



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:22 PM GMT

PDB ID : 1AHV  
Title : STRUCTURE OF THE OCTAMERIC FLAVOENZYME VANILLYL-ALCOHOL OXIDASE IN COMPLEX WITH 2-NITRO-P-CRESOL  
Authors : Mattevi, A.  
Deposited on : 1997-04-10  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

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

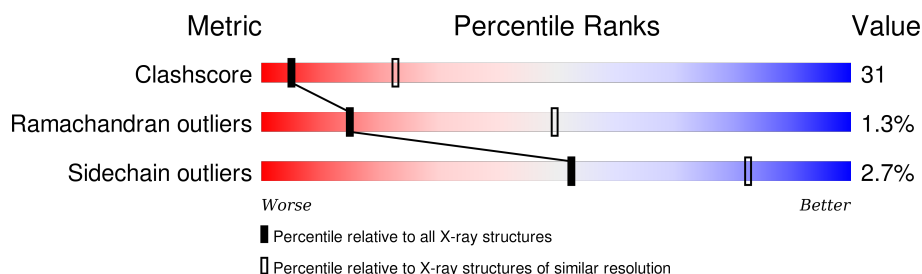
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	
1	B	560	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NCR	A	601	-	-	X	-
3	NCR	B	601	-	-	X	-

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8910 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

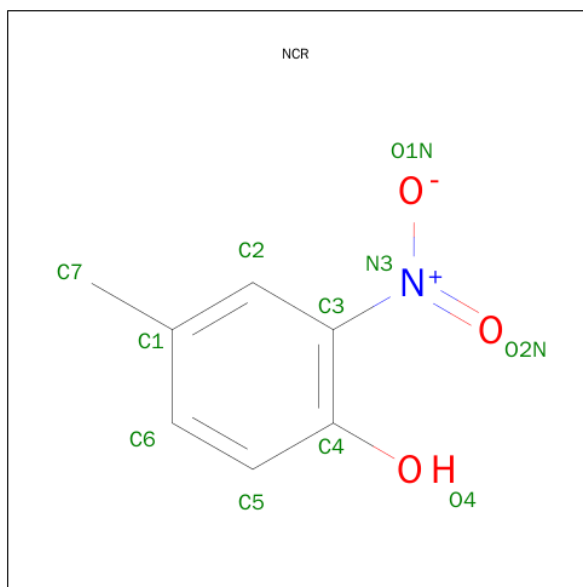
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			
1	B	555	Total	C	N	O	S	28	0	0
			4391	2817	751	799	24			

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



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

- Molecule 3 is 2-NITRO-P-CRESOL (three-letter code: NCR) (formula:  $C_7H_7NO_3$ ).



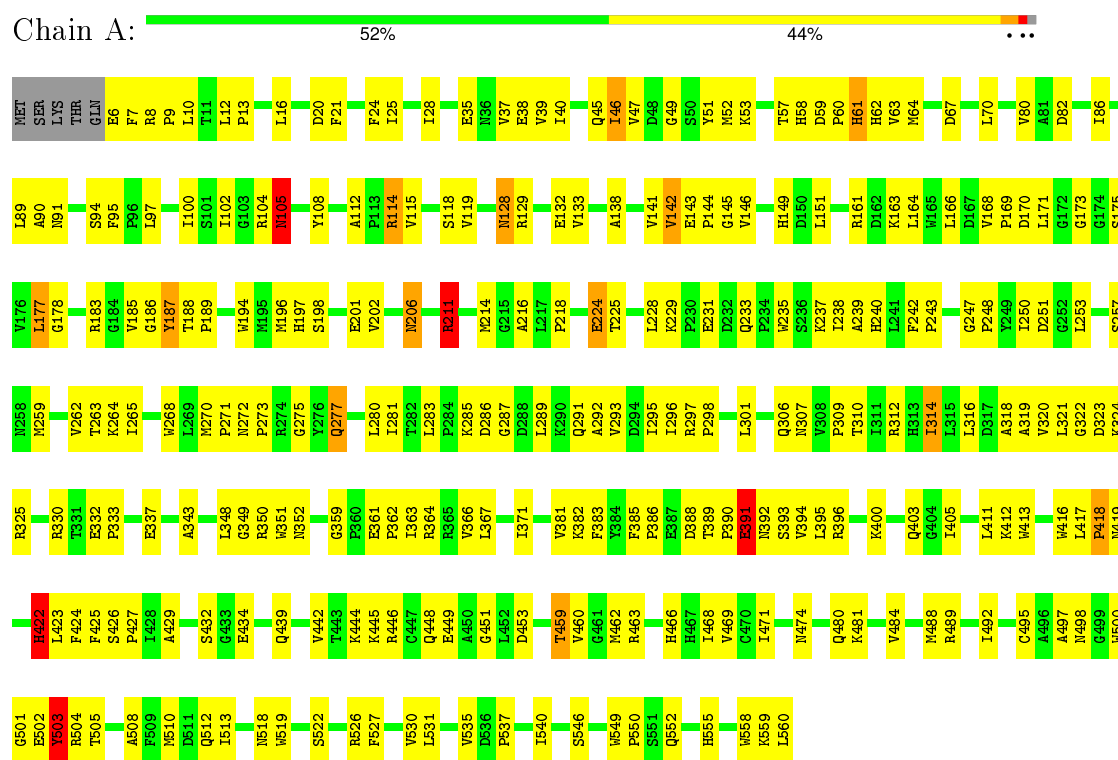
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	1	3		
3	B	1	Total	C	N	O	0	0
			11	7	1	3		

### 3 Residue-property plots

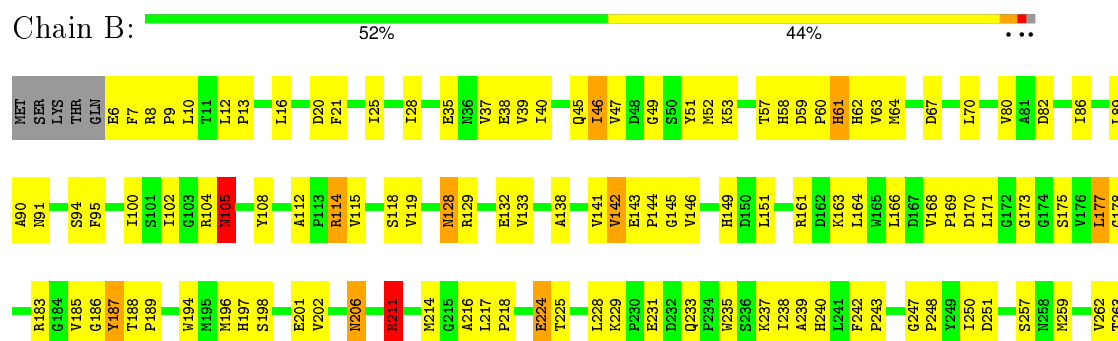
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

#### • Molecule 1: VANILLYL-ALCOHOL OXIDASE



#### • Molecule 1: VANILLYL-ALCOHOL OXIDASE



T505	P427	E337	K264
A508	I428	E337	L265
F509	A429	A343	W268
W510	K430	A343	
D511	Y431	L348	P271
Q512	S432	G349	N272
I513	G433	R350	P273
	E434	W351	R274
		N352	G275
N518	Q439	N352	Y276
W519			Q277
S522	V442	G359	
	T443	P360	
R526	K444	E361	L280
F527	K445	P362	L281
	R446	I363	T282
	G447	R364	L283
V530	Q448	R365	P284
L531	E449	V366	K285
V535	G451	L367	G287
D536	L452	L371	D288
P537	D453		L289
		V381	K290
I540	T459	R382	Q291
	V460	F383	A292
S546	G461	F384	V293
W549	M462	F385	D294
P550	R463	P386	L295
S551	M465	E387	L296
Q552	R466	D388	R297
		T389	P298
H555	R467	P390	
	I468	E391	L301
W558	V469	N392	
K559	C470	S393	Q306
L560	I471	V394	N307
		L395	V308
	N474	R396	P309
			T310
		K400	T311
	Q480		R312
	K481		H313
	V484	Q403	I314
		I405	L315
	M488		L316
	R489	L411	D317
		W412	A318
	I492	W413	A319
			V320
	C495	W416	L321
	A496	L417	G322
	A497	P418	D323
	N498	W419	K324
	G499		R325
	W500	R422	
	E501	L423	R330
	E502	F424	T331
	W503	F425	E332
	E504	C426	P232

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.62Å 140.62Å 132.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10	Depositor
% Data completeness (in resolution range)	94.3 (30.00-3.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.62	Depositor
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.205 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8910	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  > 5	RMSZ	# Z  > 5
1	A	0.33	0/4511	1.02	13/6131 (0.2%)
1	B	0.33	0/4511	1.02	13/6131 (0.2%)
All	All	0.33	0/9022	1.02	26/12262 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	TYR	N-CA-C	7.66	131.68	111.00
1	B	187	TYR	N-CA-C	7.65	131.66	111.00
1	B	7	PHE	N-CA-C	7.37	130.89	111.00
1	A	7	PHE	N-CA-C	7.36	130.87	111.00
1	B	129	ARG	N-CA-C	6.96	129.79	111.00
1	A	129	ARG	N-CA-C	6.96	129.79	111.00
1	A	211	ARG	N-CA-CB	6.56	122.41	110.60
1	B	211	ARG	N-CA-CB	6.53	122.35	110.60
1	B	459	THR	N-CA-C	-5.99	94.84	111.00
1	A	459	THR	N-CA-C	-5.96	94.89	111.00
1	A	518	ASN	N-CA-C	5.60	126.13	111.00
1	B	518	ASN	N-CA-C	5.60	126.12	111.00
1	A	422	HIS	CB-CA-C	5.31	121.03	110.40
1	A	142	VAL	CB-CA-C	-5.31	101.31	111.40
1	B	422	HIS	CB-CA-C	5.31	121.02	110.40
1	B	142	VAL	CB-CA-C	-5.31	101.32	111.40
1	B	314	ILE	CB-CA-C	-5.15	101.30	111.60
1	A	314	ILE	CB-CA-C	-5.14	101.33	111.60
1	A	558	TRP	N-CA-C	5.14	124.87	111.00
1	B	173	GLY	N-CA-C	5.13	125.94	113.10
1	A	173	GLY	N-CA-C	5.12	125.90	113.10
1	B	558	TRP	N-CA-C	5.11	124.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	503	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	B	250	ILE	N-CA-C	5.04	124.62	111.00
1	A	250	ILE	N-CA-C	5.03	124.58	111.00
1	B	503	TYR	CB-CG-CD2	-5.02	117.99	121.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4391	0	4330	278	0
1	B	4391	0	4330	278	0
2	A	53	0	29	6	0
2	B	53	0	29	6	0
3	A	11	0	6	6	0
3	B	11	0	6	7	0
All	All	8910	0	8730	539	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 31.

All (539) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:MET:HE1	1:A:546:SER:H	1.16	1.10
1:A:314:ILE:HD11	1:A:350:ARG:HG3	1.32	1.08
1:B:314:ILE:HD11	1:B:350:ARG:HG3	1.32	1.08
2:A:600:FAD:H8A	2:A:600:FAD:H51A	1.38	1.02
2:B:600:FAD:H51A	2:B:600:FAD:H8A	1.38	1.02
1:B:510:MET:HE1	1:B:546:SER:H	1.25	1.01
1:A:202:VAL:HG12	1:A:262:VAL:HA	1.52	0.92
1:B:202:VAL:HG12	1:B:262:VAL:HA	1.52	0.92
1:A:95:PHE:CE1	1:A:119:VAL:HG23	2.05	0.91
1:B:61:HIS:CD2	1:B:422:HIS:HD1	1.89	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.05	0.90
1:A:61:HIS:CD2	1:A:422:HIS:HD1	1.89	0.89
1:A:314:ILE:HD11	1:A:350:ARG:CG	2.03	0.89
1:A:505:THR:HG21	1:A:513:ILE:HD12	1.55	0.89
1:B:297:ARG:HH21	1:B:432:SER:HA	1.37	0.89
1:B:325:ARG:NH2	1:B:418:PRO:HG3	1.88	0.88
1:A:163:LYS:HE2	1:A:163:LYS:HA	1.56	0.88
1:B:314:ILE:HD11	1:B:350:ARG:CG	2.03	0.88
1:A:297:ARG:HH21	1:A:432:SER:HA	1.37	0.87
1:A:325:ARG:NH2	1:A:418:PRO:HG3	1.88	0.87
1:B:505:THR:HG21	1:B:513:ILE:HD12	1.55	0.86
1:B:163:LYS:HA	1:B:163:LYS:HE2	1.56	0.85
1:A:463:ARG:NH1	1:B:138:ALA:HB3	1.93	0.84
1:A:349:GLY:H	1:A:352:ASN:HD21	1.23	0.84
1:B:349:GLY:H	1:B:352:ASN:HD21	1.23	0.84
1:A:277:GLN:HA	1:A:277:GLN:HE21	1.43	0.83
1:B:28:ILE:HD13	1:B:89:LEU:HD12	1.61	0.83
1:A:9:PRO:HG2	1:A:12:LEU:HD21	1.61	0.83
1:A:80:VAL:HB	1:A:231:GLU:HG3	1.61	0.82
1:B:80:VAL:HB	1:B:231:GLU:HG3	1.61	0.82
1:A:61:HIS:CD2	1:A:422:HIS:H	1.97	0.81
1:A:9:PRO:HG2	1:A:12:LEU:CD2	2.10	0.81
1:B:9:PRO:HG2	1:B:12:LEU:HD21	1.60	0.81
1:B:277:GLN:HE21	1:B:277:GLN:HA	1.43	0.81
1:B:40:ILE:HD11	1:B:57:THR:HG22	1.62	0.81
1:A:16:LEU:HD11	1:A:20:ASP:HB2	1.61	0.81
1:B:61:HIS:CD2	1:B:422:HIS:H	1.97	0.81
1:B:16:LEU:HD11	1:B:20:ASP:HB2	1.60	0.81
1:B:9:PRO:HG2	1:B:12:LEU:CD2	2.10	0.81
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.62	0.80
1:A:259:MET:CE	1:A:535:VAL:HG21	2.12	0.80
1:B:259:MET:CE	1:B:535:VAL:HG21	2.12	0.80
1:B:425:PHE:CE2	1:B:427:PRO:HG3	2.16	0.80
1:A:28:ILE:HD13	1:A:89:LEU:HD12	1.61	0.80
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.62	0.80
1:A:248:PRO:HG3	1:B:257:SER:HB3	1.64	0.80
1:A:510:MET:HE1	1:A:546:SER:N	1.96	0.80
1:A:463:ARG:HH12	1:B:138:ALA:HB3	1.46	0.80
1:A:40:ILE:HD11	1:A:57:THR:HG22	1.62	0.80
1:A:16:LEU:HD11	1:A:20:ASP:CB	2.11	0.80
1:B:16:LEU:HD11	1:B:20:ASP:CB	2.11	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:PHE:CE2	1:A:427:PRO:HG3	2.16	0.79
1:A:359:GLY:O	1:A:364:ARG:HD3	1.84	0.78
1:B:359:GLY:O	1:B:364:ARG:HD3	1.84	0.78
1:A:312:ARG:HH21	1:A:316:LEU:HD21	1.48	0.77
1:B:312:ARG:HH21	1:B:316:LEU:HD21	1.48	0.77
1:A:257:SER:HB3	1:B:248:PRO:HG3	1.66	0.77
1:A:519:TRP:CZ3	1:B:211:ARG:HD3	2.19	0.77
1:B:510:MET:CE	1:B:546:SER:H	1.98	0.77
1:A:489:ARG:HG2	1:A:512:GLN:OE1	1.86	0.76
1:B:489:ARG:HG2	1:B:512:GLN:OE1	1.85	0.76
1:A:138:ALA:HB3	1:B:463:ARG:NH1	2.00	0.76
1:A:138:ALA:HB3	1:B:463:ARG:HH12	1.50	0.75
1:B:349:GLY:N	1:B:352:ASN:HD21	1.84	0.75
1:A:349:GLY:N	1:A:352:ASN:HD21	1.84	0.75
1:B:292:ALA:O	1:B:296:ILE:HG13	1.87	0.74
1:A:510:MET:CE	1:A:546:SER:H	1.98	0.73
1:B:105:ASN:HA	2:B:600:FAD:H5'2	1.71	0.73
1:B:526:ARG:O	1:B:530:VAL:HG23	1.89	0.73
1:A:503:TYR:CZ	1:A:504:ARG:HD3	2.24	0.73
1:A:292:ALA:O	1:A:296:ILE:HG13	1.87	0.73
1:A:105:ASN:HA	2:A:600:FAD:H5'2	1.71	0.73
1:A:519:TRP:CH2	1:B:211:ARG:HD3	2.22	0.73
1:A:526:ARG:O	1:A:530:VAL:HG23	1.88	0.73
1:A:161:ARG:O	1:A:161:ARG:HD3	1.89	0.73
1:B:161:ARG:O	1:B:161:ARG:HD3	1.89	0.73
1:B:503:TYR:CZ	1:B:504:ARG:HD3	2.24	0.72
1:B:206:ASN:H	1:B:206:ASN:HD22	1.37	0.72
1:A:28:ILE:CD1	1:A:89:LEU:HD12	2.20	0.72
1:B:40:ILE:HA	1:B:45:GLN:OE1	1.91	0.71
1:B:9:PRO:HG3	1:B:21:PHE:CZ	2.25	0.71
1:A:40:ILE:HA	1:A:45:GLN:OE1	1.91	0.71
1:A:9:PRO:HG3	1:A:21:PHE:CZ	2.25	0.71
1:A:142:VAL:HG12	1:A:143:GLU:O	1.91	0.71
1:B:28:ILE:CD1	1:B:89:LEU:HD12	2.20	0.70
1:B:142:VAL:HG12	1:B:143:GLU:O	1.91	0.70
1:A:310:THR:HG22	1:A:459:THR:HA	1.74	0.70
1:A:206:ASN:HD22	1:A:206:ASN:H	1.37	0.70
1:B:505:THR:HG21	1:B:513:ILE:CD1	2.22	0.69
1:B:151:LEU:CD2	1:B:166:LEU:HD21	2.22	0.69
1:B:206:ASN:ND2	1:B:206:ASN:H	1.90	0.69
1:A:206:ASN:H	1:A:206:ASN:ND2	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:THR:HG22	1:B:459:THR:HA	1.74	0.69
1:A:151:LEU:CD2	1:A:166:LEU:HD21	2.22	0.69
1:A:337:GLU:N	1:A:337:GLU:OE1	2.26	0.68
1:A:320:VAL:O	1:A:412:LYS:HE2	1.93	0.68
1:B:427:PRO:HA	1:B:501:GLY:O	1.93	0.68
1:A:427:PRO:HA	1:A:501:GLY:O	1.94	0.68
1:A:188:THR:HB	1:A:189:PRO:HD2	1.76	0.68
1:B:362:PRO:O	1:B:366:VAL:HG23	1.94	0.68
1:B:320:VAL:O	1:B:412:LYS:HE2	1.93	0.68
1:A:505:THR:HG21	1:A:513:ILE:CD1	2.23	0.67
1:A:362:PRO:O	1:A:366:VAL:HG23	1.94	0.67
1:A:291:GLN:O	1:A:295:ILE:HG13	1.94	0.67
1:B:337:GLU:N	1:B:337:GLU:OE1	2.26	0.67
1:B:489:ARG:NH2	1:B:508:ALA:O	2.28	0.67
1:B:537:PRO:O	1:B:552:GLN:NE2	2.27	0.67
1:A:489:ARG:NH2	1:A:508:ALA:O	2.28	0.67
1:A:537:PRO:O	1:A:552:GLN:NE2	2.27	0.66
1:A:389:THR:HB	1:A:390:PRO:HD2	1.78	0.66
1:B:188:THR:HB	1:B:189:PRO:HD2	1.76	0.66
1:B:389:THR:HB	1:B:390:PRO:HD2	1.78	0.66
1:B:349:GLY:H	1:B:352:ASN:ND2	1.94	0.66
1:B:291:GLN:O	1:B:295:ILE:HG13	1.94	0.66
1:A:505:THR:CG2	1:A:513:ILE:HD12	2.26	0.66
1:B:445:LYS:NZ	1:B:449:GLU:OE2	2.29	0.65
1:A:463:ARG:HH12	1:B:138:ALA:CB	2.10	0.65
1:A:247:GLY:O	1:B:183:ARG:NH2	2.20	0.65
1:B:286:ASP:HB2	1:B:350:ARG:HD3	1.78	0.65
1:A:161:ARG:NH2	1:A:403:GLN:O	2.30	0.65
1:B:161:ARG:NH2	1:B:403:GLN:O	2.30	0.65
1:A:211:ARG:HD3	1:B:519:TRP:CH2	2.32	0.64
1:A:259:MET:HE3	1:A:535:VAL:HG21	1.77	0.64
1:A:211:ARG:HD3	1:B:519:TRP:CZ3	2.33	0.64
1:B:151:LEU:HG	1:B:166:LEU:HD21	1.79	0.64
1:A:349:GLY:H	1:A:352:ASN:ND2	1.94	0.64
1:A:445:LYS:NZ	1:A:449:GLU:OE2	2.29	0.64
1:A:91:ASN:ND2	1:A:540:ILE:HG13	2.13	0.64
1:A:40:ILE:HD11	1:A:57:THR:CG2	2.28	0.63
1:A:314:ILE:CD1	1:A:350:ARG:HG3	2.20	0.63
1:B:163:LYS:O	1:B:164:LEU:HD23	1.97	0.63
1:A:286:ASP:HB2	1:A:350:ARG:HD3	1.78	0.63
1:B:259:MET:HE3	1:B:535:VAL:HG21	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HG	1:A:166:LEU:HD21	1.79	0.63
1:A:163:LYS:O	1:A:164:LEU:HD23	1.97	0.63
1:B:40:ILE:HD11	1:B:57:THR:CG2	2.28	0.63
1:B:216:ALA:O	1:B:218:PRO:HD3	1.99	0.63
1:B:510:MET:HE1	1:B:546:SER:N	2.05	0.63
1:B:505:THR:CG2	1:B:513:ILE:HD12	2.26	0.63
1:B:259:MET:HE1	1:B:535:VAL:HG21	1.81	0.63
1:A:10:LEU:O	1:A:10:LEU:HD23	1.99	0.63
1:B:91:ASN:ND2	1:B:540:ILE:HG13	2.13	0.63
1:A:495:CYS:HB3	1:A:500:TRP:HB2	1.81	0.62
1:A:216:ALA:O	1:A:218:PRO:HD3	1.99	0.62
1:A:444:LYS:O	1:A:448:GLN:HG2	1.99	0.62
1:B:314:ILE:HD11	1:B:350:ARG:HA	1.81	0.62
1:B:444:LYS:O	1:B:448:GLN:HG2	1.99	0.62
1:B:277:GLN:HE21	1:B:277:GLN:CA	2.13	0.62
1:B:425:PHE:HB3	1:B:469:VAL:HB	1.82	0.62
1:B:194:TRP:O	1:B:197:HIS:HD2	1.82	0.61
1:A:194:TRP:O	1:A:197:HIS:HD2	1.82	0.61
2:B:600:FAD:N5	3:B:601:NCR:H73	2.15	0.61
1:B:277:GLN:NE2	1:B:277:GLN:HA	2.14	0.61
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.82	0.61
1:B:35:GLU:H	1:B:35:GLU:CD	2.04	0.61
1:A:468:ILE:HD13	3:A:601:NCR:C3	2.30	0.61
1:B:497:ALA:C	1:B:498:ASN:HD22	2.03	0.61
1:A:61:HIS:HD2	1:A:422:HIS:HD1	1.46	0.61
1:B:10:LEU:HD23	1:B:10:LEU:O	1.99	0.61
2:A:600:FAD:N5	3:A:601:NCR:H73	2.15	0.61
1:A:425:PHE:HB3	1:A:469:VAL:HB	1.82	0.61
1:A:183:ARG:NH2	1:B:247:GLY:O	2.28	0.61
1:A:314:ILE:HD11	1:A:350:ARG:HA	1.81	0.61
1:B:468:ILE:HD13	3:B:601:NCR:C3	2.30	0.61
1:B:495:CYS:HB3	1:B:500:TRP:HB2	1.81	0.60
1:A:105:ASN:HD21	1:A:504:ARG:HH21	1.49	0.60
1:A:35:GLU:H	1:A:35:GLU:CD	2.03	0.60
1:B:314:ILE:CD1	1:B:350:ARG:HA	2.31	0.60
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.82	0.60
1:A:277:GLN:HE21	1:A:277:GLN:CA	2.13	0.60
1:B:309:PRO:HD2	1:B:460:VAL:HB	1.82	0.60
1:A:314:ILE:CD1	1:A:350:ARG:HA	2.32	0.60
1:A:58:HIS:O	1:A:60:PRO:HD3	2.02	0.60
1:A:259:MET:HE1	1:A:535:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:HIS:O	1:B:60:PRO:HD3	2.02	0.59
1:B:229:LYS:O	1:B:233:GLN:HG3	2.02	0.59
1:A:309:PRO:HD2	1:A:460:VAL:HB	1.82	0.59
1:A:497:ALA:C	1:A:498:ASN:HD22	2.03	0.59
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.84	0.59
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.84	0.59
1:A:277:GLN:NE2	1:A:277:GLN:HA	2.14	0.59
1:B:105:ASN:HD21	1:B:504:ARG:HH21	1.50	0.59
1:A:82:ASP:O	1:A:86:ILE:HG13	2.03	0.59
1:B:12:LEU:HB3	1:B:13:PRO:HD2	1.84	0.59
1:A:363:ILE:HD12	1:B:363:ILE:HD12	1.85	0.58
1:A:224:GLU:CD	1:A:224:GLU:H	2.07	0.58
1:A:229:LYS:O	1:A:233:GLN:HG3	2.02	0.58
1:A:12:LEU:HB3	1:A:13:PRO:CD	2.33	0.58
1:B:434:GLU:HA	1:B:434:GLU:OE1	2.03	0.58
1:A:434:GLU:OE1	1:A:434:GLU:HA	2.03	0.58
1:A:325:ARG:HH21	1:A:418:PRO:HG3	1.69	0.58
1:A:351:TRP:O	1:A:352:ASN:ND2	2.36	0.58
1:A:301:LEU:HB3	1:B:271:PRO:HG3	1.85	0.58
1:B:28:ILE:HD13	1:B:89:LEU:CD1	2.33	0.58
1:B:224:GLU:H	1:B:224:GLU:CD	2.07	0.58
1:B:82:ASP:O	1:B:86:ILE:HG13	2.03	0.58
1:B:351:TRP:O	1:B:352:ASN:ND2	2.36	0.58
1:A:138:ALA:CB	1:B:463:ARG:HH12	2.15	0.57
1:B:35:GLU:OE1	1:B:35:GLU:N	2.29	0.57
1:A:214:MET:HB2	1:A:239:ALA:HA	1.87	0.57
1:B:332:GLU:HB3	1:B:333:PRO:HD2	1.87	0.57
1:B:12:LEU:HB3	1:B:13:PRO:CD	2.33	0.57
1:A:12:LEU:HB3	1:A:13:PRO:HD2	1.84	0.57
1:A:332:GLU:HB3	1:A:333:PRO:HD2	1.87	0.57
1:A:257:SER:CB	1:B:248:PRO:HG3	2.34	0.57
1:B:128:ASN:HD22	1:B:145:GLY:HA3	1.70	0.57
1:B:343:ALA:HB1	1:B:348:LEU:O	2.04	0.57
1:A:163:LYS:HA	1:A:163:LYS:CE	2.33	0.56
1:B:163:LYS:CA	1:B:163:LYS:HE2	2.34	0.56
1:A:128:ASN:HD22	1:A:145:GLY:HA3	1.70	0.56
1:B:61:HIS:HD2	1:B:422:HIS:HD1	1.45	0.56
1:A:163:LYS:HE2	1:A:163:LYS:CA	2.34	0.56
1:B:151:LEU:CG	1:B:166:LEU:HD21	2.35	0.56
1:A:151:LEU:CG	1:A:166:LEU:HD21	2.35	0.56
1:B:446:ARG:HD3	1:B:449:GLU:OE1	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASN:O	1:A:474:ASN:HA	2.06	0.56
1:B:16:LEU:CD1	1:B:20:ASP:HB2	2.34	0.56
1:A:46:ILE:HG22	1:A:46:ILE:O	2.06	0.56
1:B:214:MET:HB2	1:B:239:ALA:HA	1.86	0.56
1:A:343:ALA:HB1	1:A:348:LEU:O	2.04	0.56
1:A:446:ARG:HD3	1:A:449:GLU:OE1	2.06	0.56
1:A:248:PRO:HG3	1:B:257:SER:CB	2.35	0.56
1:A:35:GLU:OE1	1:A:35:GLU:N	2.29	0.56
1:B:177:LEU:HD12	1:B:177:LEU:C	2.27	0.56
1:B:46:ILE:O	1:B:46:ILE:HG22	2.06	0.56
1:B:314:ILE:CD1	1:B:350:ARG:HG3	2.20	0.55
1:B:419:ASN:O	1:B:474:ASN:HA	2.06	0.55
1:B:142:VAL:HG13	1:B:146:VAL:CG2	2.37	0.55
1:A:555:HIS:CD2	1:A:559:LYS:HE3	2.41	0.55
1:A:318:ALA:O	1:A:322:GLY:N	2.38	0.55
1:B:325:ARG:HH21	1:B:418:PRO:HG3	1.69	0.55
1:B:555:HIS:CD2	1:B:559:LYS:HE3	2.41	0.55
1:A:94:SER:HA	1:A:540:ILE:HD11	1.88	0.55
1:B:555:HIS:HB3	1:B:559:LYS:HE3	1.88	0.55
1:A:37:VAL:HG12	1:A:38:GLU:N	2.21	0.55
1:A:555:HIS:HB3	1:A:559:LYS:HE3	1.88	0.55
1:A:16:LEU:CD1	1:A:20:ASP:HB2	2.34	0.55
1:A:312:ARG:HH11	1:A:394:VAL:HG11	1.72	0.55
1:B:312:ARG:HH11	1:B:394:VAL:HG11	1.72	0.55
1:A:142:VAL:HG13	1:A:146:VAL:CG2	2.37	0.55
1:A:177:LEU:C	1:A:177:LEU:HD12	2.26	0.55
1:B:37:VAL:HG12	1:B:38:GLU:N	2.21	0.55
1:A:286:ASP:CA	1:A:350:ARG:HD3	2.37	0.55
1:B:163:LYS:HA	1:B:163:LYS:CE	2.34	0.55
1:A:552:GLN:OE1	1:A:552:GLN:N	2.27	0.55
1:A:391:GLU:HA	1:A:396:ARG:HD2	1.89	0.55
1:B:471:ILE:N	1:B:471:ILE:HD12	2.22	0.55
1:A:459:THR:OG1	1:A:466:HIS:HB2	2.07	0.55
1:B:552:GLN:OE1	1:B:552:GLN:N	2.27	0.55
1:B:142:VAL:HG13	1:B:146:VAL:HG21	1.89	0.54
1:A:285:LYS:HG2	1:A:287:GLY:H	1.72	0.54
1:B:286:ASP:HB2	1:B:350:ARG:CZ	2.37	0.54
1:B:286:ASP:CA	1:B:350:ARG:HD3	2.37	0.54
1:B:459:THR:OG1	1:B:466:HIS:HB2	2.07	0.54
1:B:318:ALA:O	1:B:322:GLY:N	2.38	0.54
1:A:314:ILE:HG12	1:A:350:ARG:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ILE:HD13	1:A:89:LEU:CD1	2.33	0.54
1:A:286:ASP:HB2	1:A:350:ARG:CZ	2.37	0.54
1:B:94:SER:HA	1:B:540:ILE:HD11	1.88	0.54
1:A:471:ILE:HD12	1:A:471:ILE:N	2.22	0.54
1:B:314:ILE:HG12	1:B:350:ARG:HA	1.90	0.54
1:B:391:GLU:HA	1:B:396:ARG:HD2	1.89	0.54
1:B:281:ILE:HG23	1:B:381:VAL:CG2	2.38	0.54
1:B:188:THR:HB	1:B:189:PRO:CD	2.38	0.54
1:B:413:TRP:CZ2	2:B:600:FAD:HM72	2.43	0.53
1:A:418:PRO:HB2	1:A:474:ASN:ND2	2.23	0.53
1:A:142:VAL:HG13	1:A:146:VAL:HG21	1.89	0.53
1:A:16:LEU:HD11	1:A:20:ASP:HB3	1.91	0.53
1:A:281:ILE:HG23	1:A:381:VAL:CG2	2.38	0.53
1:A:271:PRO:HG3	1:B:301:LEU:HB3	1.89	0.53
1:B:286:ASP:N	1:B:350:ARG:HD3	2.24	0.53
1:B:418:PRO:HB2	1:B:474:ASN:ND2	2.23	0.53
1:B:8:ARG:HG3	1:B:8:ARG:O	2.08	0.53
1:B:361:GLU:HB3	1:B:362:PRO:HD3	1.91	0.53
1:A:102:ILE:HB	2:A:600:FAD:O2P	2.08	0.53
1:A:413:TRP:CZ2	2:A:600:FAD:HM72	2.43	0.53
1:B:504:ARG:O	1:B:505:THR:HG23	2.08	0.53
1:A:361:GLU:HB3	1:A:362:PRO:HD3	1.91	0.53
1:A:286:ASP:N	1:A:350:ARG:HD3	2.24	0.53
1:A:63:VAL:HG23	1:A:64:MET:N	2.23	0.53
1:A:188:THR:HB	1:A:189:PRO:CD	2.38	0.53
1:B:285:LYS:HG2	1:B:287:GLY:H	1.72	0.53
1:B:63:VAL:HG23	1:B:64:MET:N	2.23	0.53
1:A:498:ASN:O	1:B:237:LYS:HE2	2.08	0.52
1:A:177:LEU:HD12	1:A:178:GLY:N	2.24	0.52
1:B:367:LEU:O	1:B:371:ILE:HG13	2.09	0.52
1:B:102:ILE:HB	2:B:600:FAD:O2P	2.09	0.52
1:A:504:ARG:O	1:A:505:THR:HG23	2.08	0.52
1:B:171:LEU:HD11	1:B:411:LEU:HD23	1.92	0.52
1:B:312:ARG:HH21	1:B:316:LEU:CD2	2.22	0.52
1:B:51:TYR:O	1:B:104:ARG:HD3	2.10	0.52
1:A:51:TYR:O	1:A:104:ARG:HD3	2.10	0.52
1:A:225:THR:O	1:A:228:LEU:HD13	2.10	0.52
1:B:225:THR:O	1:B:228:LEU:HD13	2.10	0.52
1:A:171:LEU:HD11	1:A:411:LEU:HD23	1.92	0.52
1:A:312:ARG:HH21	1:A:316:LEU:CD2	2.22	0.51
1:B:197:HIS:HE1	1:B:251:ASP:OD2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ILE:CG1	1:B:350:ARG:HA	2.40	0.51
1:B:177:LEU:HD12	1:B:178:GLY:N	2.25	0.51
1:B:52:MET:C	1:B:53:LYS:HG3	2.29	0.51
1:A:185:VAL:HG12	1:A:186:GLY:N	2.25	0.51
1:B:185:VAL:HG12	1:B:186:GLY:N	2.25	0.51
1:A:52:MET:C	1:A:53:LYS:HG3	2.29	0.51
1:A:197:HIS:HE1	1:A:251:ASP:OD2	1.94	0.51
1:B:489:ARG:HH22	1:B:560:LEU:HD22	1.76	0.51
1:B:281:ILE:HG12	1:B:383:PHE:CD1	2.46	0.51
1:A:8:ARG:O	1:A:8:ARG:HG3	2.08	0.51
1:A:445:LYS:HZ2	1:A:449:GLU:CD	2.14	0.51
1:A:314:ILE:CG1	1:A:350:ARG:HA	2.40	0.51
1:A:489:ARG:HH22	1:A:560:LEU:HD22	1.76	0.51
1:B:100:ILE:HG13	1:B:100:ILE:O	2.10	0.51
1:A:281:ILE:HG12	1:A:383:PHE:CD1	2.46	0.50
1:A:202:VAL:HG12	1:A:262:VAL:CA	2.35	0.50
1:B:144:PRO:HD3	1:B:263:THR:O	2.11	0.50
1:B:67:ASP:O	1:B:70:LEU:HD22	2.11	0.50
1:A:367:LEU:O	1:A:371:ILE:HG13	2.09	0.50
1:B:297:ARG:HH21	1:B:432:SER:CA	2.19	0.50
1:B:301:LEU:HD23	1:B:462:MET:HE3	1.92	0.50
1:A:67:ASP:O	1:A:70:LEU:HD22	2.11	0.50
1:B:201:GLU:OE2	1:B:264:LYS:HE2	2.12	0.50
1:B:400:LYS:HB3	1:B:405:ILE:HB	1.92	0.50
1:B:21:PHE:CZ	1:B:25:ILE:HG13	2.47	0.50
1:A:128:ASN:HA	1:A:145:GLY:HA3	1.94	0.50
1:A:400:LYS:HB3	1:A:405:ILE:HB	1.92	0.50
1:A:144:PRO:HD3	1:A:263:THR:O	2.11	0.50
1:A:286:ASP:CB	1:A:350:ARG:HD3	2.42	0.50
1:A:390:PRO:HB2	1:A:392:ASN:OD1	2.11	0.50
1:A:185:VAL:HB	3:A:601:NCR:O1N	2.12	0.50
1:A:527:PHE:CE2	1:A:531:LEU:HD11	2.47	0.50
1:B:527:PHE:CE2	1:B:531:LEU:HD11	2.47	0.50
1:B:108:TYR:OH	3:B:601:NCR:H5	2.12	0.50
1:B:16:LEU:HD11	1:B:20:ASP:HB3	1.91	0.50
1:A:289:LEU:HD22	1:A:351:TRP:CZ2	2.46	0.50
1:B:289:LEU:HD22	1:B:351:TRP:CZ2	2.46	0.50
1:A:488:MET:O	1:A:492:ILE:HG13	2.12	0.50
1:B:63:VAL:HG23	1:B:64:MET:HG3	1.94	0.50
1:A:100:ILE:HG13	1:A:100:ILE:O	2.10	0.50
1:A:519:TRP:CH2	1:B:211:ARG:CD	2.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:MET:O	1:B:492:ILE:HG13	2.12	0.49
1:A:6:GLU:CB	1:A:39:VAL:HG21	2.42	0.49
1:B:128:ASN:HA	1:B:145:GLY:HA3	1.94	0.49
1:A:187:TYR:O	1:A:307:ASN:HB2	2.13	0.49
1:B:6:GLU:CB	1:B:39:VAL:HG21	2.42	0.49
1:B:185:VAL:HB	3:B:601:NCR:O1N	2.12	0.49
1:A:108:TYR:OH	3:A:601:NCR:H5	2.12	0.49
1:B:390:PRO:HB2	1:B:392:ASN:OD1	2.12	0.49
1:A:21:PHE:CZ	1:A:25:ILE:HG13	2.47	0.49
1:A:201:GLU:OE2	1:A:264:LYS:HE2	2.12	0.49
1:A:416:TRP:CD1	1:A:417:LEU:CD1	2.96	0.49
1:A:63:VAL:HG23	1:A:64:MET:HG3	1.94	0.49
1:A:238:ILE:O	1:A:238:ILE:HG22	2.13	0.49
1:B:238:ILE:HG22	1:B:238:ILE:O	2.13	0.49
1:B:187:TYR:O	1:B:307:ASN:HB2	2.13	0.48
1:B:416:TRP:CD1	1:B:417:LEU:CD1	2.96	0.48
1:A:416:TRP:HD1	1:A:417:LEU:CD1	2.26	0.48
1:B:211:ARG:HG2	1:B:235:TRP:CH2	2.49	0.48
1:B:289:LEU:O	1:B:293:VAL:HG23	2.13	0.48
1:B:286:ASP:CB	1:B:350:ARG:HD3	2.42	0.48
1:B:416:TRP:HD1	1:B:417:LEU:CD1	2.26	0.48
1:A:90:ALA:O	1:A:94:SER:N	2.47	0.48
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.96	0.48
1:A:289:LEU:O	1:A:293:VAL:HG23	2.14	0.48
1:A:280:LEU:HB2	1:A:395:LEU:HD22	1.96	0.48
1:A:196:MET:HE3	1:A:268:TRP:HE3	1.78	0.48
1:B:468:ILE:CD1	3:B:601:NCR:C3	2.92	0.48
1:B:417:LEU:HB3	1:B:418:PRO:HD2	1.96	0.48
2:A:600:FAD:C8A	2:A:600:FAD:H51A	2.28	0.47
1:B:286:ASP:HB2	1:B:350:ARG:CD	2.43	0.47
1:A:91:ASN:HD22	1:A:540:ILE:HG13	1.79	0.47
1:A:468:ILE:CD1	3:A:601:NCR:C3	2.92	0.47
1:A:211:ARG:HG2	1:A:235:TRP:CH2	2.48	0.47
1:B:132:GLU:HG2	1:B:133:VAL:N	2.30	0.47
1:A:312:ARG:NH1	1:A:394:VAL:HG11	2.30	0.47
1:B:445:LYS:HZ2	1:B:449:GLU:CD	2.18	0.47
1:A:177:LEU:CB	1:A:265:ILE:HG21	2.44	0.47
1:A:297:ARG:N	1:A:298:PRO:HD2	2.29	0.47
1:B:275:GLY:HA3	1:B:359:GLY:O	2.15	0.47
1:A:312:ARG:NH2	1:A:316:LEU:HD21	2.24	0.47
1:A:333:PRO:HA	1:A:453:ASP:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG13	1:A:118:SER:OG	2.15	0.47
1:B:333:PRO:HA	1:B:453:ASP:OD1	2.15	0.47
1:B:177:LEU:CB	1:B:265:ILE:HG21	2.44	0.47
1:A:285:LYS:HG2	1:A:286:ASP:N	2.30	0.47
1:B:91:ASN:HD22	1:B:540:ILE:HG13	1.79	0.47
1:A:301:LEU:HD23	1:A:462:MET:HE3	1.97	0.46
1:B:9:PRO:HG2	1:B:12:LEU:HD23	1.94	0.46
1:A:439:GLN:O	1:A:442:VAL:HG12	2.16	0.46
1:A:9:PRO:CG	1:A:12:LEU:HD21	2.41	0.46
1:B:429:ALA:HB2	1:B:439:GLN:NE2	2.30	0.46
1:B:297:ARG:N	1:B:298:PRO:HD2	2.29	0.46
1:B:306:GLN:NE2	1:B:367:LEU:CD1	2.79	0.46
1:B:439:GLN:O	1:B:442:VAL:HG12	2.15	0.46
1:B:225:THR:C	1:B:228:LEU:HD13	2.36	0.46
1:A:306:GLN:NE2	1:A:367:LEU:CD1	2.79	0.46
1:A:429:ALA:HB2	1:A:439:GLN:NE2	2.30	0.46
1:B:312:ARG:NH1	1:B:394:VAL:HG11	2.30	0.46
1:A:132:GLU:HG2	1:A:133:VAL:N	2.30	0.46
1:B:189:PRO:HD3	1:B:307:ASN:HB3	1.98	0.46
1:B:115:VAL:HG13	1:B:118:SER:OG	2.15	0.46
1:A:469:VAL:HG12	1:A:471:ILE:HD12	1.98	0.46
1:A:550:PRO:HB2	1:A:552:GLN:OE1	2.16	0.46
1:A:286:ASP:HB2	1:A:350:ARG:CD	2.43	0.46
1:A:333:PRO:HD3	1:A:451:GLY:O	2.16	0.46
1:A:225:THR:C	1:A:228:LEU:HD13	2.36	0.46
1:A:9:PRO:HG2	1:A:12:LEU:HD23	1.94	0.45
1:A:231:GLU:OE1	1:A:231:GLU:N	2.37	0.45
1:A:189:PRO:HD3	1:A:307:ASN:HB3	1.97	0.45
1:B:333:PRO:HD3	1:B:451:GLY:O	2.16	0.45
1:B:90:ALA:O	1:B:94:SER:N	2.47	0.45
1:B:280:LEU:HB2	1:B:395:LEU:HD22	1.96	0.45
1:A:275:GLY:HA3	1:A:359:GLY:O	2.15	0.45
1:B:550:PRO:HB2	1:B:552:GLN:OE1	2.16	0.45
1:A:185:VAL:CG1	1:A:186:GLY:N	2.79	0.45
1:B:312:ARG:NH2	1:B:316:LEU:HD21	2.24	0.45
1:B:63:VAL:CG2	1:B:64:MET:N	2.79	0.45
1:B:285:LYS:HG2	1:B:286:ASP:N	2.30	0.45
1:A:198:SER:O	1:A:240:HIS:HD2	2.00	0.45
1:B:198:SER:O	1:B:240:HIS:HD2	2.00	0.45
1:B:185:VAL:CG1	1:B:186:GLY:N	2.79	0.45
1:A:61:HIS:CD2	1:A:422:HIS:N	2.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:LEU:HD21	1:B:488:MET:HG3	1.98	0.45
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.77	0.45
1:A:503:TYR:OH	1:A:504:ARG:HD3	2.17	0.45
1:B:142:VAL:HG12	1:B:143:GLU:N	2.32	0.45
1:A:9:PRO:HG3	1:A:21:PHE:CE1	2.51	0.45
1:A:312:ARG:NH2	1:A:316:LEU:CD2	2.80	0.45
1:B:231:GLU:OE1	1:B:231:GLU:N	2.37	0.44
1:B:9:PRO:HG3	1:B:21:PHE:CE1	2.51	0.44
1:A:206:ASN:HD22	1:A:206:ASN:N	2.10	0.44
1:B:47:VAL:HG23	1:B:47:VAL:O	2.18	0.44
1:B:312:ARG:NH2	1:B:316:LEU:CD2	2.80	0.44
1:A:47:VAL:O	1:A:47:VAL:HG23	2.18	0.44
1:B:59:ASP:OD2	1:B:62:HIS:HA	2.17	0.44
1:A:102:ILE:HA	1:A:102:ILE:HD13	1.84	0.44
1:A:61:HIS:CD2	1:A:422:HIS:ND1	2.73	0.44
1:A:283:LEU:HD13	1:A:292:ALA:HB2	1.98	0.44
1:B:177:LEU:HB2	1:B:265:ILE:HG21	1.99	0.44
1:A:423:LEU:HD21	1:A:488:MET:HG3	1.98	0.44
1:B:283:LEU:HD13	1:B:292:ALA:HB2	1.98	0.44
1:A:63:VAL:CG2	1:A:64:MET:N	2.80	0.44
1:A:59:ASP:OD2	1:A:62:HIS:HA	2.17	0.44
1:B:480:GLN:O	1:B:484:VAL:HG23	2.17	0.44
2:B:600:FAD:H51A	2:B:600:FAD:C8A	2.28	0.44
1:B:277:GLN:OE1	1:B:385:PHE:HD2	2.01	0.44
1:B:469:VAL:HG12	1:B:471:ILE:HD12	1.98	0.44
1:B:503:TYR:OH	1:B:504:ARG:HD3	2.17	0.44
1:A:142:VAL:HG12	1:A:143:GLU:N	2.32	0.43
1:A:552:GLN:CD	1:A:552:GLN:H	2.17	0.43
1:B:8:ARG:HA	1:B:9:PRO:HD3	1.75	0.43
1:B:58:HIS:HA	1:B:112:ALA:HB2	1.99	0.43
1:A:63:VAL:O	1:A:481:LYS:HD3	2.18	0.43
1:B:9:PRO:CG	1:B:12:LEU:HD21	2.41	0.43
1:A:58:HIS:HA	1:A:112:ALA:HB2	1.99	0.43
1:A:177:LEU:HB2	1:A:265:ILE:HG21	1.99	0.43
1:A:480:GLN:O	1:A:484:VAL:HG23	2.17	0.43
1:B:552:GLN:CD	1:B:552:GLN:H	2.17	0.43
1:A:349:GLY:CA	1:A:352:ASN:HD21	2.31	0.43
1:A:253:LEU:O	1:A:257:SER:OG	2.30	0.43
1:A:555:HIS:HD2	1:A:559:LYS:HE3	1.83	0.43
1:A:141:VAL:C	1:A:142:VAL:HG23	2.39	0.43
1:B:555:HIS:HD2	1:B:559:LYS:HE3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:VAL:HG11	1:B:423:LEU:HD22	2.01	0.43
1:A:277:GLN:OE1	1:A:385:PHE:HD2	2.01	0.43
1:B:522:SER:O	1:B:526:ARG:HG2	2.19	0.43
1:B:503:TYR:CZ	1:B:504:ARG:CD	2.99	0.43
1:B:63:VAL:O	1:B:481:LYS:HD3	2.18	0.43
1:A:426:SER:O	1:A:502:GLU:HA	2.19	0.43
1:A:142:VAL:CG1	1:A:143:GLU:N	2.82	0.42
1:B:426:SER:O	1:B:502:GLU:HA	2.19	0.42
1:A:382:LYS:HE3	1:A:382:LYS:HB3	1.85	0.42
1:A:503:TYR:CZ	1:A:504:ARG:CD	2.99	0.42
1:B:61:HIS:CD2	1:B:422:HIS:N	2.77	0.42
1:A:237:LYS:HE2	1:B:498:ASN:O	2.19	0.42
1:A:114:ARG:NH1	1:A:549:TRP:HZ2	2.18	0.42
1:A:40:ILE:CD1	1:A:57:THR:CG2	2.98	0.42
1:A:142:VAL:CG1	1:A:146:VAL:HB	2.49	0.42
1:B:202:VAL:HG12	1:B:262:VAL:CA	2.34	0.42
1:B:323:ASP:OD1	1:B:324:LYS:N	2.53	0.42
1:A:323:ASP:OD1	1:A:324:LYS:N	2.53	0.42
1:B:142:VAL:CG1	1:B:146:VAL:HB	2.49	0.42
1:A:522:SER:O	1:A:526:ARG:HG2	2.19	0.42
1:A:281:ILE:HG12	1:A:383:PHE:HD1	1.84	0.42
1:B:393:SER:OG	1:B:396:ARG:HG3	2.19	0.42
1:A:97:LEU:HA	1:A:97:LEU:HD23	1.78	0.42
1:A:285:LYS:CG	1:A:286:ASP:N	2.83	0.42
1:B:349:GLY:CA	1:B:352:ASN:HD21	2.31	0.42
1:A:393:SER:OG	1:A:396:ARG:HG3	2.19	0.42
1:A:319:ALA:HB3	1:A:413:TRP:HB2	2.02	0.41
1:B:319:ALA:HB3	1:B:413:TRP:HB2	2.02	0.41
1:B:61:HIS:CD2	1:B:422:HIS:ND1	2.73	0.41
1:A:63:VAL:HG11	1:A:423:LEU:HD22	2.01	0.41
1:B:503:TYR:OH	3:B:601:NCR:O4	2.24	0.41
1:B:141:VAL:C	1:B:142:VAL:HG23	2.39	0.41
1:A:242:PHE:HA	1:A:243:PRO:HD3	1.65	0.41
1:B:418:PRO:HB2	1:B:474:ASN:HD22	1.86	0.41
1:A:425:PHE:CE2	1:A:427:PRO:CG	2.97	0.41
1:B:324:LYS:HB2	1:B:416:TRP:CE2	2.56	0.41
1:A:324:LYS:HB2	1:A:416:TRP:CE2	2.56	0.41
1:B:206:ASN:N	1:B:206:ASN:HD22	2.10	0.41
1:A:330:ARG:HG2	1:A:332:GLU:H	1.85	0.41
1:B:177:LEU:HD23	1:B:265:ILE:HG22	2.02	0.41
1:B:168:VAL:HB	1:B:169:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:MET:HE3	1:B:268:TRP:HE3	1.85	0.41
1:B:319:ALA:CB	1:B:413:TRP:HB2	2.51	0.41
1:B:201:GLU:HG2	1:B:263:THR:OG1	2.21	0.41
1:A:416:TRP:CD1	1:A:417:LEU:HD12	2.55	0.41
1:B:171:LEU:CD1	1:B:411:LEU:CD2	2.99	0.41
1:A:319:ALA:CB	1:A:413:TRP:HB2	2.51	0.41
1:A:424:PHE:CZ	3:A:601:NCR:H6	2.56	0.41
1:B:297:ARG:HA	1:B:431:VAL:HG11	2.03	0.41
1:B:416:TRP:CD1	1:B:417:LEU:HD12	2.55	0.41
1:A:297:ARG:HH21	1:A:432:SER:CA	2.19	0.41
1:B:40:ILE:CD1	1:B:57:THR:CG2	2.98	0.41
1:B:281:ILE:HG12	1:B:383:PHE:HD1	1.84	0.41
1:A:201:GLU:CD	1:A:264:LYS:HE2	2.41	0.41
1:B:428:ILE:HG22	1:B:429:ALA:N	2.36	0.41
1:B:114:ARG:NH1	1:B:549:TRP:HZ2	2.18	0.41
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.77	0.41
1:A:168:VAL:HB	1:A:169:PRO:HD2	2.03	0.41
1:A:177:LEU:HD23	1:A:265:ILE:HG22	2.02	0.41
1:B:272:ASN:OD1	1:B:273:PRO:HD2	2.20	0.41
1:B:285:LYS:CG	1:B:286:ASP:N	2.83	0.40
1:A:206:ASN:N	1:A:206:ASN:ND2	2.62	0.40
1:B:217:LEU:HA	1:B:217:LEU:HD12	1.69	0.40
1:A:24:PHE:HE2	1:A:119:VAL:HG21	1.86	0.40
1:A:270:MET:HA	1:A:271:PRO:HD2	1.77	0.40
1:B:201:GLU:CD	1:B:264:LYS:HE2	2.41	0.40
1:A:201:GLU:HG2	1:A:263:THR:OG1	2.21	0.40
1:A:272:ASN:OD1	1:A:273:PRO:HD2	2.20	0.40
1:B:284:PRO:HG2	1:B:288:ASP:OD2	2.22	0.40
1:B:424:PHE:CZ	3:B:601:NCR:H6	2.56	0.40
1:B:297:ARG:N	1:B:298:PRO:CD	2.85	0.40
1:A:171:LEU:CD1	1:A:411:LEU:CD2	2.99	0.40
1:A:171:LEU:HD13	1:A:411:LEU:HD21	2.03	0.40
1:A:242:PHE:HB2	1:B:464:GLU:HG2	2.03	0.40
1:B:330:ARG:HG2	1:B:332:GLU:H	1.85	0.40
1:B:171:LEU:HD13	1:B:411:LEU:HD21	2.03	0.40
1:B:242:PHE:HA	1:B:243:PRO:HD3	1.65	0.40
1:B:142:VAL:CG1	1:B:143:GLU:N	2.82	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	553/560 (99%)	510 (92%)	36 (6%)	7 (1%)	15	50
1	B	553/560 (99%)	509 (92%)	37 (7%)	7 (1%)	15	50
All	All	1106/1120 (99%)	1019 (92%)	73 (7%)	14 (1%)	15	50

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ILE
1	A	49	GLY
1	A	170	ASP
1	A	418	PRO
1	B	49	GLY
1	B	170	ASP
1	B	418	PRO
1	A	391	GLU
1	B	46	ILE
1	B	391	GLU
1	A	388	ASP
1	B	388	ASP
1	A	105	ASN
1	B	105	ASN

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	475/482 (98%)	462 (97%)	13 (3%)	52	82
1	B	475/482 (98%)	462 (97%)	13 (3%)	52	82
All	All	950/964 (98%)	924 (97%)	26 (3%)	52	82

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	105	ASN
1	A	114	ARG
1	A	128	ASN
1	A	149	HIS
1	A	177	LEU
1	A	206	ASN
1	A	211	ARG
1	A	224	GLU
1	A	277	GLN
1	A	391	GLU
1	A	422	HIS
1	A	503	TYR
1	B	61	HIS
1	B	105	ASN
1	B	114	ARG
1	B	128	ASN
1	B	149	HIS
1	B	177	LEU
1	B	206	ASN
1	B	211	ARG
1	B	224	GLU
1	B	277	GLN
1	B	391	GLU
1	B	422	HIS
1	B	503	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	84	GLN
1	A	91	ASN
1	A	105	ASN

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Mol	Chain	Res	Type
1	A	128	ASN
1	A	152	HIS
1	A	197	HIS
1	A	206	ASN
1	A	240	HIS
1	A	277	GLN
1	A	306	GLN
1	A	352	ASN
1	A	485	GLN
1	A	498	ASN
1	A	520	ASN
1	B	61	HIS
1	B	84	GLN
1	B	91	ASN
1	B	105	ASN
1	B	128	ASN
1	B	152	HIS
1	B	197	HIS
1	B	206	ASN
1	B	240	HIS
1	B	277	GLN
1	B	306	GLN
1	B	352	ASN
1	B	485	GLN
1	B	498	ASN
1	B	520	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	FAD	A	600	1	48,58,58	0.85	1 (2%)	54,89,89	1.47	3 (5%)
3	NCR	A	601	-	8,11,11	0.69	0	8,15,15	1.07	0
2	FAD	B	600	1	48,58,58	0.85	1 (2%)	54,89,89	1.47	3 (5%)
3	NCR	B	601	-	8,11,11	0.70	0	8,15,15	1.07	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	600	1	-	0/30/50/50	0/6/6/6
3	NCR	A	601	-	-	0/3/4/4	0/1/1/1
2	FAD	B	600	1	-	0/30/50/50	0/6/6/6
3	NCR	B	601	-	-	0/3/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C4-N3	3.36	1.39	1.33
2	B	600	FAD	C4-N3	3.37	1.39	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	C4X-C4-N3	-5.29	116.36	123.59
2	B	600	FAD	C4X-C4-N3	-5.25	116.41	123.59
2	B	600	FAD	C4X-C10-N10	-2.10	119.28	120.52
2	A	600	FAD	C4X-C10-N10	-2.05	119.31	120.52
2	B	600	FAD	C4-N3-C2	7.26	121.52	115.25
2	A	600	FAD	C4-N3-C2	7.28	121.54	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	6	0
3	A	601	NCR	6	0
2	B	600	FAD	6	0
3	B	601	NCR	7	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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