



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:49 AM GMT

PDB ID : 3JSX  
Title : X-ray Crystal structure of NAD(P)H: Quinone Oxidoreductase-1 (NQO1)  
bound to the coumarin-based inhibitor AS1  
Authors : Dunstan, M.S.; Levy, C.; Leys, D.  
Deposited on : 2009-09-11  
Resolution : 2.45 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<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) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

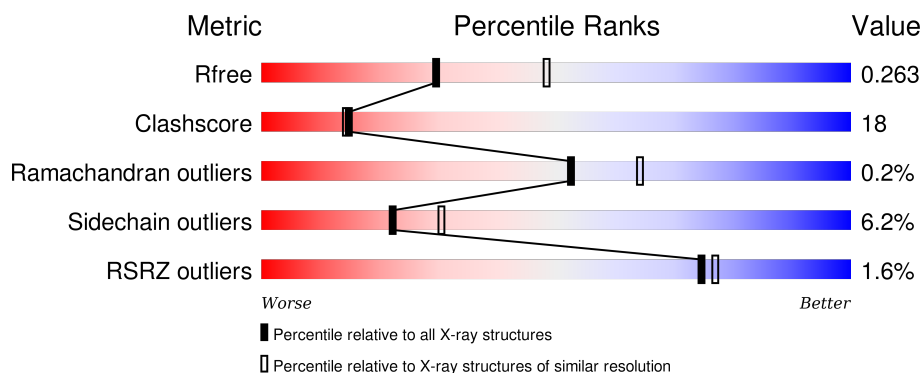
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	273	<div> <div>62%</div> <div>32%</div> <div>..</div> </div>
1	B	273	<div> <div>70%</div> <div>27%</div> <div>..</div> </div>
1	C	273	<div> <div>66%</div> <div>29%</div> <div>..</div> </div>
1	D	273	<div> <div>69%</div> <div>27%</div> <div>..</div> </div>
1	E	273	<div> <div>71%</div> <div>24%</div> <div>..</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	273	
1	G	273	
1	H	273	

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
3	CC2	B	547	-	-	X	-

## 2 Entry composition

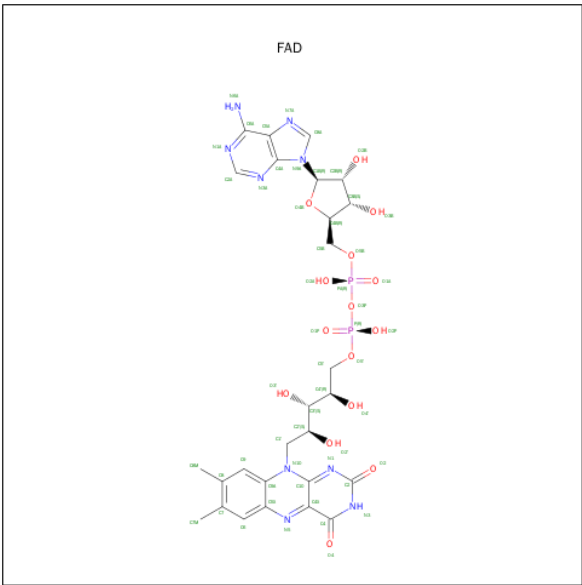
There are 4 unique types of molecules in this entry. The entry contains 18234 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NAD(P)H dehydrogenase [quinone] 1.

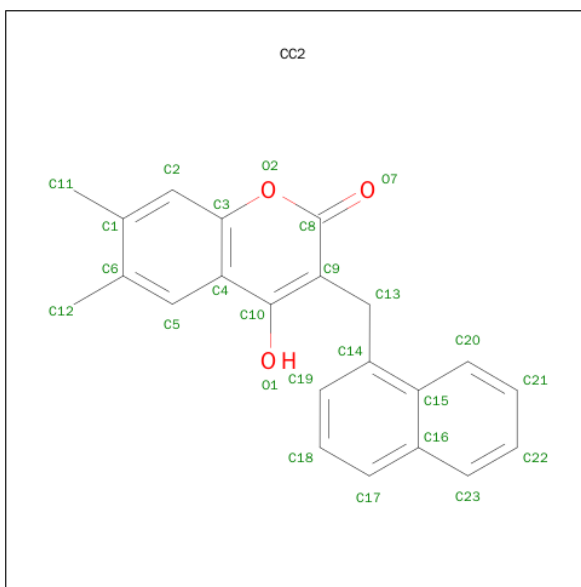
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	270	Total	C	N	O	S	0	0	0
			2147	1397	358	385	7			
1	B	270	Total	C	N	O	S	0	0	0
			2147	1397	358	385	7			
1	C	270	Total	C	N	O	S	0	0	0
			2147	1397	358	385	7			
1	D	270	Total	C	N	O	S	0	0	0
			2147	1397	358	385	7			
1	E	270	Total	C	N	O	S	0	0	0
			2147	1397	358	385	7			
1	F	270	Total	C	N	O	S	0	0	0
			2147	1397	358	385	7			
1	G	270	Total	C	N	O	S	0	0	0
			2147	1397	358	385	7			
1	H	270	Total	C	N	O	S	0	0	0
			2147	1397	358	385	7			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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	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	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is 4-HYDROXY-6,7-DIMETHYL-3-(NAPHTHALEN-1-YLMETHYL)-2H-CHROMEN-2-ONE (three-letter code: CC2) (formula: C<sub>22</sub>H<sub>18</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 25 22 3	0	0
3	B	1	Total C O 25 22 3	0	0
3	C	1	Total C O 25 22 3	0	0
3	D	1	Total C O 25 22 3	0	0
3	E	1	Total C O 25 22 3	0	0
3	F	1	Total C O 25 22 3	0	0
3	G	1	Total C O 25 22 3	0	0
3	H	1	Total C O 25 22 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	66	Total O 66 66	0	0
4	B	66	Total O 66 66	0	0
4	C	70	Total O 70 70	0	0
4	D	59	Total O 59 59	0	0

*Continued on next page...*

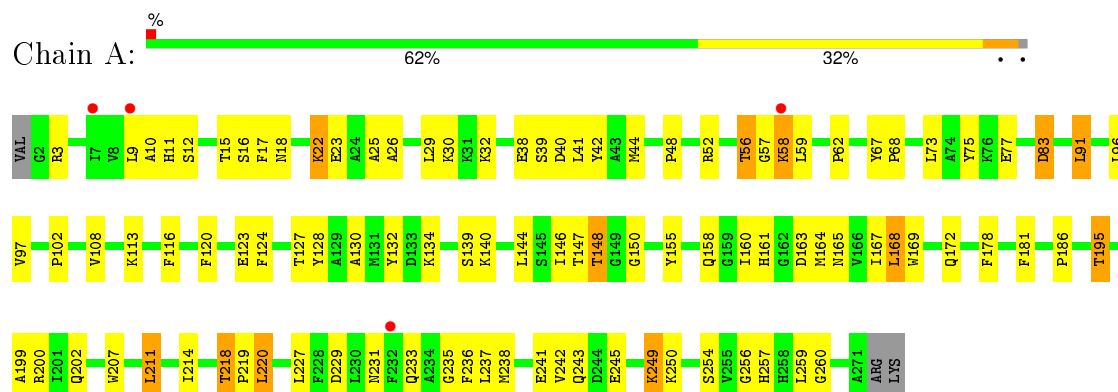
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	37	Total 37	O 37	0	0
4	F	41	Total 41	O 41	0	0
4	G	54	Total 54	O 54	0	0
4	H	41	Total 41	O 41	0	0

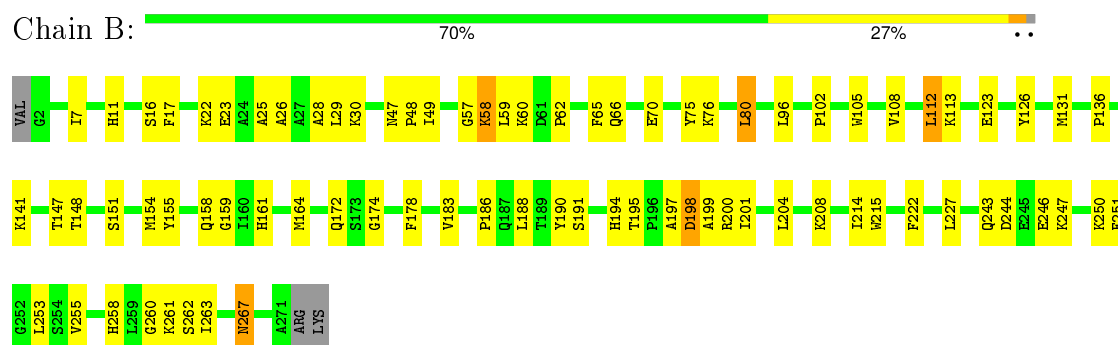
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

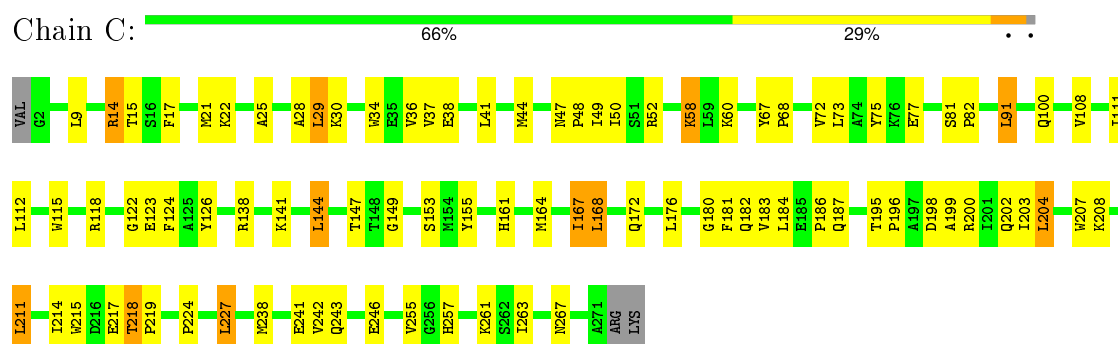
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



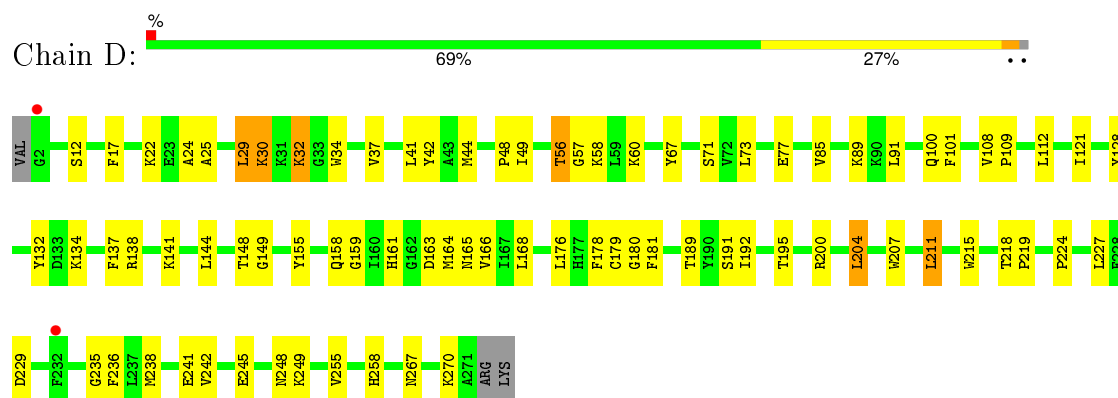
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



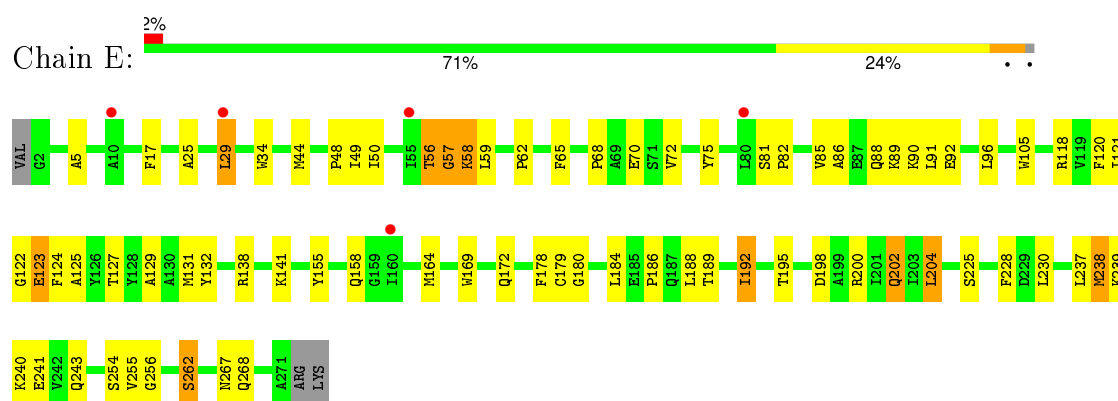
- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



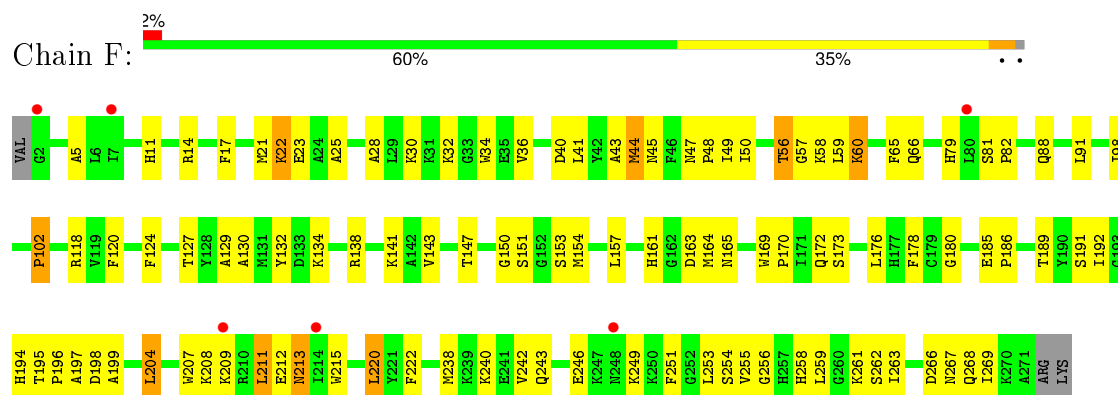
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1



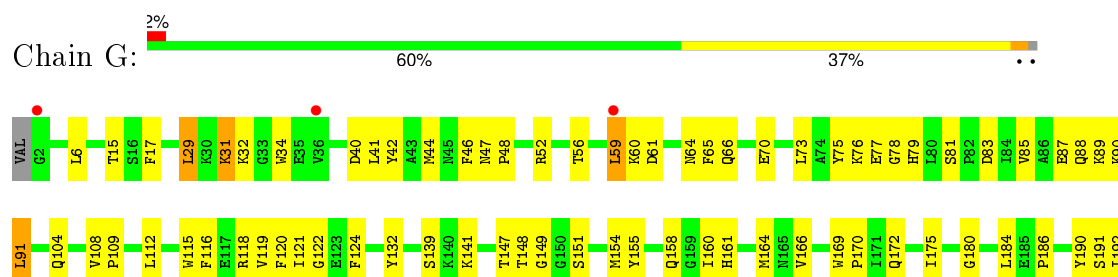
• Molecule 1: NAD(P)H dehydrogenase [quinone] 1



• Molecule 1: NAD(P)H dehydrogenase [quinone] 1

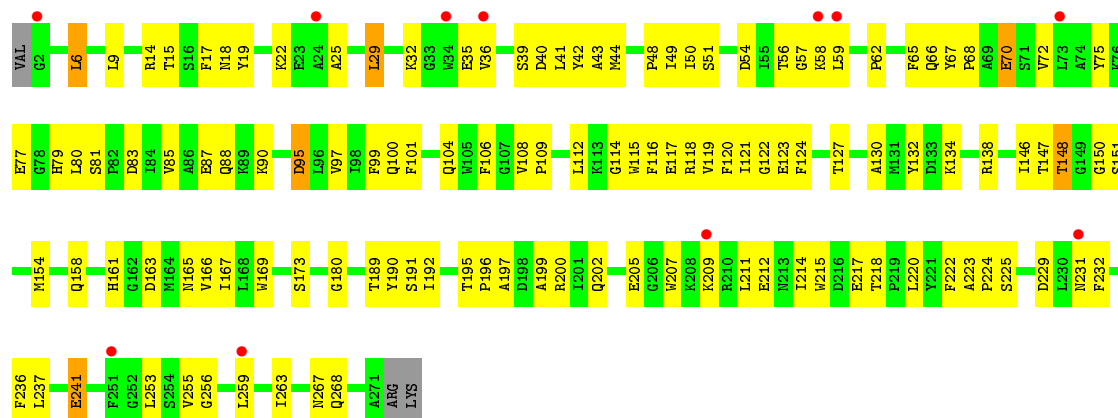


• Molecule 1: NAD(P)H dehydrogenase [quinone] 1





- Molecule 1: NAD(P)H dehydrogenase [quinone] 1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.04Å 209.94Å 102.08Å 90.00° 109.93° 90.00°	Depositor
Resolution (Å)	47.95 – 2.45 47.95 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.95-2.45) 99.1 (47.95-2.45)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.206 , 0.269 0.203 , 0.263	Depositor DCC
$R_{free}$ test set	5063 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.9	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.6	EDS
Estimated twinning fraction	0.199 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 101125 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18234	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, CC2

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	0.43	0/2205	0.59	0/2980
1	B	0.46	0/2205	0.58	0/2980
1	C	0.45	0/2205	0.58	0/2980
1	D	0.46	0/2205	0.58	0/2980
1	E	0.40	0/2205	0.54	0/2980
1	F	0.41	0/2205	0.57	0/2980
1	G	0.41	0/2205	0.56	0/2980
1	H	0.40	0/2205	0.55	0/2980
All	All	0.43	0/17640	0.57	0/23840

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2147	0	2141	90	0
1	B	2147	0	2141	79	0
1	C	2147	0	2141	80	0
1	D	2147	0	2141	67	0
1	E	2147	0	2141	70	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2147	0	2141	89	0
1	G	2147	0	2141	75	0
1	H	2147	0	2141	99	0
2	A	53	0	31	7	0
2	B	53	0	31	10	0
2	C	53	0	31	6	0
2	D	53	0	31	6	0
2	E	53	0	31	4	0
2	F	53	0	31	4	0
2	G	53	0	31	2	0
2	H	53	0	31	9	0
3	A	25	0	17	1	0
3	B	25	0	18	10	0
3	C	25	0	17	4	0
3	D	25	0	17	2	0
3	E	25	0	18	3	0
3	F	25	0	18	3	0
3	G	25	0	18	2	0
3	H	25	0	17	3	0
4	A	66	0	0	2	0
4	B	66	0	0	0	0
4	C	70	0	0	2	0
4	D	59	0	0	4	0
4	E	37	0	0	4	0
4	F	41	0	0	2	0
4	G	54	0	0	2	0
4	H	41	0	0	2	0
All	All	18234	0	17516	626	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 18.

All (626) 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:E:228:PHE:HA	4:E:361:HOH:O	1.37	1.22
1:F:151:SER:H	1:F:154:MET:HE3	1.08	1.12
1:F:17:PHE:HB2	2:F:601:FAD:H52A	1.13	1.11
1:B:17:PHE:HB2	2:B:601:FAD:H52A	1.13	1.07
1:E:238:MET:HA	4:E:361:HOH:O	1.54	1.05
1:C:14:ARG:HH11	1:C:14:ARG:HG3	1.25	1.02

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLN:HG2	1:B:243:GLN:HE21	1.26	1.01
1:B:172:GLN:HG2	1:B:183:VAL:HG11	1.43	1.00
1:B:194:HIS:CE1	3:B:547:CC2:H21	1.98	0.97
1:E:141:LYS:HD3	1:E:184:LEU:HD11	1.48	0.93
1:H:50:ILE:HD12	1:H:117:GLU:HB3	1.50	0.92
1:C:243:GLN:HE21	1:D:158:GLN:HG2	1.36	0.90
1:G:148:THR:HG22	1:G:190:TYR:HA	1.54	0.90
1:H:130:ALA:HB1	1:H:134:LYS:HB2	1.54	0.89
1:B:147:THR:OG1	2:B:601:FAD:H5'2	1.73	0.88
1:F:17:PHE:CB	2:F:601:FAD:H52A	2.01	0.88
1:A:158:GLN:HG2	1:B:243:GLN:NE2	1.90	0.86
1:E:172:GLN:HE22	1:E:186:PRO:HG3	1.42	0.83
1:B:17:PHE:HB2	2:B:601:FAD:C5B	2.06	0.83
1:B:148:THR:HG22	1:B:190:TYR:HA	1.60	0.83
1:G:47:ASN:HB3	1:G:118:ARG:NH1	1.94	0.83
1:F:151:SER:H	1:F:154:MET:CE	1.92	0.82
1:C:17:PHE:HB2	2:C:601:FAD:H52A	1.61	0.81
1:A:9:LEU:HD22	1:A:22:LYS:HG2	1.62	0.81
1:H:127:THR:HG22	1:H:130:ALA:H	1.45	0.81
1:A:164:MET:HE3	1:A:167:ILE:HB	1.63	0.80
1:H:65:PHE:CE1	1:H:70:GLU:HG2	2.17	0.80
1:F:151:SER:N	1:F:154:MET:HE3	1.93	0.80
1:C:224:PRO:HD2	1:C:227:LEU:HD22	1.63	0.80
1:A:113:LYS:NZ	1:B:105:TRP:HB2	1.97	0.79
1:A:147:THR:OG1	2:A:601:FAD:H5'2	1.83	0.79
1:E:169:TRP:CZ2	1:E:256:GLY:HA3	2.19	0.78
1:G:65:PHE:CE1	1:G:70:GLU:HG2	2.17	0.78
1:E:56:THR:HG22	1:E:57:GLY:H	1.48	0.78
1:A:163:ASP:OD2	1:A:165:ASN:HB2	1.83	0.78
1:E:267:ASN:ND2	1:E:268:GLN:HE21	1.83	0.77
1:G:65:PHE:HE1	1:G:70:GLU:HG2	1.46	0.77
1:B:7:ILE:HG21	1:B:22:LYS:HG2	1.65	0.77
1:C:243:GLN:NE2	1:D:158:GLN:HG2	2.01	0.76
1:G:198:ASP:HA	1:G:201:ILE:HD13	1.67	0.76
1:F:132:TYR:OH	1:H:161:HIS:HD2	1.68	0.75
1:C:48:PRO:HG3	1:D:49:ILE:HD11	1.68	0.75
1:E:17:PHE:HB2	2:E:601:FAD:H52A	1.67	0.75
1:B:147:THR:HG1	2:B:601:FAD:H5'2	1.48	0.75
1:H:147:THR:OG1	2:H:601:FAD:H5'2	1.86	0.74
1:F:60:LYS:HD3	1:F:60:LYS:O	1.88	0.74
1:C:255:VAL:HG23	1:C:267:ASN:HD22	1.53	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:LYS:HD3	1:E:58:LYS:N	2.02	0.74
1:E:58:LYS:H	1:E:58:LYS:HD3	1.52	0.74
1:C:58:LYS:HD3	1:C:58:LYS:H	1.54	0.73
1:A:164:MET:HE2	1:A:168:LEU:HD13	1.69	0.73
1:C:172:GLN:HG2	1:C:183:VAL:HG11	1.70	0.73
1:A:17:PHE:HB2	2:A:601:FAD:H51A	1.71	0.72
1:G:56:THR:HG23	1:G:79:HIS:O	1.88	0.72
1:B:17:PHE:CB	2:B:601:FAD:H52A	2.07	0.72
1:G:246:GLU:OE1	1:G:249:LYS:HD2	1.90	0.72
1:B:161:HIS:HE1	3:B:547:CC2:O7	1.73	0.72
1:F:153:SER:OG	1:H:237:LEU:HD21	1.90	0.71
1:D:85:VAL:O	1:D:89:LYS:HG2	1.90	0.71
1:E:132:TYR:OH	1:G:161:HIS:HD2	1.72	0.71
1:A:164:MET:CE	1:A:168:LEU:HD13	2.20	0.71
1:C:164:MET:SD	1:C:168:LEU:HD13	2.31	0.71
1:A:128:TYR:HE1	3:B:547:CC2:HO1	1.38	0.69
1:F:169:TRP:CZ2	1:F:256:GLY:HA3	2.27	0.69
1:H:138:ARG:HA	1:H:180:GLY:O	1.92	0.69
1:A:9:LEU:HD12	1:A:10:ALA:H	1.58	0.69
1:B:255:VAL:HG23	1:B:267:ASN:HD22	1.58	0.68
1:E:75:TYR:CZ	1:E:124:PHE:HB2	2.28	0.68
1:F:25:ALA:HB2	1:F:207:TRP:HE1	1.59	0.68
1:G:255:VAL:HG23	1:G:267:ASN:HD22	1.58	0.68
1:C:17:PHE:HB2	2:C:601:FAD:C5B	2.24	0.68
1:A:257:HIS:HD2	4:A:326:HOH:O	1.77	0.67
1:C:144:LEU:HD22	1:C:172:GLN:HE21	1.59	0.67
1:F:204:LEU:O	1:F:208:LYS:HG3	1.93	0.67
1:H:173:SER:HB2	1:H:222:PHE:CE1	2.28	0.67
1:H:108:VAL:HG13	1:H:112:LEU:HB3	1.76	0.67
1:B:148:THR:CG2	1:B:190:TYR:HA	2.25	0.67
1:C:14:ARG:HH11	1:C:14:ARG:CG	2.06	0.66
1:E:255:VAL:HG23	1:E:267:ASN:HD22	1.60	0.66
1:H:81:SER:O	1:H:85:VAL:HG23	1.96	0.66
1:G:31:LYS:HG3	1:G:32:LYS:N	2.10	0.66
1:C:176:LEU:O	1:C:181:PHE:HB2	1.95	0.66
1:C:50:ILE:HG22	1:C:118:ARG:HG2	1.77	0.66
1:G:41:LEU:HA	1:G:44:MET:HE2	1.78	0.66
1:D:17:PHE:HB2	2:D:601:FAD:H52A	1.78	0.66
1:H:17:PHE:HB2	2:H:601:FAD:H52A	1.78	0.65
1:H:255:VAL:HG23	1:H:267:ASN:HD22	1.62	0.65
1:A:148:THR:CG2	1:A:150:GLY:O	2.44	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:THR:HG22	1:D:57:GLY:N	2.12	0.65
1:F:141:LYS:HD2	1:F:215:TRP:CE3	2.31	0.65
1:B:25:ALA:O	1:B:29:LEU:HB2	1.97	0.65
1:F:172:GLN:HE22	1:F:186:PRO:HG3	1.62	0.65
1:E:17:PHE:HB2	2:E:601:FAD:C5B	2.25	0.65
1:H:173:SER:HB2	1:H:222:PHE:HE1	1.62	0.65
1:H:14:ARG:HA	1:H:19:TYR:CD1	2.31	0.64
1:A:200:ARG:NH1	2:A:601:FAD:N3A	2.45	0.64
1:F:138:ARG:HA	1:F:180:GLY:O	1.97	0.64
1:E:237:LEU:O	4:E:361:HOH:O	2.14	0.64
1:F:258:HIS:CE1	1:H:263:ILE:HD12	2.32	0.64
1:H:88:GLN:HG2	1:H:124:PHE:CE2	2.32	0.64
2:B:601:FAD:H9	2:B:601:FAD:O2'	1.97	0.64
1:F:246:GLU:HA	1:F:249:LYS:HG3	1.79	0.64
1:B:255:VAL:HA	1:B:263:ILE:HD13	1.79	0.64
1:A:48:PRO:HG3	1:B:49:ILE:HD11	1.80	0.64
1:H:18:ASN:ND2	1:H:100:GLN:HE21	1.96	0.63
1:B:250:LYS:HE2	1:B:251:PHE:CE2	2.34	0.63
1:D:17:PHE:HB2	2:D:601:FAD:C5B	2.29	0.63
1:H:148:THR:HG22	1:H:190:TYR:HA	1.81	0.62
1:D:67:TYR:O	1:D:71:SER:HB3	1.99	0.62
1:B:108:VAL:HG13	1:B:112:LEU:HB3	1.80	0.62
1:E:56:THR:HG22	1:E:57:GLY:N	2.14	0.61
1:G:116:PHE:O	1:G:120:PHE:HB2	2.00	0.61
1:F:25:ALA:HA	1:F:211:LEU:HD23	1.83	0.61
1:F:91:LEU:HD21	1:F:120:PHE:HE1	1.65	0.61
1:B:198:ASP:HA	1:B:201:ILE:HD13	1.82	0.61
1:B:151:SER:OG	1:B:154:MET:HG3	2.00	0.61
1:A:260:GLY:O	1:B:262:SER:OG	2.16	0.61
1:H:50:ILE:HG12	1:H:67:TYR:CZ	2.36	0.61
1:H:17:PHE:HB2	2:H:601:FAD:C5B	2.31	0.61
1:D:73:LEU:HD11	1:D:77:GLU:OE2	2.00	0.61
1:B:59:LEU:HB2	1:B:62:PRO:HG3	1.83	0.61
1:A:3:ARG:HH11	1:A:3:ARG:HG2	1.66	0.61
1:F:189:THR:CG2	1:F:192:ILE:HD13	2.30	0.60
1:F:154:MET:O	1:F:161:HIS:HB2	2.01	0.60
1:H:40:ASP:HB3	1:H:43:ALA:HB3	1.84	0.60
1:A:113:LYS:HZ1	1:B:105:TRP:HB2	1.65	0.60
1:C:108:VAL:HG22	1:C:112:LEU:HD23	1.83	0.60
1:F:60:LYS:HD3	1:F:60:LYS:C	2.21	0.60
1:C:58:LYS:N	1:C:58:LYS:HD3	2.15	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:TYR:CZ	1:A:124:PHE:HB2	2.37	0.60
1:H:77:GLU:HB3	1:H:79:HIS:CD2	2.37	0.59
1:H:229:ASP:O	1:H:236:PHE:HA	2.03	0.59
1:A:16:SER:HA	2:A:601:FAD:O1A	2.02	0.59
1:H:207:TRP:O	1:H:211:LEU:HG	2.01	0.59
1:A:200:ARG:NH1	2:A:601:FAD:H1B	2.17	0.59
1:E:49:ILE:HD11	1:G:48:PRO:HG2	1.83	0.59
1:A:128:TYR:HD1	3:B:547:CC2:C18	2.16	0.59
1:G:77:GLU:O	1:G:79:HIS:HD2	1.85	0.59
1:H:220:LEU:HD21	1:H:268:GLN:O	2.02	0.59
1:D:41:LEU:HA	1:D:44:MET:HE3	1.85	0.59
1:H:39:SER:HA	1:H:44:MET:HE1	1.84	0.59
1:C:25:ALA:HA	1:C:211:LEU:HD23	1.84	0.59
2:E:601:FAD:H9	2:E:601:FAD:O2'	2.03	0.58
1:H:75:TYR:CZ	1:H:124:PHE:HB2	2.38	0.58
1:G:52:ARG:HB3	1:G:59:LEU:HD21	1.84	0.58
1:A:41:LEU:HA	1:A:44:MET:HE3	1.85	0.58
1:C:147:THR:OG1	2:C:601:FAD:H5'2	2.04	0.58
1:E:241:GLU:CD	1:E:241:GLU:H	2.04	0.58
1:G:17:PHE:HB2	2:G:601:FAD:H51A	1.85	0.58
1:A:144:LEU:HD23	1:A:146:ILE:HD11	1.85	0.58
1:C:122:GLY:O	1:C:124:PHE:N	2.34	0.58
1:C:50:ILE:CG2	1:C:118:ARG:HG2	2.34	0.58
1:F:243:GLN:NE2	1:H:158:GLN:HG2	2.19	0.58
1:E:239:LYS:O	1:E:243:GLN:HG3	2.03	0.58
1:H:50:ILE:HG13	1:H:118:ARG:HG2	1.84	0.58
1:A:249:LYS:HD3	1:A:250:LYS:N	2.18	0.57
1:C:198:ASP:O	1:C:202:GLN:HG2	2.04	0.57
1:A:128:TYR:HE1	3:B:547:CC2:O1	1.86	0.57
1:C:238:MET:CE	1:C:242:VAL:HG12	2.34	0.57
1:H:32:LYS:HG3	1:H:212:GLU:HA	1.85	0.57
1:A:56:THR:HG22	1:A:57:GLY:N	2.17	0.57
1:G:47:ASN:HB3	1:G:118:ARG:HH12	1.69	0.57
1:G:81:SER:O	1:G:85:VAL:HG23	2.04	0.57
1:G:42:TYR:HB2	4:G:281:HOH:O	2.04	0.57
1:C:21:MET:HG3	1:C:207:TRP:CD1	2.39	0.57
1:F:25:ALA:HB2	1:F:207:TRP:NE1	2.19	0.57
1:H:54:ASP:OD1	4:H:290:HOH:O	2.18	0.57
1:C:17:PHE:CZ	1:C:204:LEU:HD13	2.40	0.57
2:D:601:FAD:O4'	2:D:601:FAD:O2'	2.13	0.57
1:A:22:LYS:HE3	1:A:23:GLU:OE1	2.05	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LYS:HE3	1:B:215:TRP:CE2	2.40	0.57
1:A:25:ALA:HB2	1:A:207:TRP:HE1	1.70	0.56
1:G:148:THR:CG2	1:G:190:TYR:HA	2.33	0.56
1:H:39:SER:HA	1:H:44:MET:CE	2.35	0.56
1:A:75:TYR:CE1	1:A:124:PHE:HB2	2.41	0.56
1:E:48:PRO:HG2	1:E:49:ILE:HD12	1.88	0.56
1:H:116:PHE:O	1:H:120:PHE:HB2	2.05	0.56
2:D:601:FAD:HO4'	2:D:601:FAD:HO2'	1.47	0.56
1:F:164:MET:O	1:F:164:MET:HG3	2.05	0.56
1:A:231:ASN:OD1	1:A:233:GLN:HB2	2.06	0.56
1:G:66:GLN:O	1:G:70:GLU:HB2	2.05	0.56
1:D:138:ARG:HA	1:D:180:GLY:O	2.05	0.56
1:E:138:ARG:HA	1:E:180:GLY:O	2.05	0.56
1:G:147:THR:OG1	2:G:601:FAD:H5'2	2.05	0.56
1:D:108:VAL:HG13	1:D:112:LEU:HB3	1.87	0.56
1:B:197:ALA:O	1:B:201:ILE:CD1	2.53	0.56
1:H:253:LEU:N	1:H:253:LEU:HD12	2.21	0.56
1:D:161:HIS:HE1	3:D:547:CC2:O7	1.89	0.56
1:G:214:ILE:HD12	1:G:217:GLU:OE1	2.06	0.55
1:C:186:PRO:HD2	4:C:300:HOH:O	2.06	0.55
3:E:547:CC2:O7	3:E:547:CC2:H19	2.05	0.55
1:F:141:LYS:HD2	1:F:215:TRP:CZ3	2.41	0.55
1:G:184:LEU:HD12	1:G:184:LEU:N	2.22	0.55
1:E:131:MET:HE2	1:E:178:PHE:HE1	1.72	0.55
1:E:225:SER:HB2	1:E:230:LEU:HD21	1.89	0.55
1:A:202:GLN:HB3	1:H:202:GLN:HB3	1.89	0.55
1:A:172:GLN:HE22	1:A:186:PRO:HD3	1.72	0.55
1:C:9:LEU:HD22	1:C:22:LYS:HD2	1.88	0.55
1:C:155:TYR:HB3	1:C:164:MET:HB2	1.89	0.54
1:F:173:SER:HB2	1:F:222:PHE:CE1	2.42	0.54
1:G:242:VAL:O	1:G:246:GLU:HG2	2.07	0.54
1:B:201:ILE:H	1:B:201:ILE:HD12	1.73	0.54
1:F:48:PRO:HG3	1:H:49:ILE:HD11	1.90	0.54
1:A:241:GLU:O	1:A:245:GLU:HG3	2.07	0.54
1:A:148:THR:HG21	1:A:150:GLY:O	2.07	0.54
1:A:140:LYS:HB2	1:A:181:PHE:CE1	2.42	0.54
1:D:195:THR:O	1:D:200:ARG:HD3	2.07	0.54
1:D:248:ASN:HB2	4:D:339:HOH:O	2.08	0.54
1:H:81:SER:HB3	1:H:83:ASP:OD1	2.08	0.54
1:A:195:THR:HG22	1:A:199:ALA:HB3	1.90	0.54
1:E:237:LEU:HD22	1:G:158:GLN:HB2	1.90	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LYS:HZ2	1:B:105:TRP:HB2	1.69	0.54
1:H:215:TRP:O	1:H:215:TRP:CD1	2.61	0.54
1:G:252:GLY:HA3	1:G:258:HIS:HA	1.90	0.54
1:A:229:ASP:O	1:A:236:PHE:HA	2.08	0.54
1:F:249:LYS:NZ	4:F:280:HOH:O	2.41	0.53
1:F:91:LEU:HD21	1:F:120:PHE:CE1	2.43	0.53
1:C:161:HIS:HD2	1:D:132:TYR:OH	1.90	0.53
1:B:11:HIS:NE2	2:B:601:FAD:O2P	2.41	0.53
1:C:164:MET:SD	1:C:167:ILE:HD12	2.49	0.53
1:C:14:ARG:HG3	1:C:14:ARG:NH1	2.03	0.53
1:E:155:TYR:HB3	1:E:164:MET:HB2	1.90	0.53
1:A:160:ILE:O	1:A:160:ILE:HG13	2.07	0.53
1:A:59:LEU:HB2	1:A:62:PRO:HG3	1.90	0.53
2:H:601:FAD:H9	2:H:601:FAD:O2'	2.09	0.53
1:B:201:ILE:HD12	1:B:201:ILE:N	2.23	0.53
1:B:197:ALA:HA	1:B:200:ARG:CZ	2.38	0.53
1:D:12:SER:HB3	1:D:42:TYR:CE1	2.44	0.53
1:D:148:THR:HG23	2:D:601:FAD:O2	2.09	0.53
1:F:59:LEU:HD13	1:F:65:PHE:CD1	2.44	0.53
1:E:238:MET:CA	4:E:361:HOH:O	2.31	0.52
1:B:75:TYR:HA	1:B:80:LEU:HD22	1.90	0.52
1:B:194:HIS:CE1	3:B:547:CC2:C21	2.82	0.52
1:F:132:TYR:CD1	1:F:178:PHE:HA	2.44	0.52
1:G:172:GLN:HE22	1:G:186:PRO:HG3	1.73	0.52
1:G:83:ASP:O	1:G:87:GLU:HG2	2.08	0.52
1:B:58:LYS:H	1:B:58:LYS:HD2	1.74	0.52
1:H:68:PRO:O	1:H:72:VAL:HG23	2.08	0.52
1:G:31:LYS:HG3	1:G:32:LYS:H	1.73	0.52
1:H:169:TRP:CZ2	1:H:256:GLY:HA3	2.44	0.52
1:A:26:ALA:O	1:A:30:LYS:HG3	2.09	0.52
1:G:196:PRO:O	1:G:199:ALA:HB3	2.10	0.52
1:B:65:PHE:CE1	1:B:70:GLU:HG2	2.45	0.52
1:G:161:HIS:HE1	3:G:547:CC2:O7	1.92	0.52
1:A:39:SER:HB3	1:A:44:MET:HE1	1.92	0.52
1:F:40:ASP:O	1:F:44:MET:HG3	2.09	0.52
1:F:169:TRP:HB3	1:F:170:PRO:HD3	1.92	0.52
1:G:75:TYR:CZ	1:G:124:PHE:HB2	2.45	0.52
1:C:196:PRO:O	1:C:199:ALA:HB3	2.10	0.52
1:B:131:MET:HE2	1:B:178:PHE:HE1	1.75	0.52
1:G:151:SER:OG	1:G:154:MET:HG3	2.10	0.52
1:B:197:ALA:O	1:B:201:ILE:HD12	2.09	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:LYS:HD3	1:D:73:LEU:CD2	2.40	0.51
1:H:83:ASP:O	1:H:87:GLU:HG2	2.10	0.51
1:A:41:LEU:HD23	1:A:44:MET:CE	2.40	0.51
1:F:147:THR:OG1	2:F:601:FAD:H5'2	2.11	0.51
1:H:77:GLU:HB3	1:H:79:HIS:NE2	2.25	0.51
1:G:199:ALA:O	1:G:203:ILE:HG13	2.10	0.51
1:B:148:THR:HG23	1:B:191:SER:H	1.75	0.51
1:C:164:MET:SD	1:C:167:ILE:CD1	2.98	0.51
1:E:198:ASP:O	1:E:202:GLN:HG2	2.11	0.51
1:E:59:LEU:HD13	1:E:65:PHE:CD1	2.45	0.51
1:A:40:ASP:N	1:A:44:MET:HE2	2.26	0.51
1:C:238:MET:HE2	1:C:242:VAL:HG12	1.93	0.51
1:D:141:LYS:HG3	1:D:215:TRP:CZ3	2.45	0.51
1:G:141:LYS:HB3	1:G:184:LEU:HD11	1.93	0.51
1:G:169:TRP:CZ2	1:G:256:GLY:HA3	2.45	0.51
1:D:238:MET:HE2	1:D:242:VAL:HG12	1.91	0.51
1:H:65:PHE:HE1	1:H:70:GLU:HG2	1.72	0.51
1:D:229:ASP:O	1:D:236:PHE:HA	2.11	0.51
1:E:89:LYS:O	1:E:92:GLU:HB2	2.10	0.51
1:H:66:GLN:HG3	1:H:68:PRO:HD2	1.92	0.50
1:F:32:LYS:HE3	1:F:212:GLU:HB3	1.93	0.50
1:B:26:ALA:O	1:B:30:LYS:HG3	2.10	0.50
1:D:176:LEU:O	1:D:181:PHE:HB2	2.11	0.50
1:F:50:ILE:CG2	1:F:118:ARG:HG2	2.41	0.50
1:F:50:ILE:HG22	1:F:118:ARG:HG2	1.94	0.50
1:A:211:LEU:O	1:A:214:ILE:HG22	2.11	0.50
1:E:81:SER:O	1:E:85:VAL:HG23	2.11	0.50
1:G:204:LEU:O	1:G:208:LYS:HG2	2.12	0.50
1:F:169:TRP:CD1	1:H:166:VAL:HG11	2.46	0.50
1:H:108:VAL:HG12	1:H:109:PRO:O	2.11	0.50
1:F:246:GLU:CD	1:F:253:LEU:HD11	2.32	0.50
1:D:25:ALA:O	1:D:29:LEU:HD23	2.11	0.50
1:F:259:LEU:HB2	1:F:261:LYS:HE2	1.93	0.50
1:H:95:ASP:HB3	1:H:215:TRP:CZ3	2.47	0.50
1:E:195:THR:O	1:E:200:ARG:HD3	2.11	0.50
1:A:161:HIS:HE1	3:A:547:CC2:O7	1.95	0.50
1:H:9:LEU:HD22	1:H:22:LYS:HD3	1.92	0.49
2:E:601:FAD:H3B	2:E:601:FAD:O1A	2.12	0.49
1:H:253:LEU:H	1:H:253:LEU:HD12	1.77	0.49
1:F:251:PHE:CD1	1:F:262:SER:HB2	2.47	0.49
1:A:148:THR:HG22	1:A:150:GLY:O	2.10	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:LEU:HD21	1:D:176:LEU:HD11	1.94	0.49
1:D:137:PHE:CD2	1:D:179:CYS:HB3	2.47	0.49
1:A:254:SER:HB2	1:A:257:HIS:HB2	1.94	0.49
1:A:164:MET:HE3	1:A:167:ILE:CB	2.38	0.49
1:G:40:ASP:O	1:G:44:MET:HG3	2.12	0.49
1:E:49:ILE:HD11	1:G:48:PRO:CG	2.42	0.49
3:B:547:CC2:C8	3:B:547:CC2:H19	2.42	0.49
1:A:257:HIS:HE1	1:B:159:GLY:O	1.95	0.49
1:B:195:THR:HG22	1:B:199:ALA:HB3	1.94	0.49
1:E:29:LEU:HD12	1:E:34:TRP:CD1	2.48	0.49
1:A:39:SER:C	1:A:44:MET:HE2	2.33	0.49
1:B:131:MET:HE2	1:B:178:PHE:CE1	2.48	0.49
1:H:95:ASP:HB3	1:H:215:TRP:CH2	2.48	0.49
1:E:48:PRO:HG2	1:E:49:ILE:CD1	2.43	0.49
1:C:29:LEU:O	1:C:34:TRP:HB2	2.13	0.49
1:H:127:THR:HG22	1:H:130:ALA:N	2.21	0.48
2:H:601:FAD:C4	3:H:547:CC2:C2	2.91	0.48
1:D:29:LEU:HD21	1:D:211:LEU:HG	1.95	0.48
1:A:67:TYR:N	1:A:68:PRO:CD	2.76	0.48
1:H:134:LYS:HE2	1:H:225:SER:OG	2.14	0.48
1:C:167:ILE:C	1:C:167:ILE:HD13	2.33	0.48
1:H:151:SER:OG	1:H:154:MET:HG3	2.14	0.48
1:F:255:VAL:HG22	1:F:263:ILE:HG21	1.95	0.48
1:C:122:GLY:C	1:C:124:PHE:H	2.15	0.48
1:C:122:GLY:HA2	1:C:126:TYR:CE2	2.48	0.48
1:F:173:SER:HB2	1:F:222:PHE:HE1	1.78	0.48
1:D:238:MET:CE	1:D:242:VAL:HG12	2.43	0.48
1:C:91:LEU:HD21	1:C:115:TRP:CH2	2.49	0.48
3:C:547:CC2:H19	3:C:547:CC2:C8	2.43	0.48
1:C:60:LYS:O	1:C:60:LYS:HG3	2.14	0.48
1:H:122:GLY:O	1:H:123:GLU:HB3	2.13	0.48
1:F:189:THR:HG21	1:F:192:ILE:HD13	1.95	0.48
1:C:241:GLU:HG2	1:C:242:VAL:H	1.78	0.48
1:B:246:GLU:O	1:B:261:LYS:NZ	2.46	0.48
1:D:158:GLN:NE2	4:D:344:HOH:O	2.47	0.48
1:A:3:ARG:NH1	1:A:3:ARG:HG2	2.29	0.48
1:A:249:LYS:HD3	1:A:250:LYS:H	1.78	0.48
1:B:76:LYS:HE3	1:B:123:GLU:OE1	2.14	0.47
1:G:184:LEU:CD1	1:G:184:LEU:N	2.76	0.47
1:E:59:LEU:HD13	1:E:65:PHE:HD1	1.80	0.47
1:F:56:THR:CG2	1:F:57:GLY:N	2.77	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ARG:HA	1:C:180:GLY:O	2.14	0.47
1:B:23:GLU:HA	1:B:23:GLU:OE1	2.14	0.47
1:C:263:ILE:HD12	1:D:258:HIS:CE1	2.50	0.47
1:A:238:MET:HE3	1:A:243:GLN:HG2	1.95	0.47
1:E:131:MET:CE	1:E:178:PHE:HE1	2.26	0.47
1:A:169:TRP:CZ2	1:A:256:GLY:HA3	2.49	0.47
1:D:71:SER:OG	1:D:121:ILE:HD12	2.14	0.47
1:F:194:HIS:CE1	1:H:232:PHE:CZ	3.02	0.47
1:H:197:ALA:HA	1:H:200:ARG:NH1	2.30	0.47
1:B:194:HIS:HE1	3:B:547:CC2:H21	1.67	0.47
1:C:147:THR:HG1	2:C:601:FAD:H5'2	1.79	0.47
1:A:200:ARG:NH1	2:A:601:FAD:C1B	2.78	0.47
1:C:164:MET:SD	1:C:168:LEU:CD1	3.03	0.47
1:C:214:ILE:O	1:C:217:GLU:HG3	2.14	0.47
1:D:255:VAL:HG23	1:D:267:ASN:HD22	1.79	0.47
1:H:214:ILE:HG23	1:H:215:TRP:N	2.29	0.47
1:F:40:ASP:HB3	1:F:43:ALA:HB3	1.97	0.47
1:H:56:THR:HG22	1:H:57:GLY:N	2.29	0.47
1:C:14:ARG:NH1	1:C:14:ARG:CG	2.69	0.47
1:E:132:TYR:OH	1:G:161:HIS:CD2	2.60	0.47
1:F:185:GLU:HG2	1:F:269:ILE:O	2.15	0.47
1:B:141:LYS:HE3	1:B:215:TRP:CZ2	2.50	0.47
1:E:91:LEU:HD21	1:E:120:PHE:CE1	2.50	0.47
1:A:132:TYR:OH	1:B:161:HIS:HD2	1.98	0.47
1:C:141:LYS:HD2	1:C:215:TRP:CE3	2.50	0.47
1:E:120:PHE:HA	1:E:125:ALA:HB2	1.97	0.47
1:C:153:SER:OG	1:D:235:GLY:O	2.33	0.47
1:D:60:LYS:HD3	1:D:73:LEU:HD21	1.96	0.46
1:E:59:LEU:HB2	1:E:62:PRO:HG3	1.97	0.46
1:B:258:HIS:CD2	1:B:260:GLY:H	2.33	0.46
3:C:547:CC2:H19	3:C:547:CC2:O7	2.15	0.46
1:G:121:ILE:HG22	1:G:122:GLY:N	2.31	0.46
1:H:189:THR:CG2	1:H:192:ILE:HD13	2.45	0.46
1:G:61:ASP:OD2	1:G:64:ASN:HB3	2.15	0.46
1:A:128:TYR:HD1	3:B:547:CC2:C19	2.28	0.46
1:F:22:LYS:HD2	1:F:22:LYS:C	2.35	0.46
1:D:24:ALA:HB2	1:D:204:LEU:HD12	1.97	0.46
1:D:155:TYR:HB3	1:D:164:MET:HB2	1.96	0.46
1:A:73:LEU:HD11	1:A:77:GLU:OE2	2.15	0.46
1:H:6:LEU:HD13	1:H:90:LYS:HB3	1.95	0.46
1:F:169:TRP:CD1	1:H:166:VAL:CG1	2.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ALA:O	1:E:90:LYS:HG3	2.15	0.46
1:G:266:ASP:HB3	1:G:270:LYS:HB2	1.97	0.46
1:C:30:LYS:HE3	1:C:36:VAL:HB	1.97	0.46
1:G:91:LEU:HD21	1:G:120:PHE:HE1	1.81	0.46
1:G:172:GLN:NE2	4:G:291:HOH:O	2.48	0.46
3:G:547:CC2:C8	3:G:547:CC2:H19	2.45	0.46
1:F:212:GLU:HB2	1:F:213:ASN:ND2	2.30	0.46
1:G:202:GLN:HA	1:G:202:GLN:NE2	2.30	0.46
1:D:137:PHE:HB2	1:D:179:CYS:O	2.16	0.46
1:C:73:LEU:HD11	1:C:77:GLU:CD	2.36	0.46
1:H:106:PHE:HD1	1:H:167:ILE:HD13	1.80	0.46
4:A:311:HOH:O	1:B:222:PHE:HB3	2.15	0.46
1:H:148:THR:HG23	1:H:150:GLY:O	2.16	0.45
1:D:30:LYS:HE3	1:D:30:LYS:HB3	1.50	0.45
1:C:111:ILE:HD12	1:D:49:ILE:HD13	1.99	0.45
1:B:59:LEU:HD12	1:B:62:PRO:HB3	1.97	0.45
1:A:32:LYS:HD3	1:A:32:LYS:HA	1.78	0.45
1:E:81:SER:HA	1:E:82:PRO:HD3	1.86	0.45
1:F:88:GLN:HG2	1:F:124:PHE:CE2	2.52	0.45
1:G:115:TRP:O	1:G:119:VAL:HB	2.17	0.45
1:F:163:ASP:OD2	1:F:165:ASN:HB2	2.16	0.45
1:G:31:LYS:CG	1:G:32:LYS:N	2.78	0.45
1:F:48:PRO:HD2	1:F:49:ILE:HG13	1.98	0.45
1:G:169:TRP:HB3	1:G:170:PRO:HD3	1.99	0.45
1:A:130:ALA:HB1	1:A:134:LYS:O	2.16	0.45
1:A:96:LEU:HD12	1:A:97:VAL:N	2.32	0.45
1:C:67:TYR:N	1:C:68:PRO:CD	2.79	0.45
1:D:108:VAL:HG13	1:D:112:LEU:HD23	1.98	0.45
1:D:218:THR:HA	1:D:219:PRO:HD3	1.77	0.45
1:E:56:THR:O	1:E:57:GLY:C	2.54	0.45
1:B:66:GLN:O	1:B:70:GLU:HB2	2.16	0.45
1:F:191:SER:HB2	1:F:194:HIS:HB2	1.97	0.45
1:C:214:ILE:HD12	1:C:217:GLU:OE2	2.17	0.45
1:E:158:GLN:HG2	1:G:243:GLN:NE2	2.31	0.45
1:C:37:VAL:HG12	1:C:38:GLU:N	2.30	0.45
1:H:77:GLU:CB	1:H:79:HIS:CD2	2.99	0.45
1:F:165:ASN:HD21	1:F:266:ASP:HA	1.82	0.45
1:C:257:HIS:HD2	4:C:324:HOH:O	1.99	0.45
1:H:42:TYR:HB2	4:H:276:HOH:O	2.16	0.45
1:E:169:TRP:CE2	1:E:256:GLY:HA3	2.51	0.45
1:G:255:VAL:O	1:G:258:HIS:HD2	2.00	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:VAL:CG1	1:D:112:LEU:HB3	2.47	0.45
1:G:155:TYR:HB3	1:G:164:MET:HB2	1.99	0.45
1:A:12:SER:HB3	1:A:42:TYR:CE1	2.52	0.45
1:C:49:ILE:HD11	1:D:48:PRO:HG3	1.98	0.45
1:H:70:GLU:OE2	1:H:70:GLU:HA	2.15	0.45
1:C:224:PRO:HD2	1:C:227:LEU:CD2	2.39	0.45
1:C:172:GLN:HG2	1:C:183:VAL:CG1	2.46	0.45
1:E:164:MET:HG3	1:E:164:MET:O	2.17	0.45
1:B:65:PHE:HE1	1:B:70:GLU:HG2	1.81	0.45
1:D:163:ASP:OD2	1:D:165:ASN:HB2	2.16	0.45
1:H:121:ILE:HG22	1:H:122:GLY:N	2.32	0.45
1:H:163:ASP:OD2	1:H:165:ASN:HB2	2.17	0.45
1:H:101:PHE:CZ	1:H:146:ILE:HG12	2.52	0.45
2:C:601:FAD:H2B	2:C:601:FAD:H8A	1.78	0.44
1:F:255:VAL:H	1:F:267:ASN:ND2	2.16	0.44
1:E:25:ALA:O	1:E:29:LEU:HD22	2.17	0.44
1:E:5:ALA:HA	1:E:96:LEU:O	2.17	0.44
1:E:68:PRO:O	1:E:72:VAL:HG23	2.17	0.44
1:C:246:GLU:O	1:C:261:LYS:NZ	2.50	0.44
1:E:127:THR:HG22	1:E:129:ALA:H	1.83	0.44
1:F:150:GLY:HA2	1:F:154:MET:HE1	1.97	0.44
1:F:132:TYR:OH	1:H:161:HIS:CD2	2.58	0.44
2:H:601:FAD:O4	3:H:547:CC2:H11B	2.17	0.44
1:D:71:SER:OG	1:D:121:ILE:HG23	2.17	0.44
1:B:174:GLY:O	1:B:178:PHE:HB2	2.18	0.44
1:G:6:LEU:HD13	1:G:90:LYS:HB3	1.99	0.44
1:E:105:TRP:HB3	1:G:175:ILE:HG12	2.00	0.44
1:B:186:PRO:HB2	1:B:188:LEU:HD21	1.99	0.44
1:D:32:LYS:HD2	1:D:32:LYS:HA	1.82	0.44
1:C:214:ILE:HG23	1:C:215:TRP:N	2.33	0.44
1:B:244:ASP:HA	1:B:247:LYS:HD3	2.00	0.44
3:F:547:CC2:H19	3:F:547:CC2:O7	2.17	0.44
1:F:192:ILE:HA	1:F:192:ILE:HD12	1.87	0.44
1:F:255:VAL:HG23	1:F:267:ASN:HB3	2.00	0.44
1:F:98:ILE:HG12	1:F:143:VAL:CG1	2.48	0.44
1:D:17:PHE:HB2	2:D:601:FAD:H51A	2.00	0.44
1:H:51:SER:O	1:H:54:ASP:HB2	2.17	0.44
1:H:115:TRP:O	1:H:119:VAL:HB	2.18	0.44
1:C:202:GLN:HB3	1:E:202:GLN:HB3	2.00	0.44
1:A:120:PHE:HB3	1:B:105:TRP:CZ2	2.52	0.43
1:C:167:ILE:HD13	1:C:168:LEU:N	2.33	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:157:LEU:O	1:H:259:LEU:HD23	2.18	0.43
1:A:227:LEU:HB3	1:A:242:VAL:HG11	2.00	0.43
1:F:161:HIS:HE1	3:F:547:CC2:O7	2.02	0.43
1:B:194:HIS:HE1	3:B:547:CC2:C21	2.28	0.43
1:F:172:GLN:NE2	4:F:297:HOH:O	2.42	0.43
1:B:58:LYS:N	1:B:58:LYS:HD2	2.32	0.43
1:F:56:THR:HB	1:F:79:HIS:O	2.17	0.43
1:C:257:HIS:HE1	1:D:159:GLY:O	2.01	0.43
1:G:104:GLN:OE1	1:G:109:PRO:HB3	2.18	0.43
1:A:48:PRO:CG	1:B:49:ILE:HD11	2.48	0.43
1:C:75:TYR:CZ	1:C:124:PHE:HB2	2.53	0.43
1:D:12:SER:HB3	1:D:42:TYR:CD1	2.53	0.43
1:B:7:ILE:CG2	1:B:22:LYS:HG2	2.42	0.43
1:H:161:HIS:HE1	3:H:547:CC2:O7	2.02	0.43
1:F:194:HIS:CE1	1:H:232:PHE:HZ	2.36	0.43
1:G:160:ILE:HG13	1:G:160:ILE:O	2.19	0.43
1:H:104:GLN:HA	2:H:601:FAD:C5X	2.49	0.43
1:C:218:THR:HA	1:C:219:PRO:HD3	1.87	0.43
3:E:547:CC2:C8	3:E:547:CC2:H19	2.49	0.43
1:H:72:VAL:HG22	1:H:122:GLY:HA3	2.00	0.43
1:E:262:SER:HA	1:G:261:LYS:O	2.19	0.43
1:H:66:GLN:O	1:H:70:GLU:HB2	2.18	0.43
1:F:196:PRO:O	1:F:199:ALA:HB3	2.19	0.43
1:H:195:THR:O	1:H:196:PRO:C	2.57	0.43
1:C:47:ASN:HA	1:C:48:PRO:HD3	1.89	0.43
1:G:227:LEU:HD23	1:G:242:VAL:HG11	2.01	0.43
1:B:214:ILE:HG23	1:B:215:TRP:N	2.33	0.43
1:H:241:GLU:HG3	1:H:241:GLU:H	1.56	0.43
1:B:147:THR:HG1	2:B:601:FAD:C5'	2.27	0.42
1:A:11:HIS:CE1	1:A:16:SER:HB3	2.54	0.42
1:A:108:VAL:O	1:B:113:LYS:NZ	2.51	0.42
1:A:164:MET:HE1	1:A:168:LEU:HD13	1.97	0.42
1:A:11:HIS:CD2	1:A:18:ASN:HB2	2.54	0.42
1:E:169:TRP:CD1	1:G:166:VAL:HG11	2.54	0.42
1:H:18:ASN:HD22	1:H:100:GLN:HE21	1.66	0.42
1:C:28:ALA:HB2	1:C:208:LYS:HB3	2.01	0.42
1:G:149:GLY:O	1:G:191:SER:HA	2.19	0.42
1:B:126:TYR:HA	1:B:136:PRO:HD2	2.01	0.42
1:C:72:VAL:O	1:C:75:TYR:HB3	2.19	0.42
1:B:155:TYR:HB3	1:B:164:MET:HB2	2.01	0.42
1:A:22:LYS:NZ	1:A:38:GLU:OE2	2.52	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:GLU:HA	1:F:186:PRO:HD3	1.85	0.42
1:B:250:LYS:HE2	1:B:251:PHE:CZ	2.55	0.42
1:D:67:TYR:O	1:D:71:SER:CB	2.67	0.42
1:G:85:VAL:O	1:G:89:LYS:HG3	2.19	0.42
1:C:21:MET:HG2	1:C:100:GLN:OE1	2.19	0.42
1:F:5:ALA:HB2	1:F:34:TRP:CE3	2.54	0.42
1:G:29:LEU:HB3	1:G:34:TRP:HB2	2.02	0.42
1:H:35:GLU:HG2	1:H:36:VAL:N	2.34	0.42
1:H:104:GLN:HA	2:H:601:FAD:N5	2.35	0.42
1:H:18:ASN:HD22	1:H:100:GLN:HG3	1.84	0.42
3:D:547:CC2:C8	3:D:547:CC2:H19	2.45	0.42
1:D:132:TYR:CD1	1:D:178:PHE:HA	2.54	0.42
1:C:91:LEU:HA	1:C:91:LEU:HD13	1.76	0.42
1:C:182:GLN:HE21	1:C:219:PRO:HG2	1.85	0.42
1:H:195:THR:HG22	1:H:199:ALA:HB3	2.02	0.42
1:H:25:ALA:O	1:H:29:LEU:HD22	2.19	0.42
1:E:118:ARG:O	1:E:121:ILE:HD11	2.19	0.42
1:F:127:THR:HG22	1:F:129:ALA:H	1.85	0.42
1:G:229:ASP:OD1	1:G:239:LYS:HG2	2.20	0.42
1:E:75:TYR:CE1	1:E:124:PHE:HB2	2.53	0.42
1:E:65:PHE:CE1	1:E:70:GLU:HG3	2.55	0.42
1:E:91:LEU:HD21	1:E:120:PHE:HE1	1.85	0.42
1:F:195:THR:HA	1:F:196:PRO:HD3	1.78	0.42
1:D:270:LYS:HD3	1:D:270:LYS:HA	1.83	0.42
1:B:11:HIS:CE1	1:B:16:SER:HB3	2.54	0.42
1:F:172:GLN:HA	1:F:176:LEU:HD12	2.02	0.42
1:D:132:TYR:O	1:D:134:LYS:N	2.52	0.42
1:D:25:ALA:O	1:D:29:LEU:CD2	2.68	0.42
1:A:96:LEU:HD12	1:A:97:VAL:H	1.85	0.42
3:F:547:CC2:H13	3:F:547:CC2:H20	1.67	0.42
1:A:116:PHE:O	1:A:120:PHE:HB2	2.19	0.42
1:B:141:LYS:HE3	1:B:215:TRP:CD2	2.55	0.42
1:A:235:GLY:O	1:A:236:PHE:HB2	2.20	0.42
1:E:200:ARG:O	1:E:204:LEU:HD22	2.19	0.42
1:H:122:GLY:O	1:H:123:GLU:CB	2.68	0.42
1:C:47:ASN:O	1:C:118:ARG:HD3	2.19	0.42
1:B:255:VAL:H	1:B:267:ASN:ND2	2.17	0.42
1:A:254:SER:HB2	1:A:257:HIS:H	1.85	0.42
3:E:547:CC2:H20	3:E:547:CC2:H13	1.75	0.42
1:G:227:LEU:HG	1:G:242:VAL:HG21	2.02	0.41
1:G:88:GLN:HG2	1:G:124:PHE:CE2	2.54	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:220:LEU:HD21	1:F:268:GLN:O	2.20	0.41
1:D:100:GLN:O	1:D:101:PHE:HB3	2.19	0.41
1:D:224:PRO:HD2	1:D:227:LEU:HD22	2.02	0.41
1:H:48:PRO:O	1:H:114:GLY:HA3	2.20	0.41
1:D:37:VAL:HG21	4:D:338:HOH:O	2.19	0.41
1:G:207:TRP:O	1:G:211:LEU:HG	2.20	0.41
1:F:161:HIS:HD2	1:H:132:TYR:OH	2.01	0.41
1:H:255:VAL:H	1:H:267:ASN:ND2	2.18	0.41
1:A:220:LEU:HD12	1:A:220:LEU:HA	1.87	0.41
1:G:132:TYR:O	1:G:180:GLY:HA2	2.19	0.41
1:D:25:ALA:HB2	1:D:207:TRP:HE1	1.86	0.41
1:E:125:ALA:O	1:E:179:CYS:HB3	2.20	0.41
1:F:30:LYS:NZ	1:F:36:VAL:HB	2.35	0.41
1:B:28:ALA:HB2	1:B:208:LYS:HE3	2.03	0.41
1:G:60:LYS:HD2	1:G:73:LEU:HD22	2.01	0.41
1:B:102:PRO:HB3	2:B:601:FAD:H5'1	2.02	0.41
1:E:88:GLN:HG2	1:E:124:PHE:CE2	2.55	0.41
1:C:199:ALA:O	1:C:202:GLN:HB2	2.20	0.41
1:D:108:VAL:HA	1:D:109:PRO:HD3	1.96	0.41
1:E:122:GLY:O	1:E:123:GLU:CB	2.69	0.41
1:F:81:SER:HA	1:F:82:PRO:HD2	1.77	0.41
1:E:131:MET:CE	1:E:178:PHE:CE1	3.03	0.41
1:F:47:ASN:HB3	1:F:118:ARG:NH1	2.36	0.41
1:D:29:LEU:CD2	1:D:211:LEU:HG	2.51	0.41
1:H:189:THR:HG21	1:H:192:ILE:HD13	2.01	0.41
1:D:241:GLU:O	1:D:245:GLU:HG3	2.21	0.41
1:F:130:ALA:HB1	1:F:134:LYS:HB2	2.01	0.41
1:B:17:PHE:CZ	1:B:204:LEU:HD13	2.56	0.41
1:A:132:TYR:CD1	1:A:178:PHE:HA	2.55	0.41
1:C:149:GLY:N	2:C:601:FAD:H2'	2.34	0.41
1:F:28:ALA:HB2	1:F:208:LYS:HE3	2.01	0.41
1:D:148:THR:CG2	1:D:149:GLY:N	2.83	0.41
1:A:41:LEU:HD23	1:A:44:MET:HE1	2.01	0.41
1:F:267:ASN:ND2	1:F:268:GLN:HE21	2.19	0.41
3:C:547:CC2:H20	3:C:547:CC2:H13	1.78	0.41
1:F:238:MET:HB3	1:F:238:MET:HE3	1.82	0.41
1:A:164:MET:CE	1:A:164:MET:O	2.69	0.41
1:E:132:TYR:CD1	1:E:178:PHE:HA	2.56	0.41
1:D:163:ASP:CG	1:D:165:ASN:HB2	2.41	0.41
1:A:218:THR:HA	1:A:219:PRO:HD3	1.79	0.41
1:B:47:ASN:HA	1:B:48:PRO:HD3	1.58	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LYS:O	1:A:58:LYS:HE2	2.19	0.41
1:D:189:THR:CG2	1:D:192:ILE:HD13	2.51	0.41
1:H:211:LEU:HA	1:H:214:ILE:HB	2.01	0.41
1:B:96:LEU:HA	1:B:141:LYS:O	2.21	0.41
1:B:204:LEU:HD12	1:B:204:LEU:HA	1.79	0.41
1:A:164:MET:HG3	1:A:164:MET:O	2.20	0.41
1:A:102:PRO:HB3	2:A:601:FAD:H5'1	2.02	0.41
1:H:148:THR:HG21	1:H:190:TYR:HD1	1.86	0.41
1:F:164:MET:O	1:F:164:MET:CG	2.69	0.41
1:B:186:PRO:HB2	1:B:188:LEU:CD2	2.51	0.41
1:E:50:ILE:HG22	1:E:118:ARG:HG2	2.02	0.41
1:F:11:HIS:CD2	1:F:102:PRO:HG3	2.56	0.41
1:D:249:LYS:NZ	4:D:309:HOH:O	2.54	0.41
1:C:200:ARG:HA	1:C:203:ILE:HD12	2.02	0.41
1:H:97:VAL:HG12	1:H:99:PHE:CE2	2.56	0.41
1:F:17:PHE:H	2:F:601:FAD:C5B	2.34	0.41
2:B:601:FAD:H8A	2:B:601:FAD:H2B	1.91	0.41
1:E:58:LYS:H	1:E:58:LYS:CD	2.28	0.41
1:H:214:ILE:O	1:H:217:GLU:HG3	2.20	0.41
1:C:187:GLN:HG2	1:C:207:TRP:CE3	2.56	0.41
3:C:547:CC2:C17	1:D:128:TYR:HB3	2.51	0.41
1:G:46:PHE:CE2	1:G:47:ASN:O	2.74	0.40
2:H:601:FAD:H2B	2:H:601:FAD:H8A	1.96	0.40
1:F:47:ASN:HA	1:F:48:PRO:HD3	1.81	0.40
1:D:29:LEU:HD12	1:D:34:TRP:CG	2.57	0.40
1:A:238:MET:HB3	1:A:243:GLN:CG	2.51	0.40
1:E:44:MET:HE1	1:E:90:LYS:NZ	2.36	0.40
1:E:121:ILE:HG22	1:E:122:GLY:N	2.36	0.40
1:G:76:LYS:C	1:G:78:GLY:H	2.24	0.40
1:E:238:MET:HB3	1:E:243:GLN:HG2	2.03	0.40
1:A:155:TYR:HB3	1:A:164:MET:HB2	2.03	0.40
1:C:108:VAL:HG13	1:C:112:LEU:HB3	2.03	0.40
1:C:195:THR:HA	1:C:196:PRO:HD3	1.87	0.40
1:F:22:LYS:HG3	1:F:23:GLU:N	2.36	0.40
1:A:52:ARG:H	1:A:52:ARG:HG2	1.58	0.40
1:H:223:ALA:HA	1:H:224:PRO:HD3	1.88	0.40
1:E:189:THR:HG22	1:E:192:ILE:HG12	2.03	0.40
1:F:238:MET:HE3	1:F:242:VAL:HG12	2.03	0.40
1:H:59:LEU:O	1:H:62:PRO:HD3	2.21	0.40
1:A:91:LEU:HA	1:A:91:LEU:HD12	1.75	0.40
1:B:60:LYS:NZ	1:F:240:LYS:HE3	2.36	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:VAL:H	1:G:267:ASN:ND2	2.18	0.40
1:H:202:GLN:O	1:H:205:GLU:HB2	2.22	0.40
1:G:108:VAL:HG13	1:G:112:LEU:HB3	2.04	0.40
1:G:229:ASP:O	1:G:236:PHE:HA	2.22	0.40
1:C:81:SER:HA	1:C:82:PRO:HD3	1.94	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	268/273 (98%)	247 (92%)	20 (8%)	1 (0%)	39	49
1	B	268/273 (98%)	242 (90%)	25 (9%)	1 (0%)	39	49
1	C	268/273 (98%)	246 (92%)	22 (8%)	0	100	100
1	D	268/273 (98%)	249 (93%)	19 (7%)	0	100	100
1	E	268/273 (98%)	243 (91%)	23 (9%)	2 (1%)	26	32
1	F	268/273 (98%)	249 (93%)	18 (7%)	1 (0%)	39	49
1	G	268/273 (98%)	240 (90%)	28 (10%)	0	100	100
1	H	268/273 (98%)	246 (92%)	22 (8%)	0	100	100
All	All	2144/2184 (98%)	1962 (92%)	177 (8%)	5 (0%)	52	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
1	E	56	THR
1	E	57	GLY
1	B	57	GLY
1	F	197	ALA

### 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	224/227 (99%)	205 (92%)	19 (8%)	13	16
1	B	224/227 (99%)	216 (96%)	8 (4%)	42	58
1	C	224/227 (99%)	207 (92%)	17 (8%)	16	21
1	D	224/227 (99%)	212 (95%)	12 (5%)	27	38
1	E	224/227 (99%)	213 (95%)	11 (5%)	31	43
1	F	224/227 (99%)	206 (92%)	18 (8%)	15	19
1	G	224/227 (99%)	211 (94%)	13 (6%)	25	34
1	H	224/227 (99%)	210 (94%)	14 (6%)	22	30
All	All	1792/1816 (99%)	1680 (94%)	112 (6%)	22	30

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	22	LYS
1	A	29	LEU
1	A	56	THR
1	A	58	LYS
1	A	83	ASP
1	A	91	LEU
1	A	123	GLU
1	A	127	THR
1	A	139	SER
1	A	148	THR
1	A	168	LEU
1	A	195	THR
1	A	211	LEU
1	A	218	THR
1	A	220	LEU
1	A	237	LEU
1	A	249	LYS
1	A	259	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	58	LYS
1	B	80	LEU
1	B	112	LEU
1	B	158	GLN
1	B	198	ASP
1	B	227	LEU
1	B	253	LEU
1	B	267	ASN
1	C	14	ARG
1	C	15	THR
1	C	29	LEU
1	C	41	LEU
1	C	44	MET
1	C	52	ARG
1	C	58	LYS
1	C	91	LEU
1	C	123	GLU
1	C	144	LEU
1	C	167	ILE
1	C	168	LEU
1	C	184	LEU
1	C	204	LEU
1	C	211	LEU
1	C	218	THR
1	C	227	LEU
1	D	22	LYS
1	D	29	LEU
1	D	30	LYS
1	D	32	LYS
1	D	56	THR
1	D	58	LYS
1	D	91	LEU
1	D	166	VAL
1	D	168	LEU
1	D	191	SER
1	D	204	LEU
1	D	211	LEU
1	E	29	LEU
1	E	58	LYS
1	E	123	GLU
1	E	188	LEU
1	E	192	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	202	GLN
1	E	204	LEU
1	E	238	MET
1	E	240	LYS
1	E	254	SER
1	E	262	SER
1	F	14	ARG
1	F	21	MET
1	F	22	LYS
1	F	41	LEU
1	F	44	MET
1	F	45	ASN
1	F	56	THR
1	F	58	LYS
1	F	60	LYS
1	F	66	GLN
1	F	102	PRO
1	F	198	ASP
1	F	204	LEU
1	F	209	LYS
1	F	211	LEU
1	F	213	ASN
1	F	220	LEU
1	F	254	SER
1	G	15	THR
1	G	29	LEU
1	G	31	LYS
1	G	59	LEU
1	G	91	LEU
1	G	139	SER
1	G	192	ILE
1	G	218	THR
1	G	220	LEU
1	G	230	LEU
1	G	233	GLN
1	G	254	SER
1	G	270	LYS
1	H	6	LEU
1	H	15	THR
1	H	29	LEU
1	H	41	LEU
1	H	58	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	H	70	GLU
1	H	80	LEU
1	H	95	ASP
1	H	148	THR
1	H	191	SER
1	H	209	LYS
1	H	218	THR
1	H	231	ASN
1	H	241	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	161	HIS
1	A	172	GLN
1	A	243	GLN
1	A	257	HIS
1	A	267	ASN
1	A	268	GLN
1	B	66	GLN
1	B	100	GLN
1	B	161	HIS
1	B	172	GLN
1	B	194	HIS
1	B	243	GLN
1	B	257	HIS
1	B	258	HIS
1	B	267	ASN
1	C	161	HIS
1	C	172	GLN
1	C	182	GLN
1	C	194	HIS
1	C	243	GLN
1	C	257	HIS
1	C	267	ASN
1	C	268	GLN
1	D	161	HIS
1	D	172	GLN
1	D	243	GLN
1	D	257	HIS
1	D	267	ASN
1	D	268	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	66	GLN
1	E	79	HIS
1	E	88	GLN
1	E	161	HIS
1	E	172	GLN
1	E	202	GLN
1	E	243	GLN
1	E	267	ASN
1	F	45	ASN
1	F	66	GLN
1	F	161	HIS
1	F	172	GLN
1	F	177	HIS
1	F	194	HIS
1	F	213	ASN
1	F	257	HIS
1	F	267	ASN
1	G	64	ASN
1	G	79	HIS
1	G	161	HIS
1	G	172	GLN
1	G	202	GLN
1	G	257	HIS
1	G	267	ASN
1	G	268	GLN
1	H	18	ASN
1	H	79	HIS
1	H	161	HIS
1	H	213	ASN
1	H	243	GLN
1	H	257	HIS
1	H	267	ASN
1	H	268	GLN

### 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](#)

16 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$
3	CC2	A	547	-	27,28,28	1.07	1 (3%)	33,41,41	1.17	4 (12%)
2	FAD	A	601	-	48,58,58	1.19	4 (8%)	54,89,89	2.78	12 (22%)
3	CC2	B	547	-	27,28,28	0.89	0	33,41,41	1.01	1 (3%)
2	FAD	B	601	-	48,58,58	1.23	6 (12%)	54,89,89	2.34	11 (20%)
3	CC2	C	547	-	27,28,28	0.95	0	33,41,41	0.96	1 (3%)
2	FAD	C	601	-	48,58,58	1.24	6 (12%)	54,89,89	2.38	11 (20%)
3	CC2	D	547	-	27,28,28	0.90	0	33,41,41	1.19	1 (3%)
2	FAD	D	601	-	48,58,58	1.37	5 (10%)	54,89,89	2.40	14 (25%)
3	CC2	E	547	-	27,28,28	0.93	0	33,41,41	0.89	1 (3%)
2	FAD	E	601	-	48,58,58	1.16	5 (10%)	54,89,89	2.22	9 (16%)
3	CC2	F	547	-	27,28,28	0.96	0	33,41,41	0.95	1 (3%)
2	FAD	F	601	-	48,58,58	1.23	5 (10%)	54,89,89	2.41	11 (20%)
3	CC2	G	547	-	27,28,28	0.98	1 (3%)	33,41,41	1.13	4 (12%)
2	FAD	G	601	-	48,58,58	1.18	5 (10%)	54,89,89	2.58	13 (24%)
3	CC2	H	547	-	27,28,28	1.08	0	33,41,41	1.00	1 (3%)
2	FAD	H	601	-	48,58,58	1.24	6 (12%)	54,89,89	2.44	11 (20%)

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
3	CC2	A	547	-	-	0/4/4/4	0/4/4/4
2	FAD	A	601	-	-	0/30/50/50	0/6/6/6
3	CC2	B	547	-	-	0/4/4/4	0/4/4/4
2	FAD	B	601	-	-	0/30/50/50	0/6/6/6
3	CC2	C	547	-	-	0/4/4/4	0/4/4/4
2	FAD	C	601	-	-	0/30/50/50	0/6/6/6
3	CC2	D	547	-	-	0/4/4/4	0/4/4/4
2	FAD	D	601	-	-	0/30/50/50	0/6/6/6
3	CC2	E	547	-	-	0/4/4/4	0/4/4/4
2	FAD	E	601	-	-	0/30/50/50	0/6/6/6
3	CC2	F	547	-	-	0/4/4/4	0/4/4/4
2	FAD	F	601	-	-	0/30/50/50	0/6/6/6
3	CC2	G	547	-	-	0/4/4/4	0/4/4/4
2	FAD	G	601	-	-	0/30/50/50	0/6/6/6
3	CC2	H	547	-	-	0/4/4/4	0/4/4/4
2	FAD	H	601	-	-	0/30/50/50	0/6/6/6

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	547	CC2	C4-C3	-2.28	1.38	1.41
2	B	601	FAD	C4'-C3'	-2.23	1.48	1.53
2	C	601	FAD	C6-C5X	-2.04	1.38	1.41
3	G	547	CC2	C15-C16	-2.02	1.39	1.42
2	G	601	FAD	C2A-N1A	2.11	1.37	1.33
2	E	601	FAD	C1'-N10	2.14	1.50	1.48
2	H	601	FAD	C10-N1	2.15	1.39	1.35
2	F	601	FAD	C2A-N1A	2.19	1.38	1.33
2	E	601	FAD	C2A-N1A	2.26	1.38	1.33
2	B	601	FAD	C2A-N1A	2.38	1.38	1.33
2	H	601	FAD	C2A-N1A	2.39	1.38	1.33
2	F	601	FAD	C4X-N5	2.41	1.37	1.33
2	C	601	FAD	C1'-N10	2.51	1.51	1.48
2	B	601	FAD	C4-N3	2.52	1.37	1.33
2	G	601	FAD	C4-N3	2.58	1.37	1.33
2	D	601	FAD	C4-N3	2.58	1.37	1.33
2	C	601	FAD	C2A-N1A	2.60	1.38	1.33
2	H	601	FAD	C4-N3	2.71	1.38	1.33
2	H	601	FAD	C4X-N5	2.72	1.37	1.33
2	C	601	FAD	C4X-N5	2.75	1.37	1.33
2	B	601	FAD	C1'-N10	2.76	1.51	1.48
2	H	601	FAD	C1'-N10	2.76	1.51	1.48
2	B	601	FAD	C4X-N5	2.77	1.37	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	FAD	C4X-N5	2.77	1.37	1.33
2	A	601	FAD	C4X-N5	2.79	1.37	1.33
2	A	601	FAD	C2A-N1A	2.80	1.39	1.33
2	C	601	FAD	C4-N3	2.81	1.38	1.33
2	A	601	FAD	C4-N3	2.81	1.38	1.33
2	D	601	FAD	C2A-N1A	2.90	1.39	1.33
2	F	601	FAD	C4-N3	2.99	1.38	1.33
2	E	601	FAD	C4-N3	3.00	1.38	1.33
2	G	601	FAD	C1'-N10	3.08	1.51	1.48
2	E	601	FAD	C4X-N5	3.15	1.38	1.33
2	F	601	FAD	C2A-N3A	3.30	1.38	1.32
2	E	601	FAD	C2A-N3A	3.31	1.38	1.32
2	G	601	FAD	C2A-N3A	3.41	1.38	1.32
2	B	601	FAD	C2A-N3A	3.42	1.38	1.32
2	F	601	FAD	C1'-N10	3.44	1.52	1.48
2	C	601	FAD	C2A-N3A	3.47	1.38	1.32
2	D	601	FAD	C4X-N5	3.56	1.38	1.33
2	H	601	FAD	C2A-N3A	3.61	1.38	1.32
2	A	601	FAD	C2A-N3A	3.65	1.38	1.32
2	D	601	FAD	C2A-N3A	3.85	1.39	1.32
2	D	601	FAD	C1'-N10	4.10	1.52	1.48

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C1'-N10-C9A	-11.90	105.50	118.86
2	C	601	FAD	N3A-C2A-N1A	-11.68	119.95	128.89
2	H	601	FAD	N3A-C2A-N1A	-11.62	120.00	128.89
2	B	601	FAD	N3A-C2A-N1A	-11.38	120.18	128.89
2	E	601	FAD	N3A-C2A-N1A	-11.36	120.20	128.89
2	G	601	FAD	N3A-C2A-N1A	-11.31	120.24	128.89
2	F	601	FAD	N3A-C2A-N1A	-11.18	120.34	128.89
2	A	601	FAD	N3A-C2A-N1A	-11.08	120.41	128.89
2	D	601	FAD	N3A-C2A-N1A	-10.32	120.99	128.89
2	G	601	FAD	C1'-N10-C9A	-9.48	108.22	118.86
2	F	601	FAD	C1'-N10-C9A	-7.85	110.05	118.86
2	H	601	FAD	C1'-N10-C9A	-7.57	110.36	118.86
2	C	601	FAD	C1'-N10-C9A	-6.97	111.03	118.86
2	B	601	FAD	C1'-N10-C9A	-6.88	111.14	118.86
2	D	601	FAD	C1'-N10-C9A	-5.59	112.59	118.86
2	A	601	FAD	C1'-C2'-C3'	-5.02	95.45	109.82
2	F	601	FAD	C2B-C1B-N9A	-4.26	107.79	114.29

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	FAD	C1'-N10-C9A	-4.25	114.09	118.86
2	H	601	FAD	C2B-C1B-N9A	-3.75	108.56	114.29
2	D	601	FAD	C2B-C1B-N9A	-3.51	108.93	114.29
2	G	601	FAD	C2B-C1B-N9A	-3.37	109.15	114.29
2	G	601	FAD	C4X-C4-N3	-3.34	119.03	123.59
2	D	601	FAD	P-O3P-PA	-3.26	123.58	132.73
2	C	601	FAD	C2B-C1B-N9A	-3.24	109.34	114.29
2	E	601	FAD	C4X-C4-N3	-3.03	119.44	123.59
2	F	601	FAD	C4X-C4-N3	-2.98	119.51	123.59
2	A	601	FAD	O4'-C4'-C5'	-2.87	103.93	110.19
2	C	601	FAD	C4X-C4-N3	-2.83	119.72	123.59
2	D	601	FAD	C4X-C4-N3	-2.82	119.73	123.59
2	E	601	FAD	C2B-C1B-N9A	-2.62	110.30	114.29
2	G	601	FAD	C4A-C5A-N7A	-2.59	107.10	109.48
2	B	601	FAD	C4A-C5A-N7A	-2.57	107.11	109.48
2	B	601	FAD	C4X-C4-N3	-2.53	120.13	123.59
2	A	601	FAD	O3P-P-O5'	-2.49	96.33	102.94
2	H	601	FAD	C4X-C4-N3	-2.49	120.18	123.59
3	A	547	CC2	C14-C13-C9	-2.48	106.75	114.33
2	C	601	FAD	C5B-C4B-C3B	-2.45	105.50	115.21
2	D	601	FAD	O3'-C3'-C4'	-2.40	102.71	108.75
2	B	601	FAD	O4'-C4'-C3'	-2.36	103.09	109.02
3	G	547	CC2	C14-C13-C9	-2.35	107.16	114.33
2	H	601	FAD	C1B-N9A-C4A	-2.35	123.40	126.94
2	H	601	FAD	C4A-C5A-N7A	-2.24	107.42	109.48
2	C	601	FAD	P-O3P-PA	-2.23	126.47	132.73
2	E	601	FAD	C1B-N9A-C4A	-2.18	123.65	126.94
2	H	601	FAD	P-O3P-PA	-2.15	126.69	132.73
2	B	601	FAD	C1B-N9A-C4A	-2.13	123.73	126.94
2	A	601	FAD	C4X-C4-N3	-2.04	120.80	123.59
2	G	601	FAD	O3'-C3'-C4'	-2.03	103.64	108.75
3	E	547	CC2	O1-C10-C4	2.00	120.63	116.52
3	G	547	CC2	C20-C15-C16	2.02	120.55	117.91
2	D	601	FAD	O2P-P-O3P	2.02	114.26	105.09
2	C	601	FAD	C4X-C10-N10	2.05	121.72	120.52
3	A	547	CC2	O1-C10-C9	2.08	121.48	118.90
2	F	601	FAD	O3P-P-O5'	2.09	108.49	102.94
3	A	547	CC2	C5-C4-C3	2.10	118.93	116.42
2	G	601	FAD	C4X-C10-N10	2.11	121.76	120.52
2	C	601	FAD	O2A-PA-O3P	2.15	114.87	105.09
3	F	547	CC2	O1-C10-C4	2.16	120.96	116.52
2	G	601	FAD	O2P-P-O3P	2.17	114.95	105.09

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	O5B-PA-O1A	2.20	118.16	109.62
2	H	601	FAD	O4B-C1B-N9A	2.22	112.75	108.10
3	G	547	CC2	C8-C9-C10	2.31	121.01	117.90
2	F	601	FAD	C4-C4X-C10	2.32	121.42	119.94
2	A	601	FAD	O2P-P-O3P	2.34	115.69	105.09
2	C	601	FAD	O3P-P-O5'	2.34	109.14	102.94
2	B	601	FAD	C4X-C10-N10	2.34	121.90	120.52
2	D	601	FAD	C4X-N5-C5X	2.41	119.54	116.76
2	E	601	FAD	O3P-P-O5'	2.43	109.39	102.94
2	A	601	FAD	C4X-N5-C5X	2.46	119.59	116.76
2	B	601	FAD	C6-C5X-C9A	2.47	122.22	118.98
3	B	547	CC2	C5-C4-C3	2.48	119.39	116.42
2	F	601	FAD	O3P-PA-O5B	2.49	109.55	102.94
2	G	601	FAD	O2A-PA-O3P	2.49	116.41	105.09
2	D	601	FAD	C4X-C10-N10	2.53	122.01	120.52
2	F	601	FAD	C4X-C10-N10	2.57	122.03	120.52
2	H	601	FAD	O2A-PA-O3P	2.63	117.03	105.09
2	D	601	FAD	O4B-C1B-N9A	2.71	113.77	108.10
3	C	547	CC2	C5-C4-C3	2.71	119.66	116.42
2	A	601	FAD	O2'-C2'-C1'	2.74	116.67	109.94
2	D	601	FAD	O3'-C3'-C2'	2.80	115.80	108.75
2	G	601	FAD	C4X-N5-C5X	2.90	120.10	116.76
2	E	601	FAD	C4X-N5-C5X	2.94	120.15	116.76
2	A	601	FAD	O3'-C3'-C4'	2.95	116.19	108.75
3	H	547	CC2	C5-C4-C3	2.96	119.96	116.42
2	B	601	FAD	C4X-N5-C5X	3.10	120.33	116.76
2	B	601	FAD	C5X-C9A-N10	3.13	120.00	117.62
3	G	547	CC2	O1-C10-C4	3.16	123.02	116.52
2	F	601	FAD	C4X-N5-C5X	3.18	120.42	116.76
2	G	601	FAD	O4B-C1B-N9A	3.28	114.97	108.10
3	A	547	CC2	C13-C9-C10	3.50	122.95	119.58
2	E	601	FAD	C5X-C9A-N10	3.54	120.31	117.62
2	F	601	FAD	C5X-C9A-N10	3.59	120.34	117.62
2	A	601	FAD	C5X-C9A-N10	3.71	120.44	117.62
2	C	601	FAD	C5X-C9A-N10	3.92	120.60	117.62
3	D	547	CC2	C13-C9-C10	4.36	123.78	119.58
2	G	601	FAD	C5X-C9A-N10	4.45	121.00	117.62
2	H	601	FAD	C5X-C9A-N10	4.45	121.00	117.62
2	B	601	FAD	C4-N3-C2	4.47	119.11	115.25
2	F	601	FAD	C4-N3-C2	4.80	119.39	115.25
2	C	601	FAD	C4-N3-C2	5.17	119.72	115.25
2	D	601	FAD	C5X-C9A-N10	5.18	121.55	117.62

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	601	FAD	C4-N3-C2	5.35	119.87	115.25
2	A	601	FAD	C4-N3-C2	5.48	119.98	115.25
2	G	601	FAD	C4-N3-C2	5.58	120.07	115.25
2	E	601	FAD	C4-N3-C2	5.59	120.08	115.25
2	D	601	FAD	C4-N3-C2	6.15	120.56	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 74 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	547	CC2	1	0
2	A	601	FAD	7	0
3	B	547	CC2	10	0
2	B	601	FAD	10	0
3	C	547	CC2	4	0
2	C	601	FAD	6	0
3	D	547	CC2	2	0
2	D	601	FAD	6	0
3	E	547	CC2	3	0
2	E	601	FAD	4	0
3	F	547	CC2	3	0
2	F	601	FAD	4	0
3	G	547	CC2	2	0
2	G	601	FAD	2	0
3	H	547	CC2	3	0
2	H	601	FAD	9	0

## 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	270/273 (98%)	0.14	4 (1%) 76 78	42, 61, 78, 92	0
1	B	270/273 (98%)	0.01	0 100 100	42, 56, 75, 87	0
1	C	270/273 (98%)	-0.01	0 100 100	41, 57, 75, 91	0
1	D	270/273 (98%)	0.08	2 (0%) 89 90	42, 59, 78, 90	0
1	E	270/273 (98%)	0.14	5 (1%) 70 72	51, 67, 89, 98	0
1	F	270/273 (98%)	0.18	6 (2%) 65 68	50, 66, 87, 102	0
1	G	270/273 (98%)	0.21	6 (2%) 65 68	50, 69, 95, 105	0
1	H	270/273 (98%)	0.34	11 (4%) 41 44	51, 70, 93, 105	0
All	All	2160/2184 (98%)	0.14	34 (1%) 74 77	41, 63, 87, 105	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	2	GLY	10.7
1	F	2	GLY	5.3
1	G	2	GLY	4.7
1	H	59	LEU	3.9
1	A	232	PHE	3.2
1	F	209	LYS	3.0
1	E	29	LEU	2.9
1	G	259	LEU	2.9
1	H	73	LEU	2.7
1	G	230	LEU	2.7
1	D	2	GLY	2.6
1	E	10	ALA	2.6
1	H	58	LYS	2.5
1	H	251	PHE	2.5
1	G	59	LEU	2.5
1	A	7	ILE	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	248	ASN	2.4
1	G	253	LEU	2.4
1	D	232	PHE	2.3
1	E	55	ILE	2.3
1	F	214	ILE	2.3
1	A	58	LYS	2.3
1	H	36	VAL	2.3
1	E	160	ILE	2.3
1	H	24	ALA	2.2
1	A	9	LEU	2.2
1	H	34	TRP	2.2
1	E	80	LEU	2.2
1	H	209	LYS	2.1
1	G	36	VAL	2.1
1	F	7	ILE	2.1
1	H	231	ASN	2.0
1	F	80	LEU	2.0
1	H	259	LEU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	CC2	F	547	25/25	0.94	0.23	1.41	59,68,81,82	0
3	CC2	C	547	25/25	0.93	0.21	0.87	52,62,85,89	0
3	CC2	B	547	25/25	0.91	0.22	0.70	57,66,87,89	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CC2	A	547	25/25	0.96	0.16	0.12	44,49,53,56	0
3	CC2	G	547	25/25	0.97	0.17	0.10	53,56,59,60	0
3	CC2	E	547	25/25	0.95	0.16	0.03	60,68,81,85	0
2	FAD	B	601	53/53	0.96	0.14	-0.25	46,58,66,68	0
2	FAD	F	601	53/53	0.94	0.15	-0.27	53,62,69,76	0
2	FAD	D	601	53/53	0.97	0.14	-0.39	42,50,62,68	0
2	FAD	H	601	53/53	0.96	0.15	-0.43	43,56,69,73	0
3	CC2	H	547	25/25	0.96	0.15	-0.54	51,55,58,60	0
2	FAD	C	601	53/53	0.96	0.14	-0.55	39,54,63,69	0
3	CC2	D	547	25/25	0.97	0.14	-0.57	46,51,54,55	0
2	FAD	A	601	53/53	0.97	0.15	-0.61	42,49,61,64	0
2	FAD	G	601	53/53	0.97	0.14	-0.65	42,54,62,68	0
2	FAD	E	601	53/53	0.96	0.15	-0.92	56,63,73,80	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.