA	1:A:156:GLU:O	2.16	0.45
1:A:83:VAL:HA	1:A:87:PHE:CD2	2.52	0.45
1:C:197:HIS:CD2	1:D:193:LEU:HD22	2.51	0.45
1:B:411:ILE:HG22	1:B:411:ILE:O	2.15	0.45
1:B:310:ARG:HA	1:B:310:ARG:HD2	1.73	0.45
1:C:172:ASP:HA	1:C:175:LEU:CD2	2.47	0.45
1:C:265:TYR:HB3	1:C:357:GLY:HA2	1.98	0.45
1:D:164:VAL:CG1	1:D:165:THR:N	2.80	0.45
1:B:275:GLU:HB2	1:B:324:PHE:CD2	2.50	0.45
1:D:106:ARG:O	1:D:110:ILE:HG13	2.17	0.45
1:D:411:ILE:O	1:D:412:VAL:CG1	2.54	0.45
1:C:15:ASP:HA	1:C:156:GLU:O	2.17	0.45
2:D:1700:FAD:H8A	2:D:1700:FAD:C5B	2.39	0.45
1:D:333:TYR:O	1:D:336:THR:HB	2.17	0.45
1:B:403:LYS:O	1:B:403:LYS:HG3	2.17	0.45
1:C:139:ASN:HD21	1:C:142:SER:CB	2.29	0.45
1:B:211:ASN:HD22	1:B:211:ASN:HA	1.61	0.45
1:B:43:ASN:HB3	1:B:46:LYS:HB2	1.99	0.44
1:B:47:SER:O	1:B:51:VAL:HG23	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:227:MET:HE3	1:D:244:LEU:HG	1.99	0.44
1:D:295:ASP:O	1:D:299:ARG:HG3	2.16	0.44
1:B:428:VAL:O	1:B:431:VAL:HG12	2.17	0.44
1:B:400:TYR:CE1	1:B:401:LYS:HG3	2.52	0.44
1:D:213:ASN:HB3	2:D:1700:FAD:O2P	2.17	0.44
1:C:403:LYS:O	1:C:403:LYS:HG3	2.17	0.44
1:B:300:MET:HG3	1:B:384:TRP:CZ2	2.52	0.44
1:B:16:ASN:HB3	1:B:19:LEU:HB3	1.99	0.44
1:A:363:ARG:HE	1:A:363:ARG:HB2	1.56	0.44
1:C:83:VAL:HA	1:C:87:PHE:CD2	2.51	0.44
1:B:139:ASN:ND2	1:B:142:SER:CB	2.81	0.44
1:A:7:PHE:O	1:A:8:ARG:HG3	2.16	0.44
1:D:262:GLY:C	1:D:263:HIS:HD2	2.21	0.44
1:D:411:ILE:HG13	1:D:412:VAL:HG22	1.98	0.44
1:B:237:LYS:HB3	4:B:5141:HOH:O	2.18	0.44
1:D:310:ARG:HA	1:D:310:ARG:HD2	1.71	0.44
1:D:9:ARG:HG2	1:D:221:LYS:O	2.18	0.43
1:B:139:ASN:H	1:B:139:ASN:ND2	2.15	0.43
1:D:217:SER:OG	1:D:218:PRO:HD3	2.19	0.43
1:B:45:TYR:CZ	1:B:332:ARG:HG3	2.53	0.43
1:C:172:ASP:HA	1:C:175:LEU:HD23	2.00	0.43
1:B:80:GLU:OE2	1:B:109:LYS:HD2	2.19	0.43
1:C:312:ARG:HH22	1:C:340:ASP:CG	2.21	0.43
1:A:265:TYR:HB3	1:A:357:GLY:HA2	2.01	0.43
1:C:333:TYR:O	1:C:336:THR:HB	2.18	0.43
2:C:1600:FAD:O4B	3:C:3003:MPD:H12	2.19	0.43
1:D:277:ASN:O	1:D:279:SER:N	2.52	0.43
1:A:227:MET:CE	1:A:244:LEU:HG	2.48	0.43
1:A:399:ILE:HA	1:A:402:THR:HG22	2.01	0.43
1:D:139:ASN:ND2	1:D:142:SER:CB	2.82	0.43
1:D:39:GLN:NE2	2:D:1800:FAD:H5'2	2.34	0.43
1:C:317:PHE:CE1	1:C:364:VAL:HA	2.54	0.43
1:B:15:ASP:HA	1:B:156:GLU:O	2.19	0.43
1:A:48:GLU:HB3	1:A:180:ILE:CG2	2.49	0.43
1:A:211:ASN:HA	1:A:211:ASN:HD22	1.59	0.43
1:D:198:ARG:HD3	4:D:5138:HOH:O	2.18	0.43
1:A:312:ARG:HH22	1:A:340:ASP:CG	2.22	0.42
1:D:47:SER:O	1:D:51:VAL:HG23	2.19	0.42
1:C:227:MET:HE3	1:C:244:LEU:HG	2.01	0.42
1:D:265:TYR:HB3	1:D:357:GLY:HA2	2.01	0.42
1:D:243:GLU:HA	1:D:246:TRP:HD1	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ARG:HG2	1:D:115:GLU:OE2	2.19	0.42
1:A:169:MET:HB3	4:A:5166:HOH:O	2.19	0.42
1:A:43:ASN:HB3	1:A:46:LYS:HB2	2.01	0.42
1:A:403:LYS:HG3	1:A:403:LYS:O	2.19	0.42
1:C:170:ASN:OD1	1:C:172:ASP:HB2	2.18	0.42
1:D:317:PHE:CE1	1:D:364:VAL:HA	2.55	0.42
1:D:15:ASP:HA	1:D:156:GLU:O	2.19	0.42
1:B:263:HIS:ND1	1:B:267:ARG:NH2	2.68	0.42
1:C:237:LYS:HB3	4:C:5042:HOH:O	2.20	0.42
1:D:111:ARG:CZ	1:D:121:PHE:HD2	2.33	0.42
1:A:18:GLY:N	1:A:96:ASN:HD21	2.10	0.42
1:A:415:LEU:CD1	1:A:419:ASN:HD21	2.32	0.42
1:A:100:THR:HB	3:A:3001:MPD:HM3	2.00	0.42
1:D:16:ASN:ND2	1:D:19:LEU:H	2.18	0.42
1:A:238:GLU:CD	1:A:238:GLU:N	2.73	0.42
1:C:139:ASN:N	1:C:139:ASN:ND2	2.67	0.42
1:D:16:ASN:HB3	1:D:19:LEU:HB3	2.02	0.42
1:A:317:PHE:CE1	1:A:364:VAL:HA	2.54	0.42
1:C:238:GLU:CD	1:C:238:GLU:N	2.73	0.42
1:D:268:GLU:HG2	1:D:429:LYS:NZ	2.35	0.41
1:B:7:PHE:O	1:B:8:ARG:HG3	2.20	0.41
1:B:389:LYS:O	1:B:389:LYS:HD2	2.20	0.41
1:B:139:ASN:ND2	1:B:142:SER:HB3	2.34	0.41
1:B:101:PRO:HB2	3:B:3002:MPD:O2	2.20	0.41
1:A:139:ASN:ND2	1:A:142:SER:HB3	2.35	0.41
1:D:131:PRO:HD2	1:D:134:LEU:HD12	2.01	0.41
1:D:335:ALA:HA	1:D:341:TYR:CD2	2.55	0.41
1:A:335:ALA:HA	1:A:341:TYR:CD2	2.55	0.41
1:B:398:SER:O	1:B:400:TYR:N	2.53	0.41
1:D:83:VAL:HA	1:D:87:PHE:CD2	2.55	0.41
1:B:277:ASN:ND2	1:B:280:TYR:CG	2.84	0.41
1:A:131:PRO:HD2	1:A:134:LEU:HD12	2.03	0.41
1:D:426:LYS:O	1:D:429:LYS:HB2	2.21	0.41
1:D:300:MET:HG2	1:D:304:THR:CG2	2.50	0.41
1:B:415:LEU:CD1	1:B:419:ASN:HD21	2.33	0.41
1:D:179:LYS:C	1:D:180:ILE:HG13	2.40	0.41
1:D:363:ARG:HE	1:D:363:ARG:HB2	1.59	0.41
1:B:269:TYR:C	1:B:271:ASN:H	2.23	0.41
1:B:349:ASN:HB3	2:B:1300:FAD:C8	2.50	0.41
1:D:15:ASP:OD1	1:D:155:PRO:HA	2.20	0.41
1:B:4:ILE:HG13	1:B:90:VAL:HG21	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLN:NE2	2:B:1400:FAD:H5'2	2.35	0.41
1:D:101:PRO:HD2	3:D:3004:MPD:O2	2.21	0.41
1:D:81:LYS:O	1:D:85:ARG:HG3	2.20	0.41
1:D:94:TYR:CE2	1:D:122:LYS:HD3	2.56	0.41
1:C:277:ASN:HD21	1:C:279:SER:HB3	1.86	0.41
1:D:375:ASP:OD1	1:D:380:PHE:HB3	2.20	0.41
1:B:266:ARG:HH11	1:B:360:TYR:HD1	1.66	0.41
1:A:39:GLN:HE22	2:A:1200:FAD:H5'2	1.85	0.41
1:A:16:ASN:ND2	1:A:19:LEU:H	2.18	0.41
1:C:389:LYS:O	1:C:389:LYS:HD2	2.20	0.41
1:C:111:ARG:CZ	1:C:121:PHE:HD2	2.34	0.41
1:D:266:ARG:HH11	1:D:360:TYR:HD1	1.69	0.41
1:C:15:ASP:OD1	1:C:155:PRO:HA	2.20	0.41
1:C:335:ALA:HA	1:C:341:TYR:CD2	2.56	0.41
1:A:197:HIS:CD2	1:B:193:LEU:HD22	2.56	0.41
1:B:363:ARG:HB2	1:B:363:ARG:HE	1.60	0.41
1:B:111:ARG:CZ	1:B:121:PHE:HD2	2.34	0.40
1:D:111:ARG:HG3	1:D:111:ARG:HH11	1.87	0.40
1:D:32:VAL:CG1	1:D:33:PHE:N	2.84	0.40
1:A:81:LYS:O	1:A:85:ARG:HG3	2.21	0.40
1:A:300:MET:HG2	1:A:304:THR:CG2	2.50	0.40
1:C:16:ASN:ND2	1:C:19:LEU:H	2.20	0.40
1:A:100:THR:HB	3:A:3001:MPD:CM	2.51	0.40
1:D:139:ASN:ND2	1:D:139:ASN:H	2.15	0.40
1:C:39:GLN:NE2	2:C:1600:FAD:H5'2	2.36	0.40
1:B:269:TYR:CZ	1:B:429:LYS:HD3	2.57	0.40
1:C:310:ARG:HD2	1:C:310:ARG:HA	1.76	0.40
1:C:275:GLU:HB2	1:C:324:PHE:CD2	2.54	0.40
1:D:238:GLU:N	1:D:238:GLU:CD	2.74	0.40
1:A:237:LYS:HB3	4:A:5139:HOH:O	2.22	0.40
1:B:318:PHE:O	1:B:322:VAL:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	426/440 (97%)	396 (93%)	26 (6%)	4 (1%)	21	55
1	B	429/440 (98%)	399 (93%)	24 (6%)	6 (1%)	14	42
1	C	426/440 (97%)	399 (94%)	23 (5%)	4 (1%)	21	55
1	D	428/440 (97%)	397 (93%)	25 (6%)	6 (1%)	14	42
All	All	1709/1760 (97%)	1591 (93%)	98 (6%)	20 (1%)	16	47

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	HIS
1	A	403	LYS
1	B	136	HIS
1	B	168	SER
1	C	136	HIS
1	C	403	LYS
1	D	136	HIS
1	D	168	SER
1	D	278	GLU
1	D	403	LYS
1	B	278	GLU
1	B	403	LYS
1	D	412	VAL
1	B	399	ILE
1	C	278	GLU
1	A	278	GLU
1	A	399	ILE
1	D	399	ILE
1	B	412	VAL
1	C	399	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	392/403 (97%)	372 (95%)	20 (5%)	29	63
1	B	394/403 (98%)	376 (95%)	18 (5%)	33	67
1	C	392/403 (97%)	375 (96%)	17 (4%)	35	70
1	D	393/403 (98%)	373 (95%)	20 (5%)	29	63
All	All	1571/1612 (98%)	1496 (95%)	75 (5%)	31	66

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	9	ARG
1	A	16	ASN
1	A	106	ARG
1	A	139	ASN
1	A	158	MET
1	A	175	LEU
1	A	190	ARG
1	A	211	ASN
1	A	238	GLU
1	A	248	ASP
1	A	278	GLU
1	A	288	ARG
1	A	291	TYR
1	A	315	VAL
1	A	336	THR
1	A	338	LEU
1	A	353	ILE
1	A	370	GLN
1	A	377	GLU
1	B	8	ARG
1	B	16	ASN
1	B	139	ASN
1	B	158	MET
1	B	175	LEU
1	B	190	ARG
1	B	211	ASN
1	B	238	GLU
1	B	248	ASP
1	B	278	GLU
1	B	288	ARG
1	B	291	TYR
1	B	336	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	338	LEU
1	B	353	ILE
1	B	355	SER
1	B	370	GLN
1	B	377	GLU
1	C	8	ARG
1	C	16	ASN
1	C	139	ASN
1	C	158	MET
1	C	175	LEU
1	C	190	ARG
1	C	211	ASN
1	C	238	GLU
1	C	248	ASP
1	C	278	GLU
1	C	288	ARG
1	C	315	VAL
1	C	336	THR
1	C	338	LEU
1	C	353	ILE
1	C	370	GLN
1	C	377	GLU
1	D	8	ARG
1	D	16	ASN
1	D	139	ASN
1	D	158	MET
1	D	172	ASP
1	D	175	LEU
1	D	190	ARG
1	D	211	ASN
1	D	238	GLU
1	D	248	ASP
1	D	268	GLU
1	D	278	GLU
1	D	288	ARG
1	D	291	TYR
1	D	336	THR
1	D	338	LEU
1	D	353	ILE
1	D	370	GLN
1	D	377	GLU
1	D	429	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	96	ASN
1	A	139	ASN
1	A	145	ASN
1	A	211	ASN
1	A	263	HIS
1	A	271	ASN
1	A	419	ASN
1	A	427	ASN
1	B	16	ASN
1	B	96	ASN
1	B	139	ASN
1	B	145	ASN
1	B	211	ASN
1	B	271	ASN
1	B	419	ASN
1	C	16	ASN
1	C	96	ASN
1	C	139	ASN
1	C	145	ASN
1	C	211	ASN
1	C	263	HIS
1	C	271	ASN
1	C	419	ASN
1	D	16	ASN
1	D	96	ASN
1	D	139	ASN
1	D	145	ASN
1	D	263	HIS
1	D	271	ASN
1	D	419	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	A	1100	-	48,58,58	1.37	5 (10%)	54,89,89	2.15	11 (20%)
2	FAD	A	1200	-	48,58,58	1.38	5 (10%)	54,89,89	2.11	12 (22%)
3	MPD	A	3001	-	6,7,7	0.40	0	7,10,10	0.46	0
3	MPD	A	3005	-	6,7,7	0.38	0	7,10,10	0.40	0
2	FAD	B	1300	-	48,58,58	1.38	5 (10%)	54,89,89	2.14	11 (20%)
2	FAD	B	1400	-	48,58,58	1.38	5 (10%)	54,89,89	2.17	14 (25%)
3	MPD	B	3002	-	6,7,7	0.53	0	7,10,10	0.41	0
2	FAD	C	1500	-	48,58,58	1.39	5 (10%)	54,89,89	2.17	12 (22%)
2	FAD	C	1600	-	48,58,58	1.37	5 (10%)	54,89,89	2.08	12 (22%)
3	MPD	C	3003	-	6,7,7	0.49	0	7,10,10	0.52	0
3	MPD	C	3006	-	6,7,7	0.38	0	7,10,10	0.45	0
2	FAD	D	1700	-	48,58,58	1.38	5 (10%)	54,89,89	2.15	12 (22%)
2	FAD	D	1800	-	48,58,58	1.37	5 (10%)	54,89,89	2.12	14 (25%)
3	MPD	D	3004	-	6,7,7	0.40	0	7,10,10	0.47	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
2	FAD	A	1100	-	-	0/30/50/50	0/6/6/6
2	FAD	A	1200	-	-	0/30/50/50	0/6/6/6
3	MPD	A	3001	-	-	0/5/5/5	0/0/0/0
3	MPD	A	3005	-	-	0/5/5/5	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	1300	-	-	0/30/50/50	0/6/6/6
2	FAD	B	1400	-	-	0/30/50/50	0/6/6/6
3	MPD	B	3002	-	-	0/5/5/5	0/0/0/0
2	FAD	C	1500	-	-	0/30/50/50	0/6/6/6
2	FAD	C	1600	-	-	0/30/50/50	0/6/6/6
3	MPD	C	3003	-	-	0/5/5/5	0/0/0/0
3	MPD	C	3006	-	-	0/5/5/5	0/0/0/0
2	FAD	D	1700	-	-	0/30/50/50	0/6/6/6
2	FAD	D	1800	-	-	0/30/50/50	0/6/6/6
3	MPD	D	3004	-	-	0/5/5/5	0/0/0/0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1400	FAD	O4B-C1B	2.40	1.44	1.41
2	C	1600	FAD	O4B-C1B	2.40	1.44	1.41
2	D	1800	FAD	O4B-C1B	2.43	1.44	1.41
2	A	1100	FAD	O4B-C1B	2.47	1.44	1.41
2	A	1200	FAD	O4B-C1B	2.48	1.44	1.41
2	B	1300	FAD	O4B-C1B	2.50	1.44	1.41
2	C	1500	FAD	O4B-C1B	2.52	1.44	1.41
2	D	1700	FAD	O4B-C1B	2.53	1.44	1.41
2	B	1400	FAD	C10-N1	2.90	1.40	1.35
2	A	1200	FAD	C10-N1	2.93	1.40	1.35
2	D	1800	FAD	C10-N1	2.94	1.40	1.35
2	C	1600	FAD	C10-N1	2.97	1.40	1.35
2	A	1100	FAD	C10-N1	2.98	1.40	1.35
2	C	1500	FAD	C10-N1	3.00	1.40	1.35
2	D	1700	FAD	C10-N1	3.00	1.40	1.35
2	B	1300	FAD	C10-N1	3.03	1.40	1.35
2	A	1200	FAD	C5X-N5	3.25	1.40	1.35
2	C	1600	FAD	C5X-N5	3.25	1.40	1.35
2	A	1100	FAD	C5X-N5	3.26	1.40	1.35
2	B	1300	FAD	C5X-N5	3.26	1.40	1.35
2	D	1700	FAD	C5X-N5	3.28	1.40	1.35
2	C	1500	FAD	C5X-N5	3.30	1.40	1.35
2	B	1400	FAD	C5X-N5	3.32	1.40	1.35
2	D	1800	FAD	C5X-N5	3.33	1.40	1.35
2	D	1700	FAD	C4-N3	3.92	1.40	1.33
2	A	1100	FAD	C4-N3	3.95	1.40	1.33
2	D	1800	FAD	C4-N3	3.96	1.40	1.33
2	C	1500	FAD	C4-N3	3.97	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1400	FAD	C4-N3	3.97	1.40	1.33
2	B	1300	FAD	C4-N3	3.99	1.40	1.33
2	C	1600	FAD	C4-N3	4.00	1.40	1.33
2	A	1200	FAD	C4-N3	4.04	1.40	1.33
2	A	1100	FAD	C4X-N5	4.50	1.40	1.33
2	D	1700	FAD	C4X-N5	4.51	1.40	1.33
2	B	1300	FAD	C4X-N5	4.51	1.40	1.33
2	C	1600	FAD	C4X-N5	4.54	1.40	1.33
2	D	1800	FAD	C4X-N5	4.56	1.40	1.33
2	B	1400	FAD	C4X-N5	4.59	1.40	1.33
2	C	1500	FAD	C4X-N5	4.61	1.40	1.33
2	A	1200	FAD	C4X-N5	4.65	1.40	1.33

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1500	FAD	N3A-C2A-N1A	-10.39	120.94	128.89
2	B	1300	FAD	N3A-C2A-N1A	-10.37	120.95	128.89
2	D	1700	FAD	N3A-C2A-N1A	-10.34	120.97	128.89
2	A	1100	FAD	N3A-C2A-N1A	-10.32	121.00	128.89
2	B	1400	FAD	N3A-C2A-N1A	-10.04	121.20	128.89
2	A	1200	FAD	N3A-C2A-N1A	-9.89	121.33	128.89
2	D	1800	FAD	N3A-C2A-N1A	-9.84	121.36	128.89
2	C	1600	FAD	N3A-C2A-N1A	-9.69	121.47	128.89
2	D	1800	FAD	O3P-PA-O5B	-4.38	91.33	102.94
2	B	1400	FAD	O3P-PA-O5B	-4.32	91.47	102.94
2	B	1300	FAD	O3P-PA-O5B	-4.17	91.88	102.94
2	D	1700	FAD	O3P-PA-O5B	-4.16	91.90	102.94
2	A	1200	FAD	O3P-PA-O5B	-4.15	91.94	102.94
2	C	1500	FAD	O3P-PA-O5B	-4.04	92.21	102.94
2	A	1100	FAD	O3P-PA-O5B	-3.98	92.38	102.94
2	A	1100	FAD	O5B-PA-O1A	-3.76	95.04	109.62
2	C	1500	FAD	O5B-PA-O1A	-3.72	95.19	109.62
2	C	1600	FAD	O3P-PA-O5B	-3.69	93.15	102.94
2	A	1100	FAD	P-O3P-PA	-3.69	122.37	132.73
2	D	1800	FAD	P-O3P-PA	-3.68	122.40	132.73
2	B	1300	FAD	O5B-PA-O1A	-3.61	95.62	109.62
2	D	1700	FAD	O5B-PA-O1A	-3.59	95.66	109.62
2	B	1400	FAD	P-O3P-PA	-3.52	122.84	132.73
2	C	1500	FAD	P-O3P-PA	-3.47	122.99	132.73
2	B	1300	FAD	P-O3P-PA	-3.46	123.01	132.73
2	A	1200	FAD	P-O3P-PA	-3.44	123.08	132.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1200	FAD	O5B-PA-O1A	-3.41	96.38	109.62
2	D	1700	FAD	P-O3P-PA	-3.25	123.60	132.73
2	C	1600	FAD	O5B-PA-O1A	-3.25	97.01	109.62
2	C	1600	FAD	P-O3P-PA	-3.23	123.66	132.73
2	B	1400	FAD	O5B-PA-O1A	-3.21	97.17	109.62
2	D	1800	FAD	O5B-PA-O1A	-3.17	97.33	109.62
2	A	1200	FAD	C4X-C4-N3	-2.56	120.08	123.59
2	D	1800	FAD	C2B-C1B-N9A	-2.54	110.42	114.29
2	C	1600	FAD	C4X-C4-N3	-2.49	120.18	123.59
2	D	1700	FAD	C4X-C4-N3	-2.47	120.21	123.59
2	C	1500	FAD	C2B-C1B-N9A	-2.45	110.54	114.29
2	B	1400	FAD	C4X-C4-N3	-2.44	120.25	123.59
2	C	1500	FAD	C4X-C4-N3	-2.41	120.30	123.59
2	A	1100	FAD	C4X-C4-N3	-2.38	120.33	123.59
2	B	1300	FAD	C4X-C4-N3	-2.36	120.36	123.59
2	D	1800	FAD	C4A-C5A-N7A	-2.34	107.33	109.48
2	D	1800	FAD	C4X-C4-N3	-2.32	120.42	123.59
2	D	1700	FAD	C4A-C5A-N7A	-2.29	107.37	109.48
2	B	1400	FAD	C2B-C1B-N9A	-2.22	110.90	114.29
2	A	1100	FAD	C4A-C5A-N7A	-2.21	107.44	109.48
2	C	1500	FAD	C4A-C5A-N7A	-2.20	107.45	109.48
2	B	1400	FAD	C4A-C5A-N7A	-2.20	107.46	109.48
2	C	1600	FAD	O2A-PA-O5B	-2.19	97.40	108.46
2	A	1200	FAD	O2A-PA-O5B	-2.13	97.70	108.46
2	C	1600	FAD	C4A-C5A-N7A	-2.13	107.52	109.48
2	B	1300	FAD	C4A-C5A-N7A	-2.13	107.52	109.48
2	A	1200	FAD	C4A-C5A-N7A	-2.09	107.56	109.48
2	D	1700	FAD	O2A-PA-O5B	-2.04	98.17	108.46
2	B	1400	FAD	O2A-PA-O5B	-2.04	98.19	108.46
2	D	1800	FAD	O2A-PA-O5B	-2.03	98.25	108.46
2	D	1800	FAD	C1'-N10-C9A	2.02	121.13	118.86
2	B	1400	FAD	C1'-N10-C9A	2.14	121.27	118.86
2	C	1500	FAD	O2A-PA-O1A	2.26	124.77	112.53
2	A	1200	FAD	O2A-PA-O1A	2.28	124.88	112.53
2	D	1700	FAD	O2A-PA-O1A	2.29	124.94	112.53
2	C	1600	FAD	O2A-PA-O1A	2.31	125.03	112.53
2	A	1100	FAD	O2A-PA-O1A	2.32	125.09	112.53
2	B	1300	FAD	O2A-PA-O1A	2.33	125.15	112.53
2	B	1400	FAD	O2A-PA-O1A	2.36	125.30	112.53
2	D	1800	FAD	O2A-PA-O1A	2.40	125.51	112.53
2	A	1200	FAD	O2A-PA-O3P	2.52	116.52	105.09
2	C	1600	FAD	O2A-PA-O3P	2.54	116.61	105.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1800	FAD	C5X-C9A-N10	2.54	119.55	117.62
2	B	1400	FAD	C5X-C9A-N10	2.59	119.59	117.62
2	B	1300	FAD	O2A-PA-O3P	2.61	116.92	105.09
2	A	1100	FAD	O2A-PA-O3P	2.62	116.96	105.09
2	C	1500	FAD	O2A-PA-O3P	2.62	116.97	105.09
2	A	1200	FAD	C5X-C9A-N10	2.63	119.62	117.62
2	D	1700	FAD	O2A-PA-O3P	2.65	117.09	105.09
2	B	1400	FAD	O2A-PA-O3P	2.69	117.31	105.09
2	D	1700	FAD	C5X-C9A-N10	2.70	119.67	117.62
2	D	1800	FAD	O2A-PA-O3P	2.70	117.36	105.09
2	B	1300	FAD	C5X-C9A-N10	2.72	119.69	117.62
2	C	1600	FAD	C5X-C9A-N10	2.78	119.73	117.62
2	C	1500	FAD	C5X-C9A-N10	2.90	119.82	117.62
2	A	1100	FAD	C5X-C9A-N10	2.92	119.84	117.62
2	A	1100	FAD	C4X-N5-C5X	3.01	120.23	116.76
2	D	1800	FAD	C4X-N5-C5X	3.09	120.32	116.76
2	A	1200	FAD	C4X-N5-C5X	3.12	120.36	116.76
2	C	1500	FAD	C4X-N5-C5X	3.18	120.42	116.76
2	D	1700	FAD	C4X-N5-C5X	3.27	120.52	116.76
2	B	1400	FAD	C4X-N5-C5X	3.29	120.55	116.76
2	B	1300	FAD	C4X-N5-C5X	3.30	120.56	116.76
2	C	1600	FAD	C4X-N5-C5X	3.33	120.59	116.76
2	A	1100	FAD	C4-N3-C2	4.93	119.51	115.25
2	C	1500	FAD	C4-N3-C2	5.16	119.71	115.25
2	B	1300	FAD	C4-N3-C2	5.18	119.73	115.25
2	D	1700	FAD	C4-N3-C2	5.31	119.84	115.25
2	C	1600	FAD	C4-N3-C2	5.43	119.94	115.25
2	D	1800	FAD	C4-N3-C2	5.52	120.02	115.25
2	A	1200	FAD	C4-N3-C2	5.71	120.18	115.25
2	B	1400	FAD	C4-N3-C2	6.07	120.50	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1100	FAD	3	0
2	A	1200	FAD	3	0
3	A	3001	MPD	4	0
3	A	3005	MPD	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1300	FAD	3	0
2	B	1400	FAD	3	0
3	B	3002	MPD	3	0
2	C	1500	FAD	3	0
2	C	1600	FAD	2	0
3	C	3003	MPD	2	0
3	C	3006	MPD	1	0
2	D	1700	FAD	5	0
2	D	1800	FAD	2	0
3	D	3004	MPD	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.