

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	1KF6
Title	:	E. coli Quinol-Fumarate Reductase with Bound Inhibitor HQNO
Authors	:	Iverson, T.M.; Luna-Chavez, C.; Croal, L.R.; Cecchini, G.; Rees, D.C.
Deposited on	:	2001-11-19
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org* A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.70 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.



Motric	Whole archive	Similar resolution				
WIEUTC	$(\# \mathbf{Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$				
Clashscore	141614	3122(2.70-2.70)				
Ramachandran outliers	138981	3069(2.70-2.70)				
Sidechain outliers	138945	3069 (2.70-2.70)				

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of ch	ain
1	А	602	71%	22% · ·
1	М	602	50%	42% • •
2	В	243	78%	20% ·
2	Ν	243	51%	44% •
3	С	130	65%	29% · ·
3	0	130	61%	35% 5%
4	D	119	61%	34% ••
4	Р	119	49%	48% •



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
12	SF4	N	246	-	-	Х	-
7	ACT	N	803	-	-	Х	-
9	1PE	А	705	-	Х	-	-



2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 17071 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.

- Chain ZeroOcc AltConf Trace Mol Residues Atoms Total С Ν 0 S 1 0 0 0 А 577 27754448 802 840 31С Ν Total S 0 1 Μ 0 0 0 577 4448 2775802 840 31
- Molecule 1 is a protein called FUMARATE REDUCTASE FLAVOPROTEIN.

• Molecule 2 is a protein called FUMARATE REDUCTASE IRON-SULFUR PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	р	242	Total	С	Ν	0	S	0	0	0
Δ	2 Б	240	1888	1189	323	357	19	0		
9	N 942		Total	С	Ν	0	S	0	0	0
Δ	IN	243	1888	1189	323	357	19	0	0	0

• Molecule 3 is a protein called FUMARATE REDUCTASE 15 KDA HYDROPHOBIC PROTEIN.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
2	C	120	Total	С	Ν	0	S	0	0	0
0	U	130	1058	720	166	169	3	0		
2	0	120	Total	С	Ν	0	S	0	0	0
0	0	130	1058	720	166	169	3			

• Molecule 4 is a protein called FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Л	110	Total	С	Ν	0	S	0	0	0
4	4 D	119	926	626	151	142	7	0	0	
4	D	110	Total	С	Ν	0	S	0	0	0
4		119	926	626	151	142	7	0		U

• Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	1	Total K 1 1	0	0
5	М	1	Total K 1 1	0	0

• Molecule 6 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 9 & 4 & 5 \end{array}$	0	0
6	М	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 9 & 4 & 5 \end{array}$	0	0

• Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0
7	Ν	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 4 & 2 & 2 \end{array}$	0	0

• Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
0	Λ	1	Total	С	Ν	Ο	Р	0	0
o A	1	53	27	9	15	2	0	0	
0	М	1	Total	С	Ν	Ο	Р	0	0
0	111	L	53	27	9	15	2	0	0

• Molecule 9 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
9	А	1	Total 16	C 10	O 6	0	0

• Molecule 10 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	В	1	TotalFeS422	0	0
10	Ν	1	TotalFeS422	0	0

• Molecule 11 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe $_3S_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	В	1	TotalFeS734	0	0
11	Ν	1	TotalFeS734	0	0

• Molecule 12 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	В	1	TotalFeS844	0	0
12	Ν	1	TotalFeS844	0	0

• Molecule 13 is 2-HEPTYL-4-HYDROXY QUINOLINE N-OXIDE (three-letter code: HQO) (formula: $C_{16}H_{21}NO_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf		
13	С	1	Total 19	C 16	N 1	O 2	0	0



Mol	Chain	Residues	A	Aton	ns		ZeroOcc	AltConf
13	Ν	1	Total 19	C 16	N 1	$\begin{array}{c} 0\\2\end{array}$	0	0

• Molecule 14 is O-DODECANYL OCTAETHYLENE GLYCOL (three-letter code: CE1) (formula: C₂₈H₅₈O₉).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	Ο	1	Total C O 37 28 9	0	0
14	О	1	Total C O 37 28 9	0	0
14	О	1	Total C O 37 28 9	0	0
14	Р	1	Total C O 37 28 9	0	0
14	Р	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 37 & 28 & 9 \end{array}$	0	0

• Molecule 15 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	А	10	Total O 10 10	0	0
15	В	1	Total O 1 1	0	0
15	М	4	Total O 4 4	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	Ν	1	Total O 1 1	0	0



Residue-property plots (i) 3

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: FUMARATE REDUCTASE FLAVOPROTEIN Chain A: 22% 71% 50% 42%

Note EDS was not executed.



• Molecule 2: FUMARATE REDUCTASE IRON-SULFUR PROTEIN







• Molecule 4: FUMARATE REDUCTASE 13 KDA HYDROPHOBIC PROTEIN





4 Data and refinement statistics (i)

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

Property	Value	Source	
Space group	P 21 21 21	Depositor	
Cell constants	96.50Å 137.84Å 273.45Å	Depositor	
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor	
Resolution (Å)	20.00 - 2.70	Depositor	
% Data completeness	(Not available) $(20.00-2.70)$	Depositor	
(in resolution range)	(1101 available) (20.00 2.10)	Depositor	
R_{merge}	(Not available)	Depositor	
R _{sym}	(Not available)	Depositor	
Refinement program	CNS, REFMAC	Depositor	
R, R_{free}	0.231 , 0.280	Depositor	
Estimated twinning fraction	No twinning to report.	Xtriage	
Total number of atoms	17071	wwPDB-VP	
Average B, all atoms $(Å^2)$	55.0	wwPDB-VP	



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: FES, ACT, FAD, SF4, CE1, OAA, F3S, K, 1PE, HQO

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).

Mal	Chain	Bo	ond lengths	B	ond angles
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.81	0/4540	0.98	10/6139~(0.2%)
1	М	0.53	1/4540~(0.0%)	0.81	2/6139~(0.0%)
2	В	0.78	1/1931~(0.1%)	0.92	7/2617~(0.3%)
2	Ν	0.59	0/1931	0.81	1/2617~(0.0%)
3	С	0.77	3/1094~(0.3%)	0.87	2/1496~(0.1%)
3	0	0.68	3/1094~(0.3%)	0.79	1/1496~(0.1%)
4	D	0.78	1/956~(0.1%)	0.89	1/1303~(0.1%)
4	Р	0.70	2/956~(0.2%)	0.82	0/1303
All	All	0.70	11/17042~(0.1%)	0.88	24/23110~(0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	С	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
4	D	118	ILE	C-OXT	11.65	1.45	1.23
4	Р	118	ILE	C-OXT	8.01	1.38	1.23
2	В	65	CYS	CB-SG	-7.99	1.68	1.82
3	С	65	ASN	C-O	-7.42	1.09	1.23
3	0	104	GLY	C-O	-6.55	1.13	1.23
4	Р	118	ILE	CA-CB	6.31	1.69	1.54
3	С	130	TRP	C-OXT	6.25	1.35	1.23
3	0	130	TRP	CA-CB	6.17	1.67	1.53
3	0	65	ASN	C-O	-5.51	1.12	1.23
1	М	359	GLY	C-O	5.23	1.32	1.23



Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
3	С	104	GLY	CA-C	-5.09	1.43	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	485	ARG	NE-CZ-NH2	-7.24	116.68	120.30
4	D	7	ARG	NE-CZ-NH2	-7.24	116.68	120.30
2	В	191	ARG	NE-CZ-NH1	-6.88	116.86	120.30
3	С	28	ARG	NE-CZ-NH2	-6.71	116.95	120.30
2	В	65	CYS	N-CA-CB	-6.56	98.79	110.60
1	М	151	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	А	477	ASP	CB-CG-OD1	6.42	124.08	118.30
1	А	18	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	А	114	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	А	18	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	В	184	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	А	467	ARG	NE-CZ-NH2	-5.83	117.39	120.30
2	В	64	SER	C-N-CA	5.76	136.09	121.70
1	М	529	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	В	65	CYS	N-CA-C	5.56	126.00	111.00
2	В	65	CYS	CB-CA-C	-5.54	99.32	110.40
3	С	28	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	А	364	ASP	CB-CG-OD1	5.47	123.22	118.30
2	В	83	ASP	CB-CG-OD2	5.25	123.02	118.30
1	А	317	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	390	ARG	NE-CZ-NH2	5.18	122.89	120.30
2	Ν	191	ARG	NE-CZ-NH2	-5.08	117.76	120.30
3	0	104	GLY	CA-C-O	-5.06	111.49	120.60
1	А	68	ASP	CB-CG-OD2	-5.00	113.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	С	65	ASN	Peptide,Mainchain

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	4448	0	4335	119	0
1	М	4448	0	4335	253	0
2	В	1888	0	1837	44	0
2	Ν	1888	0	1837	108	0
3	С	1058	0	1108	47	0
3	0	1058	0	1108	48	0
4	D	926	0	971	47	0
4	Р	926	0	971	65	0
5	А	1	0	0	0	0
5	М	1	0	0	0	0
6	А	9	0	2	2	0
6	М	9	0	2	0	0
7	А	4	0	3	0	0
7	В	4	0	3	0	0
7	Ν	4	0	3	2	0
8	А	53	0	31	8	0
8	М	53	0	31	8	0
9	А	16	0	20	5	0
10	В	4	0	0	0	0
10	N	4	0	0	0	0
11	В	7	0	0	0	0
11	Ν	7	0	0	1	0
12	В	8	0	0	0	0
12	Ν	8	0	0	4	0
13	С	19	0	20	3	0
13	N	19	0	20	2	0
14	0	111	0	174	0	0
14	Р	74	0	116	5	0
15	A	10	0	0	1	0
15	В	1	0	0	0	0
15	М	4	0	0	0	0
15	N	1	0	0	0	0
All	All	17071	0	16927	659	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 19.

All (659) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



Atom_1	Atom_2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:44:HIS:NE2	8:A:721:FAD:HM82	1.21	1.44	
1:M:44:HIS:NE2	8:M:821:FAD:HM82	1.18	1.42	
1:A:44:HIS:NE2	8:A:721:FAD:C8M	1.89	1.33	
1:M:44:HIS:NE2	8:M:821:FAD:C8M	1.98	1.27	
1:A:44:HIS:CE1	8:A:721:FAD:HM82	1.86	1.08	
1:M:421:ASN:HD22	1:M:424:ALA:HB2	1.17	1.04	
3:C:12:THR:HG22	3:C:14:THR:H	1.18	1.03	
1:M:465:ILE:HD13	1:M:465:ILE:H	1.29	0.97	
2:N:116:ILE:HG21	2:N:176:ALA:HB2	1.47	0.96	
1:M:44:HIS:CE1	8:M:821:FAD:HM82	2.01	0.95	
1:M:197:ARG:HD2	1:M:206:GLY:HA2	1.48	0.95	
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.52	0.92	
2:N:189:LYS:H	2:N:189:LYS:HD3	1.34	0.91	
1:M:469:PRO:HG3	1:M:534:ARG:HH21	1.36	0.90	
3:O:75:THR:HG22	4:P:32:ILE:HD13	1.56	0.87	
2:N:54:ARG:HE	2:N:103:VAL:HG13	1.39	0.87	
1:M:304:ILE:HD12	1:M:304:ILE:H	1.40	0.86	
2:N:15:PRO:HB2	3:O:5:LYS:H	1.41	0.85	
1:M:316:LEU:HB3	1:M:319:LEU:HD12	1.59	0.85	
1:M:447:ASN:HD21	1:M:449:ALA:HB3	1.42	0.84	
1:M:7:LEU:HD21	1:M:411:THR:HA	1.60	0.84	
1:M:421:ASN:HD22	1:M:424:ALA:CB	1.91	0.83	
12:N:246:SF4:FE3	12:N:246:SF4:S2	1.69	0.83	
3:O:19:LEU:H	3:O:19:LEU:HD23	1.44	0.83	
1:A:413:ARG:HH11	1:A:413:ARG:HB2	1.43	0.82	
3:C:104:GLY:HA2	3:C:107:PRO:HD2	1.62	0.82	
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.62	0.81	
1:M:155:HIS:CD2	1:M:174:ASN:HA	2.15	0.81	
1:M:549:LYS:HD2	1:M:565:TYR:HB3	1.62	0.81	
3:O:126:VAL:HA	3:O:130:TRP:HB3	1.65	0.79	
1:M:174:ASN:HD22	1:M:177:GLU:H	1.27	0.79	
1:A:44:HIS:NE2	8:A:721:FAD:HM81	1.96	0.78	
2:N:113:LEU:HD11	2:N:175:LEU:HD22	1.65	0.78	
1:A:292:GLN:HE22	9:A:705:1PE:H261	1.51	0.75	
1:M:236:LEU:HD22	1:M:339:VAL:HG11	1.67	0.75	
2:N:116:ILE:HG21	2:N:176:ALA:CB	2.16	0.75	
2:N:141:LYS:NZ	3:O:95:ASN:HB3	2.01	0.75	
12:N:246:SF4:FE4	12:N:246:SF4:S1	1.77	0.75	
4:P:51:TYR:HD1	4:P:52:GLU:HG3	1.49	0.75	
2:N:206:PHE:HD1	13:N:800:HQO:H112	1.52	0.74	
4:D:67:LEU:O	4:D:71:ILE:HG13	1.86	0.74	
1:M:42:ARG:HH21	2:N:150:ASN:HB2	1.51	0.74	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:M:311:VAL:HG12	1:M:312:VAL:O	1.88	0.74
1:M:437:LYS:HG2	1:M:441:ASN:HD21	1.51	0.74
4:P:105:ALA:O	4:P:109:VAL:HG23	1.88	0.74
2:N:141:LYS:HZ1	3:O:95:ASN:HB3	1.53	0.73
1:M:465:ILE:HD13	1:M:465:ILE:N	2.03	0.73
1:M:152:PHE:HB3	1:M:155:HIS:ND1	2.02	0.73
2:B:225:GLN:HE22	13:C:700:HQO:H111	1.53	0.73
1:M:437:LYS:HG2	1:M:441:ASN:ND2	2.04	0.73
3:O:106:GLU:HB2	3:O:107:PRO:HD3	1.69	0.72
3:O:97:ILE:HD13	3:O:102:LYS:HA	1.70	0.72
1:M:488:ARG:NH1	1:M:488:ARG:HB3	2.04	0.72
1:M:251:GLY:HA2	1:M:277:PRO:HG2	1.70	0.72
1:M:88:HIS:O	1:M:401:VAL:HG22	1.89	0.72
2:N:11:VAL:HG21	2:N:91:GLU:HG2	1.70	0.72
14:P:810:CE1:H171	14:P:810:CE1:H211	1.72	0.72
4:P:104:ALA:O	4:P:108:THR:OG1	2.08	0.72
1:A:42:ARG:HG2	2:B:64:SER:HB3	1.71	0.71
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.54	0.71
3:C:19:LEU:HD12	3:C:20:PRO:HD2	1.72	0.71
3:C:12:THR:HG22	3:C:14:THR:N	2.02	0.71
3:O:50:LYS:HD2	4:P:117:THR:HG22	1.72	0.71
3:O:130:TRP:O	4:P:53:ARG:NH2	2.24	0.70
3:O:50:LYS:HD2	4:P:117:THR:CG2	2.21	0.70
4:P:60:SER:O	4:P:64:ARG:HG3	1.91	0.70
1:M:316:LEU:HD22	1:M:319:LEU:HD11	1.73	0.70
1:M:545:VAL:HG12	1:M:546:ASN:ND2	2.06	0.70
1:M:447:ASN:HD22	1:M:450:LYS:HG2	1.57	0.69
1:M:497:VAL:HG21	2:N:15:PRO:HG2	1.73	0.69
3:C:50:LYS:HB3	4:D:118:ILE:HG22	1.74	0.69
4:P:51:TYR:CD1	4:P:52:GLU:HG3	2.27	0.69
1:M:89:CYS:N	1:M:90:PRO:HD2	2.07	0.69
1:M:465:ILE:H	1:M:465:ILE:CD1	1.95	0.69
2:B:225:GLN:NE2	13:C:700:HQO:H111	2.07	0.69
1:A:413:ARG:HH11	1:A:413:ARG:CB	2.05	0.69
1:M:187:ALA:HB2	1:M:414:ALA:HB2	1.74	0.69
1:A:323:LYS:HG3	1:A:327:ARG:HH11	1.58	0.69
3:C:15:TRP:O	3:C:18:LYS:HG2	1.92	0.69
1:M:99:TRP:CD2	1:M:142:THR:HG21	2.27	0.69
1:A:484:GLU:HG3	1:A:488:ARG:NH1	2.08	0.69
3:O:120:THR:HG23	4:P:30:VAL:HB	1.76	0.68
1:A:390:ARG:HH22	6:A:702:OAA:C4	2.07	0.68



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:M:1:GLN:HG2	1:M:2:THR:H	1.57	0.68
1:M:447:ASN:ND2	1:M:449:ALA:HB3	2.08	0.68
1:M:549:LYS:HA	1:M:568:VAL:HG23	1.76	0.68
1:A:413:ARG:HB2	1:A:413:ARG:NH1	2.08	0.68
1:M:435:ARG:HA	1:M:438:ASP:OD2	1.94	0.68
1:M:421:ASN:ND2	1:M:424:ALA:HB2	2.01	0.67
1:M:342:ASP:HB3	1:M:345:LYS:HB3	1.77	0.67
1:A:484:GLU:HG3	1:A:488:ARG:HH12	1.60	0.67
2:B:222:ALA:HB2	3:C:92:LYS:HE3	1.77	0.67
3:C:33:VAL:HA	4:D:82:MET:CE	2.25	0.66
4:D:20:GLY:HA2	4:D:73:LEU:HB3	1.77	0.66
3:O:86:TRP:HE1	4:P:22:MET:CE	2.09	0.66
1:M:174:ASN:ND2	1:M:177:GLU:HG2	2.09	0.66
1:M:332:CYS:HA	1:M:343:PRO:HG2	1.78	0.66
3:C:50:LYS:HE2	3:C:50:LYS:HA	1.77	0.66
4:P:48:ALA:HA	4:P:53:ARG:HD3	1.78	0.66
4:P:72:VAL:HG11	4:P:108:THR:HG23	1.77	0.66
3:O:75:THR:HG22	4:P:32:ILE:CD1	2.25	0.66
4:P:7:ARG:HG2	4:P:8:SER:N	2.10	0.66
3:O:86:TRP:HE1	4:P:22:MET:HE2	1.62	0.65
1:M:84:TYR:HE2	1:M:405:LEU:HD22	1.61	0.65
2:N:196:ASN:ND2	2:N:234:ASP:OD1	2.30	0.65
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.78	0.65
1:A:197:ARG:HD2	1:A:206:GLY:HA2	1.79	0.65
2:N:225:GLN:O	2:N:229:VAL:HG23	1.97	0.64
1:M:89:CYS:H	1:M:90:PRO:HD2	1.60	0.64
1:M:444:GLY:HA3	1:M:488:ARG:O	1.98	0.64
2:N:13:TYR:HB2	2:N:21:PRO:HB3	1.79	0.64
1:A:27:ASN:ND2	1:A:30:ALA:HB2	2.12	0.64
4:D:0:MET:HG2	4:D:1:ILE:H	1.63	0.64
4:P:77:CYS:O	4:P:81:ARG:HG3	1.97	0.64
1:A:324:LEU:CD1	1:A:344:VAL:HG22	2.28	0.64
1:M:217:LEU:HG	1:M:555:ARG:HB3	1.78	0.63
1:M:391:LEU:O	1:M:394:ASN:HB2	1.98	0.63
1:M:275:GLY:O	1:M:277:PRO:HD3	1.99	0.63
3:O:60:VAL:O	3:O:64:GLN:HG3	1.99	0.63
2:B:16:GLU:OE2	3:C:3:LYS:HD2	1.98	0.63
1:M:251:GLY:HA2	1:M:277:PRO:CG	2.28	0.63
1:M:327:ARG:O	1:M:328:LEU:HD23	1.98	0.63
1:M:435:ARG:HH12	1:M:439:LEU:HD22	1.64	0.63
2:N:57:CYS:HB3	2:N:62:CYS:HB3	1.79	0.63



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:279:ASN:O	1:A:280:LYS:HB2	1.99	0.62
4:P:24:SER:O	4:P:28:ALA:HB3	1.99	0.62
1:M:436:LEU:O	1:M:440:VAL:HG23	1.99	0.62
2:N:135:THR:HG23	2:N:136:PRO:HD2	1.82	0.62
1:M:202:ASN:HA	1:M:353:THR:HG22	1.82	0.62
2:N:206:PHE:CE1	2:N:225:GLN:HG3	2.35	0.62
1:M:41:MET:HB2	1:M:137:HIS:CE1	2.34	0.62
1:M:199:TYR:CE1	1:M:229:VAL:HG11	2.35	0.61
1:M:51:GLY:HA2	1:M:131:THR:HG21	1.82	0.61
1:M:332:CYS:O	1:M:336:LYS:HG3	2.00	0.61
3:C:130:TRP:N	3:C:130:TRP:CD1	2.69	0.61
4:D:48:ALA:O	4:D:53:ARG:HD3	2.00	0.61
1:M:444:GLY:HA3	1:M:488:ARG:C	2.21	0.61
4:D:13:PHE:HE2	4:D:97:LYS:HE2	1.65	0.61
3:O:18:LYS:HD2	3:O:19:LEU:HD22	1.81	0.61
1:A:336:LYS:O	1:A:340:GLY:HA2	2.00	0.60
4:P:22:MET:O	4:P:26:ILE:HD13	2.01	0.60
3:C:33:VAL:HA	4:D:82:MET:HE3	1.83	0.60
2:N:236:LEU:HD23	2:N:236:LEU:C	2.22	0.60
1:M:11:GLY:O	1:M:16:GLY:HA3	2.01	0.60
1:M:82:VAL:HG22	1:M:385:LEU:HD12	1.82	0.60
1:M:192:THR:OG1	1:M:212:GLY:HA3	2.02	0.60
2:N:206:PHE:CD1	13:N:800:HQO:H112	2.33	0.60
1:A:358:MET:HE3	1:A:389:ASN:HA	1.83	0.60
4:D:63:GLY:O	4:D:67:LEU:HD23	2.02	0.59
1:A:94:THR:HG23	2:B:131:THR:HG22	1.83	0.59
4:D:86:MET:HE3	4:D:86:MET:HA	1.83	0.59
1:M:92:GLU:HB3	1:M:400:VAL:HB	1.83	0.59
1:M:195:ALA:O	1:M:198:VAL:HG22	2.02	0.59
1:A:28:PRO:HA	1:A:148:GLN:HE21	1.65	0.59
1:M:156:PHE:CD2	1:M:503:LEU:HD22	2.37	0.59
1:A:148:GLN:OE1	1:A:148:GLN:N	2.30	0.59
1:M:96:LEU:HD21	1:M:139:LEU:HD21	1.85	0.59
1:A:343:PRO:HG3	1:A:348:ILE:HD11	1.85	0.59
3:O:50:LYS:HG3	4:P:118:ILE:HA	1.84	0.59
1:A:372:LYS:HE3	1:A:413:ARG:HE	1.67	0.59
2:B:57:CYS:O	2:B:58:ARG:HB2	2.02	0.59
4:D:78:GLY:O	4:D:82:MET:HG3	2.03	0.59
1:M:84:TYR:CE2	1:M:405:LEU:HD22	2.38	0.59
1:A:289:LYS:NZ	9:A:705:1PE:H262	2.18	0.59
2:N:44:LYS:HD3	2:N:51:LEU:O	2.03	0.58



	• • • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:232:HIS:HD2	1:A:234:THR:H	1.50	0.58
1:M:44:HIS:CE1	1:M:204:ASN:HA	2.38	0.58
2:N:116:ILE:HG22	2:N:191:ARG:HD3	1.86	0.58
1:A:200:ARG:NH1	1:A:201:TYR:OH	2.37	0.58
1:A:358:MET:CE	1:A:389:ASN:HA	2.33	0.58
2:B:241:LYS:HG3	2:B:241:LYS:O	2.02	0.58
1:M:181:VAL:HG12	1:M:182:GLN:H	1.67	0.58
1:M:331:ILE:HD12	1:M:331:ILE:H	1.69	0.58
1:A:103:TRP:O	2:B:139:MET:HE1	2.04	0.58
2:N:157:ALA:HB1	2:N:209:TYR:CD2	2.38	0.58
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.86	0.58
2:N:54:ARG:NE	2:N:103:VAL:HG13	2.13	0.58
3:O:36:VAL:HG11	4:P:82:MET:HE1	1.85	0.58
3:O:106:GLU:H	3:O:106:GLU:CD	2.08	0.58
1:M:499:ASN:HD22	1:M:499:ASN:C	2.06	0.57
3:O:36:VAL:HG11	4:P:82:MET:CE	2.33	0.57
3:O:98:VAL:HG23	3:O:103:MET:HB2	1.85	0.57
1:A:556:ASP:HB2	1:A:558:ASP:OD2	2.04	0.57
1:M:448:TRP:CH2	1:M:504:TYR:HB3	2.38	0.57
1:M:341:VAL:HG13	1:M:346:GLU:HB2	1.86	0.57
4:P:9:ASP:C	4:P:11:PRO:HD2	2.24	0.57
1:A:366:ASN:HB3	1:A:409:GLN:HG3	1.84	0.57
4:P:64:ARG:HB3	4:P:115:VAL:HG22	1.87	0.57
1:M:181:VAL:HG12	1:M:182:GLN:N	2.19	0.57
1:A:324:LEU:HD12	1:A:344:VAL:HG22	1.86	0.57
2:B:157:ALA:HB1	2:B:209:TYR:CD2	2.39	0.57
2:N:11:VAL:CG2	2:N:91:GLU:HG2	2.34	0.57
1:M:209:THR:O	1:M:209:THR:HG22	2.04	0.57
2:B:206:PHE:HD1	13:C:700:HQO:H112	1.69	0.56
1:A:462:GLY:HA3	1:A:475:THR:OG1	2.05	0.56
4:D:68:PHE:HD1	4:D:111:THR:HG22	1.70	0.56
2:N:2:GLU:OE1	2:N:2:GLU:HA	2.04	0.56
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.88	0.56
1:M:304:ILE:HG12	1:M:313:TYR:HE2	1.71	0.56
4:P:76:TRP:NE1	14:P:810:CE1:H362	2.21	0.56
3:C:33:VAL:HG22	4:D:82:MET:CE	2.36	0.56
1:M:510:HIS:O	1:M:514:VAL:HG23	2.06	0.56
2:B:188:LYS:NZ	2:B:230:GLU:HG3	2.20	0.56
4:D:83:HIS:O	4:D:86:MET:HB2	2.06	0.56
1:M:358:MET:SD	1:M:390:ARG:N	2.79	0.56
3:0:104:GLY:0	3:O:107:PRO:HD2	2.06	0.55



	A A A	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:M:545:VAL:C	1:M:546:ASN:HD22	2.08	0.55
2:N:135:THR:HG22	2:N:137:ALA:H	1.71	0.55
1:A:321:GLU:OE1	1:A:321:GLU:HA	2.06	0.55
1:M:102:PRO:HB2	2:N:139:MET:CE	2.36	0.55
1:M:152:PHE:O	1:M:155:HIS:HB2	2.06	0.55
1:M:260:TYR:CE1	1:M:264:GLN:NE2	2.75	0.55
4:P:112:LEU:O	4:P:116:VAL:HG22	2.07	0.55
3:C:50:LYS:HD3	4:D:118:ILE:HG22	1.88	0.55
1:M:435:ARG:O	1:M:438:ASP:HB2	2.07	0.55
3:O:19:LEU:HD21	3:O:22:TYR:CE2	2.41	0.55
1:A:250:GLU:HB3	1:A:319:LEU:HD11	1.89	0.55
4:D:112:LEU:O	4:D:116:VAL:HG22	2.06	0.55
1:M:311:VAL:HG11	1:M:349:PRO:HB2	1.89	0.55
1:M:323:LYS:HG2	1:M:327:ARG:HH21	1.71	0.55
2:N:201:VAL:HG23	2:N:202:TRP:N	2.21	0.55
3:O:19:LEU:H	3:O:19:LEU:CD2	2.19	0.55
3:C:106:GLU:CD	3:C:106:GLU:H	2.10	0.55
2:N:21:PRO:HD2	3:O:7:TYR:CE2	2.42	0.55
2:B:2:GLU:HA	2:B:2:GLU:OE2	2.06	0.55
2:B:8:ILE:HD11	2:B:81:LEU:HD11	1.89	0.55
1:M:62:PHE:HB3	1:M:86:VAL:HG23	1.89	0.55
2:N:202:TRP:CZ2	4:P:11:PRO:HG3	2.42	0.54
1:A:182:GLN:OE1	1:A:184:ARG:NH1	2.33	0.54
1:A:323:LYS:HG3	1:A:327:ARG:NH1	2.22	0.54
1:A:527:GLU:OE1	1:A:529:ARG:HD2	2.07	0.54
2:B:155:TYR:CE2	2:B:169:GLY:HA3	2.43	0.54
1:M:162:VAL:HG22	1:M:167:VAL:HA	1.89	0.54
1:M:219:HIS:O	1:M:371:ILE:HD11	2.07	0.54
3:O:70:ILE:O	3:O:73:LEU:HB2	2.07	0.54
1:M:168:ARG:HD3	1:M:425:ILE:CD1	2.37	0.54
2:B:32:ALA:O	2:B:82:ARG:NH1	2.40	0.54
3:C:50:LYS:HB3	4:D:118:ILE:CG2	2.36	0.54
4:P:72:VAL:CG1	4:P:108:THR:HG23	2.38	0.54
1:A:341:VAL:HG13	1:A:346:GLU:HB2	1.88	0.54
1:M:242:LEU:HD12	1:M:243:MET:N	2.22	0.54
1:M:253:ILE:HA	1:M:283:GLU:HG2	1.90	0.54
2:N:81:LEU:N	2:N:81:LEU:HD12	2.22	0.54
2:B:57:CYS:HB3	2:B:62:CYS:HB3	1.90	0.54
1:M:551:THR:HG23	1:M:563:LEU:HD22	1.90	0.54
4:P:3:PRO:O	4:P:4:ASN:C	2.46	0.54
1:A:7:LEU:HD21	1:A:32:ILE:HG12	1.90	0.54



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:M:95:GLN:OE1	1:M:98:LEU:HD12	2.07	0.54
1:M:308:ARG:NH1	1:M:339:VAL:HG12	2.23	0.54
1:M:217:LEU:HG	1:M:555:ARG:CB	2.39	0.53
1:A:11:GLY:O	1:A:16:GLY:HA3	2.08	0.53
1:A:184:ARG:HG2	1:A:184:ARG:NH1	2.22	0.53
1:M:331:ILE:HD12	1:M:331:ILE:N	2.23	0.53
1:M:76:LEU:HD12	1:M:388:ALA:HB2	1.90	0.53
2:N:134:GLN:NE2	2:N:184:ARG:HD3	2.23	0.53
4:P:73:LEU:HB2	4:P:74:PRO:HD3	1.90	0.53
4:P:117:THR:O	4:P:118:ILE:C	2.46	0.53
3:C:98:VAL:HG23	3:C:98:VAL:O	2.08	0.53
4:D:98:TRP:NE1	14:P:810:CE1:H141	2.24	0.53
1:M:147:PRO:HD2	1:M:148:GLN:OE1	2.09	0.53
1:M:311:VAL:HG11	1:M:349:PRO:CB	2.39	0.53
1:A:192:THR:OG1	1:A:212:GLY:HA3	2.08	0.53
1:A:200:ARG:HG3	1:A:457:LEU:HD23	1.91	0.53
1:M:7:LEU:HD12	1:M:23:ALA:HB1	1.91	0.53
4:P:102:GLY:HA2	14:P:710:CE1:H42	1.91	0.53
1:M:425:ILE:O	1:M:428:GLN:HB2	2.09	0.52
1:M:81:VAL:HG21	1:M:383:VAL:O	2.09	0.52
1:M:168:ARG:HD3	1:M:425:ILE:HD11	1.91	0.52
1:M:545:VAL:HG12	1:M:546:ASN:HD22	1.74	0.52
1:A:90:PRO:HB2	15:A:758:HOH:O	2.09	0.52
1:M:151:ARG:NH1	1:M:153:ASP:OD2	2.43	0.52
1:M:331:ILE:H	1:M:331:ILE:CD1	2.23	0.52
2:N:9:GLU:HG3	2:N:25:PHE:CZ	2.44	0.52
4:P:39:LEU:HD13	4:P:49:LEU:HB3	1.90	0.52
1:A:436:LEU:O	1:A:440:VAL:HG23	2.10	0.52
2:B:242:PRO:HG3	4:P:94:PRO:HD3	1.89	0.52
1:M:58:ASP:C	1:M:60:ASP:H	2.11	0.52
1:M:242:LEU:HD23	8:M:821:FAD:HM73	1.91	0.52
4:P:10:GLU:N	4:P:11:PRO:CD	2.73	0.52
1:A:118:GLY:HA2	1:A:279:ASN:HD21	1.73	0.52
4:D:13:PHE:CE2	4:D:97:LYS:HE2	2.45	0.52
2:N:139:MET:HA	2:N:142:TYR:CE2	2.45	0.52
1:A:292:GLN:NE2	9:A:705:1PE:H261	2.21	0.52
2:B:229:VAL:HG12	2:B:233:LYS:HE3	1.92	0.52
3:C:50:LYS:CB	4:D:118:ILE:HG22	2.40	0.52
2:N:169:GLY:O	2:N:173:ILE:HG13	2.10	0.52
1:A:232:HIS:CE1	1:A:242:LEU:HD11	2.45	0.52
1:M:10:VAL:HG13	1:M:157:VAL:HG21	1.91	0.52



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:N:97:PRO:HG2	2:N:105:ASP:HB3	1.92	0.52	
2:N:233:LYS:O	2:N:237:ILE:HD13	2.10	0.52	
3:C:113:TRP:O	3:C:117:VAL:HG23	2.09	0.52	
1:M:122:GLU:H	1:M:122:GLU:CD	2.13	0.52	
1:M:7:LEU:HD11	1:M:411:THR:OG1	2.10	0.51	
1:M:328:LEU:N	1:M:329:PRO:HD3	2.24	0.51	
1:A:356:TYR:CE2	1:A:390:ARG:HD3	2.45	0.51	
2:N:28:VAL:HG22	2:N:43:ILE:HD11	1.92	0.51	
1:M:467:ARG:NH1	1:M:532:HIS:ND1	2.58	0.51	
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.45	0.51	
1:M:227:GLU:HB2	1:M:522:ALA:HB2	1.93	0.51	
1:M:546:ASN:HD22	1:M:546:ASN:N	2.06	0.51	
3:C:59:PHE:CE1	3:C:63:LEU:HD11	2.46	0.51	
1:M:98:LEU:HD11	2:N:127:ALA:HA	1.92	0.51	
1:M:328:LEU:N	1:M:329:PRO:CD	2.74	0.51	
2:N:113:LEU:CD1	2:N:175:LEU:HD22	2.39	0.51	
4:D:93:VAL:N	2:N:243:ARG:O	2.42	0.51	
1:M:171:VAL:HG11	1:M:432:VAL:HG11	1.93	0.51	
2:N:28:VAL:CG2	2:N:43:ILE:HD11	2.41	0.51	
2:N:198:GLN:O	2:N:203:SER:HB2	2.10	0.51	
3:C:50:LYS:CG	4:D:118:ILE:HG22	2.41	0.50	
4:D:73:LEU:HB2	4:D:74:PRO:HD3	1.93	0.50	
1:M:145:GLN:O	1:M:147:PRO:HD3	2.12	0.50	
1:M:296:HIS:ND1	1:M:299:ARG:NH2	2.59	0.50	
1:M:308:ARG:HH12	1:M:339:VAL:HG12	1.76	0.50	
3:O:33:VAL:O	3:O:36:VAL:HG22	2.11	0.50	
1:M:0:MET:SD	1:M:182:GLN:HB2	2.51	0.50	
1:M:21:ILE:HG21	1:M:99:TRP:CH2	2.47	0.50	
1:M:158:LEU:HD11	1:M:436:LEU:HD22	1.93	0.50	
1:M:413:ARG:NH1	1:M:413:ARG:HB2	2.26	0.50	
1:M:311:VAL:HG13	1:M:350:VAL:O	2.11	0.50	
2:N:241:LYS:O	2:N:243:ARG:HG3	2.12	0.50	
1:A:42:ARG:CG	2:B:64:SER:HB3	2.42	0.50	
1:M:39:TYR:HE2	2:N:54:ARG:HH12	1.59	0.50	
1:M:174:ASN:ND2	1:M:177:GLU:H	2.03	0.50	
2:B:234:ASP:OD1	4:D:7:ARG:NH2	2.44	0.50	
3:C:50:LYS:HD2	4:D:118:ILE:O	2.11	0.50	
1:M:171:VAL:HB	1:M:432:VAL:HG11	1.94	0.50	
1:M:435:ARG:NH1	1:M:439:LEU:HB2	2.27	0.50	
1:M:75:TRP:O	1:M:568:VAL:HG11	2.12	0.49	
1:A:316:LEU:O	1:A:319:LEU:HB2	2.10	0.49	



		Interatomic	Clash	
Atom-1	Atom-1 Atom-2		overlap (Å)	
1:M:162:VAL:HG13	1:M:166:HIS:O	2.12	0.49	
1:M:330:PHE:HB3	1:M:331:ILE:HD12	1.94	0.49	
3:0:118:VAL:O	3:O:122:VAL:HG23	2.12	0.49	
4:P:118:ILE:HG23	4:P:118:ILE:OXT	2.11	0.49	
3:C:127:ALA:O	3:C:128:LEU:HD23	2.12	0.49	
1:A:159:ASP:OD2	1:A:160:ILE:N	2.46	0.49	
1:M:42:ARG:HD2	2:N:64:SER:OG	2.13	0.49	
1:M:66:PHE:HD1	1:M:82:VAL:HG12	1.78	0.49	
1:M:196:GLY:HA3	1:M:204:ASN:OD1	2.13	0.49	
1:M:316:LEU:HB3	1:M:319:LEU:CD1	2.35	0.49	
2:N:92:ALA:HB1	2:N:104:VAL:CG1	2.42	0.49	
2:N:96:PHE:HB3	2:N:104:VAL:HB	1.94	0.49	
2:N:189:LYS:H	2:N:189:LYS:CD	2.12	0.49	
3:O:33:VAL:HB	3:0:34:PRO:CD	2.34	0.49	
3:C:33:VAL:HG22	4:D:82:MET:HE2	1.92	0.49	
1:M:102:PRO:HB2	2:N:139:MET:HE1	1.95	0.49	
4:D:10:GLU:N	4:D:11:PRO:HD2	2.27	0.49	
1:M:187:ALA:CB	1:M:414:ALA:HB2	2.41	0.49	
1:M:304:ILE:HD12	1:M:304:ILE:N	2.18	0.49	
2:N:180:ASN:OD1	2:N:188:LYS:HA	2.12	0.49	
4:P:28:ALA:N	4:P:29:PRO:HD2	2.28	0.49	
1:M:141:GLN:HB3	2:N:118:PRO:O	2.13	0.49	
1:M:488:ARG:HB3	1:M:488:ARG:HH11	1.75	0.49	
1:A:549:LYS:HD2	1:A:565:TYR:HB3	1.95	0.49	
1:M:100:GLY:O	1:M:101:CYS:C	2.52	0.49	
1:M:104:SER:O	1:M:105:ARG:HD3	2.12	0.49	
1:M:155:HIS:HD2	1:M:174:ASN:HA	1.74	0.49	
1:A:317:ARG:C	1:A:319:LEU:H	2.17	0.49	
1:M:171:VAL:CG1	1:M:432:VAL:HG11	2.42	0.49	
2:N:159:PRO:HG2	2:N:207:VAL:HG21	1.94	0.49	
3:O:90:ALA:N	3:O:91:PRO:HD2	2.28	0.49	
3:0:127:ALA:O	3:O:128:LEU:HD23	2.13	0.49	
4:P:55:LEU:CD1	4:P:118:ILE:HD11	2.43	0.49	
1:M:435:ARG:HH12	1:M:439:LEU:CD2	2.25	0.48	
1:M:549:LYS:HD2	1:M:565:TYR:CB	2.39	0.48	
2:N:201:VAL:CG2	2:N:202:TRP:N	2.76	0.48	
1:A:115:ARG:HD3	1:A:279:ASN:ND2	2.28	0.48	
1:M:213:MET:CE	1:M:380:CYS:HA	2.43	0.48	
1:M:236:LEU:HD22	1:M:339:VAL:CG1	2.41	0.48	
1:A:109:GLY:HA2	2:B:134:GLN:O	2.13	0.48	
1:M:304:ILE:HG22	1:M:305:SER:N	2.28	0.48	



	A A A	Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
4:P:86:MET:HE3	4:P:91:ILE:HB	1.95	0.48	
1:A:44:HIS:NE2	8:A:721:FAD:C8	2.73	0.48	
2:B:201:VAL:HG23	2:B:202:TRP:N	2.28	0.48	
1:A:196:GLY:HA3	1:A:204:ASN:OD1	2.14	0.48	
1:A:448:TRP:CH2	1:A:504:TYR:HB3	2.49	0.48	
1:M:62:PHE:CD2	1:M:87:HIS:HA	2.49	0.48	
2:N:175:LEU:O	2:N:178:ARG:HB3	2.13	0.48	
1:A:556:ASP:OD2	1:A:562:ARG:NE	2.43	0.48	
4:D:93:VAL:HA	4:D:94:PRO:HD2	1.73	0.48	
1:A:85:PHE:CD2	1:A:385:LEU:HD11	2.49	0.48	
1:M:1:GLN:HG2	1:M:2:THR:N	2.27	0.48	
4:P:39:LEU:HB2	4:P:49:LEU:HD13	1.96	0.48	
4:P:70:MET:O	4:P:74:PRO:HG2	2.13	0.48	
3:C:75:THR:HG22	4:D:32:ILE:HD13	1.96	0.48	
1:M:159:ASP:OD2	1:M:160:ILE:N	2.47	0.48	
1:M:469:PRO:HG3	1:M:534:ARG:NH2	2.16	0.48	
1:M:35:ILE:CD1	1:M:155:HIS:HB3	2.44	0.48	
3:O:91:PRO:C	3:O:93:ALA:H	2.16	0.48	
1:M:63:GLU:O	1:M:66:PHE:HB3	2.14	0.47	
1:M:130:LYS:O	1:M:133:PHE:HB3	2.14	0.47	
2:N:54:ARG:O	2:N:55:TRP:HB3	2.15	0.47	
1:M:165:GLY:O	1:M:372:LYS:HB2	2.13	0.47	
1:M:382:SER:C	1:M:384:GLY:H	2.17	0.47	
1:A:224:ARG:NH2	1:A:382:SER:O	2.41	0.47	
1:A:439:LEU:HD12	1:A:442:GLN:NE2	2.29	0.47	
2:N:81:LEU:H	2:N:81:LEU:CD1	2.27	0.47	
2:B:149:ILE:HG13	2:B:151:CYS:HB3	1.96	0.47	
1:M:184:ARG:NH2	1:M:426:GLU:HG2	2.29	0.47	
1:M:66:PHE:CD1	1:M:82:VAL:HG12	2.50	0.47	
1:M:286:PRO:O	1:M:290:VAL:HG23	2.15	0.47	
1:M:311:VAL:HG12	1:M:312:VAL:N	2.30	0.47	
1:M:499:ASN:HD21	1:M:501:ASP:HB3	1.79	0.47	
2:N:194:GLN:HE22	4:P:1:ILE:HG21	1.79	0.47	
2:B:28:VAL:HG12	2:B:29:PRO:O	2.14	0.47	
2:B:113:LEU:HD23	2:B:113:LEU:O	2.13	0.47	
1:A:377:VAL:HG21	1:A:403:GLY:HA2	1.97	0.47	
1:M:493:ASP:OD1	2:N:50:ASP:HB3	2.15	0.47	
2:N:135:THR:CG2	2:N:136:PRO:HD2	2.45	0.47	
2:B:195:LEU:O	2:B:201:VAL:HG22	2.15	0.47	
1:M:479:LEU:HB3	1:M:516:GLU:HG2	1.97	0.47	
1:A:89:CYS:HB2	1:A:90:PRO:HD3	1.96	0.47	



	• • • • • •	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
3:C:31:THR:O	3:C:34:PRO:HD2	2.15	0.47	
3:C:53:PRO:HD3	4:D:51:TYR:CZ	2.50	0.47	
3:O:39:SER:OG	4:P:71:ILE:O	2.33	0.47	
2:B:135:THR:O	2:B:136:PRO:C	2.52	0.47	
1:A:151:ARG:NH2	2:B:114:GLU:OE2	2.48	0.46	
3:C:50:LYS:CD	4:D:118:ILE:HG22	2.46	0.46	
4:P:79:LEU:HD23	4:P:82:MET:CE	2.45	0.46	
1:A:244:THR:H	1:A:331:ILE:HD11	1.79	0.46	
1:M:232:HIS:O	1:M:352:PRO:HA	2.15	0.46	
2:N:160:GLN:NE2	2:N:205:THR:OG1	2.47	0.46	
4:P:10:GLU:N	4:P:11:PRO:HD2	2.30	0.46	
1:A:232:HIS:NE2	1:A:242:LEU:HD11	2.30	0.46	
1:A:287:ARG:H	9:A:705:1PE:H122	1.81	0.46	
1:M:247:CYS:CB	1:M:314:LEU:HD21	2.46	0.46	
1:M:393:SER:HA	8:M:821:FAD:O2	2.15	0.46	
1:A:184:ARG:NH1	1:A:184:ARG:CG	2.78	0.46	
2:B:188:LYS:HZ1	2:B:230:GLU:HG3	1.81	0.46	
4:D:64:ARG:NH1	4:D:117:THR:HG23	2.30	0.46	
1:M:479:LEU:O	1:M:483:GLN:HG2	2.16	0.46	
1:A:142:THR:O	1:A:145:GLN:HG2	2.15	0.46	
1:A:244:THR:HG22	1:A:331:ILE:HG13	1.97	0.46	
4:P:39:LEU:N	4:P:40:PRO:HD2	2.30	0.46	
2:N:133:ILE:O	2:N:133:ILE:HG22	2.14	0.46	
2:N:145:PHE:HA	2:N:218:VAL:HG13	1.97	0.46	
1:M:364:ASP:CG	1:M:366:ASN:H	2.19	0.46	
2:N:214:CYS:SG	12:N:246:SF4:S1	3.14	0.46	
4:P:109:VAL:O	4:P:112:LEU:HB3	2.16	0.46	
1:M:40:PRO:HB2	1:M:140:PHE:CD1	2.51	0.46	
2:N:15:PRO:CB	3:O:5:LYS:H	2.18	0.46	
1:M:174:ASN:ND2	1:M:177:GLU:CG	2.77	0.46	
2:N:158:CYS:HA	2:N:159:PRO:HD3	1.85	0.46	
1:M:263:LEU:CD1	1:M:283:GLU:HA	2.45	0.45	
1:M:304:ILE:H	1:M:304:ILE:CD1	2.16	0.45	
2:N:81:LEU:HD12	2:N:81:LEU:H	1.81	0.45	
2:N:167:PHE:CD1	2:N:203:SER:HB3	2.51	0.45	
1:A:40:PRO:HB2	1:A:140:PHE:CD1	2.51	0.45	
1:A:206:GLY:HA3	2:B:55:TRP:CH2	2.51	0.45	
1:M:315:ASP:OD1	1:M:317:ARG:HG3	2.15	0.45	
1:M:448:TRP:CG	1:M:449:ALA:N	2.84	0.45	
2:N:41:GLY:CA	7:N:803:ACT:H2	2.46	0.45	
1:A:536:ASP:O	1:A:539:CYS:HB2	2.16	0.45	



		Interatomic	Clash	
Atom-1	Atom-2		overlap (Å)	
1:A:546:ASN:O	1:A:549:LYS:HE2	2.16	0.45	
3:C:49:LEU:HG	4:D:55:LEU:HD12	1.98	0.45	
4:D:24:SER:O	4:D:28:ALA:HB3	2.15	0.45	
4:P:93:VAL:HA	4:P:94:PRO:HD2	1.78	0.45	
1:A:176:MET:HG3	3:C:4:ARG:HD3	1.98	0.45	
1:A:202:ASN:HA	1:A:353:THR:HG22	1.99	0.45	
4:D:48:ALA:HA	4:D:53:ARG:HD3	1.98	0.45	
1:M:396:LEU:HG	8:M:821:FAD:C2	2.46	0.45	
2:N:39:ALA:O	2:N:43:ILE:HG12	2.16	0.45	
4:P:95:ALA:HB1	4:P:98:TRP:HB2	1.98	0.45	
1:M:279:ASN:O	1:M:280:LYS:HB2	2.17	0.45	
1:M:158:LEU:O	1:M:159:ASP:HB2	2.17	0.45	
1:M:546:ASN:O	1:M:549:LYS:HE3	2.17	0.45	
1:A:342:ASP:C	1:A:344:VAL:H	2.20	0.45	
1:M:93:MET:HB3	1:M:125:TRP:CE3	2.50	0.45	
1:M:162:VAL:HG13	1:M:166:HIS:C	2.37	0.45	
1:A:317:ARG:O	1:A:319:LEU:N	2.50	0.45	
1:A:366:ASN:O	1:A:367:CYS:HB2	2.16	0.45	
1:A:385:LEU:HD23	1:A:386:HIS:CE1	2.52	0.45	
3:O:36:VAL:HG23	3:O:37:TRP:N	2.32	0.45	
4:P:9:ASP:OD2	4:P:9:ASP:N	2.49	0.45	
1:A:332:CYS:O	1:A:336:LYS:HG3	2.17	0.45	
3:C:90:ALA:N	3:C:91:PRO:CD	2.80	0.45	
1:M:114:ARG:C	1:M:122:GLU:HB2	2.36	0.45	
1:M:320:GLY:O	1:M:324:LEU:HB2	2.17	0.45	
1:M:498:PHE:CD2	2:N:103:VAL:HG21	2.51	0.45	
2:N:12:ARG:NH2	2:N:101:ASP:OD1	2.49	0.45	
1:A:141:GLN:HB3	2:B:118:PRO:O	2.17	0.45	
1:A:448:TRP:CG	1:A:449:ALA:N	2.85	0.45	
4:D:86:MET:CE	4:D:91:ILE:HD12	2.47	0.45	
4:P:51:TYR:CD1	4:P:52:GLU:N	2.82	0.44	
1:A:45:THR:O	1:A:132:GLY:HA3	2.16	0.44	
4:D:64:ARG:HH12	4:D:117:THR:HG23	1.82	0.44	
1:M:239:SER:OG	1:M:241:ILE:HG13	2.17	0.44	
1:M:488:ARG:HB3	1:M:488:ARG:CZ	2.46	0.44	
2:N:119:TYR:CE1	2:N:121:ILE:HD11	2.52	0.44	
2:N:162:GLY:HA3	3:O:11:MET:CE	2.47	0.44	
2:N:235:PHE:CE1	4:P:9:ASP:HA	2.51	0.44	
4:P:30:VAL:O	4:P:33:LEU:HB3	2.17	0.44	
1:A:93:MET:HB3	1:A:125:TRP:CZ3	2.52	0.44	
2:B:7:LYS:HE2	2:B:25:PHE:CD2	2.52	0.44	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:N:155:TYR:CZ	2:N:169:GLY:HA3	2.53	0.44	
1:M:17:LEU:O	1:M:21:ILE:HG13	2.18	0.44	
1:M:9:ILE:HD13	1:M:19:ALA:HB3	2.00	0.44	
1:M:38:VAL:O	1:M:39:TYR:C	2.56	0.44	
1:M:96:LEU:HD23	1:M:96:LEU:HA	1.86	0.44	
1:A:0:MET:SD	1:A:182:GLN:HG3	2.58	0.44	
3:C:123:ILE:HD12	4:D:30:VAL:HG11	2.00	0.44	
1:M:102:PRO:HB2	2:N:139:MET:HE3	1.99	0.44	
1:M:326:GLU:HG2	1:M:326:GLU:O	2.18	0.44	
4:D:92:HIS:HB3	2:N:243:ARG:CB	2.48	0.44	
3:0:114:ALA:O	3:O:118:VAL:HG23	2.18	0.44	
1:A:324:LEU:HD23	1:A:328:LEU:HD12	2.00	0.44	
1:M:41:MET:CE	2:N:150:ASN:HD22	2.31	0.44	
4:P:64:ARG:O	4:P:115:VAL:HG21	2.17	0.44	
1:A:356:TYR:HE1	8:A:721:FAD:O3'	2.01	0.43	
2:B:209:TYR:CZ	3:C:19:LEU:HD21	2.53	0.43	
1:M:44:HIS:NE2	8:M:821:FAD:HM81	2.18	0.43	
1:M:89:CYS:N	1:M:90:PRO:CD	2.78	0.43	
1:M:171:VAL:CB	1:M:432:VAL:HG11	2.48	0.43	
1:M:488:ARG:HH11	1:M:488:ARG:CB	2.29	0.43	
4:P:55:LEU:HD12	4:P:118:ILE:HD11	1.99	0.43	
3:O:84:LYS:HE2	3:O:88:GLU:OE2	2.17	0.43	
1:A:244:THR:HG22	1:A:331:ILE:CG1	2.49	0.43	
4:D:114:GLY:O	4:D:117:THR:HA	2.18	0.43	
1:M:46:VAL:HG23	1:M:133:PHE:HA	2.00	0.43	
1:M:335:ALA:HA	1:M:339:VAL:HG22	2.00	0.43	
1:M:435:ARG:O	1:M:435:ARG:HD2	2.18	0.43	
1:M:546:ASN:ND2	1:M:546:ASN:N	2.66	0.43	
1:M:382:SER:O	1:M:384:GLY:N	2.51	0.43	
1:M:548:LEU:HD12	1:M:568:VAL:HG21	1.99	0.43	
1:A:232:HIS:CD2	1:A:234:THR:H	2.33	0.43	
2:B:136:PRO:HB2	3:C:100:ASP:OD1	2.17	0.43	
3:C:37:TRP:CZ2	3:C:41:GLU:OE1	2.72	0.43	
1:M:21:ILE:O	1:M:25:GLN:HG3	2.19	0.43	
1:M:329:PRO:HG2	1:M:330:PHE:H	1.83	0.43	
2:N:75:LEU:HD11	2:N:215:PRO:HG3	2.00	0.43	
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.54	0.43	
2:N:197:SER:HB2	4:P:5:PRO:HG2	2.00	0.43	
1:A:273:PRO:O	1:A:274:LEU:C	2.57	0.43	
1:A:328:LEU:N	1:A:329:PRO:CD	2.81	0.43	
1:A:253:ILE:HG13	1:A:315:ASP:HB3	1.99	0.43	



		Interatomic	Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
1:A:289:LYS:HZ3	9:A:705:1PE:H262	1.84	0.43	
1:M:311:VAL:CG1	1:M:312:VAL:N	2.81	0.43	
2:N:35:SER:O	2:N:38:ASP:HB2	2.19	0.43	
2:N:149:ILE:HG23	2:N:216:LYS:HG3	1.99	0.43	
1:M:239:SER:CB	1:M:241:ILE:HG13	2.49	0.43	
2:N:82:ARG:HG3	2:N:83:ASP:OD1	2.19	0.43	
2:N:221:ALA:O	2:N:225:GLN:HG2	2.19	0.43	
1:A:204:ASN:N	1:A:204:ASN:HD22	2.17	0.43	
2:B:73:PRO:HG2	2:B:213:VAL:HG11	2.01	0.43	
3:C:49:LEU:HG	4:D:55:LEU:CD1	2.49	0.43	
4:D:53:ARG:HH11	4:D:53:ARG:HG2	1.84	0.43	
1:M:382:SER:C	1:M:384:GLY:N	2.73	0.43	
2:N:57:CYS:O	2:N:59:MET:HG2	2.19	0.43	
1:A:78:GLU:OE2	1:A:568:VAL:HA	2.19	0.42	
1:M:0:MET:O	1:M:1:GLN:HB2	2.19	0.42	
1:M:499:ASN:C	1:M:499:ASN:ND2	2.72	0.42	
2:N:36:LEU:HD23	2:N:76:ALA:CB	2.49	0.42	
2:N:135:THR:HG22	2:N:137:ALA:N	2.33	0.42	
1:A:346:GLU:HB3	1:A:347:PRO:CD	2.49	0.42	
4:D:4:ASN:HD21	4:P:6:LYS:HE3	1.84	0.42	
2:N:81:LEU:N	2:N:81:LEU:CD1	2.82	0.42	
2:N:110:ILE:O	2:N:114:GLU:HG3	2.19	0.42	
1:A:89:CYS:N	1:A:90:PRO:CD	2.81	0.42	
4:D:64:ARG:NH1	4:D:115:VAL:O	2.51	0.42	
1:A:120:LYS:HG2	1:A:121:ILE:HD13	2.01	0.42	
2:B:188:LYS:NZ	2:B:230:GLU:CG	2.81	0.42	
1:M:44:HIS:NE2	8:M:821:FAD:C8	2.78	0.42	
4:P:35:VAL:O	4:P:40:PRO:HD3	2.19	0.42	
1:A:243:MET:HA	1:A:331:ILE:HD12	2.01	0.42	
4:D:30:VAL:HG13	4:D:31:MET:N	2.34	0.42	
4:D:36:GLY:C	4:D:37:ILE:HG13	2.40	0.42	
1:M:365:GLN:O	1:M:366:ASN:ND2	2.48	0.42	
1:M:481:GLU:O	1:M:485:ARG:HG2	2.18	0.42	
1:M:548:LEU:HD21	1:M:575:PRO:HG3	2.02	0.42	
4:P:10:GLU:OE2	4:P:80:HIS:HE1	2.02	0.42	
4:P:68:PHE:CE1	4:P:72:VAL:HG21	2.55	0.42	
1:A:42:ARG:HD2	1:A:42:ARG:N	2.35	0.42	
1:A:379:GLU:HB2	8:A:721:FAD:H5'2	2.02	0.42	
2:B:6:LEU:HD23	2:B:81:LEU:HD13	2.02	0.42	
1:M:469:PRO:CD	1:M:536:ASP:HB3	2.50	0.42	
1:M:469:PRO:HA	1:M:523:MET:HE3	2.02	0.42	



			Clash	
Atom-1	Atom-2	distance (\AA)	overlap (Å)	
2:N:137:ALA:HB2	3:O:100:ASP:OD1	2.20	0.42	
3:O:59:PHE:O	3:O:62:PHE:HB3	2.20	0.42	
1:M:92:GLU:HG3	1:M:400:VAL:O	2.20	0.42	
1:M:100:GLY:O	2:N:184:ARG:NH2	2.51	0.42	
2:N:54:ARG:HH21	2:N:103:VAL:CG1	2.33	0.42	
1:M:85:PHE:CD2	1:M:385:LEU:HD11	2.55	0.42	
2:N:45:ASP:OD1	7:N:803:ACT:H1	2.20	0.42	
1:A:542:ARG:NH2	1:A:544:ASP:OD2	2.41	0.42	
1:M:51:GLY:O	1:M:396:LEU:HD12	2.19	0.42	
1:M:184:ARG:HH11	1:M:184:ARG:HG3	1.85	0.42	
1:M:321:GLU:HA	1:M:324:LEU:HB3	2.02	0.42	
1:M:370:ARG:HH12	1:M:554:PHE:HZ	1.67	0.42	
2:N:206:PHE:HA	11:N:245:F3S:S1	2.60	0.42	
2:B:28:VAL:HA	2:B:29:PRO:HD3	1.92	0.41	
1:M:18:ARG:HG2	1:M:400:VAL:HA	2.01	0.41	
2:N:72:VAL:HA	2:N:73:PRO:HD3	1.77	0.41	
1:M:213:MET:HE3	1:M:380:CYS:HA	2.02	0.41	
1:M:377:VAL:HG21	1:M:402:PHE:O	2.19	0.41	
2:N:188:LYS:HE2	2:N:192:MET:CE	2.50	0.41	
1:A:68:ASP:HB3	1:A:391:LEU:HD21	2.01	0.41	
2:B:8:ILE:HD11	2:B:81:LEU:CD1	2.50	0.41	
3:C:39:SER:O	3:C:43:ILE:HG13	2.21	0.41	
2:N:16:GLU:HG2	3:O:3:LYS:HG2	2.02	0.41	
3:O:28:ARG:HD2	4:P:81:ARG:HH22	1.85	0.41	
1:A:242:LEU:HD21	6:A:702:OAA:O1	2.20	0.41	
3:C:59:PHE:CZ	3:C:63:LEU:HD11	2.55	0.41	
1:M:9:ILE:HD12	1:M:20:ALA:HB2	2.03	0.41	
1:M:106:ARG:NH1	1:M:111:VAL:O	2.53	0.41	
1:M:180:LEU:HD21	1:M:436:LEU:CD2	2.51	0.41	
2:N:126:THR:OG1	2:N:129:GLN:HG3	2.21	0.41	
3:C:50:LYS:HE2	3:C:50:LYS:CA	2.49	0.41	
1:M:48:ALA:HB3	1:M:132:GLY:HA3	2.02	0.41	
2:N:151:CYS:HB2	2:N:153:LEU:HG	2.03	0.41	
4:P:96:GLY:O	4:P:97:LYS:C	2.57	0.41	
1:A:209:THR:OG1	1:A:507:GLU:HG2	2.20	0.41	
1:A:443:ASP:HA	1:A:490:ARG:HG3	2.03	0.41	
3:C:12:THR:CG2	3:C:13:SER:N	2.83	0.41	
3:C:15:TRP:CD2	3:C:16:TRP:N	2.88	0.41	
1:M:527:GLU:OE2	1:M:529:ARG:NH1	2.54	0.41	
4:P:72:VAL:HG12	4:P:76:TRP:CD1	2.56	0.41	
1:M:199:TYR:OH	1:M:229:VAL:HG21	2.21	0.41	



		Interatomic	Clash	
Atom-1	Atom-1 Atom-2		overlap (Å)	
1:M:342:ASP:HA	1:M:343:PRO:HD3	1.84	0.41	
1:M:439:LEU:O	1:M:442:GLN:HB3	2.20	0.41	
3:C:72:ASN:HD22	3:C:72:ASN:HA	1.61	0.41	
1:M:570:ILE:HG22	1:M:571:THR:N	2.35	0.41	
2:N:150:ASN:HA	12:N:246:SF4:S4	2.61	0.41	
14:P:710:CE1:H211	14:P:710:CE1:H171	2.02	0.41	
1:A:59:HIS:CD2	1:A:59:HIS:H	2.39	0.41	
2:B:188:LYS:HZ2	2:B:230:GLU:CG	2.34	0.41	
1:M:26:ALA:O	1:M:28:PRO:HD3	2.21	0.41	
1:M:233:PRO:HG2	1:M:248:ARG:HH22	1.84	0.41	
1:M:233:PRO:HG2	1:M:248:ARG:NH2	2.36	0.41	
1:M:316:LEU:O	1:M:319:LEU:HG	2.21	0.41	
2:N:214:CYS:SG	2:N:218:VAL:HG23	2.60	0.41	
3:O:47:PHE:HE2	4:P:114:GLY:HA3	1.86	0.41	
3:O:89:LEU:C	3:O:91:PRO:HD2	2.41	0.41	
1:A:57:GLN:NE2	1:A:122:GLU:HG2	2.36	0.41	
1:A:204:ASN:N	1:A:204:ASN:ND2	2.69	0.41	
2:B:134:GLN:HE21	2:B:139:MET:CE	2.35	0.41	
1:M:7:LEU:CD2	1:M:411:THR:HA	2.39	0.41	
1:M:62:PHE:HB3	1:M:86:VAL:CG2	2.50	0.41	
1:M:485:ARG:HH11	1:M:485:ARG:HB3	1.85	0.40	
2:N:56:SER:O	2:N:58:ARG:HG3	2.21	0.40	
1:A:529:ARG:NH1	1:A:542:ARG:HG2	2.36	0.40	
3:C:18:LYS:HB2	3:C:19:LEU:H	1.61	0.40	
1:M:208:VAL:O	1:M:208:VAL:HG12	2.19	0.40	
1:M:212:GLY:HA2	1:M:215:MET:HE2	2.03	0.40	
1:M:356:TYR:HD1	1:M:358:MET:HG2	1.86	0.40	
4:P:26:ILE:HG22	4:P:27:ILE:N	2.35	0.40	
1:A:48:ALA:HA	8:A:721:FAD:C6	2.51	0.40	
2:B:141:LYS:HE3	3:C:95:ASN:OD1	2.21	0.40	
3:C:65:ASN:HB3	3:C:68:ILE:H	1.86	0.40	
4:D:95:ALA:HB2	2:N:239:THR:HG22	2.03	0.40	
1:M:213:MET:HB3	1:M:223:LEU:HD21	2.04	0.40	
1:M:311:VAL:HG13	1:M:350:VAL:N	2.36	0.40	
1:M:324:LEU:O	1:M:328:LEU:N	2.47	0.40	
1:M:508:LEU:O	1:M:508:LEU:HD12	2.21	0.40	
1:A:152:PHE:HB3	1:A:155:HIS:CG	2.56	0.40	
1:M:76:LEU:HD23	1:M:76:LEU:HA	1.98	0.40	
1:M:313:TYR:CD1	1:M:347:PRO:HB2	2.57	0.40	
2:N:116:ILE:HG22	2:N:116:ILE:O	2.21	0.40	
2:N:226:GLN:HE21	2:N:226:GLN:HB2	1.62	0.40	



Atom-1 Atom-2		Interatomic distance (Å)	Clash overlap (Å)	
1:M:6:ASP:O	1:M:185:ALA:HB1	2.21	0.40	
3:O:25:TYR:HD1	3:O:28:ARG:HH21	1.69	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	Perce	entiles
1	А	575/602~(96%)	541 (94%)	30 (5%)	4 (1%)	22	46
1	М	575/602~(96%)	487 (85%)	75 (13%)	13 (2%)	6	16
2	В	241/243~(99%)	224 (93%)	16 (7%)	1 (0%)	34	60
2	N	241/243~(99%)	215 (89%)	20 (8%)	6 (2%)	5	14
3	С	128/130~(98%)	120 (94%)	4 (3%)	4 (3%)	4	9
3	Ο	128/130~(98%)	114 (89%)	12 (9%)	2 (2%)	9	24
4	D	117/119~(98%)	111 (95%)	3 (3%)	3 (3%)	5	13
4	Р	117/119~(98%)	102 (87%)	14 (12%)	1 (1%)	17	40
All	All	2122/2188~(97%)	1914 (90%)	174 (8%)	34 (2%)	9	24

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	С	18	LYS
3	С	65	ASN
1	М	244	THR
1	М	382	SER
1	А	318	HIS
1	М	79	GLN
1	М	540	THR
2	Ν	183	SER



Mol	Chain	Res	Type
3	0	18	LYS
2	В	56	SER
4	D	43	LEU
1	А	389	ASN
3	С	66	PRO
1	М	329	PRO
1	М	492	THR
2	Ν	55	TRP
2	N	93	LEU
2	N	101	ASP
3	0	99	LYS
1	А	244	THR
1	М	119	MET
1	М	257	LYS
1	М	344	VAL
2	Ν	56	SER
1	А	343	PRO
4	D	117	THR
1	М	318	HIS
1	М	324	LEU
2	Ν	128	ASP
1	М	444	GLY
4	Р	4	ASN
1	M	383	VAL
3	С	104	GLY
4	D	99	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
1	А	460/475~(97%)	446 (97%)	14 (3%)	41 70		
1	М	460/475~(97%)	437 (95%)	23~(5%)	24 51		
2	В	205/205~(100%)	199~(97%)	6 (3%)	42 71		
2	Ν	205/205~(100%)	195~(95%)	10 (5%)	25 52		



Mol	Chain	Analysed	Rotameric Outliers		Percentiles		
3	С	111/111 (100%)	107~(96%)	4 (4%)	35	64	
3	Ο	111/111 (100%)	108~(97%)	3~(3%)	44	74	
4	D	97/97~(100%)	94~(97%)	3~(3%)	40	69	
4	Р	97/97~(100%)	95~(98%)	2(2%)	53	80	
All	All	1746/1776~(98%)	1681 (96%)	65~(4%)	34	63	

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All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	42	ARG
1	А	74	ASP
1	А	93	MET
1	А	184	ARG
1	А	197	ARG
1	А	200	ARG
1	А	319	LEU
1	А	325	HIS
1	А	327	ARG
1	А	358	MET
1	А	413	ARG
1	А	498	PHE
1	А	528	SER
1	А	560	THR
2	В	65	CYS
2	В	81	LEU
2	В	128	ASP
2	В	178	ARG
2	В	206	PHE
2	В	212	GLU
3	С	39	SER
3	С	50	LYS
3	С	84	LYS
3	С	92	LYS
4	D	0	MET
4	D	86	MET
4	D	118	ILE
1	М	74	ASP
1	М	93	MET
1	М	122	GLU
1	М	126	PHE
1	М	137	HIS



Mol	Chain	Res	Type
1	М	143	SER
1	М	155	HIS
1	М	156	PHE
1	М	163	ASP
1	М	164	ASP
1	М	197	ARG
1	М	227	GLU
1	М	243	MET
1	М	330	PHE
1	М	375	PHE
1	М	389	ASN
1	М	413	ARG
1	М	465	ILE
1	М	470	GLU
1	М	485	ARG
1	М	498	PHE
1	М	499	ASN
1	М	558	ASP
2	N	46	ASN
2	Ν	50	ASP
2	N	100	ARG
2	N	128	ASP
2	N	148	CYS
2	N	178	ARG
2	Ν	185	ASP
2	N	189	LYS
2	Ν	206	PHE
2	N	226	GLN
3	0	5	LYS
3	0	37	TRP
3	0	39	SER
4	Р	7	ARG
4	Р	51	TYR

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

Mol	Chain	Res	Type
1	А	87	HIS
1	А	141	GLN
1	А	232	HIS
1	А	279	ASN
1	А	292	GLN



Mol	Chain	Res	Type
1	А	434	GLN
1	А	442	GLN
2	В	134	GLN
2	В	194	GLN
3	С	51	ASN
3	С	72	ASN
4	D	4	ASN
4	D	59	GLN
1	М	1	GLN
1	М	27	ASN
1	М	137	HIS
1	М	174	ASN
1	М	204	ASN
1	М	292	GLN
1	М	394	ASN
1	М	409	GLN
1	М	421	ASN
1	М	434	GLN
1	М	441	ASN
1	М	447	ASN
1	М	499	ASN
1	М	520	HIS
1	М	546	ASN
2	Ν	95	ASN
2	Ν	129	GLN
2	Ν	150	ASN
2	Ν	160	GLN
2	Ν	177	HIS
2	N	186	HIS
2	N	226	GLN
3	0	72	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 2 are monoatomic - leaving 21 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).

Mal	Type	Chain	Bos	Link	Bond lengths		Bond angles			
WIOI	туре	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
12	SF4	В	246	2	0,12,12	-	-	-		
14	CE1	Ο	812	-	36,36,36	1.11	0	35,35,35	1.89	15 (42%)
8	FAD	М	821	-	53,58,58	1.40	6 (11%)	68,89,89	1.46	9 (13%)
9	1PE	А	705	-	15,15,15	1.63	0	14,14,14	2.29	10 (71%)
14	CE1	Ο	813	-	36,36,36	1.18	0	35,35,35	1.95	15 (42%)
14	CE1	Р	710	-	36,36,36	1.10	0	35,35,35	1.91	15 (42%)
14	CE1	Ο	811	-	36,36,36	1.11	0	35,35,35	1.97	15 (42%)
7	ACT	N	803	-	3,3,3	1.14	0	3,3,3	1.05	0
14	CE1	Р	810	-	36,36,36	1.10	0	35,35,35	1.99	15 (42%)
13	HQO	С	700	-	20,20,20	<mark>3.05</mark>	8 (40%)	18,26,26	1.18	1 (5%)
7	ACT	А	703	-	3,3,3	0.91	0	3,3,3	1.32	0
7	ACT	В	704	-	3,3,3	0.76	0	3,3,3	1.00	0
11	F3S	Ν	245	2	0,9,9	-	-	-		
6	OAA	А	702	-	8,8,8	1.28	1 (12%)	$9,\!10,\!10$	1.84	2 (22%)
13	HQO	Ν	800	-	20,20,20	<mark>3.05</mark>	8 (40%)	18,26,26	1.18	1 (5%)
6	OAA	М	802	-	8,8,8	1.27	1 (12%)	9,10,10	1.85	2 (22%)
12	SF4	N	246	2	0,12,12	-	-	-		
10	FES	N	244	2	0,4,4	-	-	-		
10	FES	В	244	2	0,4,4	-	-	-		
11	F3S	В	245	2	0,9,9	-	_	-		
8	FAD	А	721	-	53, 58, 58	1.46	11 (20%)	68,89,89	1.48	12 (17%)

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



$1 \mathrm{KF6}$

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	SF4	В	246	2	_	_	0/6/5/5
10	FES	В	244	2	-	-	0/1/1/1
14	CE1	0	812	-	-	18/34/34/34	-
13	HQO	С	700	-	-	3/7/7/7	0/2/2/2
11	F3S	N	245	2	-	-	0/3/3/3
6	OAA	А	702	-	-	4/8/8/8	-
8	FAD	М	821	-	-	5/30/50/50	0/6/6/6
9	1PE	А	705	-	-	8/13/13/13	-
13	HQO	N	800	-	-	3/7/7/7	0/2/2/2
14	CE1	0	813	-	-	14/34/34/34	-
6	OAA	М	802	-	-	4/8/8/8	-
14	CE1	Р	710	-	-	17/34/34/34	-
14	CE1	0	811	-	-	18/34/34/34	-
12	SF4	N	246	2	-	-	0/6/5/5
11	F3S	В	245	2	-	-	0/3/3/3
14	CE1	Р	810	-	-	16/34/34/34	-
8	FAD	А	721	-	-	6/30/50/50	0/6/6/6
10	FES	N	244	2	-	-	0/1/1/1

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Ν	800	HQO	O4-N1	-11.24	1.23	1.38
13	С	700	HQO	O4-N1	-11.24	1.23	1.38
8	М	821	FAD	O4B-C1B	3.91	1.46	1.41
8	М	821	FAD	C4A-N3A	3.77	1.40	1.35
8	А	721	FAD	C10-N10	3.53	1.45	1.37
13	С	700	HQO	O1-C1	-3.51	1.26	1.36
13	Ν	800	HQO	O1-C1	-3.50	1.26	1.36
8	М	821	FAD	C5'-C4'	3.48	1.56	1.51
13	Ν	800	HQO	C11-C3	-3.22	1.42	1.50
13	С	700	HQO	C11-C3	-3.21	1.42	1.50
8	А	721	FAD	C10-N1	2.91	1.39	1.33
8	М	821	FAD	C10-N10	2.74	1.43	1.37
8	А	721	FAD	C9-C9A	2.71	1.44	1.39
8	А	721	FAD	C4X-N5	2.66	1.35	1.30
13	Ν	800	HQO	C2-C3	2.61	1.43	1.38
13	С	700	HQO	C2-C3	2.60	1.43	1.38



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	А	721	FAD	C4-N3	2.55	1.43	1.38
13	N	800	HQO	C7-C6	2.52	1.42	1.36
13	С	700	HQO	C7-C6	2.51	1.42	1.36
8	А	721	FAD	C2A-N3A	2.43	1.36	1.32
13	N	800	HQO	C8-C9	2.41	1.42	1.36
6	М	802	OAA	O2-C1	2.37	1.38	1.30
13	С	700	HQO	C8-C9	2.36	1.42	1.36
6	А	702	OAA	O2-C1	2.36	1.38	1.30
8	А	721	FAD	C2B-C1B	-2.33	1.50	1.53
8	М	821	FAD	C9-C8	2.31	1.43	1.39
8	А	721	FAD	O4B-C1B	2.19	1.44	1.41
13	Ν	800	HQO	C8-C7	2.18	1.43	1.38
13	Ν	800	HQO	C10-C5	2.18	1.46	1.42
13	С	700	HQO	C8-C7	2.17	1.43	1.38
8	М	821	FAD	C4X-N5	2.17	1.35	1.30
13	С	700	HQO	C10-C5	2.16	1.46	1.42
8	А	721	FAD	P-O5'	-2.12	1.50	1.59
8	A	721	FAD	C5A-N7A	-2.05	1.32	1.39
8	А	721	FAD	C9A-C5X	2.02	1.44	1.41

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
8	М	821	FAD	N3A-C2A-N1A	-5.72	119.73	128.68
14	Р	810	CE1	O28-C27-C26	4.64	131.30	110.39
8	М	821	FAD	C4-N3-C2	-3.91	118.42	125.64
6	М	802	OAA	O3-C3-C2	3.66	125.88	120.58
6	А	702	OAA	O3-C3-C2	3.65	125.86	120.58
13	С	700	HQO	O1-C1-C10	3.62	120.83	116.31
13	N	800	HQO	O1-C1-C10	3.61	120.82	116.31
8	А	721	FAD	C4-N3-C2	-3.53	119.13	125.64
8	А	721	FAD	N3A-C2A-N1A	-3.52	123.17	128.68
14	0	813	CE1	O22-C23-C24	3.23	124.96	110.39
14	0	811	CE1	O19-C18-C17	3.22	124.92	110.39
14	Р	710	CE1	O28-C27-C26	3.19	124.76	110.39
14	0	813	CE1	O22-C21-C20	3.19	124.76	110.39
14	0	812	CE1	O22-C21-C20	3.18	124.73	110.39
8	А	721	FAD	C5'-C4'-C3'	3.17	118.34	112.20
14	0	812	CE1	O22-C23-C24	3.15	124.61	110.39
14	0	812	CE1	O13-C14-C15	3.15	124.59	110.39
6	М	802	OAA	C2-C3-C4	-3.14	112.55	117.85
6	А	702	OAA	C2-C3-C4	-3.13	112.56	117.85



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
14	Р	810	CE1	O28-C29-C30	3.13	124.49	110.39
14	Р	810	CE1	O13-C14-C15	3.12	124.48	110.39
14	Р	710	CE1	O25-C24-C23	3.11	124.41	110.39
14	0	811	CE1	O16-C17-C18	3.10	124.38	110.39
14	0	811	CE1	O22-C23-C24	3.10	124.37	110.39
8	А	721	FAD	C10-N1-C2	3.08	123.06	116.90
14	0	813	CE1	O34-C35-C36	3.06	123.52	110.07
14	0	811	CE1	O16-C15-C14	3.06	124.19	110.39
14	0	812	CE1	O16-C15-C14	3.03	124.07	110.39
8	А	721	FAD	C5X-N5-C4X	3.02	123.09	118.07
8	М	821	FAD	C4X-C4-N3	3.02	120.85	113.19
14	Р	710	CE1	O13-C14-C15	3.01	123.97	110.39
14	Р	810	CE1	O22-C23-C24	3.01	123.96	110.39
14	0	813	CE1	O19-C18-C17	3.00	123.92	110.39
8	А	721	FAD	O3'-C3'-C2'	-2.99	101.58	108.81
14	Р	710	CE1	O22-C23-C24	2.98	123.85	110.39
8	М	821	FAD	C5X-N5-C4X	2.97	123.02	118.07
9	А	705	1PE	OH5-C25-C15	2.94	123.65	110.39
14	Р	710	CE1	O34-C33-C32	2.93	123.60	110.39
14	0	812	CE1	O34-C35-C36 2.91		122.85	110.07
14	0	813	CE1	O25-C24-C23	2.90	123.49	110.39
14	Р	810	CE1	O25-C24-C23	2.90	123.46	110.39
14	0	813	CE1	O16-C15-C14	2.89	123.43	110.39
9	А	705	1PE	OH3-C22-C12	2.89	122.76	110.07
14	0	812	CE1	O19-C18-C17	2.88	123.40	110.39
14	0	813	CE1	O25-C26-C27	2.86	123.31	110.39
14	0	813	CE1	O31-C32-C33	2.85	123.25	110.39
14	0	812	CE1	O34-C33-C32	2.83	123.15	110.39
14	0	811	CE1	O31-C32-C33	2.82	123.11	110.39
9	А	705	1PE	OH4-C24-C14	2.80	123.03	110.39
14	0	813	CE1	O28-C29-C30	2.80	123.01	110.39
14	0	811	CE1	O19-C20-C21	2.79	122.99	110.39
9	А	705	1PE	OH4-C13-C23	2.78	122.95	110.39
14	Р	710	CE1	O16-C15-C14	2.76	122.84	110.39
14	0	811	CE1	O22-C21-C20	2.75	122.77	110.39
14	0	811	CE1	O34-C35-C36	2.74	122.12	110.07
14	0	811	CE1	O25-C24-C23	2.74	122.75	110.39
14	Р	710	CE1	O19-C20-C21	2.72	122.68	110.39
14	0	811	CE1	O34-C33-C32	2.72	122.68	110.39
14	Р	710	CE1	O34-C35-C36	2.72	122.03	110.07
14	0	812	CE1	O16-C17-C18	2.70	$1\overline{22.57}$	110.39
14	Р	810	CE1	O34-C33-C32	2.70	122.57	110.39



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
14	0	812	CE1	O31-C32-C33	2.70	122.57	110.39
14	Р	810	CE1	O31-C30-C29	2.68	122.50	110.39
14	0	813	CE1	O13-C14-C15	2.66	122.41	110.39
14	Р	810	CE1	O22-C21-C20	2.64	122.32	110.39
14	Р	810	CE1	O16-C17-C18	2.64	122.28	110.39
14	0	813	CE1	O34-C33-C32	2.63	122.25	110.39
14	Р	810	CE1	O34-C35-C36	2.63	121.61	110.07
8	А	721	FAD	C4X-C4-N3	2.62	119.84	113.19
8	А	721	FAD	C9A-C5X-N5	-2.61	119.60	122.43
14	0	812	CE1	O31-C30-C29	2.61	122.14	110.39
9	А	705	1PE	OH3-C23-C13	2.61	122.14	110.39
8	М	821	FAD	C9A-C5X-N5	-2.60	119.60	122.43
14	0	812	CE1	O25-C24-C23	2.60	122.11	110.39
8	А	721	FAD	O4-C4-C4X	-2.60	119.71	126.60
14	0	811	CE1	O28-C27-C26	2.60	122.10	110.39
9	А	705	1PE	OH6-C15-C25	2.58	122.04	110.39
14	Р	810	CE1	O19-C20-C21	2.58	122.03	110.39
14	0	811	CE1	O13-C14-C15	2.57	121.98	110.39
14	0	811	CE1	O31-C30-C29	2.56	121.95	110.39
9	А	705	1PE	OH6-C26-C16	2.55	121.29	110.07
14	0	811	CE1	O28-C29-C30	2.55	121.88	110.39
14	0	813	CE1	O28-C27-C26	2.53	121.82	110.39
14	Р	710	CE1	O31-C30-C29	2.53	121.80	110.39
14	0	813	CE1	O31-C30-C29	2.52	121.77	110.39
8	А	721	FAD	C4X-C10-N1	-2.51	118.89	124.73
14	Р	710	CE1	O22-C21-C20	2.50	121.67	110.39
14	Р	710	CE1	O28-C29-C30	2.49	121.62	110.39
14	Р	810	CE1	O16-C15-C14	2.49	121.62	110.39
8	М	821	FAD	C10-N1-C2	2.49	121.87	116.90
14	Р	710	CE1	O31-C32-C33	2.47	121.54	110.39
8	А	721	FAD	P-O3P-PA	2.47	141.29	132.83
14	0	811	CE1	O25-C26-C27	2.46	121.48	110.39
14	Р	710	CE1	O19-C18-C17	2.44	121.39	110.39
14	Р	710	CE1	O25-C26-C27	2.41	121.24	110.39
14	Р	810	CE1	O31-C32-C33	2.40	121.24	110.39
9	A	705	1PE	OH5-C14-C24	2.37	121.09	110.39
14	0	813	CE1	C10-C11-C12	-2.34	103.11	113.49
8	М	821	FAD	O4-C4-C4X	-2.33	120.43	126.60
14	0	812	CE1	O28-C27-C26	2.32	120.86	110.39
14	0	812	CE1	O28-C29-C30	2.31	120.80	110.39
14	0	813	CE1	O16-C17-C18	2.31	120.79	110.39
14	0	812	CE1	O25-C26-C27	2.27	120.64	110.39



$1 \mathrm{KF6}$

Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
14	Р	710	CE1	O16-C17-C18	2.26	120.59	110.39
14	0	812	CE1	O19-C20-C21	2.26	120.57	110.39
14	Р	810	CE1	O19-C18-C17	2.25	120.53	110.39
14	Р	810	CE1	O25-C26-C27	2.22	120.38	110.39
8	М	821	FAD	P-O3P-PA	2.21	140.41	132.83
9	А	705	1PE	OH2-C12-C22	2.13	124.19	111.81
8	М	821	FAD	C5'-C4'-C3'	2.12	116.30	112.20
8	А	721	FAD	C10-C4X-N5	-2.05	120.50	124.86
9	А	705	1PE	OH7-C16-C26	2.01	123.48	111.81

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	А	702	OAA	O3-C3-C4-O4
6	А	702	OAA	O3-C3-C4-O5
6	А	702	OAA	C2-C3-C4-O5
6	М	802	OAA	O3-C3-C4-O4
6	М	802	OAA	O3-C3-C4-O5
6	М	802	OAA	C2-C3-C4-O5
8	А	721	FAD	N10-C1'-C2'-O2'
8	А	721	FAD	N10-C1'-C2'-C3'
8	А	721	FAD	PA-O3P-P-O5'
8	М	821	FAD	N10-C1'-C2'-O2'
8	М	821	FAD	N10-C1'-C2'-C3'
8	М	821	FAD	PA-O3P-P-O5'
14	0	811	CE1	C17-C18-O19-C20
14	0	812	CE1	O28-C29-C30-O31
14	0	813	CE1	O25-C26-C27-O28
14	Р	710	CE1	O28-C29-C30-O31
14	Р	710	CE1	O13-C14-C15-O16
14	Р	710	CE1	O22-C23-C24-O25
9	А	705	1PE	ОН7-С16-С26-ОН6
9	А	705	1PE	OH5-C14-C24-OH4
14	Р	810	CE1	O25-C26-C27-O28
14	0	811	CE1	O28-C29-C30-O31
14	0	812	CE1	O13-C14-C15-O16
13	С	700	HQO	C3-C11-C13-C12
13	N	800	HQO	C3-C11-C13-C12
14	Р	810	CE1	O34-C35-C36-O37
13	С	700	HQO	C14-C12-C13-C11
13	N	800	HQO	C14-C12-C13-C11



Mol	Chain	Res	Type	Atoms
14	0	813	CE1	C6-C7-C8-C9
14	Р	810	CE1	O28-C29-C30-O31
14	0	813	CE1	C7-C8-C9-C10
14	Р	710	CE1	O34-C35-C36-O37
14	0	811	CE1	C7-C8-C9-C10
14	Р	710	CE1	C11-C10-C9-C8
14	0	813	CE1	C3-C4-C5-C6
14	0	813	CE1	O13-C14-C15-O16
14	Р	810	CE1	O22-C23-C24-O25
14	0	812	CE1	O25-C26-C27-O28
14	0	812	CE1	C6-C7-C8-C9
14	0	812	CE1	C3-C4-C5-C6
14	Р	810	CE1	O13-C14-C15-O16
14	0	811	CE1	C3-C4-C5-C6
14	Р	710	CE1	O25-C26-C27-O28
14	Р	810	CE1	C2-C3-C4-C5
14	0	811	CE1	C6-C7-C8-C9
14	0	812	CE1	C7-C8-C9-C10
14	0	812	CE1	C2-C3-C4-C5
14	Р	810	CE1	C6-C7-C8-C9
14	0	811	CE1	O34-C35-C36-O37
9	А	705	1PE	C13-C23-OH3-C22
14	Р	810	CE1	C11-C12-O13-C14
14	0	813	CE1	C23-C24-O25-C26
14	0	812	CE1	C24-C23-O22-C21
9	А	705	1PE	C15-C25-OH5-C14
14	Р	710	CE1	C33-C32-O31-C30
14	0	813	CE1	C4-C5-C6-C7
14	Р	810	CE1	C11-C10-C9-C8
14	0	811	CE1	C36-C35-O34-C33
14	0	813	CE1	C33-C32-O31-C30
14	0	811	CE1	O22-C23-C24-O25
9	А	705	1PE	C14-C24-OH4-C13
14	0	811	CE1	O25-C26-C27-O28
14	Р	710	CE1	C4-C5-C6-C7
14	0	813	CE1	C20-C21-O22-C23
13	С	700	HQO	C12-C14-C15-C16
13	N	800	HQO	C12-C14-C15-C16
14	Р	710	CE1	C36-C35-O34-C33
6	А	702	OAA	C2-C3-C4-O4
6	М	802	OAA	C2-C3-C4-O4
14	0	813	CE1	C18-C17-O16-C15



Mol	Chain	Res	Type	Atoms
14	0	812	CE1	O34-C35-C36-O37
14	0	812	CE1	C11-C12-O13-C14
14	0	812	CE1	C4-C5-C6-C7
14	Р	710	CE1	C32-C33-O34-C35
14	Р	810	CE1	C30-C29-O28-C27
9	А	705	1PE	OH2-C12-C22-OH3
14	0	812	CE1	C32-C33-O34-C35
14	Р	810	CE1	C36-C35-O34-C33
14	Р	810	CE1	O19-C20-C21-O22
14	0	812	CE1	C33-C32-O31-C30
14	Р	810	CE1	C18-C17-O16-C15
14	Р	710	CE1	C11-C12-O13-C14
14	0	812	CE1	C30-C29-O28-C27
14	0	811	CE1	C32-C33-O34-C35
14	0	811	CE1	C20-C21-O22-C23
8	А	721	FAD	O4B-C4B-C5B-O5B
8	М	821	FAD	O4B-C4B-C5B-O5B
14	0	811	CE1	C24-C23-O22-C21
14	0	813	CE1	O28-C29-C30-O31
14	Р	810	CE1	C24-C23-O22-C21
14	0	811	CE1	C11-C12-O13-C14
14	0	813	CE1	O31-C32-C33-O34
14	0	811	CE1	O19-C20-C21-O22
14	Р	710	CE1	O19-C20-C21-O22
14	Р	710	CE1	C24-C23-O22-C21
14	Р	710	CE1	C1-C2-C3-C4
8	А	721	FAD	PA-O3P-P-O1P
8	А	721	FAD	PA-O3P-P-O2P
8	М	821	FAD	PA-O3P-P-O1P
14	0	811	CE1	O13-C14-C15-O16
14	0	812	CE1	O22-C23-C24-O25
14	0	812	CE1	O19-C20-C21-O22
14	Р	710	CE1	C6-C7-C8-C9
14	0	812	CE1	O31-C32-C33-O34
14	Р	810	CE1	O16-C17-C18-O19
14	Р	710	CE1	O16-C17-C18-O19
14	Р	710	CE1	O31-C32-C33-O34
14	0	811	CE1	C1-C2-C3-C4
14	0	811	CE1	O16-C17-C18-O19
14	Р	810	CE1	O31-C32-C33-O34
9	А	705	1PE	OH6-C15-C25-OH5
14	0	811	CE1	O31-C32-C33-O34

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Mol	Chain	Res	Type	Atoms
14	0	813	CE1	O16-C17-C18-O19
9	А	705	1PE	OH4-C13-C23-OH3
14	0	813	CE1	O19-C20-C21-O22
14	0	812	CE1	O16-C17-C18-O19

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There are no ring outliers.

11 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	М	821	FAD	8	0
9	А	705	1PE	5	0
14	Р	710	CE1	2	0
7	Ν	803	ACT	2	0
14	Р	810	CE1	3	0
13	С	700	HQO	3	0
11	Ν	245	F3S	1	0
6	А	702	OAA	2	0
13	Ν	800	HQO	2	0
12	N	246	SF4	4	0
8	А	721	FAD	8	0

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























5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.

