

Full wwPDB X-ray Structure Validation Report (i)

May 23, 2020 - 05:46 am BST

PDB ID	:	6H3O
Title	:	Alcohol oxidase from Phanerochaete chrysosporium mutant F101S
Authors	:	Nguyen, QT.; Romero, E.; Dijkman, W.P.; de Vasconcellos, S.P.; Binda, C.;
		Mattevi, A.; Fraaije, M.W.
Deposited on	:	2018-07-19
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 https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

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)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$		
R _{free}	130704	4661 (2.50-2.50)		
Clashscore	141614	$5346\ (2.50-2.50)$		
Ramachandran outliers	138981	$5231 \ (2.50-2.50)$		
Sidechain outliers	138945	5233 (2.50-2.50)		
RSRZ outliers	127900	4559(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 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% 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	А	651	76%	20%	•
1	В	651	78%	19%	
1	С	651	78%	20%	•
1	D	651	77%	20%	•
1	Е	651	76%	20%	•••
1	F	651	78%	18%	•



Mol	Chain	Length	Quality of chain		
1	G	651	76%	20%	•
1	Н	651	% 	20%	•



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 41785 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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	Δ	640	Total	С	Ν	Ο	\mathbf{S}	0	1	0
	A	049	5095	3200	904	966	25	0	L	0
1	р	647	Total	С	Ν	Ο	S	0	0	0
	D	047	5067	3184	896	962	25	0	0	0
1	C	619	Total	С	Ν	Ο	S	0	0	0
	U	040	5078	3190	900	963	25	0	0	0
1	п	640	Total	С	Ν	Ο	S	0	0	0
	D	049	5088	3196	903	964	25	0	0	U
1	F	649	Total	С	Ν	Ο	S	0	0	0
	Ľ	040	5078	3190	900	963	25	0	0	
1	Б	650	Total	С	Ν	Ο	S	0	0	0
	Г	0.00	5092	3198	904	965	25	0	0	0
1	C	619	Total	С	Ν	Ο	S	0	0	0
	G	040	5078	3190	900	963	25	0	0	0
1	ц	649	Total	С	Ν	Ο	S	0	0	0
	11	040	5078	3190	900	963	25	0		

• Molecule 1 is a protein called Alcohol oxidase.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	101	SER	PHE	engineered mutation	UNP T2M2J4
В	101	SER	PHE	engineered mutation	UNP T2M2J4
С	101	SER	PHE	engineered mutation	UNP T2M2J4
D	101	SER	PHE	engineered mutation	UNP T2M2J4
Е	101	SER	PHE	engineered mutation	UNP T2M2J4
F	101	SER	PHE	engineered mutation	UNP T2M2J4
G	101	SER	PHE	engineered mutation	UNP T2M2J4
Н	101	SER	PHE	engineered mutation	UNP T2M2J4

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





Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf
0	Λ	1	Total	С	Ν	Ο	Р	0	0
	А	L	53	27	9	15	2	0	0
0	р	1	Total	С	Ν	Ο	Р	0	0
	D	L	53	27	9	15	2	0	0
0	С	1	Total	С	Ν	Ο	Р	0	0
	U	L	53	27	9	15	2	0	0
0	D	1	Total	С	Ν	Ο	Р	0	0
		D	L	53	27	9	15	2	0
0	Г	1	Total	С	Ν	Ο	Р	0	0
		L	53	27	9	15	2	0	0
0	Б	1	Total	С	Ν	Ο	Р	0	0
	Г	L	53	27	9	15	2	0	0
0	C	1	Total	С	Ν	Ο	Р	0	0
	G		53	27	9	15	2	U	U
0	ц	1	Total	С	Ν	Ο	Р	0	0
			53	27	9	15	2	0	

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
3	Н	1	$\begin{array}{ccc} \text{Total} \text{C} \text{O} \\ 6 3 3 \end{array}$	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	75	Total O 75 75	0	0
4	В	112	Total O 112 112	0	0
4	С	95	Total O 95 95	0	0
4	D	111	Total O 111 111	0	0
4	Ε	49	Total O 49 49	0	0
4	F	78	Total O 78 78	0	0
4	G	72	TotalO7272	0	0
4	Н	103	Total O 103 103	0	0



3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.











K466 K466 K491 K491 K491 K494 K204 <th

 \bullet Molecule 1: Alcohol oxidase

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	112.07Å 203.55 Å 116.01 Å	Deperitor
a, b, c, α , β , γ	90.00° 104.64° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	49.19 - 2.50	Depositor
Resolution (A)	49.14 - 2.50	EDS
% Data completeness	98.4 (49.19-2.50)	Depositor
(in resolution range)	98.4(49.14-2.50)	EDS
R _{merge}	(Not available)	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.70 (at 2.51 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
D D	0.210 , 0.286	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.214 , 0.285	DCC
R_{free} test set	8397 reflections $(4.93%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	31.2	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , 35.7	EDS
L-test for twinning ²	$< L >=0.47, < L^2>=0.29$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	41785	wwPDB-VP
Average B, all atoms $(Å^2)$	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.

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.

 $^{^1 {\}rm Intensities}$ estimated from amplitudes.

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: GOL, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mal	Chain	Bond	lengths	Bond angles		
	Cham	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.40	0/5220	0.64	0/7088	
1	В	0.40	0/5191	0.64	0/7048	
1	С	0.40	0/5202	0.64	0/7062	
1	D	0.42	0/5213	0.66	1/7078~(0.0%)	
1	Е	0.39	0/5202	0.64	0/7062	
1	F	0.40	0/5217	0.65	0/7083	
1	G	0.39	0/5202	0.65	0/7062	
1	Н	0.40	0/5202	0.65	0/7062	
All	All	0.40	0/41649	0.65	1/56545~(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	А	0	5
1	В	0	4
1	С	0	5
1	D	0	5
1	Ε	0	7
1	F	0	9
1	G	0	11
1	Н	0	11
All	All	0	57

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	D	578	ASP	CB-CA-C	-5.72	98.96	110.40

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	203	ARG	Sidechain
1	А	224	ARG	Sidechain
1	А	265	ARG	Sidechain
1	А	321	ARG	Sidechain
1	А	571	ARG	Sidechain
1	В	203	ARG	Sidechain
1	В	321	ARG	Sidechain
1	В	431	ARG	Sidechain
1	В	462	ARG	Sidechain
1	С	203	ARG	Sidechain
1	С	224	ARG	Sidechain
1	С	228	ARG	Sidechain
1	С	474	ARG	Sidechain
1	С	83	ARG	Sidechain
1	D	106	ARG	Sidechain
1	D	228	ARG	Sidechain
1	D	321	ARG	Sidechain
1	D	368	ARG	Sidechain
1	D	651	ARG	Sidechain
1	Е	106	ARG	Sidechain
1	Е	224	ARG	Sidechain
1	Е	321	ARG	Sidechain
1	Е	44	ARG	Sidechain
1	Ε	479	ARG	Sidechain
1	Ε	61	ARG	Sidechain
1	Ε	644	ARG	Sidechain
1	F	106	ARG	Sidechain
1	F	203	ARG	Sidechain
1	F	249	ARG	Sidechain
1	F	293	ARG	Sidechain
1	F	321	ARG	Sidechain
1	F	479	ARG	Sidechain
1	F	580	ARG	Sidechain
1	F	81	ARG	Sidechain
1	F	83	ARG	Sidechain
1	G	167	ARG	Sidechain
1	G	228	ARG	Sidechain

Mol	Chain	Res	Type	Group
10101	Chain	1005	1 ypc	Gible
1	G	231	ARG	Sidechain
1	G	321	ARG	Sidechain
1	G	341	ARG	Sidechain
1	G	469	ARG	Sidechain
1	G	580	ARG	Sidechain
1	G	61	ARG	Sidechain
1	G	644	ARG	Sidechain
1	G	81	ARG	Sidechain
1	G	83	ARG	Sidechain
1	Н	106	ARG	Sidechain
1	Н	228	ARG	Sidechain
1	Н	231	ARG	Sidechain
1	Н	251	ARG	Sidechain
1	Н	321	ARG	Sidechain
1	Н	341	ARG	Sidechain
1	Н	473	ARG	Sidechain
1	Н	644	ARG	Sidechain
1	Н	81	ARG	Sidechain
1	Н	83	ARG	Sidechain
1	Н	84	ARG	Sidechain

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5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	5095	0	4969	98	0
1	В	5067	0	4944	81	0
1	С	5078	0	4957	92	0
1	D	5088	0	4963	95	0
1	Е	5078	0	4957	83	0
1	F	5092	0	4966	91	0
1	G	5078	0	4957	91	0
1	Н	5078	0	4957	96	0
2	А	53	0	31	2	0
2	В	53	0	31	3	0
2	С	53	0	31	2	0
2	D	53	0	31	3	0
2	Е	53	0	31	2	0

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	53	0	31	3	0
2	G	53	0	31	3	0
2	Н	53	0	31	3	0
3	В	6	0	8	0	0
3	Н	6	0	8	0	0
4	А	75	0	0	3	0
4	В	112	0	0	2	0
4	С	95	0	0	1	0
4	D	111	0	0	5	0
4	Ε	49	0	0	2	0
4	F	78	0	0	2	0
4	G	72	0	0	4	0
4	Н	103	0	0	4	0
All	All	41785	0	39934	663	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 8.

All (663) 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	${ m distance}~({ m \AA})$	overlap (Å)
1:D:410:HIS:ND1	1:H:514:THR:HG21	1.83	0.94
1:F:100:ASN:O	1:F:203:ARG:NH2	2.06	0.89
1:A:228:ARG:NH1	1:A:441:PRO:O	2.05	0.88
1:A:106:ARG:NH1	1:A:181:GLN:O	2.11	0.83
1:G:51:ARG:O	1:G:54:ILE:HD13	1.79	0.83
1:D:104:TYR:OH	1:D:106:ARG:HD2	1.83	0.79
1:H:228:ARG:NH2	4:H:801:HOH:O	2.16	0.78
1:B:473:ARG:NH2	1:B:536:GLU:O	2.17	0.78
1:D:35:MET:HE1	1:D:262:VAL:HG21	1.65	0.78
1:C:470:GLU:OE1	1:C:474:ARG:NH2	2.16	0.77
1:E:81:ARG:NH1	1:E:554:ASP:OD2	2.18	0.76
1:F:61:ARG:HG2	1:F:61:ARG:HH11	1.50	0.76
1:F:177:SER:HB3	1:F:180:ILE:HD13	1.67	0.75
1:B:407:TYR:H	1:B:420:THR:HG21	1.51	0.75
1:B:216:ASP:OD2	1:D:647:THR:HG22	1.87	0.74
1:F:61:ARG:CG	1:F:61:ARG:HH11	2.00	0.74
1:A:440:ASN:HD22	1:A:443:VAL:HG13	1.53	0.73
1:D:473:ARG:NH2	1:D:536:GLU:O	2.20	0.73
1:F:368:ARG:NH2	1:F:389:PHE:O	2.19	0.73
1:D:580:ARG:NH1	1:D:623:GLU:OE2	2.21	0.72

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:F:578:ASP:HB3	1:F:580:ARG:H	1.55	0.72
1:D:100:ASN:O	1:D:203:ARG:NH2	2.21	0.72
4:D:870:HOH:O	1:H:514:THR:HG22	1.89	0.71
1:H:100:ASN:HB2	2:H:701:FAD:N5	2.05	0.71
1:H:100:ASN:O	1:H:203:ARG:NH2	2.25	0.70
1:D:407:TYR:H	1:D:420:THR:HG21	1.56	0.69
1:D:180:ILE:HG22	1:D:181:GLN:NE2	2.08	0.69
1:B:269:VAL:HG13	1:B:592:VAL:HG13	1.75	0.69
1:A:438:SER:HB3	1:A:443:VAL:HG21	1.74	0.68
1:C:566:CYS:O	1:C:596:ILE:HA	1.93	0.68
1:B:104:TYR:CE1	1:B:152:ILE:HD13	2.28	0.68
1:F:48:TRP:HE3	1:F:54:ILE:HG13	1.57	0.68
1:C:564:GLY:HA2	1:C:597:CYS:O	1.94	0.68
1:F:106:ARG:NH1	1:F:181:GLN:O	2.26	0.68
1:H:566:CYS:O	1:H:596:ILE:HA	1.94	0.68
1:D:8:ASP:OD1	1:D:265:ARG:NH1	2.23	0.68
1:B:100:ASN:O	1:B:203:ARG:NH2	2.27	0.67
1:E:106:ARG:NH2	1:E:143:THR:O	2.24	0.67
1:D:409:ASP:OD2	4:D:801:HOH:O	2.13	0.67
1:E:470:GLU:HB3	1:E:474:ARG:HH21	1.60	0.67
1:A:566:CYS:HA	1:A:576:VAL:HG21	1.77	0.66
1:A:557:GLU:OE2	1:E:521:SER:OG	2.13	0.66
1:F:399:PHE:CD1	1:F:424:TYR:CD2	2.84	0.66
1:F:48:TRP:CE3	1:F:54:ILE:HG13	2.31	0.66
1:G:100:ASN:HB2	2:G:701:FAD:C5X	2.26	0.65
1:B:410:HIS:ND1	1:G:514:THR:HG21	2.10	0.65
1:B:470:GLU:OE1	1:B:474:ARG:NH2	2.29	0.65
1:A:399:PHE:CD1	1:A:424:TYR:CD2	2.84	0.65
1:E:476:ASP:OD1	1:G:251:ARG:NH1	2.30	0.65
1:A:353:LYS:HE3	1:C:202:ARG:HH12	1.62	0.65
1:G:100:ASN:HB2	2:G:701:FAD:N5	2.12	0.64
1:G:440:ASN:HD21	1:G:442:TYR:HB2	1.62	0.64
1:A:647:THR:HG22	1:C:216:ASP:OD2	1.98	0.64
1:D:405:GLY:O	1:D:420:THR:HG22	1.97	0.64
1:G:409:ASP:OD1	1:G:411:THR:HB	1.97	0.64
1:F:399:PHE:CG	1:F:424:TYR:CE2	2.86	0.64
1:G:81:ARG:NH1	1:G:554:ASP:OD2	2.31	0.64
1:A:399:PHE:CG	1:A:424:TYR:CE2	2.86	0.64
1:E:405:GLY:O	1:E:420:THR:HG22	1.97	0.63
1:G:535:ILE:HD12	1:H:251:ARG:HG2	1.81	0.63
1:C:409:ASP:OD1	1:C:411:THR:HB	1.98	0.63

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:C:399:PHE:CG	1:C:424:TYR:CE2	2.87	0.63
1:B:321:ARG:NH2	1:G:411:THR:O	2.31	0.63
1:G:513:LEU:HD23	1:G:513:LEU:N	2.14	0.63
1:C:230:SER:O	1:C:283:ARG:HD2	1.99	0.63
1:A:44:ARG:NH1	1:B:648:GLN:HE22	1.96	0.62
1:H:407:TYR:H	1:H:420:THR:HG21	1.64	0.62
1:E:370:THR:HG22	1:E:372:GLU:H	1.64	0.62
1:C:399:PHE:CD2	1:C:424:TYR:CE2	2.88	0.62
1:F:473:ARG:NH2	1:F:536:GLU:O	2.32	0.62
1:H:635:VAL:HG13	1:H:638:ALA:HB3	1.82	0.62
1:A:514[B]:THR:HG23	1:A:517:ILE:HD12	1.81	0.62
1:F:102:GLN:HG3	1:F:203:ARG:HH21	1.64	0.62
1:A:407:TYR:H	1:A:420:THR:HG21	1.65	0.62
1:A:147:ASP:HB3	1:A:643:GLY:HA2	1.82	0.62
1:A:580:ARG:NH1	1:A:623:GLU:OE2	2.33	0.62
1:E:407:TYR:H	1:E:420:THR:HG21	1.65	0.62
1:H:561:HIS:CE1	1:H:604:ASN:HA	2.35	0.62
1:E:635:VAL:HG13	1:E:638:ALA:HB3	1.81	0.61
1:H:352:GLU:OE2	1:H:651:ARG:HD2	2.00	0.61
1:D:398:MET:SD	1:D:425:LEU:HA	2.41	0.61
1:F:208:THR:HA	1:F:212:HIS:HB2	1.83	0.61
1:G:314:TYR:CD2	1:G:452:MET:HE2	2.35	0.61
1:A:474:ARG:NH2	1:A:537:ASP:OD1	2.34	0.61
1:H:80:LEU:O	1:H:83:ARG:HG2	2.01	0.61
1:A:44:ARG:HH11	1:B:648:GLN:HE22	1.48	0.60
1:G:647:THR:HG23	4:H:809:HOH:O	2.01	0.60
1:A:269:VAL:CG1	1:A:592:VAL:HG13	2.31	0.60
1:B:559:THR:O	1:B:561:HIS:CD2	2.55	0.60
1:E:140:ASN:HB2	1:E:178:ASP:OD2	2.02	0.60
1:E:217:VAL:HG23	1:E:218:GLN:HG3	1.84	0.60
1:F:578:ASP:OD2	1:F:582:ASN:HB2	2.02	0.60
1:B:69:THR:HG22	1:B:91:ASN:HB2	1.84	0.60
1:B:51:ARG:O	1:B:54:ILE:HD13	2.02	0.59
1:C:368:ARG:NH2	1:C:389:PHE:O	2.35	0.59
1:F:205:ASP:OD1	1:F:208:THR:HG23	2.02	0.59
1:C:474:ARG:HD3	1:D:251:ARG:O	2.02	0.59
1:G:203:ARG:NH1	4:G:804:HOH:O	2.35	0.59
1:E:205:ASP:OD1	1:E:208:THR:HG23	2.02	0.59
1:G:399:PHE:CG	1:G:424:TYR:CE2	2.91	0.59
1:A:100:ASN:O	1:A:203:ARG:NH2	2.35	0.59
1:C:399:PHE:CD2	1:C:424:TYR:CD2	2.91	0.59

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:D:104:TYR:CE1	1:D:152:ILE:HD13	2.37	0.59
1:E:113:ASP:OD1	1:E:121:THR:HG23	2.03	0.59
1:E:472:ALA:HA	1:E:475:MET:HE2	1.83	0.59
1:E:577:VAL:HA	1:E:582:ASN:O	2.03	0.58
1:B:580:ARG:NH1	1:B:623:GLU:OE2	2.36	0.58
1:F:228:ARG:NH2	4:F:801:HOH:O	2.37	0.58
1:B:407:TYR:H	1:B:420:THR:CG2	2.16	0.58
1:F:147:ASP:HB3	1:F:643:GLY:HA2	1.86	0.58
1:E:61:ARG:HH11	1:E:61:ARG:HB2	1.68	0.58
1:F:407:TYR:H	1:F:420:THR:HG21	1.68	0.58
1:C:512:GLY:HA2	1:F:333:LEU:O	2.04	0.57
1:C:408:ALA:HB3	1:C:413:LEU:HD11	1.86	0.57
1:C:314:TYR:CD2	1:C:452:MET:HE2	2.40	0.57
1:H:180:ILE:CD1	1:H:185:THR:HG21	2.34	0.57
1:B:83:ARG:NH2	1:B:556:VAL:O	2.35	0.57
1:G:121:THR:HB	1:G:124:ASP:OD1	2.05	0.57
1:G:459:ALA:N	1:G:460:PRO:HD2	2.20	0.57
1:F:100:ASN:HB2	2:F:701:FAD:C5X	2.35	0.56
1:E:403:VAL:HB	1:E:420:THR:HG23	1.85	0.56
1:F:106:ARG:NH2	1:F:143:THR:O	2.38	0.56
1:B:203:ARG:NH1	4:B:807:HOH:O	2.38	0.56
1:A:251:ARG:O	1:B:474:ARG:HD3	2.06	0.56
1:F:580:ARG:HH22	1:F:622:GLU:CD	2.09	0.56
1:C:100:ASN:N	1:C:203:ARG:NH2	2.53	0.56
1:G:208:THR:HA	1:G:212:HIS:HB2	1.87	0.56
1:B:227:ALA:HB1	1:B:245:TYR:CD1	2.40	0.56
1:H:314:TYR:O	1:H:424:TYR:HA	2.05	0.56
1:H:470:GLU:OE1	1:H:474:ARG:NH2	2.37	0.56
1:F:158:ILE:HG23	1:F:362:ASP:HB3	1.88	0.56
1:C:322:VAL:HG11	1:C:419:ILE:HG23	1.86	0.56
1:B:309:GLN:O	1:B:311:GLN:HG3	2.05	0.56
1:E:249:ARG:NH1	1:F:476:ASP:OD2	2.39	0.56
1:C:580:ARG:HH12	1:C:623:GLU:HG3	1.72	0.55
1:A:483:THR:HG22	1:A:497:CYS:HB2	1.87	0.55
1:D:578:ASP:HB3	1:D:580:ARG:H	1.71	0.55
1:E:44:ARG:NH2	1:E:216:ASP:OD1	2.30	0.55
1:C:470:GLU:HB3	1:C:474:ARG:HH21	1.72	0.55
1:B:280:ILE:O	1:B:284:SER:OG	2.07	0.55
1:E:231:ARG:HG3	1:E:231:ARG:HH11	1.70	0.55
1:E:10:ILE:HD12	1:E:264:ALA:HB2	1.87	0.55
1:H:100:ASN:HB2	2:H:701:FAD:C5X	2.34	0.55

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:10:ILE:HD11	1:A:262:VAL:HG22	1.88	0.55
1:F:399:PHE:CD1	1:F:424:TYR:CE2	2.95	0.55
1:D:503:GLU:OE2	1:D:503:GLU:HA	2.07	0.55
1:G:314:TYR:HD2	1:G:452:MET:HE2	1.72	0.55
1:A:514[B]:THR:HG21	1:E:408:ALA:O	2.08	0.54
1:D:315:THR:HA	1:D:423:GLN:O	2.07	0.54
1:D:409:ASP:OD1	1:D:411:THR:HB	2.07	0.54
1:E:54:ILE:O	1:E:57:ARG:HG2	2.07	0.54
1:C:347:TRP:HA	1:C:354:ALA:CB	2.37	0.54
1:C:577:VAL:HA	1:C:582:ASN:O	2.08	0.54
1:D:308:GLU:OE2	1:D:435:HIS:NE2	2.40	0.54
1:C:277:THR:HB	1:C:278:PRO:HD3	1.89	0.54
1:B:33:LYS:HD2	1:B:265:ARG:HH22	1.73	0.54
1:A:399:PHE:CD1	1:A:424:TYR:CE2	2.96	0.54
1:G:592:VAL:HG23	1:G:612:VAL:HG12	1.90	0.54
1:H:313:HIS:O	1:H:559:THR:HG23	2.07	0.54
1:A:227:ALA:HB1	1:A:245:TYR:CD1	2.42	0.54
1:B:409:ASP:OD1	1:B:411:THR:HB	2.08	0.54
1:H:20:VAL:HG22	1:H:210:TYR:CE2	2.43	0.54
1:E:251:ARG:HG3	1:F:535:ILE:HG13	1.90	0.54
1:E:399:PHE:CG	1:E:424:TYR:CE2	2.95	0.54
1:A:353:LYS:HE3	1:C:202:ARG:NH1	2.22	0.54
1:E:578:ASP:HB3	1:E:580:ARG:H	1.73	0.54
1:G:411:THR:HG21	4:G:841:HOH:O	2.08	0.54
1:A:180:ILE:HG22	1:A:181:GLN:NE2	2.22	0.53
1:D:177:SER:HB3	1:D:180:ILE:CD1	2.38	0.53
1:B:391:ASP:O	1:B:392:LYS:HD2	2.08	0.53
1:B:577:VAL:HA	1:B:582:ASN:O	2.08	0.53
1:F:54:ILE:O	1:F:54:ILE:HG12	2.07	0.53
1:G:368:ARG:NH2	1:G:389:PHE:O	2.40	0.53
1:A:314:TYR:O	1:A:424:TYR:HA	2.09	0.53
1:A:49:VAL:O	1:A:203:ARG:HD2	2.09	0.53
1:B:314:TYR:CD2	1:B:452:MET:CE	2.92	0.53
1:H:402:ILE:HD12	1:H:475:MET:HE1	1.88	0.53
1:A:149:PRO:HB2	1:A:209:ALA:HB1	1.91	0.53
1:C:177:SER:HB3	1:C:180:ILE:CD1	2.38	0.53
1:G:158:ILE:HG23	1:G:362:ASP:HB3	1.91	0.53
1:B:348:GLU:O	1:D:651:ARG:NH2	2.42	0.53
1:F:29:ASP:OD1	1:F:31:THR:HB	2.09	0.53
1:F:20:VAL:HG11	1:F:614:GLU:N	2.24	0.53
1:E:514:THR:HA	1:E:517:ILE:HD12	1.90	0.53

		Interatomic	Clash
Atom-1	Atom-2	$distance ({ m \AA})$	overlap (Å)
1:F:180:ILE:HD11	1:F:188:GLY:HA3	1.91	0.53
1:F:356:LEU:HB2	4:F:828:HOH:O	2.09	0.53
1:H:67:LYS:HE3	4:H:826:HOH:O	2.09	0.53
1:A:112:TRP:O	1:A:115:PHE:HB2	2.08	0.53
1:D:321:ARG:NH1	1:D:500:ILE:HD12	2.24	0.53
1:E:132:LEU:HD12	1:E:132:LEU:C	2.30	0.52
1:C:423:GLN:OE1	1:C:464:SER:OG	2.21	0.52
1:E:112:TRP:CZ2	1:E:611:LEU:HD23	2.43	0.52
1:H:249:ARG:HB3	1:H:251:ARG:HD3	1.91	0.52
1:A:228:ARG:HG2	1:A:228:ARG:HH11	1.73	0.52
1:H:106:ARG:HH12	1:H:143:THR:HG22	1.73	0.52
1:A:100:ASN:HB2	2:A:701:FAD:N5	2.24	0.52
1:D:213:SER:HB2	1:D:633:ALA:HB3	1.92	0.52
1:B:290:GLU:OE1	1:B:294:GLN:NE2	2.37	0.52
1:C:459:ALA:N	1:C:460:PRO:HD2	2.24	0.52
1:H:106:ARG:NH2	1:H:143:THR:O	2.42	0.52
1:E:180:ILE:HG13	1:E:185:THR:HG21	1.91	0.52
1:H:217:VAL:HG23	1:H:218:GLN:HG3	1.91	0.52
1:A:180:ILE:HG13	1:A:185:THR:HG21	1.92	0.52
1:F:128:LEU:HD22	1:F:131:ARG:CZ	2.39	0.52
1:A:177:SER:HB3	1:A:180:ILE:CD1	2.39	0.52
1:H:205:ASP:OD1	1:H:208:THR:HG23	2.09	0.52
1:H:580:ARG:HH22	1:H:622:GLU:HG3	1.75	0.52
1:C:269:VAL:CG1	1:C:592:VAL:CG1	2.88	0.52
1:A:473:ARG:NH2	1:A:536:GLU:O	2.42	0.51
1:A:577:VAL:HA	1:A:582:ASN:O	2.11	0.51
1:A:61:ARG:HD2	1:A:70:PHE:CG	2.45	0.51
1:F:9:VAL:HG22	1:F:267:MET:HB3	1.93	0.51
1:B:279:GLN:O	1:B:283:ARG:HG2	2.11	0.51
1:D:198:ARG:NH2	1:D:646:ALA:O	2.42	0.51
1:B:580:ARG:HH12	1:B:623:GLU:HG3	1.76	0.51
1:F:604:ASN:HB3	2:F:701:FAD:C2	2.41	0.51
1:D:286:VAL:HG13	1:D:303:LEU:HD12	1.92	0.51
1:G:476:ASP:OD2	1:H:249:ARG:NH1	2.44	0.51
1:F:269:VAL:HG13	1:F:592:VAL:HG13	1.93	0.51
1:B:69:THR:CG2	1:B:91:ASN:HB2	2.41	0.51
1:F:314:TYR:CD2	1:F:452:MET:CE	2.93	0.51
1:F:69:THR:HG23	1:F:91:ASN:HB2	1.93	0.51
1:B:27:TYR:CE1	1:B:633:ALA:HB2	2.46	0.51
1:E:180:ILE:HG23	1:E:366:LYS:HE3	1.93	0.51
1:A:315:THR:HA	1:A:423:GLN:O	2.11	0.51

		Interatomic	Clash	
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)	
1:A:35:MET:HE2	1:A:37:ILE:HD11	1.93	0.51	
1:A:44:ARG:NH1	1:B:648:GLN:NE2	2.59	0.50	
1:E:227:ALA:HB1	1:E:245:TYR:CD1	2.46	0.50	
1:G:604:ASN:HB3	2:G:701:FAD:C2	2.42	0.50	
1:D:282:GLU:OE1	1:D:435:HIS:ND1	2.38	0.50	
1:C:596:ILE:HD12	1:C:596:ILE:C	2.32	0.50	
1:F:80:LEU:O	1:F:83:ARG:HG2	2.11	0.50	
1:H:235:ASP:OD2	1:H:239:LYS:HB3	2.11	0.50	
1:B:348:GLU:HG3	1:D:350:SER:OG	2.11	0.50	
1:H:110:SER:OG	1:H:395:LYS:HE2	2.12	0.50	
1:E:100:ASN:O	1:E:203:ARG:NH2	2.44	0.50	
1:A:48:TRP:HA	1:A:54:ILE:HD12	1.93	0.50	
1:C:180:ILE:HG22	1:C:181:GLN:NE2	2.26	0.50	
1:E:520:GLY:HA3	1:E:522:TRP:NE1	2.27	0.50	
1:G:35:MET:HE2	1:G:37:ILE:HD11	1.93	0.50	
1:G:435:HIS:O	1:G:446:PHE:N	2.45	0.50	
1:C:552:VAL:O	1:C:556:VAL:HB	2.12	0.49	
1:G:369:PRO:CD	1:G:397:VAL:HG21	2.42	0.49	
1:B:186:ALA:HB2	1:B:394:ASP:C	2.32	0.49	
1:C:20:VAL:HG22	1:C:210:TYR:CZ	2.47	0.49	
1:B:580:ARG:HH22	1:B:622:GLU:HG3	1.77	0.49	
1:C:305:GLY:HA3	1:C:574:GLY:O	2.12	0.49	
1:C:347:TRP:HA	1:C:354:ALA:HB2	1.95	0.49	
1:D:580:ARG:HH22	1:D:622:GLU:CG	2.25	0.49	
1:B:180:ILE:CD1	1:B:185:THR:HG21	2.42	0.49	
1:C:321:ARG:NH2	1:C:414:PRO:HB2	2.27	0.49	
1:C:635:VAL:HG22	1:C:638:ALA:HB3	1.94	0.49	
1:D:104:TYR:CZ	1:D:106:ARG:HD2	2.47	0.49	
1:A:51:ARG:HB2	1:A:54:ILE:HD13	1.95	0.49	
1:C:118:GLU:OE1	1:C:579:LYS:NZ	2.31	0.49	
1:D:282:GLU:O	1:D:292:LEU:CD2	2.61	0.49	
1:E:637:HIS:CE1	1:F:648:GLN:HG3	2.47	0.49	
1:D:604:ASN:HB3	2:D:701:FAD:C2	2.42	0.49	
1:F:162:ALA:O	1:F:165:PHE:HB3	2.12	0.49	
1:F:315:THR:HA	1:F:423:GLN:O	2.13	0.49	
1:H:564:GLY:HA2	1:H:597:CYS:O	2.13	0.49	
1:A:51:ARG:NH2	4:A:801:HOH:O	2.18	0.49	
1:C:20:VAL:HG22	1:C:210:TYR:CE2	2.48	0.49	
1:D:10:ILE:HD12	1:D:264:ALA:HB2	1.95	0.49	
1:E:466:LYS:HG2	1:E:540:TYR:CZ	2.47	0.49	
1:A:251:ARG:HG2	1:B:535:ILE:HD12	1.94	0.49	

		Interatomic	Clash
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)
1:B:399:PHE:CG	1:B:424:TYR:CE2	3.00	0.49
1:B:644:ARG:HB2	1:B:644:ARG:HH11	1.77	0.49
1:C:208:THR:HA	1:C:212:HIS:HB2	1.94	0.49
1:F:314:TYR:O	1:F:424:TYR:HA	2.13	0.49
1:A:440:ASN:ND2	1:A:443:VAL:HG13	2.25	0.48
1:D:514:THR:HA	1:D:517:ILE:HD12	1.95	0.48
1:E:474:ARG:HD3	1:G:251:ARG:O	2.13	0.48
1:A:100:ASN:HB2	2:A:701:FAD:C4X	2.44	0.48
1:F:102:GLN:O	1:F:194:LYS:HA	2.12	0.48
1:G:557:GLU:HG3	4:G:801:HOH:O	2.12	0.48
1:A:472:ALA:HA	1:A:475:MET:HE3	1.96	0.48
1:C:580:ARG:NH1	1:C:623:GLU:HG3	2.28	0.48
1:D:208:THR:HA	1:D:212:HIS:HB2	1.95	0.48
1:D:314:TYR:O	1:D:424:TYR:HA	2.13	0.48
1:G:449:SER:OG	1:G:451:PHE:CD1	2.67	0.48
1:H:108:SER:O	1:H:109:ALA:C	2.52	0.48
1:G:100:ASN:O	1:G:203:ARG:NH2	2.45	0.48
1:H:580:ARG:HH22	1:H:622:GLU:CD	2.17	0.48
1:H:580:ARG:NH2	1:H:622:GLU:OE1	2.47	0.48
1:A:548:ILE:O	1:A:552:VAL:HG23	2.14	0.48
1:C:476:ASP:OD1	1:D:251:ARG:NH1	2.47	0.48
1:C:561:HIS:CE1	1:C:604:ASN:HA	2.49	0.48
1:C:100:ASN:HB2	2:C:701:FAD:N5	2.29	0.48
1:F:61:ARG:HG2	1:F:61:ARG:NH1	2.24	0.48
1:G:269:VAL:HG13	1:G:592:VAL:CG1	2.44	0.48
1:B:314:TYR:CE1	1:B:451:PHE:CD1	3.01	0.48
1:G:180:ILE:HG23	1:G:366:LYS:HD2	1.95	0.48
1:G:369:PRO:HB2	1:G:374:LEU:HD22	1.96	0.48
1:B:324:ASN:O	1:B:417:LYS:NZ	2.46	0.48
1:D:269:VAL:HG13	1:D:592:VAL:HG13	1.96	0.48
1:F:47:PRO:HG3	1:H:157:GLN:OE1	2.12	0.48
1:H:580:ARG:HH22	1:H:622:GLU:CG	2.27	0.48
1:C:519:MET:SD	1:F:557:GLU:HG2	2.53	0.48
1:D:102:GLN:HG3	1:D:203:ARG:NH2	2.29	0.47
1:E:321:ARG:HD2	1:E:499:ASP:OD1	2.14	0.47
1:F:100:ASN:HB2	2:F:701:FAD:N5	2.29	0.47
1:B:557:GLU:HG2	1:G:519:MET:SD	2.54	0.47
1:H:399:PHE:CD1	1:H:424:TYR:CE2	3.02	0.47
1:A:310:TYR:OH	1:A:312:ASP:OD2	2.19	0.47
1:A:314:TYR:CD2	1:A:452:MET:CE	2.97	0.47
1:G:229:VAL:HG13	1:G:243:VAL:HG13	1.96	0.47

Atom 1 Atom 2		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:G:470:GLU:HB3	1:G:474:ARG:HH21	1.78	0.47	
1:H:321:ARG:HG2	1:H:321:ARG:HH11	1.79	0.47	
1:A:190:GLU:HB2	4:A:836:HOH:O	2.13	0.47	
1:E:352:GLU:OE2	1:E:651:ARG:HD2	2.15	0.47	
1:G:532:ASP:O	1:G:533:LYS:C	2.52	0.47	
1:H:407:TYR:H	1:H:420:THR:CG2	2.25	0.47	
1:A:407:TYR:H	1:A:420:THR:CG2	2.26	0.47	
1:C:314:TYR:CE1	1:C:451:PHE:CD1	3.02	0.47	
1:F:177:SER:HB3	1:F:180:ILE:CD1	2.42	0.47	
1:H:161:VAL:HG13	4:H:865:HOH:O	2.15	0.47	
1:A:106:ARG:NH2	1:A:143:THR:O	2.48	0.47	
1:A:514[A]:THR:OG1	1:E:409:ASP:HA	2.14	0.47	
1:A:35:MET:CE	1:A:37:ILE:HD11	2.44	0.47	
1:B:269:VAL:CG1	1:B:592:VAL:HG13	2.42	0.47	
1:E:83:ARG:NH1	1:E:553:ALA:O	2.48	0.47	
1:F:361:ILE:HG12	1:F:403:VAL:HG22	1.96	0.47	
1:F:217:VAL:HA	1:H:645:PRO:HB2	1.96	0.47	
1:B:230:SER:O	1:B:283:ARG:HD2	2.15	0.47	
1:D:35:MET:HE1	1:D:262:VAL:CG2	2.40	0.47	
1:D:472:ALA:HA	1:D:475:MET:HE2	1.97	0.47	
1:G:95:GLY:O	1:G:96:GLY:C	2.54	0.47	
1:H:16:PRO:O	1:H:20:VAL:HG23	2.15	0.47	
1:H:35:MET:HE3	1:H:37:ILE:HG12	1.97	0.47	
1:B:8:ASP:OD1	1:B:265:ARG:NH1	2.47	0.47	
1:A:163:GLN:HE22	1:C:42:ASN:HB3	1.80	0.47	
1:E:466:LYS:HG2	1:E:540:TYR:CE1	2.50	0.47	
1:H:168:ALA:O	1:H:171:ALA:HB3	2.15	0.47	
1:H:20:VAL:HG22	1:H:210:TYR:CZ	2.50	0.47	
1:A:500:ILE:HD11	1:A:504:THR:HG22	1.96	0.46	
1:C:205:ASP:OD2	1:C:208:THR:HG23	2.15	0.46	
1:C:414:PRO:HA	1:F:413:LEU:O	2.15	0.46	
1:D:100:ASN:HB2	2:D:701:FAD:C5X	2.44	0.46	
1:E:621:ALA:O	1:E:626:LEU:N	2.39	0.46	
1:H:449:SER:HB3	1:H:451:PHE:CD1	2.50	0.46	
1:G:564:GLY:HA2	1:G:597:CYS:O	2.15	0.46	
1:G:80:LEU:O	1:G:83:ARG:HG2	2.16	0.46	
1:H:578:ASP:HB3	1:H:580:ARG:H	1.80	0.46	
1:B:414:PRO:HG2	1:B:482:LEU:HD11	1.95	0.46	
1:C:369:PRO:CD	1:C:397:VAL:HG21	2.45	0.46	
1:D:479:ARG:NH2	4:D:803:HOH:O	2.30	0.46	
1:C:54:ILE:O	1:C:57:ARG:CG	2.63	0.46	

		Interatomic	Clash
Atom-1	Atom-1 Atom-2 di		overlap (Å)
1:D:580:ARG:HH12	1:D:623:GLU:HG3	1.80	0.46
1:G:130:LYS:O	1:G:145:GLY:HA3	2.16	0.46
1:A:11:VAL:HG21	1:A:22:ALA:HB2	1.97	0.46
1:D:203:ARG:NH1	4:D:808:HOH:O	2.48	0.46
1:H:269:VAL:CG1	1:H:592:VAL:CG1	2.94	0.46
1:C:100:ASN:HB2	2:C:701:FAD:C5X	2.45	0.46
1:G:112:TRP:O	1:G:115:PHE:HB2	2.16	0.46
1:H:187:HIS:HA	1:H:366:LYS:O	2.15	0.46
1:H:44:ARG:HH22	1:H:216:ASP:CG	2.19	0.46
1:C:321:ARG:NH2	1:F:411:THR:O	2.48	0.46
1:G:369:PRO:HD3	1:G:397:VAL:HG21	1.98	0.46
1:G:370:THR:HG22	1:G:372:GLU:H	1.81	0.46
1:A:410:HIS:HA	1:A:413:LEU:HD12	1.97	0.46
1:A:48:TRP:HA	1:A:54:ILE:CD1	2.46	0.46
1:D:100:ASN:HB2	2:D:701:FAD:N5	2.30	0.46
1:F:9:VAL:O	1:F:34:VAL:HA	2.16	0.46
1:G:269:VAL:HG13	1:G:592:VAL:HG12	1.98	0.46
1:H:326:SER:O	1:H:417:LYS:HE2	2.15	0.46
1:D:410:HIS:H	1:H:514:THR:HG23	1.81	0.46
1:B:274:THR:OG1	1:B:563:LEU:HA	2.16	0.46
1:C:314:TYR:CD2	1:C:452:MET:CE	2.99	0.46
1:D:459:ALA:N	1:D:460:PRO:HD2	2.32	0.46
1:D:557:GLU:HG2	1:H:519:MET:SD	2.55	0.46
1:B:399:PHE:CD1	1:B:424:TYR:CD2	3.04	0.45
1:B:101:SER:HB2	2:B:701:FAD:O4	2.16	0.45
1:C:14:GLY:HA2	1:C:36:LEU:HD11	1.97	0.45
1:D:314:TYR:CE1	1:D:451:PHE:CD1	3.04	0.45
1:E:548:ILE:O	1:E:552:VAL:HG23	2.15	0.45
1:E:552:VAL:O	1:E:556:VAL:HB	2.15	0.45
1:F:409:ASP:OD1	1:F:411:THR:HB	2.16	0.45
1:D:282:GLU:O	1:D:292:LEU:HD21	2.16	0.45
1:D:399:PHE:CD1	1:D:424:TYR:CD2	3.05	0.45
1:D:399:PHE:CD1	1:D:424:TYR:CE2	3.05	0.45
1:G:180:ILE:HG22	1:G:181:GLN:NE2	2.31	0.45
1:F:216:ASP:HB2	1:H:647:THR:HG22	1.98	0.45
1:A:278:PRO:HB2	4:A:844:HOH:O	2.16	0.45
1:B:33:LYS:HD2	1:B:265:ARG:NH2	2.32	0.45
1:C:112:TRP:CZ2	1:C:611:LEU:HD23	2.51	0.45
1:C:269:VAL:HG13	1:C:592:VAL:HG12	1.99	0.45
1:H:235:ASP:HB3	1:H:237:ASN:H	1.82	0.45
1:B:102:GLN:O	1:B:194:LYS:HA	2.17	0.45

		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:245:TYR:CD1	1:D:245:TYR:C	2.90	0.45
1:D:566:CYS:O	1:D:596:ILE:HA	2.16	0.45
1:G:44:ARG:HH22	1:G:216:ASP:CG	2.19	0.45
1:G:599:ASP:OD1	1:G:600:ASN:N	2.39	0.45
1:H:112:TRP:O	1:H:115:PHE:HB2	2.16	0.45
1:H:506:LYS:HA	1:H:515:VAL:HG11	1.98	0.45
1:A:40:GLY:HA3	1:A:92:ILE:HA	1.98	0.45
1:A:505:ALA:HB1	1:E:411:THR:HG21	1.97	0.45
1:E:101:SER:HB2	2:E:701:FAD:O4	2.17	0.45
1:G:286:VAL:HG13	1:G:301:SER:HB3	1.99	0.45
1:H:604:ASN:HB3	2:H:701:FAD:C2	2.46	0.45
1:A:101:SER:O	1:A:359:ASN:ND2	2.40	0.45
1:D:580:ARG:NH1	1:D:623:GLU:HG3	2.32	0.45
1:E:354:ALA:HB1	4:E:808:HOH:O	2.17	0.45
1:E:370:THR:HG22	1:E:372:GLU:N	2.31	0.45
1:E:348:GLU:HG3	1:F:350:SER:OG	2.17	0.45
1:F:314:TYR:CD2	1:F:452:MET:HE3	2.52	0.45
1:C:182:ASP:O	1:C:183:LEU:HB2	2.17	0.45
1:C:80:LEU:O	1:C:83:ARG:HG2	2.17	0.45
1:F:69:THR:CG2	1:F:91:ASN:HB2	2.47	0.45
1:B:569:LYS:HB2	1:B:570:PRO:CD	2.47	0.45
1:C:405:GLY:O	1:C:420:THR:HG22	2.17	0.45
1:C:473:ARG:NH2	1:C:536:GLU:O	2.50	0.45
1:C:513:LEU:HD13	1:F:57:ARG:HB3	1.99	0.45
1:F:136:GLN:O	1:F:198:ARG:NH1	2.50	0.45
1:C:137:LYS:HB2	1:C:138:PRO:HD2	1.98	0.44
1:E:473:ARG:HD3	4:E:813:HOH:O	2.17	0.44
1:F:313:HIS:CD2	1:F:426:GLU:O	2.70	0.44
1:H:43:ASN:ND2	1:H:98:SER:OG	2.42	0.44
1:B:208:THR:HA	1:B:212:HIS:HB2	1.98	0.44
1:D:102:GLN:O	1:D:194:LYS:HA	2.18	0.44
1:E:135:TYR:CZ	1:E:144:HIS:CD2	3.05	0.44
1:E:165:PHE:CZ	1:E:364:GLY:HA2	2.53	0.44
1:H:243:VAL:HG12	1:H:262:VAL:HG13	2.00	0.44
1:D:391:ASP:O	1:D:392:LYS:HD2	2.17	0.44
1:A:578:ASP:HB3	1:A:580:ARG:H	1.83	0.44
1:D:55:TYR:CD2	1:D:101:SER:HA	2.53	0.44
1:E:604:ASN:HB3	2:E:701:FAD:C2	2.48	0.44
1:G:9:VAL:HB	1:G:34:VAL:HB	2.00	0.44
1:A:43:ASN:ND2	1:A:98:SER:OG	2.42	0.44
1:B:12:CYS:SG	1:B:243:VAL:HG21	2.58	0.44

		Interatomic	Clash	
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)	
1:B:557:GLU:CG	1:G:519:MET:SD	3.06	0.44	
1:F:102:GLN:CG	1:F:203:ARG:HH21	2.30	0.44	
1:C:147:ASP:HA	1:C:641:PRO:HB2	2.00	0.44	
1:F:87:VAL:HG22	1:F:558:THR:HB	1.99	0.44	
1:B:180:ILE:HD12	1:B:185:THR:HG21	2.00	0.44	
1:D:235:ASP:HB2	1:D:239:LYS:HB3	1.99	0.44	
1:F:314:TYR:HD2	1:F:452:MET:CE	2.31	0.44	
1:F:532:ASP:O	1:F:533:LYS:C	2.57	0.44	
1:G:411:THR:CG2	4:G:841:HOH:O	2.66	0.44	
1:G:580:ARG:O	1:G:590:LYS:NZ	2.49	0.44	
1:C:470:GLU:CB	1:C:474:ARG:HH21	2.29	0.44	
1:H:459:ALA:N	1:H:460:PRO:HD2	2.33	0.44	
1:F:251:ARG:HG2	1:H:535:ILE:HD12	1.99	0.44	
1:A:352:GLU:HG2	1:A:353:LYS:HG2	2.00	0.43	
1:A:54:ILE:O	1:A:57:ARG:HG2	2.18	0.43	
1:C:34:VAL:HG22	1:C:221:LEU:CD1	2.48	0.43	
1:C:513:LEU:CD2	1:C:513:LEU:N	2.82	0.43	
1:D:147:ASP:HB3	1:D:643:GLY:HA2	1.98	0.43	
1:F:405:GLY:O	1:F:420:THR:HG22	2.18	0.43	
1:F:120:TRP:CZ2	1:F:581:LEU:HD21	2.52	0.43	
1:G:462:ARG:NH1	462:ARG:NH1 1:G:549:ASP:OD1		0.43	
1:H:97:SER:HB2	1:H:606:TYR:CZ	2.53	0.43	
1:A:389:PHE:O	1:A:390:LYS:C	2.55	0.43	
1:D:102:GLN:CG	1:D:203:ARG:NH2	2.82	0.43	
1:E:321:ARG:HD3	1:E:500:ILE:HB	1.99	0.43	
1:E:466:LYS:O	1:E:470:GLU:HG2	2.18	0.43	
1:F:114:ASP:O	1:F:116:LYS:HG2	2.18	0.43	
1:G:102:GLN:O	1:G:194:LYS:HA	2.19	0.43	
1:A:514[A]:THR:HG21	1:E:410:HIS:HB2	2.00	0.43	
1:A:72:THR:O	1:A:73:ASP:C	2.56	0.43	
1:C:147:ASP:HB3	1:C:643:GLY:HA2	2.01	0.43	
1:D:158:ILE:HG23	1:D:362:ASP:HB3	2.00	0.43	
1:F:478:PHE:CZ	1:F:480:GLY:HA2	2.53	0.43	
1:G:399:PHE:CD1	1:G:424:TYR:CD2	3.06	0.43	
1:A:73:ASP:O	1:A:84:ARG:HD2	2.18	0.43	
1:B:315:THR:HA	1:B:423:GLN:O	2.19	0.43	
1:D:112:TRP:O	1:D:115:PHE:HB2	2.18	0.43	
1:H:569:LYS:O	1:H:575:GLY:HA3	2.17	0.43	
1:D:403:VAL:HB	1:D:420:THR:HG23	2.00	0.43	
1:D:438:SER:HB3	1:D:443:VAL:HG21	1.99	0.43	
1:E:235:ASP:HB3	1:E:237:ASN:H	1.84	0.43	

Atom 1 Atom 2		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:F:107:ALA:HB2	1:F:603:THR:HG21	1.99	0.43	
1:F:73:ASP:O	1:F:84:ARG:HD2	2.18	0.43	
1:G:103:MET:O	1:G:195:TYR:HE2	2.02	0.43	
1:G:315:THR:HA	1:G:423:GLN:O	2.19	0.43	
1:G:440:ASN:ND2	1:G:442:TYR:H	2.16	0.43	
1:F:251:ARG:NH1	1:H:476:ASP:OD1	2.50	0.43	
1:H:514:THR:HA	1:H:517:ILE:HD12	2.01	0.43	
1:B:126:LEU:N	1:B:127:PRO:CD	2.82	0.43	
1:C:279:GLN:O	1:C:283:ARG:HG2	2.18	0.43	
1:D:205:ASP:OD2	1:D:208:THR:CG2	2.66	0.43	
1:F:126:LEU:N	1:F:127:PRO:CD	2.81	0.43	
1:G:43:ASN:ND2	1:G:98:SER:OG	2.50	0.43	
1:H:406:ALA:HA	1:H:420:THR:HG22	2.01	0.43	
1:A:476:ASP:OD1	1:C:251:ARG:NH1	2.52	0.43	
1:A:69:THR:CG2	1:A:91:ASN:HB2	2.49	0.43	
1:D:411:THR:HG21	1:H:505:ALA:CB	2.49	0.43	
1:E:69:THR:CG2	1:E:91:ASN:HB2	2.49	0.43	
1:H:106:ARG:NH1	1:H:181:GLN:O	2.52	0.43	
1:G:647:THR:HG22	1:H:216:ASP:OD2	2.18	0.43	
1:B:244:ALA:HA	1:B:260:THR:O	2.18	0.43	
1:B:100:ASN:HB2	2:B:701:FAD:C4X	2.48	0.43	
1:A:350:SER:OG	1:C:348:GLU:HG3	2.19	0.43	
1:C:473:ARG:HD2	4:C:836:HOH:O	2.18	0.43	
1:C:470:GLU:HB3	1:C:474:ARG:NH2	2.33	0.43	
1:C:115:PHE:CZ	1:C:598:PRO:HD2	2.54	0.43	
1:D:465:TYR:OH	1:D:486:HIS:ND1	2.43	0.43	
1:F:269:VAL:CG1	1:F:592:VAL:HG13	2.49	0.43	
1:G:312:ASP:O	1:G:428:PRO:HG2	2.19	0.43	
1:G:49:VAL:O	1:G:203:ARG:HD2	2.19	0.43	
1:H:112:TRP:CZ2	1:H:611:LEU:HD23	2.53	0.43	
1:B:205:ASP:OD2	1:B:208:THR:HG23	2.19	0.43	
1:B:481:GLU:O	1:B:499:ASP:HA	2.18	0.43	
1:D:130:LYS:O	1:D:145:GLY:HA3	2.19	0.43	
1:D:277:THR:HB	1:D:278:PRO:HD3	1.99	0.43	
1:E:566:CYS:HA	1:E:576:VAL:HG21	2.01	0.43	
1:E:69:THR:HG22	1:E:91:ASN:HB2	2.01	0.43	
1:H:335:GLY:HA2	1:H:340:GLN:NE2	2.34	0.43	
1:D:321:ARG:NH2	1:H:411:THR:O	2.50	0.43	
1:A:277:THR:N	1:A:278:PRO:CD	2.81	0.43	
1:D:411:THR:HG22	1:D:412:LEU:CD2	2.49	0.43	
1:D:430:SER:OG	1:D:450:GLY:O	2.37	0.43	

		Interatomic	Clash	
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)	
1:E:205:ASP:OD2	1:E:207:ALA:HB3	2.19	0.43	
1:F:322:VAL:HA	1:F:477:ALA:O	2.19	0.43	
1:A:252:THR:O	1:A:253:HIS:C	2.57	0.42	
1:D:337:LYS:HD3	1:D:337:LYS:H	1.83	0.42	
1:E:147:ASP:HB3	1:E:643:GLY:HA2	2.00	0.42	
1:E:593:ASP:O	1:E:596:ILE:HG13	2.19	0.42	
1:E:593:ASP:O	1:E:612:VAL:HG11	2.18	0.42	
1:G:578:ASP:HB2	1:G:582:ASN:HB2	2.01	0.42	
1:H:231:ARG:NH2	1:H:259:GLU:OE1	2.49	0.42	
1:C:580:ARG:NH1	1:C:623:GLU:CG	2.82	0.42	
1:D:283:ARG:HA	1:D:297:ILE:HD13	2.01	0.42	
1:D:383:GLU:OE2	1:D:387:ARG:HD3	2.20	0.42	
1:F:128:LEU:HD22	1:F:131:ARG:NH2	2.35	0.42	
1:G:55:TYR:CD2	1:G:101:SER:HA	2.54	0.42	
1:H:100:ASN:N	1:H:203:ARG:NH2	2.66	0.42	
1:A:440:ASN:HD21	1:A:442:TYR:HB2	1.83	0.42	
1:C:403:VAL:HB	1:C:420:THR:CG2	2.48	0.42	
1:D:314:TYR:CE2	1:D:428:PRO:HB3	2.53	0.42	
1:E:449:SER:HB3	1:E:451:PHE:CD1	2.54	0.42	
1:G:399:PHE:CD2	1:G:424:TYR:CE2	3.08	0.42	
1:B:100:ASN:HB2	2:B:701:FAD:N5	2.35	0.42	
1:H:194:LYS:CB	1:H:196:ILE:HD12	2.49	0.42	
1:H:315:THR:HA	1:H:423:GLN:O	2.20	0.42	
1:B:515:VAL:O	1:G:60:GLN:NE2	2.48	0.42	
1:C:186:ALA:HB2	1:C:394:ASP:C	2.40	0.42	
1:E:134:ASN:HB2	1:E:148:GLY:O	2.19	0.42	
1:G:449:SER:OG	1:G:451:PHE:CG	2.72	0.42	
1:H:532:ASP:O	1:H:533:LYS:C	2.56	0.42	
1:A:182:ASP:OD1	1:A:185:THR:OG1	2.29	0.42	
1:E:217:VAL:HA	1:F:645:PRO:HB2	2.02	0.42	
1:C:513:LEU:HD13	1:F:57:ARG:HG2	2.00	0.42	
1:C:500:ILE:HG12	1:C:501:ASP:O	2.20	0.42	
1:D:277:THR:N	1:D:278:PRO:CD	2.82	0.42	
1:D:431:ARG:HG2	1:D:431:ARG:HH11	1.85	0.42	
1:D:69:THR:O	1:D:88:PRO:HA	2.20	0.42	
1:H:115:PHE:CZ	1:H:598:PRO:HD2	2.54	0.42	
1:A:269:VAL:HG13	1:A:592:VAL:CG1	2.49	0.42	
1:A:158:ILE:HG23	1:A:362:ASP:HB3	2.01	0.42	
1:B:161:VAL:HG13	4:B:860:HOH:O	2.18	0.42	
1:H:313:HIS:HE1	1:H:603:THR:O	2.02	0.42	
1:A:35:MET:HE1	1:A:262:VAL:HG11	2.02	0.42	

Atom 1			Clash	
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)	
1:A:349:VAL:HG22	1:B:349:VAL:HG11	2.01	0.42	
1:B:470:GLU:HB3	1:B:474:ARG:HH21	1.84	0.42	
1:C:35:MET:HE2	1:C:37:ILE:HD11	2.02	0.42	
1:D:519:MET:SD	1:H:557:GLU:HG2	2.60	0.42	
1:A:514[B]:THR:CG2	1:E:408:ALA:O	2.68	0.42	
1:E:431:ARG:O	1:E:450:GLY:HA3	2.19	0.42	
1:F:305:GLY:HA3	1:F:574:GLY:O	2.19	0.42	
1:G:104:TYR:HA	1:G:195:TYR:CE2	2.54	0.42	
1:G:130:LYS:HE2	1:G:142:ASP:O	2.19	0.42	
1:G:428:PRO:HD2	1:G:600:ASN:ND2	2.35	0.42	
1:A:228:ARG:HG2	1:A:228:ARG:NH1	2.34	0.42	
1:A:425:LEU:HD23	1:A:428:PRO:HB3	2.02	0.42	
1:B:81:ARG:HD3	1:B:554:ASP:OD1	2.19	0.42	
1:A:163:GLN:NE2	1:C:42:ASN:HB3	2.35	0.42	
1:E:406:ALA:HB2	1:E:418:TYR:HB2	2.02	0.42	
1:G:10:ILE:HD12	1:G:264:ALA:HB2	2.02	0.42	
1:G:69:THR:CG2	1:G:91:ASN:HB2	2.49	0.42	
1:D:57:ARG:HA	1:H:513:LEU:O	2.20	0.42	
1:H:636:PRO:O	1:H:637:HIS:HB2	2.19	0.42	
1:A:624:LEU:HB2	1:A:626:LEU:HD22	2.01	0.41	
1:B:112:TRP:CZ2	1:B:611:LEU:HD23	2.55	0.41	
1:B:411:THR:HG21	1:G:505:ALA:CB	2.49	0.41	
1:B:566:CYS:HA	1:B:576:VAL:HG21	2.02	0.41	
1:D:269:VAL:CG1	1:D:592:VAL:HG13	2.50	0.41	
1:G:44:ARG:NH2	1:G:216:ASP:OD1	2.47	0.41	
1:G:69:THR:HG23	1:G:91:ASN:HB2	2.02	0.41	
1:G:177:SER:HB3	1:G:180:ILE:CD1	2.50	0.41	
1:G:470:GLU:OE1	1:G:474:ARG:NH2	2.53	0.41	
1:G:80:LEU:O	1:G:82:GLY:N	2.53	0.41	
1:H:208:THR:HA	1:H:212:HIS:HB2	2.02	0.41	
1:C:166:LEU:HD12	1:C:166:LEU:HA	1.88	0.41	
1:C:335:GLY:HA2	1:C:340:GLN:NE2	2.35	0.41	
1:C:54:ILE:O	1:C:57:ARG:HG2	2.20	0.41	
1:C:592:VAL:O	1:C:593:ASP:HB3	2.20	0.41	
1:D:374:LEU:HA	1:D:374:LEU:HD13	1.92	0.41	
1:H:313:HIS:O	1:H:559:THR:CG2	2.68	0.41	
1:A:314:TYR:CD2	1:A:452:MET:HE1	2.56	0.41	
1:A:81:ARG:HD3	1:A:554:ASP:OD1	2.20	0.41	
1:C:177:SER:HB3	1:C:180:ILE:HD13	2.02	0.41	
1:D:303:LEU:HD21	1:D:584:TYR:HB2	2.02	0.41	
1:A:409:ASP:HA	1:E:514:THR:HB	2.02	0.41	

		Interatomic	Clash	
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)	
1:B:57:ARG:HB3	1:G:513:LEU:HB3	2.01	0.41	
1:H:321:ARG:HH11	1:H:321:ARG:CG	2.33	0.41	
1:A:43:ASN:HB2	1:A:49:VAL:HG21	2.03	0.41	
1:C:352:GLU:HG2	1:C:353:LYS:HG3	2.03	0.41	
1:E:459:ALA:N	1:E:460:PRO:HD2	2.36	0.41	
1:G:513:LEU:CD2	1:G:513:LEU:N	2.83	0.41	
1:H:473:ARG:NH2	1:H:536:GLU:O	2.53	0.41	
1:B:159:MET:SD	1:B:327:ILE:HG22	2.60	0.41	
1:B:348:GLU:CG	1:D:350:SER:OG	2.69	0.41	
1:D:197:ASN:HB3	1:D:200:THR:OG1	2.20	0.41	
1:D:35:MET:CE	1:D:262:VAL:HG21	2.44	0.41	
1:D:561:HIS:O	4:D:802:HOH:O	2.22	0.41	
1:E:205:ASP:CG	1:E:208:THR:HG23	2.41	0.41	
1:E:83:ARG:NH2	1:E:556:VAL:O	2.34	0.41	
1:F:162:ALA:HB2	1:F:362:ASP:HB2	2.03	0.41	
1:F:12:CYS:SG	1:F:243:VAL:HG21	2.61	0.41	
1:H:115:PHE:CE1	1:H:598:PRO:HD2	2.56	0.41	
1:A:177:SER:HB3	1:A:180:ILE:HD13	2.02	0.41	
1:A:513:LEU:N	1:A:513:LEU:HD23	2.36	0.41	
1:B:35:MET:HE2	1:B:37:ILE:HD11	2.01	0.41	
1:B:520:GLY:HA3	1:B:522:TRP:NE1	2.35	0.41	
1:C:369:PRO:HD2	1:C:397:VAL:HG21	2.03	0.41	
1:D:20:VAL:HG11	1:D:614:GLU:N	2.35	0.41	
1:F:438:SER:HB3	1:F:443:VAL:HG21	2.02	0.41	
1:G:289:GLY:HA3	1:G:302:ASP:OD2	2.20	0.41	
1:C:34:VAL:HG22	1:C:221:LEU:HD13	2.02	0.41	
1:D:466:LYS:O	1:D:470:GLU:HG2	2.20	0.41	
1:E:308:GLU:O	1:E:565:THR:HA	2.21	0.41	
1:F:449:SER:HB3	1:F:451:PHE:CD1	2.56	0.41	
1:G:269:VAL:CG1	1:G:592:VAL:CG1	2.99	0.41	
1:C:106:ARG:NH2	1:C:143:THR:O	2.46	0.41	
1:E:10:ILE:HD11	1:E:262:VAL:HG22	2.03	0.41	
1:E:452:MET:HE3	1:E:556:VAL:HG21	2.02	0.41	
1:E:569:LYS:HB2	1:E:570:PRO:HD2	2.01	0.41	
1:G:184:THR:O	1:G:184:THR:HG22	2.20	0.41	
1:H:208:THR:O	1:H:636:PRO:HD2	2.20	0.41	
1:A:282:GLU:O	1:A:292:LEU:CD2	2.69	0.41	
1:E:253:HIS:ND1	1:F:536:GLU:HA	2.35	0.41	
1:G:459:ALA:N	1:G:460:PRO:CD	2.82	0.41	
1:H:16:PRO:HA	1:H:206:ALA:CB	2.51	0.41	
1:B:121:THR:HG22	1:B:123:LYS:H	1.86	0.41	

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:B:121:THR:HG22	1:B:123:LYS:N	2.36	0.41
1:B:406:ALA:HA	1:B:420:THR:HG22	2.03	0.41
1:H:52:PRO:HB3	1:H:102:GLN:OE1	2.21	0.41
1:H:500:ILE:HD11	1:H:504:THR:HG22	2.03	0.41
1:A:10:ILE:HD12	1:A:264:ALA:HB2	2.03	0.40
1:F:577:VAL:HA	1:F:582:ASN:O	2.21	0.40
1:D:513:LEU:O	1:H:57:ARG:HA	2.22	0.40
1:C:134:ASN:HB3	1:C:151:ALA:HA	2.02	0.40
1:F:137:LYS:HB2	1:F:138:PRO:HD2	2.03	0.40
1:G:403:VAL:CG2	1:G:420:THR:HG23	2.50	0.40
1:H:134:ASN:HB2	1:H:148:GLY:O	2.22	0.40
1:H:314:TYR:CE2	1:H:428:PRO:HB3	2.56	0.40
1:A:321:ARG:HG2	1:A:418:TYR:CE1	2.56	0.40
1:C:269:VAL:CG1	1:C:592:VAL:HG12	2.52	0.40
1:C:72:THR:O	1:C:73:ASP:C	2.59	0.40
1:F:114:ASP:OD2	1:F:395:LYS:NZ	2.42	0.40
1:G:378:GLY:O	1:G:382:ASN:ND2	2.40	0.40
1:E:315:THR:HA	1:E:423:GLN:O	2.22	0.40
1:F:618:ASP:O	1:F:622:GLU:HG2	2.21	0.40
1:G:405:GLY:O	1:G:420:THR:HG22	2.22	0.40
1:G:474:ARG:HD3	1:H:251:ARG:O	2.21	0.40
1:C:245:TYR:O	1:C:259:GLU:HA	2.21	0.40
1:D:407:TYR:H	1:D:420:THR:CG2	2.30	0.40
1:D:470:GLU:OE1	1:D:474:ARG:NH2	2.54	0.40
1:E:106:ARG:HB2	1:E:181:GLN:HB3	2.03	0.40
1:E:446:PHE:C	1:E:446:PHE:CD1	2.95	0.40
1:F:313:HIS:NE2	1:F:426:GLU:O	2.54	0.40
1:H:106:ARG:HH12	1:H:143:THR:CG2	2.34	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	А	648/651~(100%)	607~(94%)	36~(6%)	5(1%)	19 35
1	В	645/651~(99%)	604~(94%)	40~(6%)	1 (0%)	47 68
1	С	646/651~(99%)	605~(94%)	38~(6%)	3~(0%)	29 48
1	D	647/651~(99%)	617~(95%)	29~(4%)	1 (0%)	47 68
1	Е	646/651~(99%)	614~(95%)	29~(4%)	3~(0%)	29 48
1	F	648/651~(100%)	607~(94%)	39~(6%)	2 (0%)	41 61
1	G	646/651~(99%)	608~(94%)	35~(5%)	3~(0%)	29 48
1	Н	646/651~(99%)	599~(93%)	45 (7%)	2(0%)	41 61
All	All	5172/5208~(99%)	4861 (94%)	291 (6%)	20 (0%)	34 54

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	578	ASP
1	G	81	ARG
1	А	253	HIS
1	С	593	ASP
1	D	578	ASP
1	Е	578	ASP
1	А	593	ASP
1	G	96	GLY
1	А	449	SER
1	В	198	ARG
1	F	533	LYS
1	F	578	ASP
1	G	323	SER
1	Н	235	ASP
1	А	306	VAL
1	С	235	ASP
1	С	558	THR
1	Е	414	PRO
1	Е	92	ILE
1	Н	21	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.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
1	А	548/548~(100%)	495~(90%)	53~(10%)	8	16
1	В	545/548~(100%)	498~(91%)	47 (9%)	10	20
1	С	546/548~(100%)	510~(93%)	36~(7%)	16	32
1	D	547/548~(100%)	500~(91%)	47 (9%)	10	20
1	Ε	546/548~(100%)	498~(91%)	48 (9%)	10	19
1	F	547/548~(100%)	498~(91%)	49 (9%)	9	19
1	G	546/548~(100%)	498~(91%)	48 (9%)	10	19
1	Н	546/548~(100%)	505~(92%)	41 (8%)	13	26
All	All	4371/4384~(100%)	4002 (92%)	369 (8%)	11	21

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

All (369) residues with a non-rotameric sidechain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	3	HIS
1	А	34	VAL
1	А	44	ARG
1	А	50	TYR
1	А	54	ILE
1	А	57	ARG
1	А	61	ARG
1	A	69	THR
1	А	106	ARG
1	А	126	LEU
1	А	166	LEU
1	А	180	ILE
1	А	192	TRP
1	А	194	LYS
1	А	203	ARG
1	А	228	ARG
1	А	256	LYS
1	А	262	VAL
1	A	275	LEU
1	А	283	ARG
1	A	333	LEU
1	A	337	LYS
1	A	338	ASP
1	А	341	ARG

Mol	Chain	Res	Type
1	А	348	GLU
1	А	350	SER
1	А	353	LYS
1	А	365	PHE
1	А	370	THR
1	А	371	GLU
1	А	374	LEU
1	А	391	ASP
1	А	392	LYS
1	А	393	PRO
1	А	399	PHE
1	А	411	THR
1	A	412	LEU
1	A	417	LYS
1	А	420	THR
1	A	514[A]	THR
1	А	514[B]	THR
1	А	542	GLU
1	А	546	LYS
1	А	557	GLU
1	А	578	ASP
1	А	592	VAL
1	А	600	ASN
1	А	608	SER
1	А	626	LEU
1	А	635	VAL
1	A	644	ARG
1	A	647	THR
1	A	651	ARG
1	В	5	GLU
1	В	34	VAL
1	В	44	ARG
1	В	54	ILE
1	В	57	ARG
1	В	66	ASP
1	В	69	THR
1	В	116	LYS
1	В	123	LYS
1	В	147	ASP
1	В	166	LEU
1	В	203	ARG
1	В	205	ASP

Mol	Chain	Res	Type
1	В	224	ARG
1	В	241	VAL
1	В	243	VAL
1	В	248	SER
1	В	251	ARG
1	В	275	LEU
1	В	291	LEU
1	В	333	LEU
1	В	337	LYS
1	В	348	GLU
1	В	350	SER
1	В	353	LYS
1	В	365	PHE
1	В	374	LEU
1	В	391	ASP
1	В	392	LYS
1	В	399	PHE
1	В	411	THR
1	В	420	THR
1	В	455	LYS
1	В	524	GLN
1	В	527	GLU
1	В	542	GLU
1	В	559	THR
1	В	572	GLU
1	В	587	GLN
1	В	592	VAL
1	В	604	ASN
1	В	608	SER
1	В	626	LEU
1	В	635	VAL
1	В	640	VAL
1	В	644	ARG
1	В	650	VAL
1	С	34	VAL
1	С	54	ILE
1	С	57	ARG
1	С	121	THR
1	С	126	LEU
1	С	166	LEU
1	C	180	ILE
1	C	194	LYS
	<u> </u>	-	

Mol	Chain	Res	Type
1	С	208	THR
1	С	213	SER
1	С	241	VAL
1	С	243	VAL
1	С	251	ARG
1	С	260	THR
1	С	262	VAL
1	С	291	LEU
1	С	333	LEU
1	С	341	ARG
1	С	348	GLU
1	С	365	PHE
1	С	374	LEU
1	С	392	LYS
1	С	412	LEU
1	С	433	LYS
1	С	513	LEU
1	С	527	GLU
1	С	551	TRP
1	С	587	GLN
1	С	592	VAL
1	С	618	ASP
1	С	626	LEU
1	С	635	VAL
1	С	642	THR
1	С	644	ARG
1	С	650	VAL
1	С	651	ARG
1	D	34	VAL
1	D	44	ARG
1	D	54	ILE
1	D	57	ARG
1	D	61	ARG
1	D	75	MET
1	D	106	ARG
1	D	126	LEU
1	D	166	LEU
1	D	184	THR
1	D	192	TRP
1	D	203	ARG
1	D	208	THR
1	D	213	SER

Mol	Chain	Res	Type
1	D	236	ASP
1	D	241	VAL
1	D	243	VAL
1	D	245	TYR
1	D	248	SER
1	D	251	ARG
1	D	262	VAL
1	D	263	LYS
1	D	275	LEU
1	D	298	LYS
1	D	325	GLU
1	D	333	LEU
1	D	337	LYS
1	D	338	ASP
1	D	348	GLU
1	D	353	LYS
1	D	365	PHE
1	D	371	GLU
1	D	374	LEU
1	D	380	GLU
1	D	387	ARG
1	D	399	PHE
1	D	417	LYS
1	D	420	THR
1	D	443	VAL
1	D	449	SER
1	D	474	ARG
1	D	592	VAL
1	D	626	LEU
1	D	635	VAL
1	D	644	ARG
1	D	650	VAL
1	D	651	ARG
1	Е	34	VAL
1	E	44	ARG
1	E	$5\overline{4}$	ILE
1	E	61	ARG
1	E	69	THR
1	E	75	MET
1	E	83	ARG
1	E	$10\overline{6}$	ARG
1	E	126	LEU

Mol	Chain	Res	Type
1	Е	147	ASP
1	Е	166	LEU
1	Е	194	LYS
1	Е	203	ARG
1	Е	208	THR
1	Е	228	ARG
1	Е	233	LEU
1	Е	243	VAL
1	Е	251	ARG
1	Е	263	LYS
1	Е	275	LEU
1	Е	284	SER
1	Е	291	LEU
1	Е	333	LEU
1	Е	337	LYS
1	Е	338	ASP
1	Е	348	GLU
1	Е	353	LYS
1	Е	365	PHE
1	Е	374	LEU
1	Е	380	GLU
1	Е	383	GLU
1	Е	411	THR
1	Е	420	THR
1	Е	443	VAL
1	Е	449	SER
1	Е	531	HIS
1	Е	532	ASP
1	Ε	535	ILE
1	Е	559	THR
1	Е	578	ASP
1	Е	580	ARG
1	E	$59\overline{2}$	VAL
1	E	600	ASN
1	Ε	630	THR
1	E	635	VAL
1	E	644	ARG
1	E	647	THR
1	E	651	ARG
1	F	31	THR
1	F	44	ARG
1	F	54	ILE

Mol	Chain	Res	Type
1	F	57	ARG
1	F	61	ARG
1	F	69	THR
1	F	106	ARG
1	F	116	LYS
1	F	126	LEU
1	F	166	LEU
1	F	184	THR
1	F	185	THR
1	F	192	TRP
1	F	194	LYS
1	F	208	THR
1	F	228	ARG
1	F	248	SER
1	F	262	VAL
1	F	275	LEU
1	F	295	LEU
1	F	333	LEU
1	F	337	LYS
1	F	338	ASP
1	F	348	GLU
1	F	350	SER
1	F	353	LYS
1	F	365	PHE
1	F	374	LEU
1	F	383	GLU
1	F	392	LYS
1	F	399	PHE
1	F	411	THR
1	F	420	THR
1	F	422	PHE
1	F	443	VAL
1	F	473	ARG
1	F	513	LEU
1	F	521	SER
1	F	533	LYS
1	F	534	VAL
1	F	535	ILE
1	F	559	THR
1	F	592	VAL
1	F	601	LEU
1	F	608	SER

Mol	Chain	Res	Type
1	F	635	VAL
1	F	640	VAL
1	F	644	ARG
1	F	649	GLN
1	G	34	VAL
1	G	44	ARG
1	G	54	ILE
1	G	69	THR
1	G	123	LYS
1	G	124	ASP
1	G	126	LEU
1	G	143	THR
1	G	166	LEU
1	G	180	ILE
1	G	194	LYS
1	G	198	ARG
1	G	203	ARG
1	G	224	ARG
1	G	251	ARG
1	G	256	LYS
1	G	260	THR
1	G	262	VAL
1	G	275	LEU
1	G	333	LEU
1	G	337	LYS
1	G	361	ILE
1	G	365	PHE
1	G	377	MET
1	G	380	GLU
1	G	383	GLU
1	G	391	ASP
1	G	392	LYS
1	G	411	THR
1	G	433	LYS
1	G	438	SER
1	G	449	SER
1	G	513	LEU
1	G	527	GLU
1	G	530	LYS
1	G	533	LYS
1	G	557	GLU
1	G	559	THR

Mol	Chain	Res	Type
1	G	572	GLU
1	G	578	ASP
1	G	587	GLN
1	G	592	VAL
1	G	600	ASN
1	G	618	ASP
1	G	626	LEU
1	G	635	VAL
1	G	642	THR
1	G	644	ARG
1	Н	34	VAL
1	Н	54	ILE
1	Н	57	ARG
1	Н	69	THR
1	Н	75	MET
1	Н	78	SER
1	Н	106	ARG
1	Н	126	LEU
1	Н	166	LEU
1	Н	184	THR
1	Н	203	ARG
1	Н	208	THR
1	Н	243	VAL
1	Н	253	HIS
1	Н	256	LYS
1	Н	262	VAL
1	Н	275	LEU
1	Н	291	LEU
1	Н	333	LEU
1	Н	338	ASP
1	H	348	GLU
1	H	353	LYS
1	Н	365	PHE
1	H	374	LEU
1	Н	387	ARG
1	H	$39\overline{2}$	LYS
1	Н	411	THR
1	H	417	LYS
1	H	420	THR
1	Н	443	VAL
1	H	$53\overline{0}$	LYS
1	Н	559	THR

Contr	Continuca from pretious page			
\mathbf{Mol}	Chain	\mathbf{Res}	Type	
1	Н	578	ASP	
1	Н	587	GLN	
1	Н	592	VAL	
1	Н	626	LEU	
1	Н	627	LYS	
1	Н	630	THR	
1	Н	635	VAL	
1	Н	644	ARG	
1	Н	651	ARG	

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	157	GLN
1	А	440	ASN
1	В	157	GLN
1	В	524	GLN
1	D	439	GLN
1	D	518	HIS
1	Е	531	HIS
1	F	157	GLN
1	G	324	ASN
1	G	440	ASN
1	Н	157	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mal	Tune	Chain	Dec	Tink	Bo	ond leng	\mathbf{ths}	B	ond ang	gles
	туре	Chain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
2	FAD	F	701	-	51, 58, 58	1.94	7 (13%)	$60,\!89,\!89$	2.20	13 (21%)
2	FAD	D	701	-	51, 58, 58	1.82	6 (11%)	60,89,89	2.23	15 (25%)
2	FAD	G	701	-	51, 58, 58	1.83	6 (11%)	60,89,89	2.06	14 (23%)
2	FAD	В	701	-	51, 58, 58	1.88	8 (15%)	60,89,89	2.02	12 (20%)
2	FAD	Е	701	-	51, 58, 58	1.95	7 (13%)	60,89,89	1.98	10 (16%)
2	FAD	С	701	-	51, 58, 58	1.76	6 (11%)	60,89,89	2.23	12 (20%)
2	FAD	А	701	-	51, 58, 58	1.84	7 (13%)	60,89,89	2.26	14 (23%)
3	GOL	В	702	-	$5,\!5,\!5$	0.68	0	5, 5, 5	0.71	0
3	GOL	Н	702	-	5, 5, 5	0.55	0	5, 5, 5	0.42	0
2	FAD	Н	701	-	$51,\!58,\!58$	1.98	8 (15%)	60,89,89	2.10	12 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	F	701	-	-	8/30/50/50	0/6/6/6
2	FAD	D	701	-	-	6/30/50/50	0/6/6/6
2	FAD	G	701	-	-	7/30/50/50	0/6/6/6
2	FAD	В	701	-	-	6/30/50/50	0/6/6/6
2	FAD	Е	701	-	-	$\frac{5/30}{50}$	0/6/6/6
2	FAD	С	701	-	-	$\frac{5/30}{50}$	0/6/6/6
2	FAD	А	701	-	-	8/30/50/50	0/6/6/6
3	GOL	В	702	-	-	4/4/4/4	-
3	GOL	Н	702	-	-	2/4/4/4	_
2	FAD	Н	701	-	-	4/30/50/50	0/6/6/6

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Mol	Chain	Res	Type	Atoms	7	Observed(Å)	Ideal(Å)
2	Н	701	FAD	C4X-C10	10.21	1 49	1 38
$\frac{2}{2}$	F	701	FAD	C4X-C10	9.89	1.48	1.38
2	Ē	701	FAD	C4X-C10	9.74	1.48	1.38
2	B	701	FAD	C4X-C10	9.58	1.48	1.38
$\frac{-}{2}$	G	701	FAD	C4X-C10	9.39	1.48	1.38
2	A	701	FAD	C4X-C10	9.38	1.48	1.38
2	D	701	FAD	C4X-C10	9.04	1.47	1.38
2	C	701	FAD	C4X-C10	8.51	1.47	1.38
2	F	701	FAD	C4-C4X	4.56	1.49	1.41
2	Н	701	FAD	C4-C4X	4.54	1.49	1.41
2	Е	701	FAD	C4-C4X	4.31	1.48	1.41
2	D	701	FAD	C4-C4X	4.22	1.48	1.41
2	С	701	FAD	C9A-C5X	3.99	1.50	1.42
2	В	701	FAD	C9A-C5X	3.98	1.50	1.42
2	G	701	FAD	C4-C4X	3.95	1.48	1.41
2	Е	701	FAD	C9A-N10	3.86	1.43	1.38
2	D	701	FAD	C9A-C5X	3.75	1.50	1.42
2	Е	701	FAD	C9A-C5X	3.70	1.50	1.42
2	F	701	FAD	C9A-C5X	3.70	1.50	1.42
2	С	701	FAD	C4-C4X	3.63	1.47	1.41
2	G	701	FAD	C9A-C5X	3.56	1.49	1.42
2	В	701	FAD	C4-C4X	3.53	1.47	1.41
2	Н	701	FAD	C9A-C5X	3.51	1.49	1.42
2	А	701	FAD	C8-C7	3.49	1.49	1.40
2	А	701	FAD	C9A-C5X	3.48	1.49	1.42
2	G	701	FAD	C8-C7	3.35	1.49	1.40
2	В	701	FAD	C8-C7	3.34	1.49	1.40
2	Н	701	FAD	C8-C7	3.29	1.49	1.40
2	F	701	FAD	C8-C7	3.24	1.49	1.40
2	E	701	FAD	C8-C7	3.24	1.49	1.40
2	A	701	FAD	C4-C4X	3.13	1.46	1.41
2	С	701	FAD	C8-C7	3.11	1.48	1.40
2	D	701	FAD	C8-C7	2.89	1.48	1.40
2	Н	701	FAD	C10-N1	2.87	1.36	1.33
2	D	701	FAD	C9A-N10	2.81	1.42	1.38
2	A	701	FAD	C9A-N10	2.75	1.42	1.38
2	B	701	F'AD	O4B-C1B	2.68	1.44	1.41
2	F	701	FAD	C9A-N10	2.52	1.41	1.38
2	E	701	FAD	C5A-C4A	2.48	1.47	1.40
2	C	701	FAD	C9A-N10	2.47	1.41	1.38
2	B	701	FAD	C9A-N10	2.38	1.41	1.38
2	F	701	FAD	O4B-C1B	2.37	1.44	1.41

All (55) bond length outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	$\operatorname{Observed}(\operatorname{\AA})$	Ideal(Å)
2	В	701	FAD	C5A-C4A	2.36	1.47	1.40
2	G	701	FAD	C10-N1	2.35	1.36	1.33
2	D	701	FAD	C4-N3	2.32	1.37	1.33
2	С	701	FAD	C5A-C4A	2.32	1.47	1.40
2	Η	701	FAD	C2A-N3A	2.26	1.35	1.32
2	Η	701	FAD	C9A-N10	2.26	1.41	1.38
2	G	701	FAD	C9A-N10	2.25	1.41	1.38
2	Н	701	FAD	C5A-C4A	2.17	1.46	1.40
2	Е	701	FAD	C6-C5X	-2.16	1.38	1.41
2	F	701	FAD	C5A-C4A	2.13	1.46	1.40
2	А	701	FAD	C5A-C4A	2.13	1.46	1.40
2	В	701	FAD	C2A-N3A	2.06	1.35	1.32
2	А	701	FAD	C2B-C1B	-2.03	1.50	1.53

Continued from previous page...

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	F	701	FAD	C4-N3-C2	9.28	122.97	115.14
2	А	701	FAD	C4-N3-C2	8.99	122.73	115.14
2	D	701	FAD	C4-N3-C2	8.88	122.64	115.14
2	С	701	FAD	C4-N3-C2	8.63	122.43	115.14
2	Н	701	FAD	C4-N3-C2	8.47	122.29	115.14
2	Е	701	FAD	C4-N3-C2	8.18	122.05	115.14
2	G	701	FAD	C4-N3-C2	7.77	121.70	115.14
2	С	701	FAD	C4-C4X-C10	-7.47	115.01	119.95
2	В	701	FAD	C1'-N10-C9A	7.07	123.86	118.29
2	А	701	FAD	C4-C4X-C10	-6.90	115.38	119.95
2	В	701	FAD	C4-N3-C2	6.29	120.45	115.14
2	Н	701	FAD	C4-C4X-C10	-6.27	115.80	119.95
2	В	701	FAD	C4-C4X-C10	-6.16	115.87	119.95
2	С	701	FAD	C1'-N10-C9A	6.10	123.09	118.29
2	А	701	FAD	C1'-N10-C9A	6.05	123.05	118.29
2	G	701	FAD	C4-C4X-C10	-5.80	116.11	119.95
2	D	701	FAD	C4X-N5-C5X	5.53	122.30	116.77
2	F	701	FAD	C1'-N10-C9A	5.52	122.64	118.29
2	F	701	FAD	C4-C4X-C10	-5.37	116.40	119.95
2	Е	701	FAD	C4-C4X-C10	-5.17	116.53	119.95
2	D	701	FAD	C4-C4X-C10	-5.10	116.58	119.95
2	В	701	FAD	C9A-N10-C10	-5.02	115.33	121.91
2	A	701	FAD	N3A-C2A-N1A	-4.65	121.42	128.68
2	Е	701	FAD	C1'-N10-C9A	4.65	121.95	118.29
2	С	701	FAD	C4-C4X-N5	4.58	123.83	118.60

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	Chain	l preur	Uus puye	 Atoms	7	Observed $(^{o})$	Ideal(°)
2		701		C1 N10 C0A	1.59	191.00	118 20
	D	701	FAD FAD	C1-N10-C9A	4.00	121.90	116.29
	E E	701	FAD FAD	$\begin{array}{c} C4X - N5 - C5X \\ \hline C4X - N5 - C5X \\ \hline \end{array}$	4.00	121.10 191.11	110.77
	E C	701	FAD FAD	$\frac{04A-N0-00A}{N2A}$	4.00	121.11	110.77
$\frac{2}{2}$	G	701	FAD FAD	NOA-OZA-NIA	-4.04	121.09	120.00 116.77
	G	701	FAD FAD	C4A-NO-COA	4.31	121.00	110.77
2	H D	701	FAD	UT-NIU-C9A	4.28	121.00	118.29
2	E	701	FAD	N3A-C2A-N1A	-4.27	122.00	128.08
2	F D	701	FAD	C4X-C4-N3	-4.27	117.60	123.43
2	D	701	FAD	N3A-C2A-NIA	-4.13	122.22	128.68
2	H	701	FAD	C4A-C5A-N7A	-4.12	105.11	109.40
2	G	701	FAD	C4-C4X-N5	4.08	123.26	118.60
2	D	701	FAD	C4X-C4-N3	-4.04	117.91	123.43
2	D	701	FAD	C4-C4X-N5	4.01	123.18	118.60
2	С	701	FAD	N3A-C2A-N1A	-3.96	122.49	128.68
2	F	701	FAD	C4-C4X-N5	3.90	123.06	118.60
2	F	701	FAD	C4X-N5-C5X	3.81	120.58	116.77
2	G	701	FAD	C1'-N10-C9A	3.73	121.23	118.29
2	Н	701	FAD	C4-C4X-N5	3.71	122.84	118.60
2	D	701	FAD	O3B-C3B-C4B	-3.71	100.32	111.05
2	F	701	FAD	N3A-C2A-N1A	-3.71	122.88	128.68
2	D	701	FAD	C1B-N9A-C4A	-3.70	120.14	126.64
2	Н	701	FAD	N3A-C2A-N1A	-3.68	122.92	128.68
2	F	701	FAD	C6-C5X-N5	-3.67	115.00	119.05
2	А	701	FAD	C4X-N5-C5X	3.67	120.44	116.77
2	Е	701	FAD	C4X-C4-N3	-3.60	118.51	123.43
2	Н	701	FAD	C4X-N5-C5X	3.56	120.33	116.77
2	А	701	FAD	C4-C4X-N5	3.50	122.60	118.60
2	F	701	FAD	C1B-N9A-C4A	-3.44	120.61	126.64
2	А	701	FAD	C4X-C4-N3	-3.35	118.85	123.43
2	В	701	FAD	N3A-C2A-N1A	-3.34	123.45	128.68
2	G	701	FAD	C4'-C3'-C2'	-3.34	106.42	113.36
2	G	701	FAD	P-O3P-PA	-3.24	121.70	132.83
2	Н	701	FAD	C9A-N10-C10	-3.17	117.75	121.91
2	А	701	FAD	C1B-N9A-C4A	-3.14	121.12	126.64
2	G	701	FAD	C9A-C5X-N5	-3.13	117.47	122.36
2	F	701	FAD	C9A-N10-C10	-3.13	117.81	121.91
2	Е	701	FAD	C4-C4X-N5	3.06	122.10	118.60
2	D	701	FAD	C6-C5X-N5	-3.05	115.68	119.05
2	G	701	FAD	C4X-C4-N3	-3.04	119.28	123.43
2	Н	701	FAD	C4X-C4-N3	-3.04	119.28	123.43
$\frac{1}{2}$	B	701	FAD	C4A-C5A-N7A	-2.98	106.29	109.40
2	С	701	FAD	C9A-C5X-N5	-2.92	117.79	122.36

Contin $d f_{a}$

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	701	FAD	C4X-C4-N3	-2.92	119.44	123.43
2	С	701	FAD	C1B-N9A-C4A	-2.87	121.61	126.64
2	С	701	FAD	C9A-N10-C10	-2.85	118.17	121.91
2	В	701	FAD	C4X-C4-N3	-2.82	119.58	123.43
2	G	701	FAD	C9A-N10-C10	-2.71	118.36	121.91
2	Н	701	FAD	C9A-C5X-N5	-2.69	118.15	122.36
2	В	701	FAD	C4-C4X-N5	2.66	121.64	118.60
2	Е	701	FAD	C9A-N10-C10	-2.66	118.42	121.91
2	А	701	FAD	C4A-C5A-N7A	-2.56	106.73	109.40
2	Н	701	FAD	P-O3P-PA	-2.54	124.09	132.83
2	D	701	FAD	C2A-N1A-C6A	2.50	123.03	118.75
2	G	701	FAD	C1B-N9A-C4A	-2.48	122.29	126.64
2	А	701	FAD	C2A-N1A-C6A	2.46	122.96	118.75
2	D	701	FAD	C4A-C5A-N7A	-2.45	106.85	109.40
2	В	701	FAD	C2B-C3B-C4B	2.41	107.33	102.64
2	D	701	FAD	C9A-C5X-N5	-2.40	118.60	122.36
2	А	701	FAD	C5X-C9A-N10	2.37	119.44	117.72
2	D	701	FAD	C2B-C3B-C4B	2.37	107.25	102.64
2	А	701	FAD	C9A-N10-C10	-2.35	118.83	121.91
2	F	701	FAD	C2A-N1A-C6A	2.35	122.78	118.75
2	F	701	FAD	C9A-C5X-N5	-2.35	118.68	122.36
2	С	701	FAD	P-O3P-PA	-2.34	124.79	132.83
2	Е	701	FAD	C2A-N1A-C6A	2.33	122.74	118.75
2	Е	701	FAD	P-O3P-PA	-2.32	124.88	132.83
2	А	701	FAD	O4B-C1B-C2B	-2.28	103.60	106.93
2	F	701	FAD	N6A-C6A-N1A	2.26	123.27	118.57
2	В	701	FAD	C4X-N5-C5X	2.22	118.99	116.77
2	В	701	FAD	P-O3P-PA	-2.21	125.25	132.83
2	Н	701	FAD	C1'-N10-C10	2.20	120.38	118.41
2	С	701	FAD	C2A-N1A-C6A	2.17	122.47	118.75
2	D	701	FAD	C9A-N10-C10	-2.16	119.08	121.91
2	G	701	FAD	C2A-N1A-C6A	2.15	122.43	118.75
2	В	701	FAD	C1'-N10-C10	2.05	120.24	118.41
2	А	701	FAD	C4'-C3'-C2'	-2.02	109.15	113.36
2	G	701	FAD	C4A-C5A-N7A	-2.02	107.30	109.40

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Atoms
2	F	701	FAD	N10-C1'-C2'-O2'
2	F	701	FAD	N10-C1'-C2'-C3'

Mol	Chain	Res	Type	Atoms
2	D	701	FAD	N10-C1'-C2'-O2'
2	D	701	FAD	N10-C1'-C2'-C3'
2	G	701	FAD	N10-C1'-C2'-O2'
2	G	701	FAD	N10-C1'-C2'-C3'
2	В	701	FAD	N10-C1'-C2'-O2'
2	Е	701	FAD	N10-C1'-C2'-O2'
2	С	701	FAD	N10-C1'-C2'-O2'
2	А	701	FAD	C5B-O5B-PA-O1A
2	А	701	FAD	N10-C1'-C2'-O2'
3	В	702	GOL	O1-C1-C2-C3
3	Н	702	GOL	C1-C2-C3-O3
3	В	702	GOL	O1-C1-C2-O2
3	Н	702	GOL	O2-C2-C3-O3
2	F	701	FAD	PA-O3P-P-O1P
2	G	701	FAD	PA-O3P-P-O1P
2	D	701	FAD	PA-O3P-P-O5'
2	В	701	FAD	PA-O3P-P-O5'
2	Е	701	FAD	PA-O3P-P-O5'
2	С	701	FAD	PA-O3P-P-O5'
2	А	701	FAD	PA-O3P-P-O5'
2	Н	701	FAD	PA-O3P-P-O5'
2	F	701	FAD	P-O3P-PA-O1A
2	В	701	FAD	PA-O3P-P-O1P
2	А	701	FAD	N10-C1'-C2'-C3'
3	В	702	GOL	O2-C2-C3-O3
2	G	701	FAD	P-O3P-PA-O2A
2	В	701	FAD	P-O3P-PA-O2A
2	E	701	FAD	P-O3P-PA-O2A
2	E	701	FAD	PA-O3P-P-O1P
2	С	701	FAD	P-O3P-PA-O2A
2	A	701	FAD	P-O3P-PA-O2A
2	H	701	FAD	P-O3P-PA-O1A
2	F	701	FAD	PA-O3P-P-O5'
2	G	701	FAD	PA-O3P-P-O5'
2	F	701	FAD	O4'-C4'-C5'-O5'
2	Н	701	FAD	O4'-C4'-C5'-O5'
2	D	701	FAD	O4B-C4B-C5B-O5B
2	F	701	FAD	O4B-C4B-C5B-O5B
2	G	701	FAD	O4B-C4B-C5B-O5B
2	В	701	FAD	O4B-C4B-C5B-O5B
2	С	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	F	701	FAD	P-O3P-PA-O2A
2	D	701	FAD	P-O3P-PA-O2A
2	G	701	FAD	P-O3P-PA-O1A
2	С	701	FAD	PA-O3P-P-O1P
2	А	701	FAD	P-O3P-PA-O1A
3	В	702	GOL	C1-C2-C3-O3
2	D	701	FAD	C5'-O5'-P-O1P
2	В	701	FAD	C5B-O5B-PA-O1A
2	А	701	FAD	C5'-O5'-P-O1P
2	Е	701	FAD	O4B-C4B-C5B-O5B
2	Н	701	FAD	O4B-C4B-C5B-O5B

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There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	FAD	3	0
2	D	701	FAD	3	0
2	G	701	FAD	3	0
2	В	701	FAD	3	0
2	Е	701	FAD	2	0
2	С	701	FAD	2	0
2	А	701	FAD	2	0
2	Ĥ	701	FAD	3	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 any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	А	649/651~(99%)	-0.18	4 (0%)	89	90	20, 33, 49, 73	0
1	В	647/651~(99%)	-0.19	1 (0%)	95	95	21, 30, 47, 61	0
1	С	648/651~(99%)	-0.13	3 (0%)	91	91	21, 33, 48, 60	0
1	D	649/651~(99%)	-0.19	1 (0%)	95	95	20, 30, 45, 67	0
1	Ε	648/651~(99%)	0.05	4 (0%)	89	90	22, 36, 52, 68	0
1	F	650/651~(99%)	-0.23	3 (0%)	91	91	22, 32, 49, 73	0
1	G	648/651~(99%)	-0.16	2(0%)	94	94	20, 33, 51, 66	0
1	Н	648/651~(99%)	-0.14	5 (0%)	86	87	20, 32, 49, 72	0
All	All	5187/5208~(99%)	-0.15	23 (0%)	92	93	20, 32, 49, 73	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	640	VAL	3.7
1	С	233	LEU	3.0
1	А	641	PRO	2.8
1	Е	626	LEU	2.7
1	F	387	ARG	2.6
1	G	119	GLY	2.6
1	Н	241	VAL	2.5
1	G	640	VAL	2.5
1	Н	237	ASN	2.5
1	F	341	ARG	2.3
1	В	640	VAL	2.3
1	F	534	VAL	2.2
1	Н	233	LEU	2.2
1	Е	296	GLY	2.1
1	А	75	MET	2.1
1	C	439	GLN	2.1

Mol	Chain	Chain Res Type		RSRZ
1	А	534	VAL	2.1
1	Е	257	LEU	2.1
1	Е	382	ASN	2.1
1	D	28	ALA	2.0
1	Н	285	GLY	2.0
1	Н	234	PHE	2.0
1	С	236	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} extsf{-}\mathbf{factors}(\mathbf{A}^2)$	$Q{<}0.9$
3	GOL	В	702	6/6	0.80	0.20	$30,\!31,\!32,\!32$	0
3	GOL	Н	702	6/6	0.80	0.24	$30,\!30,\!32,\!32$	0
2	FAD	Е	701	53/53	0.95	0.17	$30,\!37,\!40,\!42$	0
2	FAD	С	701	53/53	0.96	0.15	$29,\!34,\!45,\!46$	0
2	FAD	А	701	53/53	0.96	0.13	$23,\!28,\!32,\!35$	0
2	FAD	G	701	53/53	0.96	0.12	28,32,37,38	0
2	FAD	D	701	53/53	0.96	0.14	$18,\!22,\!30,\!33$	0
2	FAD	Н	701	53/53	0.96	0.14	29,31,36,37	0
2	FAD	F	701	53/53	0.97	0.12	23,26,31,32	0
2	FAD	В	701	53/53	0.97	0.12	21,26,29,32	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

6.5 Other polymers (i)

There are no such residues in this entry.

