



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2018 – 04:53 AM EST

PDB ID : 3HR4
Title : Human iNOS Reductase and Calmodulin Complex
Authors : Xia, C.; Misra, I.; Iyanaki, T.; Kim, J.J.K.
Deposited on : 2009-06-08
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030736

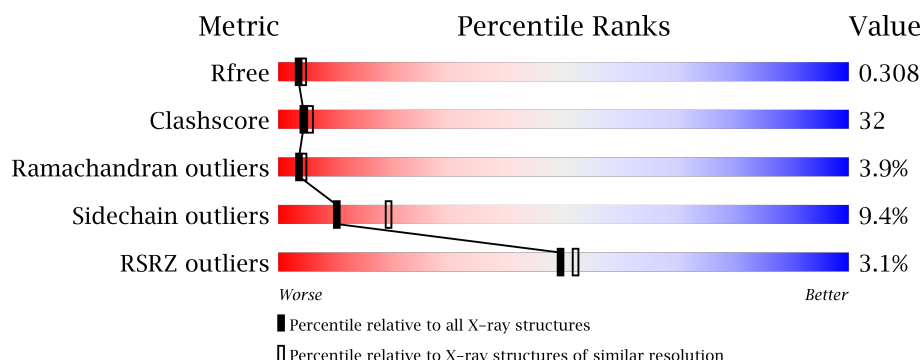
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. 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	219	
1	C	219	
1	E	219	
1	G	219	
2	B	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
2	D	149		•
2	F	149		•
2	H	149		•

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10594 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 Nitric oxide synthase, inducible.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1470	943	250	263	14			
1	C	188	Total	C	N	O	S	0	0	0
			1455	931	248	262	14			
1	E	189	Total	C	N	O	S	0	0	0
			1463	937	249	263	14			
1	G	187	Total	C	N	O	S	0	0	0
			1449	931	246	258	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	497	HIS	-	EXPRESSION TAG	UNP P35228
A	498	HIS	-	EXPRESSION TAG	UNP P35228
A	499	HIS	-	EXPRESSION TAG	UNP P35228
A	500	HIS	-	EXPRESSION TAG	UNP P35228
A	501	HIS	-	EXPRESSION TAG	UNP P35228
A	502	HIS	-	EXPRESSION TAG	UNP P35228
C	497	HIS	-	EXPRESSION TAG	UNP P35228
C	498	HIS	-	EXPRESSION TAG	UNP P35228
C	499	HIS	-	EXPRESSION TAG	UNP P35228
C	500	HIS	-	EXPRESSION TAG	UNP P35228
C	501	HIS	-	EXPRESSION TAG	UNP P35228
C	502	HIS	-	EXPRESSION TAG	UNP P35228
E	497	HIS	-	EXPRESSION TAG	UNP P35228
E	498	HIS	-	EXPRESSION TAG	UNP P35228
E	499	HIS	-	EXPRESSION TAG	UNP P35228
E	500	HIS	-	EXPRESSION TAG	UNP P35228
E	501	HIS	-	EXPRESSION TAG	UNP P35228
E	502	HIS	-	EXPRESSION TAG	UNP P35228
G	497	HIS	-	EXPRESSION TAG	UNP P35228
G	498	HIS	-	EXPRESSION TAG	UNP P35228
G	499	HIS	-	EXPRESSION TAG	UNP P35228

Continued on next page...

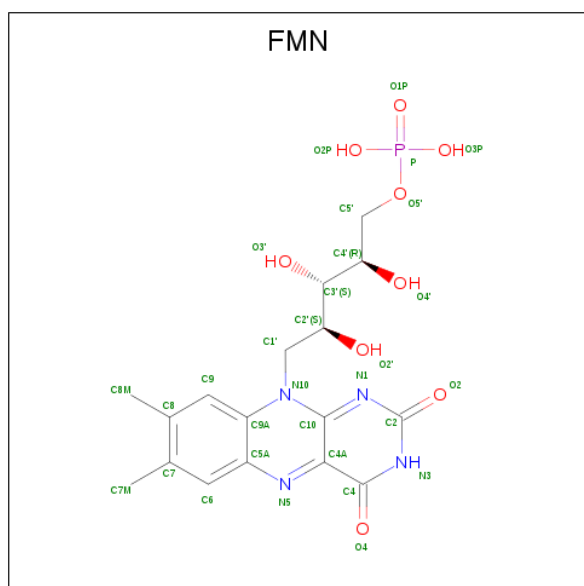
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	500	HIS	-	EXPRESSION TAG	UNP P35228
G	501	HIS	-	EXPRESSION TAG	UNP P35228
G	502	HIS	-	EXPRESSION TAG	UNP P35228

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	0	0
			1143	701	184	249	9			
2	D	145	Total	C	N	O	S	0	0	0
			1136	696	183	248	9			
2	F	145	Total	C	N	O	S	0	0	0
			1143	701	184	249	9			
2	H	145	Total	C	N	O	S	0	0	0
			1124	689	181	245	9			

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	E	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

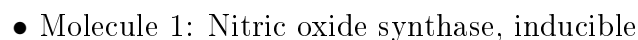
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

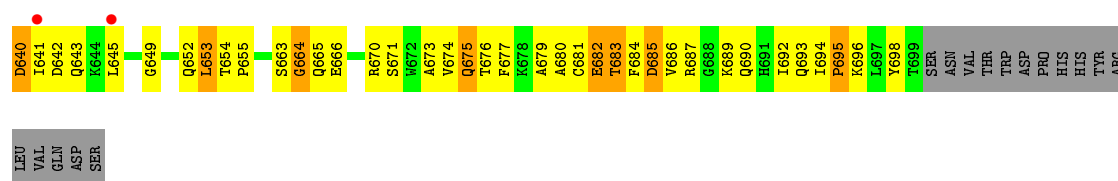
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	4	Total 4	Ca 4	0	0
4	B	4	Total 4	Ca 4	0	0
4	D	4	Total 4	Ca 4	0	0
4	F	4	Total 4	Ca 4	0	0

- Molecule 5 is water.

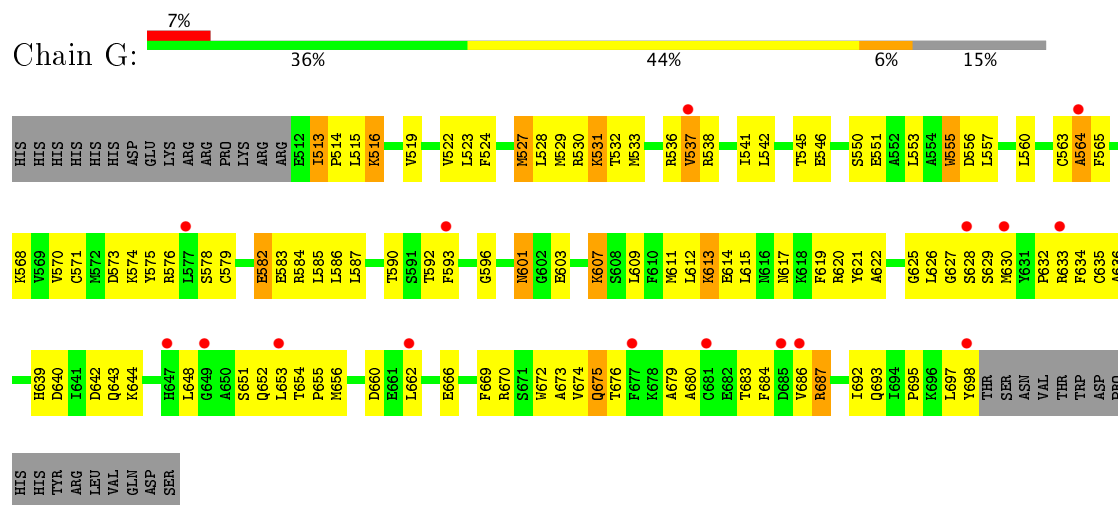
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	11	Total 11	O 11	0	0
5	B	7	Total 7	O 7	0	0
5	C	5	Total 5	O 5	0	0
5	D	23	Total 23	O 23	0	0
5	E	2	Total 2	O 2	0	0
5	F	15	Total 15	O 15	0	0
5	G	5	Total 5	O 5	0	0
5	H	3	Total 3	O 3	0	0

- Molecule 1: Nitric oxide synthase, inducible

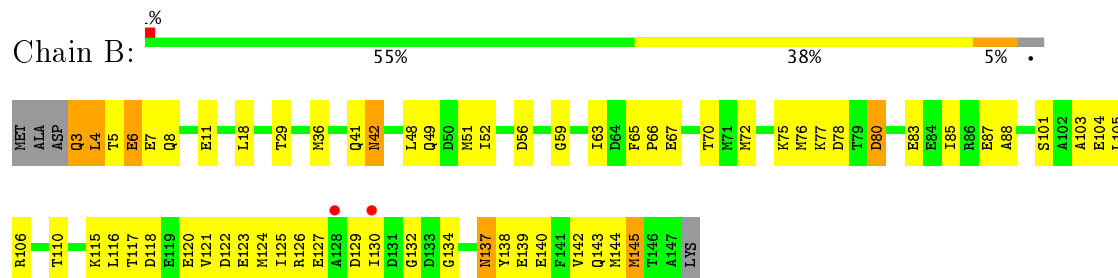




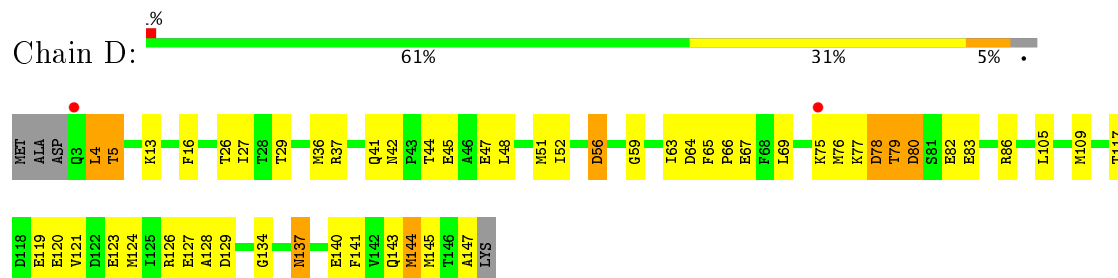
• Molecule 1: Nitric oxide synthase, inducible



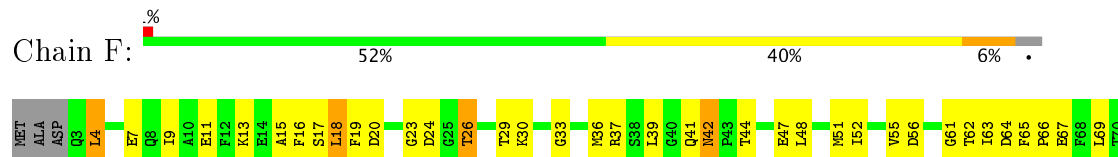
• Molecule 2: Calmodulin

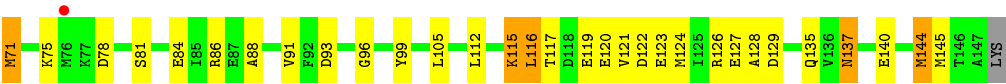


• Molecule 2: Calmodulin

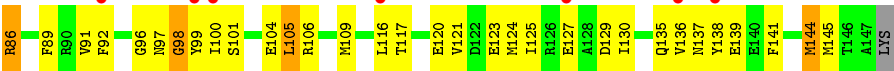
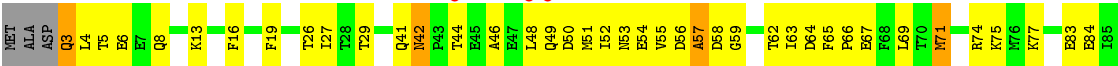


• Molecule 2: Calmodulin





● Molecule 2: Calmodulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	36.60 Å 160.84 Å 127.77 Å 90.00° 90.37° 90.00°	Depositor
Resolution (Å)	29.69 – 2.50 36.60 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (29.69-2.50) 86.8 (36.60-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.51 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.237 , 0.309 0.237 , 0.308	Depositor DCC
R_{free} test set	2213 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.051 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10594	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/1499	0.64	0/2016
1	C	0.40	0/1484	0.64	0/1997
1	E	0.40	0/1492	0.61	0/2008
1	G	0.44	1/1478 (0.1%)	0.69	2/1989 (0.1%)
2	B	0.40	0/1155	0.59	0/1551
2	D	0.46	0/1148	0.73	1/1542 (0.1%)
2	F	0.45	0/1155	0.67	0/1551
2	H	0.35	0/1136	0.58	0/1527
All	All	0.42	1/10547 (0.0%)	0.65	3/14181 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	613	LYS	C-O	-5.28	1.13	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	614	GLU	N-CA-CB	-10.18	92.28	110.60
1	G	613	LYS	N-CA-C	8.26	133.30	111.00
2	D	4	LEU	CB-CA-C	-6.56	97.73	110.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	511	ARG	Peptide

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	1470	0	1485	81	0
1	C	1455	0	1454	119	0
1	E	1463	0	1465	115	0
1	G	1449	0	1462	118	0
2	B	1143	0	1071	79	0
2	D	1136	0	1056	62	0
2	F	1143	0	1071	72	0
2	H	1124	0	1036	83	0
3	A	31	0	18	1	0
3	C	31	0	18	5	0
3	E	31	0	18	1	0
3	G	31	0	18	1	0
4	B	4	0	0	0	0
4	D	4	0	0	0	0
4	F	4	0	0	0	0
4	H	4	0	0	0	0
5	A	11	0	0	3	0
5	B	7	0	0	0	0
5	C	5	0	0	1	0
5	D	23	0	0	1	0
5	E	2	0	0	0	0
5	F	15	0	0	0	0
5	G	5	0	0	0	0
5	H	3	0	0	0	0
All	All	10594	0	10172	656	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 32.

All (656) 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)
2:D:4:LEU:O	2:D:5:THR:HG23	1.24	1.31
2:B:29:THR:HG22	2:B:52:ILE:HG13	1.39	1.05
2:H:109:MET:HE2	2:H:116:LEU:HD11	1.42	1.02
1:G:633:ARG:HB3	1:G:636:ALA:HB2	1.42	1.01
2:F:42:ASN:N	2:F:42:ASN:HD22	1.55	0.99
2:F:122:ASP:HB3	2:F:126:ARG:HH22	1.25	0.97
2:D:4:LEU:O	2:D:5:THR:CG2	2.12	0.97
1:C:583:GLU:HG2	1:C:586:LEU:HD23	1.46	0.96
2:B:137:ASN:ND2	2:B:140:GLU:H	1.65	0.94
2:H:3:GLN:HG2	2:H:4:LEU:N	1.82	0.92
1:C:633:ARG:HH11	1:C:633:ARG:HG3	1.33	0.92
1:C:598:CYS:SG	1:C:606:LYS:HD2	2.10	0.91
2:F:42:ASN:H	2:F:42:ASN:HD22	1.18	0.89
2:F:137:ASN:ND2	2:F:140:GLU:H	1.72	0.87
1:E:596:GLY:HA2	1:E:636:ALA:HB3	1.56	0.87
2:H:106:ARG:HG3	2:H:121:VAL:HG21	1.57	0.86
1:A:697:LEU:HD23	1:A:697:LEU:H	1.38	0.86
2:B:137:ASN:HD21	2:B:140:GLU:H	1.21	0.86
2:D:4:LEU:C	2:D:5:THR:HG23	1.98	0.84
1:G:513:ILE:H	1:G:513:ILE:HD13	1.42	0.83
2:F:122:ASP:HB3	2:F:126:ARG:NH2	1.93	0.83
1:G:584:ARG:HD3	1:G:684:PHE:HE2	1.43	0.83
2:F:137:ASN:HD21	2:F:140:GLU:HG3	1.44	0.82
1:A:513:ILE:N	1:A:513:ILE:HD12	1.95	0.81
1:G:522:VAL:HG21	2:H:91:VAL:HG21	1.61	0.81
2:H:29:THR:HG22	2:H:52:ILE:HG13	1.60	0.81
1:C:527:MET:HE3	2:D:75:LYS:HB2	1.62	0.81
1:G:601:ASN:HD22	1:G:601:ASN:N	1.79	0.80
2:H:137:ASN:OD1	2:H:139:GLU:N	2.15	0.80
2:D:48:LEU:HA	2:D:51:MET:HE3	1.63	0.80
1:A:598:CYS:SG	1:A:603:GLU:HG2	2.22	0.80
1:E:620:ARG:HG3	1:E:620:ARG:HH11	1.47	0.79
1:A:525:ALA:HB1	2:B:41:GLN:HE22	1.48	0.79
2:F:144:MET:HE2	2:F:144:MET:HA	1.65	0.78
1:C:579:CYS:O	1:C:582:GLU:HG2	1.83	0.77
2:H:120:GLU:O	2:H:123:GLU:HB3	1.84	0.77
1:C:584:ARG:NH1	1:C:584:ARG:HB3	2.00	0.76
2:D:105:LEU:HD12	2:D:121:VAL:HG13	1.67	0.76
1:C:553:LEU:HD21	1:C:666:GLU:OE1	1.85	0.76
2:D:29:THR:HG22	2:D:52:ILE:HG13	1.67	0.76
1:E:519:VAL:HG13	2:F:145:MET:HE2	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:42:ASN:N	2:F:42:ASN:ND2	2.28	0.76
2:H:48:LEU:HA	2:H:51:MET:HE3	1.66	0.76
1:E:582:GLU:HG2	1:E:583:GLU:N	2.01	0.76
1:C:694:ILE:HD12	1:C:698:TYR:HB2	1.67	0.76
1:C:543:PHE:HA	1:C:589:VAL:O	1.86	0.75
2:F:115:LYS:H	2:F:115:LYS:HE2	1.51	0.75
1:E:546:GLU:HG2	1:E:599:PRO:HB3	1.68	0.74
1:G:617:ASN:HD21	1:G:619:PHE:HB3	1.53	0.74
1:C:553:LEU:HD22	1:C:669:PHE:CD2	2.23	0.73
2:H:50:ASP:O	2:H:54:GLU:HG3	1.87	0.73
1:G:644:LYS:HE3	1:G:648:LEU:HD11	1.68	0.73
1:C:519:VAL:O	2:D:145:MET:HE1	1.88	0.73
2:H:48:LEU:HD23	2:H:51:MET:CE	2.18	0.73
1:E:666:GLU:HB3	1:E:670:ARG:NH1	2.03	0.73
1:G:673:ALA:HA	1:G:676:THR:HG22	1.71	0.73
1:C:546:GLU:OE2	1:C:599:PRO:HB3	1.89	0.73
1:C:654:THR:HG21	1:C:676:THR:OG1	1.89	0.73
2:B:106:ARG:O	2:B:110:THR:HG23	1.88	0.72
1:C:637:PHE:O	1:C:641:ILE:HG22	1.90	0.72
1:G:633:ARG:HB3	1:G:636:ALA:CB	2.17	0.72
2:B:139:GLU:HG2	2:B:143:GLN:HE21	1.54	0.72
2:F:29:THR:HG22	2:F:52:ILE:HG13	1.70	0.72
2:H:48:LEU:HA	2:H:51:MET:CE	2.20	0.72
2:B:42:ASN:H	2:B:42:ASN:HD22	1.38	0.72
1:C:573:ASP:OD1	1:C:574:LYS:HG2	1.90	0.72
1:A:537:VAL:HG13	1:A:565:PHE:HD2	1.55	0.71
2:F:115:LYS:HE2	2:F:115:LYS:N	2.06	0.71
1:E:670:ARG:O	1:E:674:VAL:HG23	1.91	0.70
1:C:523:LEU:HB2	2:D:145:MET:HE1	1.73	0.70
1:C:687:ARG:HG2	5:C:46:HOH:O	1.89	0.70
1:G:557:LEU:HD21	1:G:587:LEU:HD13	1.72	0.70
1:E:542:LEU:HB2	1:E:588:VAL:HG12	1.71	0.69
1:E:544:ALA:HB3	1:E:590:THR:OG1	1.91	0.69
1:C:546:GLU:HG3	1:C:593:PHE:CD1	2.27	0.69
2:D:105:LEU:HD11	2:D:124:MET:HE3	1.74	0.69
2:F:124:MET:O	2:F:127:GLU:HB3	1.92	0.69
1:A:523:LEU:HG	2:B:145:MET:CE	2.23	0.69
1:G:630:MET:O	1:G:630:MET:HG2	1.93	0.68
2:H:51:MET:HA	2:H:54:GLU:OE2	1.93	0.68
2:H:109:MET:HE2	2:H:116:LEU:CD1	2.22	0.68
1:C:633:ARG:CG	1:C:633:ARG:HH11	2.05	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:697:LEU:HD23	1:C:697:LEU:O	1.94	0.68
2:B:137:ASN:HD21	2:B:140:GLU:N	1.91	0.68
2:D:105:LEU:HD11	2:D:124:MET:CE	2.24	0.68
1:E:641:ILE:HD12	1:E:642:ASP:N	2.09	0.67
1:A:515:LEU:HD12	2:B:144:MET:HE1	1.76	0.67
1:C:542:LEU:HD12	1:C:586:LEU:HD11	1.75	0.67
1:C:572:MET:HB3	1:C:605:LEU:HD22	1.75	0.67
1:E:633:ARG:HB3	1:E:636:ALA:HB2	1.77	0.67
2:B:29:THR:CG2	2:B:52:ILE:HG13	2.21	0.67
2:F:137:ASN:HD21	2:F:140:GLU:H	1.41	0.67
1:E:537:VAL:HB	1:E:565:PHE:HD2	1.60	0.67
2:H:137:ASN:O	2:H:141:PHE:HB2	1.95	0.67
1:A:516:LYS:HG2	2:B:127:GLU:OE2	1.94	0.67
1:E:523:LEU:HB2	2:F:145:MET:HE1	1.75	0.67
1:C:527:MET:CE	2:D:75:LYS:HB2	2.25	0.66
1:C:584:ARG:HH11	1:C:584:ARG:HB3	1.60	0.66
1:E:529:MET:HG2	2:F:36:MET:CE	2.25	0.66
2:H:117:THR:O	2:H:121:VAL:HG23	1.95	0.66
1:G:529:MET:HG2	2:H:41:GLN:HG2	1.76	0.66
1:G:584:ARG:HD3	1:G:684:PHE:CE2	2.29	0.66
2:B:29:THR:HG21	2:B:49:GLN:NE2	2.11	0.65
2:B:48:LEU:HA	2:B:51:MET:HE3	1.77	0.65
2:H:109:MET:CE	2:H:116:LEU:HD11	2.24	0.65
1:G:652:GLN:NE2	1:G:655:PRO:HA	2.10	0.65
1:A:553:LEU:HD22	1:A:669:PHE:CD2	2.31	0.65
1:G:642:ASP:OD1	1:G:656:MET:HB2	1.96	0.65
2:H:49:GLN:O	2:H:53:ASN:ND2	2.30	0.65
1:G:687:ARG:HD3	1:G:687:ARG:H	1.61	0.65
2:B:85:ILE:HG12	2:B:145:MET:HE3	1.79	0.64
1:E:606:LYS:HG3	1:E:610:PHE:CE2	2.33	0.64
2:F:37:ARG:HA	2:F:41:GLN:O	1.98	0.64
2:H:105:LEU:CD1	2:H:124:MET:HE3	2.28	0.64
1:A:553:LEU:HD12	1:A:626:LEU:HD11	1.80	0.64
2:B:3:GLN:O	2:B:4:LEU:HB2	1.95	0.64
1:C:630:MET:HG2	1:C:630:MET:O	1.98	0.64
1:G:553:LEU:HD12	1:G:626:LEU:HD21	1.79	0.64
1:E:620:ARG:NH1	1:E:620:ARG:HG3	2.12	0.64
2:D:78:ASP:O	2:D:80:ASP:N	2.30	0.63
1:C:527:MET:HE3	2:D:75:LYS:CB	2.26	0.63
1:G:612:LEU:HD12	1:G:613:LYS:H	1.62	0.63
1:C:598:CYS:HB3	1:C:637:PHE:CD1	2.32	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:644:LYS:HD2	1:G:644:LYS:O	1.99	0.63
1:A:671:SER:O	1:A:675:GLN:HG2	1.98	0.63
1:E:593:PHE:O	1:E:597:ASP:HB3	1.97	0.63
1:G:530:ARG:HH22	2:H:83:GLU:HB3	1.64	0.63
2:F:37:ARG:HH11	2:F:37:ARG:HG2	1.63	0.63
1:A:673:ALA:O	1:A:676:THR:HG22	1.99	0.63
1:A:519:VAL:HG13	2:B:145:MET:SD	2.39	0.63
1:C:529:MET:HG2	2:D:36:MET:CE	2.29	0.63
1:A:553:LEU:HD22	1:A:669:PHE:CG	2.34	0.62
1:E:542:LEU:HD21	1:E:575:TYR:HB2	1.81	0.62
1:G:617:ASN:ND2	1:G:619:PHE:HB3	2.14	0.62
1:C:515:LEU:O	1:C:519:VAL:HB	1.99	0.62
2:H:92:PHE:HB3	2:H:100:ILE:HD12	1.81	0.62
1:C:627:GLY:HA2	3:C:999:FMN:H3'	1.81	0.62
2:F:44:THR:OG1	2:F:47:GLU:HG3	1.99	0.62
1:C:598:CYS:HB3	1:C:637:PHE:CE1	2.34	0.62
1:E:694:ILE:O	1:E:696:LYS:N	2.32	0.62
1:G:528:LEU:HB3	2:H:51:MET:SD	2.39	0.62
2:F:122:ASP:CB	2:F:126:ARG:HH22	2.05	0.61
2:F:15:ALA:O	2:F:18:LEU:HB2	2.00	0.61
1:G:601:ASN:ND2	1:G:601:ASN:N	2.48	0.61
1:C:697:LEU:HD22	1:C:698:TYR:CE1	2.35	0.61
2:D:79:THR:HG22	2:D:79:THR:O	1.99	0.61
1:A:666:GLU:HB3	1:A:670:ARG:NH1	2.14	0.61
2:H:3:GLN:CG	2:H:4:LEU:N	2.58	0.61
2:F:64:ASP:OD1	2:F:67:GLU:HG3	1.98	0.61
1:C:543:PHE:O	1:C:572:MET:HG3	2.00	0.61
1:E:537:VAL:HG13	1:E:584:ARG:HE	1.65	0.61
1:A:596:GLY:HA2	1:A:636:ALA:HB3	1.83	0.60
1:E:623:VAL:HG11	1:E:641:ILE:HD11	1.83	0.60
1:G:537:VAL:HG23	1:G:584:ARG:HD2	1.83	0.60
1:C:536:ARG:HD2	2:D:47:GLU:OE2	2.01	0.60
1:A:537:VAL:HG12	5:A:27:HOH:O	2.00	0.60
1:C:523:LEU:HD12	2:D:145:MET:SD	2.42	0.60
2:D:137:ASN:ND2	2:D:140:GLU:H	1.99	0.60
1:C:523:LEU:HD22	1:C:527:MET:SD	2.41	0.60
2:F:144:MET:CE	2:F:144:MET:HA	2.30	0.60
1:E:693:GLN:NE2	1:E:696:LYS:NZ	2.50	0.60
1:G:629:SER:OG	1:G:662:LEU:HD22	2.01	0.60
1:G:570:VAL:HG12	1:G:571:CYS:O	2.02	0.59
2:D:109:MET:HG3	2:D:124:MET:HE1	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:125:ILE:O	2:H:129:ASP:HB2	2.01	0.59
2:F:7:GLU:O	2:F:11:GLU:HG3	2.02	0.59
1:G:644:LYS:CE	1:G:648:LEU:HD11	2.33	0.59
1:G:620:ARG:HG2	1:G:651:SER:HB2	1.84	0.59
1:A:591:SER:HA	1:A:626:LEU:O	2.02	0.59
1:E:673:ALA:HA	1:E:676:THR:HG22	1.84	0.59
1:E:674:VAL:HG22	1:E:698:TYR:HB3	1.84	0.59
1:A:530:ARG:HG3	1:A:530:ARG:HH11	1.67	0.59
2:B:125:ILE:C	2:B:127:GLU:H	2.06	0.59
1:A:523:LEU:HG	2:B:145:MET:HE3	1.84	0.59
2:B:137:ASN:HD22	2:B:137:ASN:C	2.06	0.59
1:C:577:LEU:HG	1:C:608:SER:HB3	1.84	0.59
1:G:531:LYS:C	1:G:533:MET:H	2.05	0.59
2:H:52:ILE:HD13	2:H:63:ILE:HD11	1.85	0.59
1:C:614:GLU:HA	1:C:648:LEU:HD22	1.85	0.59
1:E:513:ILE:N	1:E:513:ILE:HD12	2.18	0.58
1:G:628:SER:N	1:G:634:PHE:HE1	2.01	0.58
2:H:4:LEU:O	2:H:4:LEU:HD23	2.02	0.58
2:F:33:GLY:O	2:F:37:ARG:HG3	2.04	0.58
1:G:519:VAL:HA	1:G:522:VAL:HG12	1.85	0.58
1:G:516:LYS:HA	1:G:519:VAL:HG12	1.85	0.58
1:C:523:LEU:HB2	2:D:145:MET:CE	2.33	0.58
1:E:588:VAL:CG2	1:E:623:VAL:HG22	2.33	0.58
1:A:515:LEU:HD12	2:B:144:MET:CE	2.34	0.58
1:C:621:TYR:CD1	1:C:650:ALA:HB1	2.39	0.58
1:E:641:ILE:C	1:E:641:ILE:HD12	2.24	0.57
1:G:670:ARG:O	1:G:674:VAL:HG23	2.04	0.57
2:H:141:PHE:O	2:H:144:MET:HB3	2.04	0.57
1:E:587:LEU:CD2	1:E:622:ALA:HB3	2.34	0.57
2:B:137:ASN:HD21	2:B:140:GLU:CB	2.17	0.57
2:B:137:ASN:HD21	2:B:140:GLU:CG	2.17	0.57
1:C:633:ARG:HG3	1:C:633:ARG:NH1	2.12	0.57
1:G:692:ILE:HD12	2:H:44:THR:HG22	1.87	0.57
2:B:121:VAL:O	2:B:125:ILE:HG13	2.03	0.57
2:D:64:ASP:OD2	2:D:67:GLU:HG3	2.05	0.57
1:G:592:THR:HG21	1:G:596:GLY:HA2	1.87	0.57
2:H:89:PHE:HB2	2:H:141:PHE:CE1	2.40	0.57
1:E:618:LYS:HD2	1:E:649:GLY:O	2.05	0.57
1:G:537:VAL:HG22	1:G:565:PHE:HD2	1.69	0.57
1:A:545:THR:HB	1:A:550:SER:HB2	1.85	0.57
2:B:103:ALA:O	2:B:106:ARG:HB3	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:666:GLU:HB3	1:E:670:ARG:HH12	1.69	0.56
2:H:16:PHE:CE1	2:H:27:ILE:HD11	2.39	0.56
1:E:542:LEU:HB2	1:E:588:VAL:CG1	2.35	0.56
1:E:547:THR:HB	3:E:999:FMN:O3P	2.05	0.56
1:G:653:LEU:HD21	1:G:679:ALA:O	2.06	0.56
1:G:622:ALA:HB1	1:G:672:TRP:HZ2	1.71	0.56
2:B:42:ASN:N	2:B:42:ASN:HD22	1.99	0.56
1:G:513:ILE:HG12	1:G:513:ILE:O	2.04	0.56
2:B:72:MET:O	2:B:76:MET:HG2	2.06	0.56
1:C:644:LYS:HE3	1:C:648:LEU:HD11	1.86	0.56
1:G:530:ARG:HH11	2:H:84:GLU:CD	2.09	0.56
1:G:687:ARG:CD	1:G:687:ARG:H	2.19	0.56
1:E:581:GLU:OE2	1:E:617:ASN:HB3	2.06	0.56
1:G:523:LEU:HD12	2:H:145:MET:CE	2.36	0.56
1:A:513:ILE:CD1	1:A:513:ILE:N	2.66	0.56
2:D:83:GLU:O	2:D:86:ARG:HB3	2.06	0.55
2:F:81:SER:HA	2:F:84:GLU:HG3	1.87	0.55
2:F:48:LEU:HA	2:F:51:MET:CE	2.36	0.55
2:H:48:LEU:HD23	2:H:51:MET:HE1	1.89	0.55
1:E:582:GLU:CG	1:E:583:GLU:N	2.69	0.55
2:B:139:GLU:O	2:B:143:GLN:HG3	2.07	0.55
1:C:628:SER:C	1:C:630:MET:H	2.10	0.55
1:C:633:ARG:HB3	1:C:636:ALA:HB2	1.89	0.55
1:E:528:LEU:HB3	2:F:51:MET:SD	2.46	0.55
2:F:137:ASN:ND2	2:F:140:GLU:HG3	2.17	0.55
1:E:576:ARG:HH12	1:E:604:LYS:NZ	2.04	0.55
1:E:515:LEU:HD12	2:F:144:MET:SD	2.47	0.55
1:C:513:ILE:HD11	1:C:517:VAL:HG12	1.89	0.55
1:C:690:GLN:HG2	1:C:691:HIS:CD2	2.43	0.55
1:G:584:ARG:O	1:G:619:PHE:HB2	2.07	0.55
1:G:673:ALA:HA	1:G:676:THR:CG2	2.35	0.55
1:E:547:THR:O	1:E:547:THR:HG22	2.07	0.54
1:G:516:LYS:HG3	2:H:144:MET:CE	2.37	0.54
1:G:673:ALA:CA	1:G:676:THR:HG22	2.35	0.54
1:C:579:CYS:HB2	1:C:582:GLU:CD	2.27	0.54
1:C:690:GLN:N	1:C:690:GLN:CD	2.60	0.54
2:D:75:LYS:C	2:D:77:LYS:H	2.11	0.54
2:B:56:ASP:OD2	2:B:59:GLY:HA2	2.08	0.54
2:D:137:ASN:HD21	2:D:140:GLU:HG3	1.72	0.54
1:G:513:ILE:N	1:G:513:ILE:HD13	2.18	0.54
2:H:105:LEU:HD11	2:H:124:MET:HE3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:HD12	2:B:144:MET:SD	2.48	0.54
1:C:529:MET:HG3	2:D:41:GLN:HB3	1.90	0.54
2:F:48:LEU:HA	2:F:51:MET:HE3	1.89	0.54
1:C:529:MET:HG2	2:D:36:MET:HE2	1.87	0.54
1:C:633:ARG:CG	1:C:633:ARG:NH1	2.67	0.54
2:F:99:TYR:HB3	2:F:135:GLN:HE21	1.72	0.54
2:F:93:ASP:OD2	2:F:96:GLY:HA2	2.07	0.54
2:H:137:ASN:OD1	2:H:138:TYR:N	2.40	0.54
1:E:537:VAL:HB	1:E:565:PHE:CD2	2.42	0.54
2:D:128:ALA:HB2	2:D:144:MET:SD	2.48	0.54
1:G:538:ARG:HH11	1:G:538:ARG:HG3	1.71	0.54
1:G:551:GLU:OE2	1:G:555:TRP:HZ3	1.90	0.54
2:F:115:LYS:CA	2:F:115:LYS:HE2	2.38	0.54
2:B:139:GLU:HG2	2:B:143:GLN:NE2	2.23	0.53
2:B:29:THR:HG22	2:B:52:ILE:CG1	2.25	0.53
1:E:570:VAL:HG12	1:E:571:CYS:O	2.09	0.53
1:E:654:THR:HG21	1:E:676:THR:CB	2.37	0.53
1:E:525:ALA:HB1	2:F:41:GLN:HE22	1.72	0.53
2:B:36:MET:HG2	2:B:41:GLN:NE2	2.23	0.53
1:C:686:VAL:O	1:C:689:LYS:HG3	2.08	0.53
2:H:69:LEU:HD13	2:H:69:LEU:O	2.08	0.53
1:A:519:VAL:HG11	2:B:145:MET:HG2	1.89	0.53
1:C:537:VAL:HB	1:C:565:PHE:HD2	1.72	0.53
2:B:63:ILE:HA	2:B:67:GLU:OE1	2.08	0.53
1:C:541:ILE:HA	1:C:587:LEU:O	2.09	0.53
2:B:137:ASN:HD21	2:B:140:GLU:HG3	1.74	0.53
2:B:83:GLU:O	2:B:87:GLU:HG3	2.09	0.53
1:A:527:MET:HE3	2:B:75:LYS:HG2	1.91	0.53
2:H:64:ASP:OD1	2:H:67:GLU:HG3	2.09	0.53
1:A:611:MET:CE	1:A:611:MET:HA	2.39	0.53
1:C:579:CYS:HB2	1:C:582:GLU:OE1	2.09	0.53
2:D:4:LEU:C	2:D:5:THR:CG2	2.68	0.53
1:E:528:LEU:O	1:E:532:THR:HG23	2.09	0.53
1:E:539:VAL:HG22	1:E:585:LEU:HB3	1.91	0.53
1:E:673:ALA:O	1:E:676:THR:HG22	2.09	0.53
1:A:585:LEU:HA	1:A:620:ARG:O	2.09	0.53
2:B:48:LEU:HD23	2:B:51:MET:HE3	1.91	0.53
1:E:533:MET:C	1:E:535:SER:H	2.11	0.53
2:F:117:THR:HG22	2:F:120:GLU:H	1.74	0.53
1:G:530:ARG:O	1:G:533:MET:HB3	2.09	0.53
2:H:100:ILE:HG12	2:H:136:VAL:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:ILE:HG13	1:A:642:ASP:N	2.22	0.52
1:E:588:VAL:HG23	1:E:623:VAL:HG22	1.90	0.52
1:A:528:LEU:O	1:A:532:THR:HG23	2.08	0.52
2:B:137:ASN:ND2	2:B:140:GLU:HB2	2.23	0.52
1:C:573:ASP:OD1	1:C:574:LYS:N	2.43	0.52
2:F:123:GLU:O	2:F:127:GLU:HB2	2.09	0.52
1:C:577:LEU:H	1:C:577:LEU:HD22	1.73	0.52
1:E:654:THR:HG21	1:E:676:THR:HB	1.90	0.52
2:F:137:ASN:HD22	2:F:137:ASN:C	2.13	0.52
2:H:101:SER:OG	2:H:104:GLU:HG3	2.09	0.52
1:G:619:PHE:HE1	1:G:621:TYR:HB3	1.73	0.52
1:E:581:GLU:OE2	1:E:617:ASN:N	2.29	0.52
1:E:519:VAL:HG13	2:F:145:MET:CE	2.37	0.52
1:A:589:VAL:HA	1:A:624:PHE:O	2.10	0.52
1:A:670:ARG:O	1:A:674:VAL:HG23	2.09	0.52
2:B:42:ASN:H	2:B:42:ASN:ND2	2.03	0.52
1:G:553:LEU:HD22	1:G:669:PHE:CD2	2.45	0.52
2:H:5:THR:HG23	2:H:8:GLN:HE21	1.74	0.52
1:C:553:LEU:HD12	1:C:626:LEU:HD21	1.91	0.52
2:D:137:ASN:HD22	2:D:137:ASN:C	2.13	0.52
1:E:529:MET:O	1:E:533:MET:HB2	2.09	0.52
1:E:606:LYS:HD2	1:E:637:PHE:CE1	2.45	0.52
1:A:529:MET:HG2	2:B:36:MET:CE	2.40	0.51
1:C:592:THR:CG2	1:C:596:GLY:HA2	2.40	0.51
2:D:117:THR:OG1	2:D:120:GLU:HG3	2.11	0.51
1:C:516:LYS:HG2	2:D:127:GLU:OE2	2.11	0.51
2:F:56:ASP:OD2	2:F:61:GLY:N	2.42	0.51
1:G:680:ALA:O	1:G:684:PHE:HD1	1.93	0.51
1:E:542:LEU:HA	1:E:570:VAL:O	2.11	0.51
1:E:679:ALA:O	1:E:683:THR:HG23	2.10	0.51
1:G:634:PHE:HZ	1:G:660:ASP:HA	1.74	0.51
1:A:628:SER:N	1:A:634:PHE:HE1	2.08	0.51
2:B:116:LEU:HB3	2:B:120:GLU:HG3	1.91	0.51
1:A:519:VAL:CG1	2:B:145:MET:SD	2.98	0.51
1:C:689:LYS:O	1:C:692:ILE:HG12	2.10	0.51
1:C:519:VAL:HG13	2:D:145:MET:CE	2.40	0.51
1:C:519:VAL:HG13	2:D:145:MET:HE2	1.91	0.51
1:C:596:GLY:HA2	1:C:636:ALA:HB3	1.93	0.51
1:G:607:LYS:O	1:G:607:LYS:HE3	2.11	0.51
1:G:620:ARG:HA	1:G:651:SER:O	2.11	0.51
2:B:65:PHE:HB3	2:B:66:PRO:HD3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:532:THR:O	1:E:535:SER:HB2	2.10	0.51
1:E:606:LYS:HG3	1:E:610:PHE:CD2	2.46	0.51
1:E:563:CYS:O	1:E:692:ILE:HD11	2.10	0.51
1:G:592:THR:CG2	1:G:596:GLY:HA2	2.41	0.51
2:B:42:ASN:ND2	2:B:42:ASN:N	2.57	0.51
1:C:682:GLU:C	1:C:684:PHE:H	2.14	0.51
2:F:39:LEU:HD21	2:F:112:LEU:HD21	1.92	0.51
1:A:606:LYS:HG3	1:A:610:PHE:HE2	1.76	0.50
1:A:690:GLN:NE2	1:A:691:HIS:ND1	2.59	0.50
1:E:619:PHE:HD1	1:E:620:ARG:O	1.94	0.50
2:F:4:LEU:HD22	2:F:9:ILE:HG13	1.93	0.50
2:H:99:TYR:HB3	2:H:135:GLN:HB3	1.94	0.50
1:A:544:ALA:HB2	1:A:572:MET:SD	2.51	0.50
1:C:533:MET:SD	1:C:566:ASN:HB2	2.51	0.50
2:H:117:THR:O	2:H:120:GLU:HG2	2.12	0.50
1:A:546:GLU:HB2	1:A:593:PHE:CZ	2.47	0.50
1:C:529:MET:HG2	2:D:36:MET:HE1	1.94	0.50
1:C:648:LEU:N	1:C:648:LEU:HD23	2.26	0.50
1:G:516:LYS:HD2	1:G:516:LYS:H	1.76	0.50
1:G:550:SER:OG	1:G:626:LEU:HD22	2.11	0.50
2:B:7:GLU:O	2:B:11:GLU:HG3	2.11	0.50
2:D:126:ARG:HG2	2:D:126:ARG:O	2.12	0.50
2:D:13:LYS:HA	2:D:65:PHE:CE1	2.47	0.50
1:G:687:ARG:NH1	1:G:687:ARG:HG3	2.27	0.50
1:G:542:LEU:HA	1:G:570:VAL:O	2.12	0.50
2:F:66:PRO:HG3	2:H:69:LEU:CD1	2.41	0.50
2:B:137:ASN:ND2	2:B:140:GLU:CB	2.75	0.50
2:F:88:ALA:O	2:F:91:VAL:HB	2.12	0.49
1:G:620:ARG:NH1	1:G:683:THR:HB	2.27	0.49
1:C:544:ALA:HB3	1:C:590:THR:OG1	2.12	0.49
2:F:69:LEU:CD1	2:H:66:PRO:HG3	2.43	0.49
1:G:575:TYR:CZ	1:G:579:CYS:HB2	2.47	0.49
2:H:105:LEU:HD13	2:H:124:MET:HE3	1.93	0.49
1:C:576:ARG:HB3	1:C:578:SER:OG	2.12	0.49
1:C:634:PHE:HA	3:C:999:FMN:O2	2.12	0.49
1:G:516:LYS:HA	1:G:519:VAL:CG1	2.42	0.49
2:B:125:ILE:C	2:B:127:GLU:N	2.66	0.49
1:E:523:LEU:HB2	2:F:145:MET:CE	2.40	0.49
1:C:695:PRO:HG2	1:C:698:TYR:CD1	2.47	0.49
1:E:596:GLY:CA	1:E:636:ALA:HB3	2.35	0.49
1:G:627:GLY:HA2	3:G:999:FMN:O2'	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:64:ASP:OD1	2:H:66:PRO:HD2	2.12	0.49
1:C:620:ARG:HG3	1:C:620:ARG:HH11	1.77	0.49
2:D:47:GLU:O	2:D:51:MET:HG3	2.12	0.49
1:G:644:LYS:NZ	1:G:648:LEU:HD21	2.27	0.49
1:C:518:LEU:O	1:C:522:VAL:HG12	2.13	0.48
1:G:546:GLU:HG3	1:G:593:PHE:CD1	2.48	0.48
1:G:612:LEU:CD1	1:G:613:LYS:H	2.24	0.48
1:C:539:VAL:O	1:C:567:PRO:HA	2.14	0.48
1:A:637:PHE:O	1:A:641:ILE:HG23	2.13	0.48
1:G:529:MET:O	1:G:533:MET:HB2	2.12	0.48
1:E:559:ALA:O	1:E:562:SER:HB2	2.13	0.48
2:F:4:LEU:CD2	2:F:9:ILE:HG13	2.43	0.48
1:G:692:ILE:HD12	2:H:44:THR:CG2	2.43	0.48
2:D:105:LEU:O	2:D:109:MET:HG2	2.13	0.48
1:E:577:LEU:HD21	1:E:608:SER:HB2	1.95	0.48
2:F:26:THR:HG22	2:F:63:ILE:O	2.14	0.48
1:G:545:THR:HB	1:G:550:SER:HB2	1.94	0.48
1:E:689:LYS:O	1:E:692:ILE:HG22	2.13	0.48
2:F:13:LYS:HG2	2:H:6:GLU:HG3	1.94	0.48
2:B:123:GLU:C	2:B:125:ILE:H	2.17	0.48
2:H:48:LEU:HD23	2:H:51:MET:HE2	1.95	0.48
2:F:55:VAL:HB	2:F:63:ILE:CD1	2.44	0.48
1:G:533:MET:O	1:G:536:ARG:HB2	2.13	0.48
1:G:538:ARG:HG3	1:G:538:ARG:NH1	2.28	0.48
1:G:575:TYR:OH	1:G:579:CYS:HB2	2.14	0.48
2:F:121:VAL:HA	2:F:124:MET:CE	2.44	0.48
1:G:523:LEU:O	1:G:527:MET:HG2	2.13	0.48
2:H:46:ALA:O	2:H:50:ASP:N	2.47	0.48
1:E:540:THR:HB	1:E:586:LEU:HD23	1.96	0.47
1:E:609:LEU:O	1:E:609:LEU:HD23	2.14	0.47
1:C:662:LEU:HD12	1:C:662:LEU:N	2.29	0.47
1:G:609:LEU:HD22	1:G:644:LYS:HE2	1.95	0.47
1:A:514:PRO:HG2	1:A:517:VAL:HB	1.96	0.47
2:F:55:VAL:HB	2:F:63:ILE:HD11	1.95	0.47
1:E:677:PHE:C	1:E:679:ALA:H	2.17	0.47
1:A:592:THR:HG22	1:A:593:PHE:N	2.29	0.47
1:A:622:ALA:HB1	1:A:654:THR:HG22	1.97	0.47
1:E:610:PHE:HB2	1:E:611:MET:CE	2.44	0.47
1:E:673:ALA:HA	1:E:676:THR:CG2	2.43	0.47
1:C:550:SER:OG	1:C:626:LEU:HD22	2.13	0.47
2:H:55:VAL:HG22	2:H:71:MET:CE	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:ASP:OD1	1:A:662:LEU:HB2	2.15	0.47
2:B:5:THR:O	2:B:6:GLU:C	2.53	0.47
2:D:129:ASP:OD1	2:D:134:GLY:N	2.47	0.47
1:C:525:ALA:HB1	2:D:41:GLN:HE22	1.80	0.47
2:F:23:GLY:O	2:H:3:GLN:NE2	2.47	0.47
1:A:696:LYS:HG3	1:A:697:LEU:N	2.30	0.47
1:C:680:ALA:O	1:C:684:PHE:HB2	2.15	0.47
2:F:13:LYS:O	2:F:16:PHE:HB3	2.15	0.47
2:H:97:ASN:CG	2:H:98:GLY:H	2.18	0.47
1:A:529:MET:HG2	2:B:36:MET:HE2	1.97	0.47
2:D:13:LYS:O	2:D:16:PHE:HB3	2.14	0.47
2:H:83:GLU:O	2:H:86:ARG:HG3	2.14	0.47
1:E:603:GLU:O	1:E:605:LEU:N	2.48	0.47
2:F:65:PHE:HB3	2:F:66:PRO:HD3	1.97	0.46
1:A:543:PHE:CE2	1:A:551:GLU:HB2	2.50	0.46
1:A:515:LEU:CD1	2:B:144:MET:HE1	2.45	0.46
1:G:687:ARG:HG3	1:G:687:ARG:HH11	1.80	0.46
1:A:546:GLU:HG2	1:A:599:PRO:HB3	1.98	0.46
2:F:105:LEU:HD13	2:F:105:LEU:O	2.14	0.46
1:G:601:ASN:ND2	1:G:601:ASN:H	2.13	0.46
2:D:78:ASP:C	2:D:80:ASP:H	2.17	0.46
1:G:601:ASN:HD22	1:G:601:ASN:H	1.60	0.46
1:A:685:ASP:OD2	1:E:682:GLU:HG3	2.16	0.46
1:E:675:GLN:O	1:E:679:ALA:HB2	2.15	0.46
1:E:663:SER:O	1:E:665:GLN:N	2.49	0.46
1:G:545:THR:HG21	1:G:551:GLU:HB2	1.96	0.46
1:C:682:GLU:O	1:C:684:PHE:N	2.49	0.46
2:D:65:PHE:HB3	2:D:66:PRO:HD3	1.97	0.46
1:A:577:LEU:HD21	1:A:605:LEU:HD12	1.98	0.46
1:C:596:GLY:CA	1:C:636:ALA:HB3	2.46	0.46
2:D:86:ARG:HG2	5:D:169:HOH:O	2.16	0.46
1:E:623:VAL:CG1	1:E:641:ILE:HD11	2.45	0.46
2:F:116:LEU:HD22	2:F:116:LEU:C	2.36	0.46
2:B:105:LEU:O	2:B:105:LEU:HD23	2.16	0.46
2:B:78:ASP:OD2	2:B:80:ASP:HB2	2.16	0.46
2:B:123:GLU:C	2:B:125:ILE:N	2.69	0.46
2:D:105:LEU:HD13	2:D:105:LEU:O	2.16	0.46
2:D:82:GLU:O	2:D:86:ARG:HB2	2.15	0.46
1:G:622:ALA:HB1	1:G:672:TRP:CZ2	2.51	0.46
1:G:642:ASP:CG	1:G:656:MET:HB2	2.37	0.46
1:G:687:ARG:HG3	2:H:46:ALA:CB	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:591:SER:O	1:E:599:PRO:HD3	2.16	0.45
1:E:643:GLN:HA	1:E:643:GLN:OE1	2.16	0.45
1:A:633:ARG:HG3	1:A:633:ARG:HH11	1.80	0.45
1:A:527:MET:CE	2:B:75:LYS:HG2	2.46	0.45
1:C:545:THR:HG1	3:C:999:FMN:P	2.39	0.45
1:E:515:LEU:HD13	1:E:515:LEU:O	2.16	0.45
1:E:673:ALA:CA	1:E:676:THR:HG22	2.46	0.45
2:H:69:LEU:C	2:H:69:LEU:HD13	2.36	0.45
1:A:514:PRO:HG2	1:A:517:VAL:CG2	2.47	0.45
1:A:519:VAL:CG1	2:B:145:MET:HG2	2.46	0.45
1:C:530:ARG:HH22	2:D:83:GLU:HG2	1.82	0.45
1:E:571:CYS:SG	1:E:573:ASP:OD1	2.75	0.45
2:B:117:THR:HG22	2:B:118:ASP:N	2.31	0.45
2:F:137:ASN:HD21	2:F:140:GLU:CG	2.23	0.45
1:E:527:MET:SD	2:F:75:LYS:HG2	2.56	0.45
1:G:531:LYS:C	1:G:533:MET:N	2.70	0.45
1:G:516:LYS:HG3	2:H:144:MET:HE1	1.99	0.45
1:G:516:LYS:HG3	2:H:144:MET:HE2	1.98	0.45
1:C:606:LYS:O	1:C:609:LEU:HB2	2.17	0.45
2:H:26:THR:HA	2:H:63:ILE:O	2.17	0.45
1:C:576:ARG:C	1:C:578:SER:N	2.70	0.45
2:F:117:THR:HG22	2:F:119:GLU:HB3	1.99	0.45
1:G:619:PHE:C	1:G:619:PHE:CD1	2.90	0.45
2:H:13:LYS:O	2:H:16:PHE:HB3	2.17	0.45
2:B:36:MET:HG2	2:B:41:GLN:HE22	1.82	0.45
1:G:531:LYS:O	1:G:533:MET:N	2.50	0.45
1:G:675:GLN:HE21	1:G:675:GLN:HA	1.82	0.45
2:B:129:ASP:OD1	2:B:134:GLY:N	2.50	0.45
1:E:524:PHE:HD2	2:F:19:PHE:CZ	2.34	0.45
1:C:536:ARG:HG2	1:C:565:PHE:HA	1.99	0.44
2:D:105:LEU:CD1	2:D:124:MET:HE3	2.45	0.44
1:E:677:PHE:C	1:E:679:ALA:N	2.71	0.44
2:H:26:THR:HB	2:H:62:THR:HB	2.00	0.44
1:A:695:PRO:HB2	1:A:698:TYR:HD1	1.82	0.44
1:E:521:ALA:O	1:E:524:PHE:HB3	2.17	0.44
2:F:117:THR:CG2	2:F:119:GLU:HB3	2.47	0.44
2:H:138:TYR:HA	2:H:141:PHE:HB3	1.99	0.44
1:E:572:MET:C	1:E:574:LYS:H	2.21	0.44
2:F:116:LEU:CD1	2:F:116:LEU:H	2.30	0.44
1:E:522:VAL:CG2	2:F:88:ALA:HB1	2.47	0.44
1:G:576:ARG:NE	1:G:578:SER:OG	2.41	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:582:GLU:O	1:G:583:GLU:HB2	2.17	0.44
1:A:513:ILE:H	1:A:513:ILE:HD12	1.79	0.44
1:A:542:LEU:HA	1:A:570:VAL:O	2.16	0.44
2:B:115:LYS:HD2	2:B:115:LYS:H	1.82	0.44
2:B:126:ARG:HB2	2:B:126:ARG:HH11	1.82	0.44
1:C:536:ARG:HG2	1:C:564:ALA:O	2.17	0.44
2:H:48:LEU:HA	2:H:51:MET:HE2	1.99	0.44
2:H:97:ASN:CG	2:H:98:GLY:N	2.71	0.44
1:A:598:CYS:HG	1:A:603:GLU:HG2	1.78	0.44
1:C:641:ILE:HD11	1:C:645:LEU:HD11	1.98	0.44
1:G:537:VAL:HG13	1:G:565:PHE:CD2	2.53	0.44
2:H:125:ILE:HG23	2:H:136:VAL:HG23	1.99	0.44
1:A:537:VAL:HA	5:A:65:HOH:O	2.16	0.44
1:C:629:SER:HB3	1:C:660:ASP:OD2	2.17	0.44
1:G:639:HIS:O	1:G:643:GLN:HB2	2.17	0.44
2:B:85:ILE:O	2:B:88:ALA:HB3	2.17	0.44
1:E:539:VAL:O	1:E:567:PRO:HA	2.18	0.44
1:E:652:GLN:NE2	1:E:655:PRO:HA	2.33	0.44
1:G:541:ILE:HG12	1:G:587:LEU:HB2	1.99	0.44
1:A:694:ILE:HB	1:A:695:PRO:CD	2.48	0.44
1:C:536:ARG:NH2	1:C:562:SER:O	2.51	0.44
1:C:577:LEU:H	1:C:577:LEU:CD2	2.30	0.44
1:E:587:LEU:HD22	1:E:622:ALA:HB3	1.99	0.44
2:F:26:THR:HG22	2:F:63:ILE:C	2.37	0.44
2:H:65:PHE:HB3	2:H:66:PRO:HD3	1.98	0.44
2:H:55:VAL:HG22	2:H:71:MET:HE3	2.00	0.44
1:C:581:GLU:CD	1:C:617:ASN:HB2	2.38	0.43
2:D:123:GLU:HA	2:D:123:GLU:OE2	2.17	0.43
2:D:29:THR:CG2	2:D:52:ILE:HG13	2.45	0.43
1:G:640:ASP:O	1:G:644:LYS:HB3	2.17	0.43
2:H:3:GLN:HB3	2:H:3:GLN:HE21	1.55	0.43
1:A:623:VAL:HG12	1:A:624:PHE:N	2.32	0.43
1:C:549:LYS:HB2	3:C:999:FMN:O3P	2.19	0.43
2:D:141:PHE:O	2:D:144:MET:HB3	2.19	0.43
1:E:653:LEU:HD13	1:E:653:LEU:O	2.18	0.43
1:G:644:LYS:NZ	1:G:648:LEU:HD11	2.33	0.43
1:A:620:ARG:HH22	1:E:687:ARG:HA	1.82	0.43
1:C:546:GLU:C	1:C:548:GLY:H	2.21	0.43
1:C:690:GLN:H	1:C:690:GLN:CD	2.20	0.43
2:D:79:THR:O	2:D:79:THR:CG2	2.67	0.43
1:E:610:PHE:HB2	1:E:611:MET:HE1	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:621:TYR:CD2	1:E:645:LEU:HD13	2.53	0.43
2:H:117:THR:HB	2:H:120:GLU:HG2	2.01	0.43
2:H:55:VAL:O	2:H:57:ALA:N	2.46	0.43
1:A:546:GLU:OE1	1:C:633:ARG:NH2	2.51	0.43
1:E:533:MET:C	1:E:535:SER:N	2.71	0.43
1:A:590:THR:O	1:A:625:GLY:HA2	2.18	0.43
2:B:137:ASN:ND2	2:B:137:ASN:C	2.71	0.43
2:B:5:THR:O	2:B:8:GLN:N	2.52	0.43
1:E:529:MET:HG2	2:F:36:MET:HE3	2.00	0.43
1:E:582:GLU:HG2	1:E:583:GLU:H	1.78	0.43
1:C:576:ARG:O	1:C:577:LEU:C	2.57	0.43
1:C:609:LEU:O	1:C:611:MET:N	2.52	0.43
1:C:519:VAL:HG13	2:D:145:MET:SD	2.59	0.43
2:D:4:LEU:O	2:D:5:THR:CB	2.65	0.43
1:E:592:THR:HG21	1:E:596:GLY:HA2	2.00	0.43
1:E:693:GLN:NE2	1:E:696:LYS:HZ3	2.15	0.43
1:G:519:VAL:O	1:G:522:VAL:HG12	2.19	0.43
1:A:659:GLY:C	1:A:665:GLN:HG3	2.38	0.43
1:C:624:PHE:CE1	1:C:669:PHE:HA	2.54	0.43
1:C:670:ARG:HG3	1:C:670:ARG:HH11	1.84	0.43
1:E:553:LEU:HD12	1:E:626:LEU:HD11	2.01	0.43
1:G:592:THR:OG1	1:G:635:CYS:HA	2.18	0.43
2:B:126:ARG:CB	2:B:126:ARG:HH11	2.32	0.43
1:E:583:GLU:HA	1:E:583:GLU:OE1	2.18	0.43
1:E:581:GLU:OE2	1:E:617:ASN:CB	2.67	0.43
1:E:680:ALA:O	1:E:684:PHE:HB2	2.19	0.43
2:B:48:LEU:HD23	2:B:51:MET:CE	2.49	0.43
1:G:568:LYS:HG3	1:G:570:VAL:HG23	2.00	0.43
1:A:694:ILE:HB	1:A:695:PRO:HD2	2.01	0.42
2:B:29:THR:HG21	2:B:49:GLN:CD	2.39	0.42
1:C:592:THR:HG21	1:C:596:GLY:HA2	2.02	0.42
1:E:619:PHE:C	1:E:619:PHE:CD1	2.92	0.42
1:E:675:GLN:O	1:E:679:ALA:CB	2.67	0.42
1:G:513:ILE:H	1:G:513:ILE:CD1	2.24	0.42
1:A:515:LEU:HD23	2:B:124:MET:HG2	2.00	0.42
1:A:577:LEU:O	1:A:578:SER:C	2.56	0.42
1:E:530:ARG:HG2	1:E:530:ARG:HH11	1.85	0.42
1:A:689:LYS:NZ	1:A:689:LYS:CB	2.82	0.42
1:E:513:ILE:CD1	1:E:513:ILE:N	2.81	0.42
1:G:615:LEU:HG	1:G:617:ASN:O	2.20	0.42
2:H:65:PHE:N	2:H:66:PRO:CD	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:GLU:O	1:A:667:ASP:C	2.58	0.42
2:B:3:GLN:CD	2:B:3:GLN:N	2.73	0.42
1:C:670:ARG:O	1:C:674:VAL:HG23	2.19	0.42
1:E:663:SER:O	1:E:664:GLY:C	2.58	0.42
1:G:522:VAL:CG2	2:H:91:VAL:HG21	2.42	0.42
2:H:41:GLN:HB2	2:H:41:GLN:HE21	1.60	0.42
2:H:57:ALA:O	2:H:59:GLY:N	2.53	0.42
1:A:587:LEU:HD22	1:A:622:ALA:HB3	2.02	0.42
1:E:610:PHE:CZ	1:E:640:ASP:HB3	2.55	0.42
1:E:681:CYS:HA	1:E:686:VAL:HG23	2.02	0.42
2:B:126:ARG:HB2	2:B:126:ARG:NH1	2.35	0.42
2:B:130:ILE:CG1	2:B:140:GLU:HG2	2.50	0.42
1:C:519:VAL:O	1:C:522:VAL:HG13	2.20	0.42
1:C:628:SER:H	3:C:999:FMN:H1'1	1.83	0.42
1:G:652:GLN:HE21	1:G:655:PRO:HA	1.82	0.42
1:A:672:TRP:HA	1:A:675:GLN:CG	2.50	0.42
2:D:56:ASP:OD2	2:D:59:GLY:HA2	2.20	0.42
2:F:17:SER:HA	2:F:20:ASP:HB3	2.02	0.42
2:F:56:ASP:OD1	2:F:62:THR:O	2.38	0.42
1:G:563:CYS:O	1:G:564:ALA:HB2	2.20	0.42
2:B:3:GLN:NE2	2:B:3:GLN:N	2.68	0.41
1:C:631:TYR:HA	1:C:632:PRO:HD3	1.91	0.41
1:C:691:HIS:O	1:C:692:ILE:C	2.58	0.41
1:E:610:PHE:HZ	1:E:640:ASP:HB3	1.85	0.41
2:F:128:ALA:HB2	2:F:144:MET:SD	2.60	0.41
1:A:545:THR:HG1	3:A:999:FMN:P	2.42	0.41
1:E:598:CYS:O	1:E:599:PRO:O	2.38	0.41
1:A:583:GLU:HG3	5:A:15:HOH:O	2.20	0.41
2:B:138:TYR:CZ	2:B:142:VAL:HG21	2.55	0.41
1:C:598:CYS:SG	1:C:606:LYS:HB2	2.61	0.41
1:G:519:VAL:HA	1:G:522:VAL:CG1	2.51	0.41
2:D:143:GLN:O	2:D:147:ALA:HB2	2.20	0.41
2:F:26:THR:HG21	2:F:62:THR:OG1	2.21	0.41
2:H:5:THR:HG23	2:H:8:GLN:NE2	2.35	0.41
1:C:697:LEU:HD23	1:C:697:LEU:C	2.41	0.41
1:G:686:VAL:O	1:G:687:ARG:C	2.57	0.41
2:F:127:GLU:O	2:F:144:MET:HE1	2.20	0.41
1:A:689:LYS:NZ	1:A:689:LYS:HB2	2.35	0.41
1:C:607:LYS:O	1:C:611:MET:HG2	2.21	0.41
1:C:638:ALA:O	1:C:641:ILE:HG23	2.20	0.41
1:C:649:GLY:O	1:C:650:ALA:C	2.59	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:675:GLN:HE21	1:G:675:GLN:CA	2.33	0.41
1:G:530:ARG:NH1	2:H:84:GLU:CD	2.73	0.41
1:A:592:THR:CG2	1:A:593:PHE:N	2.84	0.41
1:A:672:TRP:O	1:A:676:THR:HG22	2.20	0.41
1:C:692:ILE:HD12	2:D:44:THR:HG22	2.03	0.41
2:D:37:ARG:HG2	2:D:42:ASN:HD22	1.84	0.41
1:G:590:THR:O	1:G:625:GLY:HA2	2.21	0.41
1:G:653:LEU:HD11	1:G:679:ALA:HB3	2.03	0.41
2:H:42:ASN:C	2:H:42:ASN:HD22	2.24	0.41
1:G:527:MET:H	1:G:527:MET:HG2	1.68	0.41
2:H:29:THR:CG2	2:H:52:ILE:HG13	2.41	0.41
1:C:621:TYR:CE1	1:C:652:GLN:N	2.88	0.41
1:C:680:ALA:O	1:C:684:PHE:HD1	2.04	0.41
1:E:546:GLU:HB2	1:E:593:PHE:CZ	2.56	0.41
1:G:573:ASP:OD1	1:G:574:LYS:HG2	2.19	0.41
2:B:101:SER:OG	2:B:104:GLU:HG3	2.21	0.41
1:E:589:VAL:HA	1:E:624:PHE:O	2.21	0.41
1:G:524:PHE:HD2	2:H:19:PHE:CZ	2.39	0.41
1:G:579:CYS:HA	1:G:582:GLU:HG3	2.02	0.41
1:G:553:LEU:HD22	1:G:669:PHE:CG	2.56	0.41
1:A:581:GLU:OE2	1:A:617:ASN:N	2.44	0.40
1:A:528:LEU:HB3	2:B:51:MET:SD	2.61	0.40
1:C:621:TYR:CD1	1:C:621:TYR:N	2.89	0.40
1:C:670:ARG:HG3	1:C:670:ARG:NH1	2.36	0.40
1:E:537:VAL:HG21	1:E:684:PHE:CD2	2.56	0.40
1:E:561:PHE:CE1	1:E:677:PHE:HB2	2.55	0.40
1:G:644:LYS:HZ2	1:G:648:LEU:HD21	1.85	0.40
1:A:546:GLU:HG3	1:A:593:PHE:CE1	2.56	0.40
2:D:27:ILE:HB	2:D:63:ILE:HB	2.04	0.40
1:C:662:LEU:CD1	1:C:662:LEU:N	2.84	0.40
1:E:528:LEU:HD21	2:F:71:MET:CE	2.51	0.40
1:E:598:CYS:C	1:E:599:PRO:O	2.60	0.40
1:G:527:MET:CE	2:H:75:LYS:HG2	2.52	0.40
2:D:109:MET:HE3	2:D:109:MET:HA	2.03	0.40
1:G:654:THR:HG21	1:G:676:THR:HB	2.03	0.40
2:B:137:ASN:ND2	2:B:140:GLU:N	2.48	0.40
2:B:77:LYS:HA	2:B:77:LYS:HD3	1.91	0.40
1:C:696:LYS:HB2	1:C:696:LYS:HE2	1.93	0.40
2:D:137:ASN:ND2	2:D:137:ASN:C	2.75	0.40
2:H:57:ALA:C	2:H:59:GLY:H	2.24	0.40
2:H:74:ARG:O	2:H:77:LYS:HB3	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	187/219 (85%)	165 (88%)	17 (9%)	5 (3%)	6	9
1	C	186/219 (85%)	142 (76%)	34 (18%)	10 (5%)	2	2
1	E	187/219 (85%)	156 (83%)	19 (10%)	12 (6%)	1	1
1	G	185/219 (84%)	156 (84%)	22 (12%)	7 (4%)	4	4
2	B	143/149 (96%)	125 (87%)	16 (11%)	2 (1%)	13	23
2	D	143/149 (96%)	129 (90%)	10 (7%)	4 (3%)	6	8
2	F	143/149 (96%)	128 (90%)	11 (8%)	4 (3%)	6	8
2	H	143/149 (96%)	113 (79%)	22 (15%)	8 (6%)	2	2
All	All	1317/1472 (90%)	1114 (85%)	151 (12%)	52 (4%)	3	4

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	609	LEU
1	C	689	LYS
2	D	5	THR
2	D	78	ASP
2	D	79	THR
1	E	695	PRO
1	G	603	GLU
1	G	632	PRO
1	G	695	PRO
1	A	619	PHE
2	B	132	GLY
1	C	610	PHE
1	C	648	LEU
1	C	683	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	690	GLN
1	E	564	ALA
1	E	582	GLU
1	E	583	GLU
1	E	604	LYS
1	E	664	GLY
2	F	24	ASP
2	F	115	LYS
2	F	129	ASP
1	G	564	ALA
2	H	56	ASP
2	H	58	ASP
1	A	609	LEU
1	E	603	GLU
2	F	78	ASP
1	G	514	PRO
1	G	532	THR
1	A	601	ASN
1	A	695	PRO
1	E	573	ASP
1	E	685	ASP
2	H	71	MET
2	B	4	LEU
1	C	612	LEU
1	C	649	GLY
1	G	531	LYS
2	H	57	ALA
2	H	127	GLU
1	A	629	SER
1	C	607	LYS
2	D	56	ASP
1	E	599	PRO
1	E	594	GLY
1	E	632	PRO
2	H	96	GLY
2	H	130	ILE
2	H	98	GLY
1	C	548	GLY

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	157/190 (83%)	138 (88%)	19 (12%)	6	11
1	C	154/190 (81%)	137 (89%)	17 (11%)	7	13
1	E	155/190 (82%)	139 (90%)	16 (10%)	8	16
1	G	154/190 (81%)	134 (87%)	20 (13%)	5	9
2	B	124/127 (98%)	115 (93%)	9 (7%)	16	31
2	D	122/127 (96%)	114 (93%)	8 (7%)	19	36
2	F	124/127 (98%)	114 (92%)	10 (8%)	14	26
2	H	119/127 (94%)	114 (96%)	5 (4%)	34	59
All	All	1109/1268 (88%)	1005 (91%)	104 (9%)	10	19

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	515	LEU
1	A	519	VAL
1	A	523	LEU
1	A	532	THR
1	A	537	VAL
1	A	555	TRP
1	A	560	LEU
1	A	583	GLU
1	A	584	ARG
1	A	586	LEU
1	A	609	LEU
1	A	641	ILE
1	A	643	GLN
1	A	653	LEU
1	A	665	GLN
1	A	675	GLN
1	A	683	THR
1	A	696	LYS
1	A	697	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	3	GLN
2	B	6	GLU
2	B	18	LEU
2	B	42	ASN
2	B	70	THR
2	B	80	ASP
2	B	122	ASP
2	B	137	ASN
2	B	145	MET
1	C	512	GLU
1	C	519	VAL
1	C	522	VAL
1	C	523	LEU
1	C	532	THR
1	C	555	TRP
1	C	556	ASP
1	C	560	LEU
1	C	567	PRO
1	C	584	ARG
1	C	586	LEU
1	C	619	PHE
1	C	633	ARG
1	C	641	ILE
1	C	643	GLN
1	C	648	LEU
1	C	685	ASP
2	D	26	THR
2	D	45	GLU
2	D	69	LEU
2	D	76	MET
2	D	80	ASP
2	D	119	GLU
2	D	137	ASN
2	D	144	MET
1	E	523	LEU
1	E	555	TRP
1	E	560	LEU
1	E	583	GLU
1	E	586	LEU
1	E	588	VAL
1	E	609	LEU
1	E	640	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	653	LEU
1	E	671	SER
1	E	675	GLN
1	E	682	GLU
1	E	683	THR
1	E	685	ASP
1	E	690	GLN
1	E	695	PRO
2	F	4	LEU
2	F	18	LEU
2	F	26	THR
2	F	30	LYS
2	F	42	ASN
2	F	71	MET
2	F	86	ARG
2	F	116	LEU
2	F	137	ASN
2	F	144	MET
1	G	513	ILE
1	G	515	LEU
1	G	516	LYS
1	G	527	MET
1	G	537	VAL
1	G	555	TRP
1	G	556	ASP
1	G	560	LEU
1	G	582	GLU
1	G	585	LEU
1	G	586	LEU
1	G	601	ASN
1	G	607	LYS
1	G	611	MET
1	G	666	GLU
1	G	675	GLN
1	G	687	ARG
1	G	693	GLN
1	G	697	LEU
1	G	698	TYR
2	H	3	GLN
2	H	42	ASN
2	H	86	ARG
2	H	105	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	144	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	639	HIS
1	A	652	GLN
1	A	675	GLN
1	A	690	GLN
2	B	3	GLN
2	B	41	GLN
2	B	42	ASN
2	B	135	GLN
2	B	137	ASN
2	B	143	GLN
1	C	675	GLN
1	C	691	HIS
2	D	8	GLN
2	D	41	GLN
2	D	42	ASN
2	D	135	GLN
2	D	137	ASN
1	E	652	GLN
1	E	675	GLN
1	E	690	GLN
1	E	693	GLN
2	F	41	GLN
2	F	42	ASN
2	F	135	GLN
2	F	137	ASN
1	G	601	ASN
1	G	617	ASN
1	G	652	GLN
1	G	675	GLN
1	G	691	HIS
2	H	3	GLN
2	H	8	GLN
2	H	41	GLN
2	H	42	ASN
2	H	53	ASN
2	H	135	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FMN	A	999	-	31,33,33	4.94	20 (64%)	38,50,50	3.33	17 (44%)
3	FMN	C	999	-	31,33,33	4.93	20 (64%)	38,50,50	3.30	15 (39%)
3	FMN	E	999	-	31,33,33	5.02	19 (61%)	38,50,50	3.29	13 (34%)
3	FMN	G	999	-	31,33,33	4.85	20 (64%)	38,50,50	3.27	14 (36%)

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	FMN	A	999	-	-	0/16/18/18	0/3/3/3
3	FMN	C	999	-	-	0/16/18/18	0/3/3/3
3	FMN	E	999	-	-	0/16/18/18	0/3/3/3
3	FMN	G	999	-	-	0/16/18/18	0/3/3/3

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	999	FMN	C2'-C3'	-5.72	1.42	1.53
3	A	999	FMN	C2'-C3'	-5.15	1.43	1.53
3	C	999	FMN	C2'-C3'	-4.66	1.44	1.53
3	G	999	FMN	C2'-C3'	-4.51	1.44	1.53
3	E	999	FMN	O2'-C2'	-3.93	1.34	1.43
3	G	999	FMN	O2'-C2'	-3.67	1.35	1.43
3	E	999	FMN	C4-C4A	-3.50	1.34	1.41
3	A	999	FMN	C1'-N10	-3.47	1.44	1.48
3	C	999	FMN	O2'-C2'	-3.42	1.35	1.43
3	A	999	FMN	C4-C4A	-3.39	1.34	1.41
3	A	999	FMN	O2'-C2'	-3.37	1.36	1.43
3	G	999	FMN	C4-C4A	-3.25	1.35	1.41
3	E	999	FMN	C1'-N10	-3.17	1.45	1.48
3	C	999	FMN	C4-C4A	-3.15	1.35	1.41
3	G	999	FMN	C1'-N10	-3.08	1.45	1.48
3	A	999	FMN	P-O1P	-2.84	1.41	1.50
3	E	999	FMN	P-O1P	-2.62	1.41	1.50
3	G	999	FMN	P-O1P	-2.58	1.42	1.50
3	C	999	FMN	P-O1P	-2.55	1.42	1.50
3	E	999	FMN	C7M-C7	-2.48	1.46	1.51
3	A	999	FMN	C7M-C7	-2.41	1.46	1.51
3	C	999	FMN	C1'-N10	-2.38	1.45	1.48
3	C	999	FMN	C7M-C7	-2.23	1.46	1.51
3	A	999	FMN	P-O3P	-2.23	1.45	1.54
3	G	999	FMN	P-O3P	-2.18	1.45	1.54
3	G	999	FMN	C7M-C7	-2.10	1.46	1.51
3	C	999	FMN	P-O3P	-2.08	1.46	1.54
3	C	999	FMN	C5'-C4'	3.13	1.56	1.51
3	A	999	FMN	C10-N1	3.42	1.38	1.33
3	A	999	FMN	C6-C5A	3.56	1.47	1.41
3	C	999	FMN	C10-N1	3.62	1.38	1.33
3	E	999	FMN	C6-C5A	3.67	1.47	1.41
3	G	999	FMN	C6-C5A	3.91	1.47	1.41
3	G	999	FMN	C10-N1	4.02	1.38	1.33
3	C	999	FMN	C6-C5A	4.07	1.47	1.41
3	G	999	FMN	C5'-C4'	4.16	1.58	1.51
3	E	999	FMN	C10-N1	4.18	1.39	1.33
3	E	999	FMN	C5'-C4'	4.18	1.58	1.51
3	E	999	FMN	O3'-C3'	4.59	1.53	1.43
3	C	999	FMN	O3'-C3'	4.84	1.54	1.43
3	A	999	FMN	C5'-C4'	4.98	1.59	1.51
3	E	999	FMN	C6-C7	4.98	1.51	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	999	FMN	C6-C7	4.98	1.51	1.37
3	E	999	FMN	C2-N3	5.10	1.48	1.38
3	G	999	FMN	C2-N3	5.15	1.48	1.38
3	A	999	FMN	C6-C7	5.20	1.51	1.37
3	G	999	FMN	O3'-C3'	5.24	1.55	1.43
3	C	999	FMN	C2-N3	5.26	1.48	1.38
3	C	999	FMN	C6-C7	5.27	1.51	1.37
3	A	999	FMN	O3'-C3'	5.32	1.55	1.43
3	C	999	FMN	C8-C7	5.35	1.54	1.41
3	G	999	FMN	C8-C7	5.44	1.54	1.41
3	A	999	FMN	C8-C7	5.48	1.54	1.41
3	E	999	FMN	C8-C7	5.52	1.54	1.41
3	A	999	FMN	C9A-C5A	5.55	1.54	1.42
3	A	999	FMN	C2-N3	5.82	1.49	1.38
3	C	999	FMN	C9A-C5A	5.87	1.54	1.42
3	G	999	FMN	C9A-C5A	5.93	1.54	1.42
3	E	999	FMN	C9A-C5A	6.24	1.55	1.42
3	A	999	FMN	C9A-N10	8.19	1.49	1.38
3	G	999	FMN	C9A-N10	8.31	1.49	1.38
3	A	999	FMN	C9-C9A	8.75	1.59	1.40
3	G	999	FMN	C9-C9A	8.90	1.59	1.40
3	C	999	FMN	C9-C9A	8.98	1.59	1.40
3	C	999	FMN	C9A-N10	9.06	1.50	1.38
3	E	999	FMN	C9A-N10	9.20	1.50	1.38
3	A	999	FMN	C5A-N5	9.24	1.49	1.35
3	E	999	FMN	C9-C9A	9.30	1.60	1.40
3	C	999	FMN	C4-N3	9.44	1.50	1.33
3	E	999	FMN	C5A-N5	9.54	1.49	1.35
3	G	999	FMN	C4-N3	9.56	1.50	1.33
3	G	999	FMN	C5A-N5	9.81	1.50	1.35
3	E	999	FMN	C4-N3	9.91	1.51	1.33
3	A	999	FMN	C4-N3	9.96	1.51	1.33
3	C	999	FMN	C5A-N5	10.46	1.51	1.35
3	G	999	FMN	C4A-C10	11.13	1.60	1.41
3	C	999	FMN	C4A-C10	11.60	1.61	1.41
3	E	999	FMN	C4A-C10	11.63	1.61	1.41
3	A	999	FMN	C4A-C10	11.91	1.61	1.41

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	999	FMN	C7M-C7-C6	-5.27	107.14	120.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	999	FMN	C7M-C7-C6	-5.09	107.58	120.34
3	A	999	FMN	C7M-C7-C6	-5.05	107.68	120.34
3	C	999	FMN	C7M-C7-C6	-4.97	107.88	120.34
3	A	999	FMN	C4A-C4-N3	-4.59	116.95	123.48
3	G	999	FMN	C4A-C4-N3	-4.36	117.27	123.48
3	E	999	FMN	C4A-C4-N3	-4.34	117.31	123.48
3	C	999	FMN	C4A-C4-N3	-4.32	117.33	123.48
3	A	999	FMN	C9A-C5A-N5	-3.77	116.62	122.24
3	C	999	FMN	C9A-C5A-N5	-3.72	116.70	122.24
3	G	999	FMN	C9A-C5A-N5	-3.64	116.82	122.24
3	E	999	FMN	C9A-C5A-N5	-3.61	116.87	122.24
3	C	999	FMN	O5'-C5'-C4'	-3.44	100.18	109.36
3	A	999	FMN	O5'-C5'-C4'	-3.22	100.77	109.36
3	A	999	FMN	O3'-C3'-C4'	-2.82	101.84	108.82
3	A	999	FMN	O4'-C4'-C5'	-2.70	103.97	110.00
3	G	999	FMN	O5'-C5'-C4'	-2.57	102.49	109.36
3	E	999	FMN	O5'-C5'-C4'	-2.51	102.67	109.36
3	E	999	FMN	O3'-C3'-C4'	-2.36	102.98	108.82
3	A	999	FMN	C4A-C10-N10	-2.30	118.92	120.52
3	C	999	FMN	O3'-C3'-C4'	-2.11	103.59	108.82
3	G	999	FMN	O3'-C3'-C4'	-2.10	103.62	108.82
3	C	999	FMN	C4-C4A-C10	-2.04	118.32	119.96
3	G	999	FMN	C4-C4A-N5	2.18	121.07	118.68
3	C	999	FMN	C4'-C3'-C2'	2.19	118.12	113.41
3	G	999	FMN	C4'-C3'-C2'	2.20	118.15	113.41
3	A	999	FMN	O2P-P-O5'	2.23	112.67	106.73
3	E	999	FMN	C4'-C3'-C2'	2.41	118.61	113.41
3	C	999	FMN	C4-C4A-N5	2.59	121.52	118.68
3	A	999	FMN	C4'-C3'-C2'	2.96	119.79	113.41
3	A	999	FMN	O3P-P-O2P	2.97	119.61	107.61
3	C	999	FMN	O3P-P-O2P	2.98	119.62	107.61
3	G	999	FMN	O3P-P-O2P	3.00	119.70	107.61
3	E	999	FMN	O3P-P-O2P	3.13	120.25	107.61
3	E	999	FMN	C6-C5A-N5	3.20	122.72	118.97
3	A	999	FMN	C1'-N10-C9A	3.28	121.35	118.35
3	A	999	FMN	C1'-N10-C10	3.32	121.91	118.50
3	G	999	FMN	C6-C5A-N5	3.44	123.01	118.97
3	A	999	FMN	C6-C5A-N5	3.84	123.47	118.97
3	C	999	FMN	C6-C5A-N5	3.86	123.50	118.97
3	C	999	FMN	C7M-C7-C8	4.50	130.17	120.72
3	A	999	FMN	C7M-C7-C8	4.56	130.29	120.72
3	G	999	FMN	C7M-C7-C8	4.67	130.52	120.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	999	FMN	C7M-C7-C8	4.74	130.67	120.72
3	G	999	FMN	C5A-C9A-N10	5.80	121.97	117.66
3	E	999	FMN	C5A-C9A-N10	5.86	122.01	117.66
3	C	999	FMN	C5A-C9A-N10	6.10	122.19	117.66
3	C	999	FMN	C1'-N10-C9A	6.61	124.41	118.35
3	E	999	FMN	C1'-N10-C9A	6.82	124.59	118.35
3	A	999	FMN	C4A-N5-C5A	6.90	124.05	116.76
3	G	999	FMN	C1'-N10-C9A	7.08	124.83	118.35
3	E	999	FMN	C4A-N5-C5A	7.13	124.29	116.76
3	C	999	FMN	C4A-N5-C5A	7.17	124.33	116.76
3	G	999	FMN	C4A-N5-C5A	7.17	124.33	116.76
3	A	999	FMN	C5A-C9A-N10	7.17	122.98	117.66
3	A	999	FMN	C4-N3-C2	10.76	124.57	115.16
3	C	999	FMN	C4-N3-C2	10.86	124.66	115.16
3	G	999	FMN	C4-N3-C2	10.94	124.72	115.16
3	E	999	FMN	C4-N3-C2	10.95	124.73	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	FMN	1	0
3	C	999	FMN	5	0
3	E	999	FMN	1	0
3	G	999	FMN	1	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	189/219 (86%)	-0.16	0 100 100	31, 51, 72, 86	0
1	C	188/219 (85%)	0.27	7 (3%) 42 44	32, 68, 94, 102	0
1	E	189/219 (86%)	0.11	3 (1%) 72 73	41, 69, 85, 92	0
1	G	187/219 (85%)	0.64	16 (8%) 11 11	48, 81, 98, 104	0
2	B	145/149 (97%)	-0.18	2 (1%) 75 76	34, 58, 86, 97	0
2	D	145/149 (97%)	-0.11	2 (1%) 75 76	27, 43, 72, 86	0
2	F	145/149 (97%)	-0.13	1 (0%) 87 88	27, 55, 77, 87	0
2	H	145/149 (97%)	0.46	10 (6%) 18 18	52, 83, 102, 105	0
All	All	1333/1472 (90%)	0.12	41 (3%) 49 52	27, 64, 94, 105	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	686	VAL	5.1
1	G	593	PHE	4.2
1	C	593	PHE	3.7
1	G	681	CYS	3.7
2	H	92	PHE	3.4
1	G	628	SER	3.2
1	G	662	LEU	3.1
2	H	116	LEU	3.1
2	H	48	LEU	3.0
1	G	698	TYR	3.0
2	B	128	ALA	2.9
1	G	537	VAL	2.8
2	D	3	GLN	2.8
1	G	577	LEU	2.7
2	H	99	TYR	2.7
1	C	662	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	75	LYS	2.6
1	C	594	GLY	2.5
1	G	685	ASP	2.5
2	H	44	THR	2.5
1	G	647	HIS	2.4
1	E	641	ILE	2.4
1	C	615	LEU	2.4
1	G	564	ALA	2.4
1	G	633	ARG	2.4
2	H	138	TYR	2.3
1	G	649	GLY	2.3
1	C	580	LEU	2.3
1	G	653	LEU	2.3
2	H	49	GLN	2.3
2	H	136	VAL	2.3
2	H	127	GLU	2.3
1	G	677	PHE	2.2
2	H	100	ILE	2.2
1	E	645	LEU	2.2
1	C	582	GLU	2.1
1	E	577	LEU	2.1
2	B	130	ILE	2.0
1	C	691	HIS	2.0
2	F	76	MET	2.0
1	G	630	MET	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 95th percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	CA	D	203	1/1	0.97	0.16	1.51	37,37,37,37	0
4	CA	D	204	1/1	0.98	0.14	1.04	36,36,36,36	0
3	FMN	C	999	31/31	0.89	0.25	0.78	91,93,94,95	0
4	CA	F	204	1/1	0.98	0.15	0.76	39,39,39,39	0
4	CA	B	202	1/1	0.98	0.14	0.69	41,41,41,41	0
4	CA	F	203	1/1	0.98	0.12	0.50	39,39,39,39	0
3	FMN	G	999	31/31	0.88	0.25	0.42	93,97,99,99	0
4	CA	D	202	1/1	0.99	0.12	0.36	43,43,43,43	0
3	FMN	A	999	31/31	0.95	0.17	-0.05	49,55,58,59	0
3	FMN	E	999	31/31	0.96	0.16	-0.06	57,61,64,65	0
4	CA	D	201	1/1	0.99	0.12	-0.09	43,43,43,43	0
4	CA	F	201	1/1	0.97	0.14	-0.30	63,63,63,63	0
4	CA	H	201	1/1	0.94	0.13	-0.54	88,88,88,88	0
4	CA	F	202	1/1	0.94	0.09	-1.20	73,73,73,73	0
4	CA	B	201	1/1	0.99	0.12	-1.28	44,44,44,44	0
4	CA	H	202	1/1	0.99	0.09	-1.35	67,67,67,67	0
4	CA	H	204	1/1	0.96	0.10	-1.56	113,113,113,113	0
4	CA	B	204	1/1	0.80	0.06	-1.77	77,77,77,77	0
4	CA	H	203	1/1	0.90	0.04	-2.19	95,95,95,95	0
4	CA	B	203	1/1	0.98	0.05	-3.42	61,61,61,61	0

6.5 Other polymers

There are no such residues in this entry.