Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:10 PM GMT

PDB ID	:	1SEZ
Title	:	Crystal Structure of Protoporphyrinogen IX Oxidase
Authors	:	Koch, M.; Breithaupt, C.; Kiefersauer, R.; Freigang, J.; Huber, R.; Messerschmidt, A.
Deposited on	:	2004-02-19
Resolution	:	2.90 Å(reported)

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

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

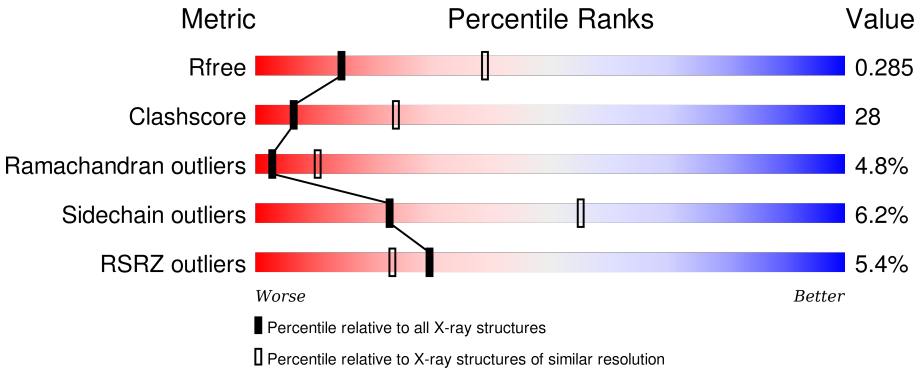
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	504	4% 53% 35% • 8%
1	B	504	6% 51% 37% • • 8%

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
4	TON	B	605	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7295 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.

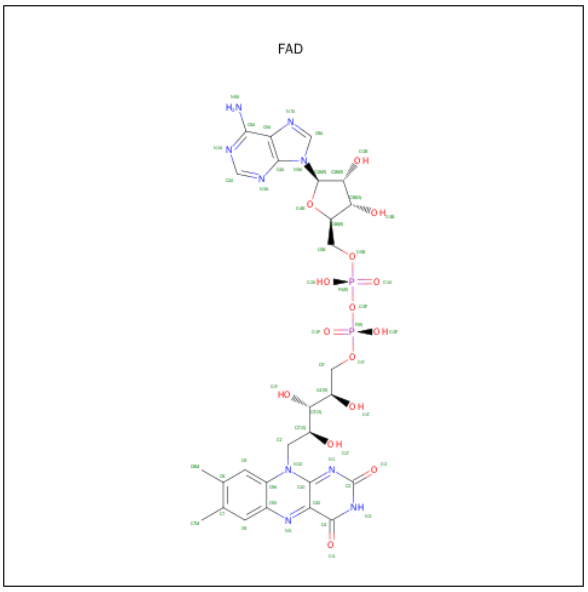
- Molecule 1 is a protein called Protoporphyrinogen oxidase, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	Se	41	0	0
			3480	2215	588	662	6	9			
1	B	465	Total	C	N	O	S	Se	165	0	0
			3480	2215	588	662	6	9			

There are 18 discrepancies between the modelled and reference sequences:

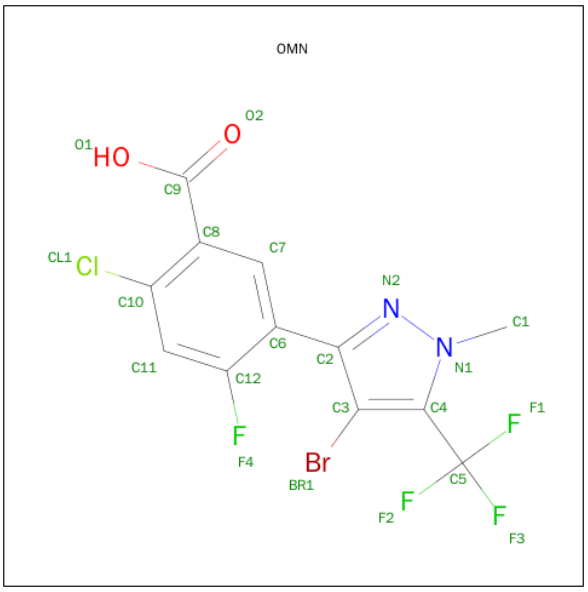
Chain	Residue	Modelled	Actual	Comment	Reference
A	69	MSE	MET	MODIFIED RESIDUE	UNP O24164
A	130	MSE	MET	MODIFIED RESIDUE	UNP O24164
A	186	MSE	MET	MODIFIED RESIDUE	UNP O24164
A	242	MSE	MET	MODIFIED RESIDUE	UNP O24164
A	302	MSE	MET	MODIFIED RESIDUE	UNP O24164
A	312	MSE	MET	MODIFIED RESIDUE	UNP O24164
A	376	MSE	MET	MODIFIED RESIDUE	UNP O24164
A	377	MSE	MET	MODIFIED RESIDUE	UNP O24164
A	456	MSE	MET	MODIFIED RESIDUE	UNP O24164
B	69	MSE	MET	MODIFIED RESIDUE	UNP O24164
B	130	MSE	MET	MODIFIED RESIDUE	UNP O24164
B	186	MSE	MET	MODIFIED RESIDUE	UNP O24164
B	242	MSE	MET	MODIFIED RESIDUE	UNP O24164
B	302	MSE	MET	MODIFIED RESIDUE	UNP O24164
B	312	MSE	MET	MODIFIED RESIDUE	UNP O24164
B	376	MSE	MET	MODIFIED RESIDUE	UNP O24164
B	377	MSE	MET	MODIFIED RESIDUE	UNP O24164
B	456	MSE	MET	MODIFIED RESIDUE	UNP O24164

- 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 4-BROMO-3-(5'-CARBOXY-4'-CHLORO-2'-FLUOROPHENYL)-1-METHYL-5-TRIFLUOROMETHYL-PYRAZOL (three-letter code: OMN) (formula: $C_{12}H_6BrClF_4N_2O_2$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Br	C	Cl	F	N	O	0	0
			22	1	12	1	4	2	2		

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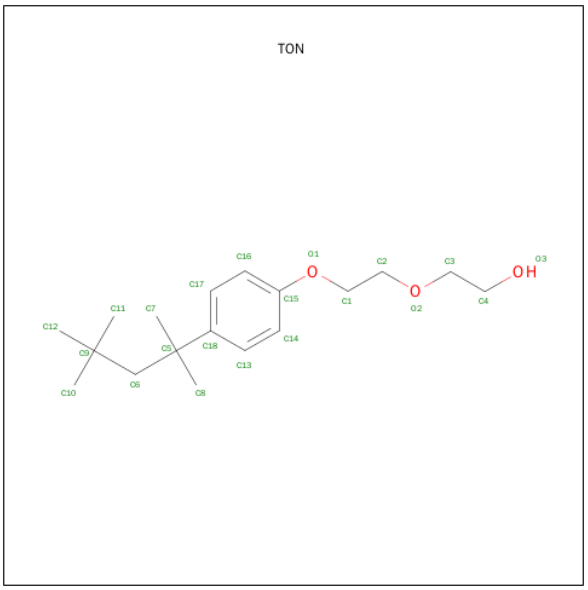
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	B	1	Total	Br	C	Cl	F	N	O	0	0
			22	1	12	1	4	2	2		

- Molecule 4 is 2-{2-[4-(1,1,3,3-TETRAMETHYLBUTYL)PHENOXY]ETHOXY}ETHANOL (three-letter code: TON) (formula: $C_{18}H_{30}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			21	18	3		
4	B	1	Total	C	O	0	0
			21	18	3		

- Molecule 5 is water.

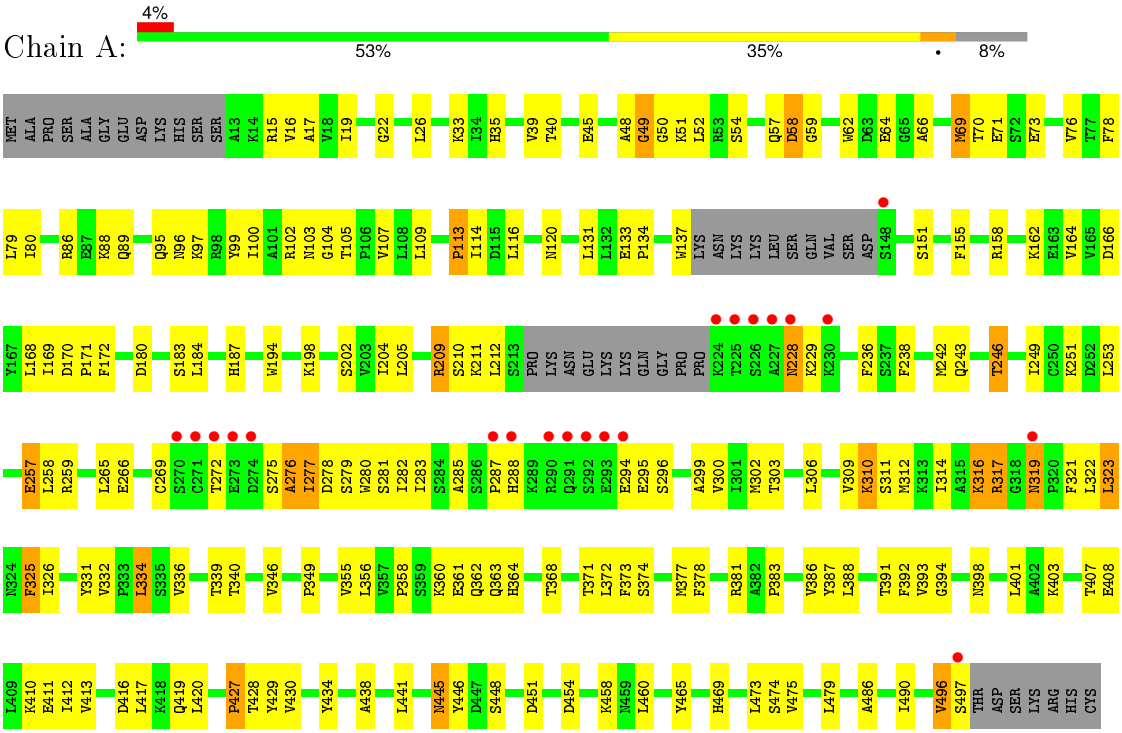
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	75	Total	O	0	0
			75	75		
5	B	68	Total	O	0	0
			68	68		

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 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.

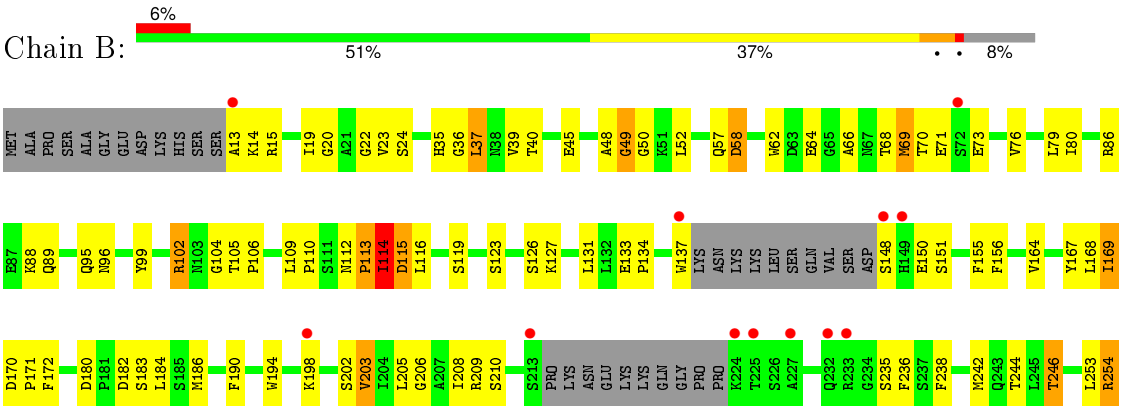
- Molecule 1: Protoporphyrinogen oxidase, mitochondrial

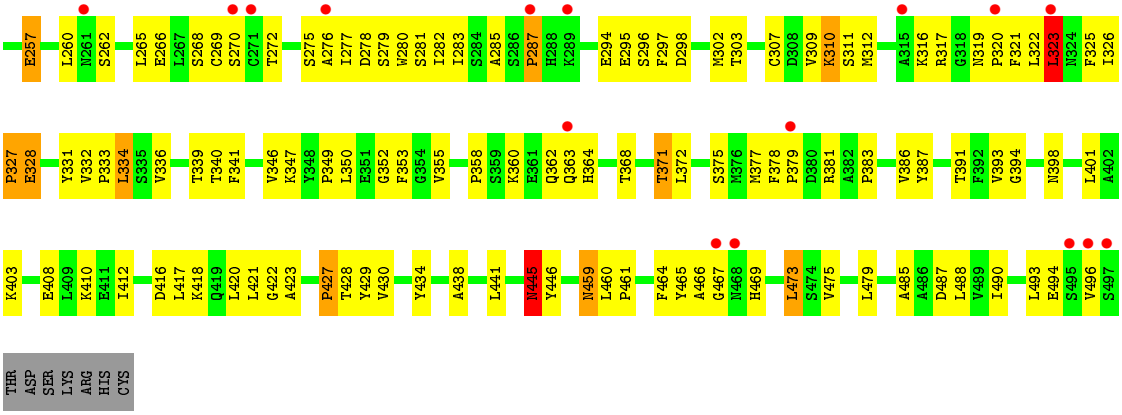
Chain A:



- Molecule 1: Protoporphyrinogen oxidase, mitochondrial

Chain B:




E257
L260 N261 S262
L265 E266 L267 S268 C269 S270 C271 T272
S275 A276 I277 D278 S279 W280 S281 I282 I283 S284 A285 S286 P287 H288 K289
E294 E295 S296 F297 D298
M302 T303
C307 D308 V309 K310 S311 M312
A315 K316 R317 G318 N319 P320 F321 L322 I323 N324 F325 I326
P327 E328
Y331 V332 P333 L334 S335 V336
T339 T340 F341
V346 K347 Y348 P349 L350 E351 G352 F353 G354 V355
P358 S359 K360 E361 Q362 Q363 H364
T368
T371 L372
S375 N376 M377 F378 P379 D380 R381 A382 P383
V386 Y387
T391 P392 V393 G394
N398
L401 A402
K403
E408 L409 K410 E411 I412
D416 L417 K418 Q419 L420 L421 G422 A423
P427 T428 Y429 V430
Y434
A438
L441
N445 Y446
N459 L460 P461
F464 Y465 A466 G467 N468 H469
L473 S474 V475
L479
A485 A486 D487 L488 V489 I490
L493 E494 S495 V496 S497
THR
ASP
SER
LYS
ARG
HIS
CYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	119.09Å 147.25Å 127.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.73 – 2.90 19.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (19.73-2.90) 99.5 (19.73-2.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.293 0.226 , 0.285	Depositor DCC
R_{free} test set	1209 reflections (5.11%)	DCC
Wilson B-factor (Å^2)	77.2	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 50.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 24891 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7295	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TON, OMN, 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	0.41	0/3539	0.62	1/4781 (0.0%)
1	B	0.41	0/3539	0.63	1/4781 (0.0%)
All	All	0.41	0/7078	0.62	2/9562 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	PRO	N-CA-CB	5.58	110.00	103.30
1	B	287	PRO	N-CA-CB	5.56	109.97	103.30

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	3480	0	3367	193	0
1	B	3480	0	3367	184	0
2	A	53	0	31	2	0
2	B	53	0	31	3	0
3	A	22	0	5	0	0
3	B	22	0	5	0	0
4	A	21	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	21	0	30	1	0
5	A	75	0	0	14	0
5	B	68	0	0	14	0
All	All	7295	0	6866	375	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 28.

All (375) 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:69:MSE:HE2	1:A:242:MSE:HE1	1.44	1.00
1:B:69:MSE:HE1	1:B:238:PHE:HE1	1.25	0.99
1:B:309:VAL:HA	1:B:312:MSE:HE3	1.47	0.95
1:A:496:VAL:HG23	1:A:497:SER:H	1.32	0.95
1:B:69:MSE:HE1	1:B:238:PHE:CE1	2.06	0.90
1:A:69:MSE:HE1	1:A:238:PHE:HE1	1.35	0.90
1:A:69:MSE:HE1	1:A:238:PHE:CE1	2.11	0.86
1:A:410:LYS:HG3	1:A:430:VAL:HG21	1.60	0.84
1:A:316:LYS:HG3	1:A:317:ARG:H	1.45	0.81
1:A:309:VAL:HA	1:A:312:MSE:HE3	1.62	0.81
1:A:460:LEU:HB2	5:A:652:HOH:O	1.81	0.81
1:A:253:LEU:HD22	1:A:257:GLU:HG2	1.64	0.79
1:B:265:LEU:HD11	1:B:285:ALA:HB2	1.65	0.78
1:B:346:VAL:HG21	1:B:387:TYR:HD1	1.46	0.78
1:A:460:LEU:HD22	5:A:652:HOH:O	1.82	0.77
1:A:209:ARG:HH11	1:A:209:ARG:HG2	1.50	0.77
1:B:69:MSE:HE2	1:B:242:MSE:HE1	1.67	0.76
1:A:69:MSE:HE2	1:A:242:MSE:CE	2.16	0.75
1:B:114:ILE:O	1:B:114:ILE:HD13	1.85	0.74
1:A:265:LEU:HD11	1:A:285:ALA:HB2	1.68	0.74
1:B:410:LYS:HG3	1:B:430:VAL:HG21	1.69	0.74
1:A:360:LYS:O	1:A:363:GLN:HG2	1.88	0.73
1:A:340:THR:O	1:A:428:THR:HB	1.89	0.73
1:A:69:MSE:HG2	1:A:70:THR:N	2.03	0.73
1:A:251:LYS:HA	1:A:251:LYS:HE2	1.69	0.73
1:B:69:MSE:HG2	1:B:70:THR:N	2.03	0.73
1:A:325:PHE:HD2	1:A:325:PHE:H	1.37	0.72
1:A:410:LYS:HE2	1:A:427:PRO:HD2	1.72	0.72
1:A:100:ILE:HD11	1:A:109:LEU:HD13	1.71	0.71
1:B:334:LEU:HD23	1:B:334:LEU:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LYS:HE3	1:B:311:SER:HB3	1.72	0.71
1:A:310:LYS:HE3	1:A:311:SER:HB3	1.72	0.71
1:A:242:MSE:HG2	5:A:660:HOH:O	1.90	0.70
1:B:332:VAL:HG23	1:B:441:LEU:HD13	1.72	0.70
1:A:340:THR:O	1:A:427:PRO:O	2.09	0.70
1:B:50:GLY:N	5:B:651:HOH:O	2.25	0.69
1:B:76:VAL:O	1:B:80:ILE:HG12	1.93	0.69
1:A:323:LEU:HA	1:A:325:PHE:CE2	2.28	0.69
1:A:331:TYR:OH	1:A:469:HIS:HE1	1.75	0.69
1:B:340:THR:O	1:B:427:PRO:O	2.10	0.68
1:B:331:TYR:OH	1:B:469:HIS:HE1	1.76	0.68
1:A:372:LEU:HD22	1:A:377:MSE:HE1	1.74	0.68
1:A:496:VAL:HG23	1:A:497:SER:N	2.08	0.67
1:B:494:GLU:O	1:B:496:VAL:HG23	1.94	0.67
1:A:411:GLU:HB2	5:A:650:HOH:O	1.95	0.67
1:A:35:HIS:ND1	1:A:35:HIS:O	2.27	0.67
1:B:340:THR:O	1:B:428:THR:HB	1.95	0.67
1:A:314:ILE:HD11	1:A:460:LEU:HD23	1.77	0.66
1:A:314:ILE:HD11	1:A:460:LEU:CD2	2.26	0.66
1:A:49:GLY:HA2	1:A:246:THR:HG21	1.78	0.66
1:B:49:GLY:HA2	5:B:651:HOH:O	1.97	0.65
1:B:418:LYS:HA	1:B:423:ALA:H	1.60	0.65
1:B:15:ARG:HB2	1:B:297:PHE:HA	1.79	0.65
1:A:334:LEU:HD23	1:A:334:LEU:O	1.96	0.65
1:B:336:VAL:HG23	5:B:644:HOH:O	1.95	0.65
1:A:316:LYS:HE2	1:A:321:PHE:HD1	1.60	0.65
1:A:228:ASN:HA	5:A:620:HOH:O	1.97	0.65
1:B:398:ASN:HD22	1:B:401:LEU:HD22	1.63	0.64
1:A:17:ALA:HB3	1:A:300:VAL:HG22	1.79	0.64
1:A:398:ASN:ND2	1:A:401:LEU:HB2	2.12	0.64
1:A:383:PRO:O	1:A:386:VAL:HG12	1.98	0.63
1:B:334:LEU:HD22	1:B:438:ALA:CB	2.29	0.63
1:B:410:LYS:HE2	1:B:427:PRO:HD2	1.81	0.63
1:A:76:VAL:O	1:A:80:ILE:HG12	1.99	0.63
1:B:198:LYS:HD3	1:B:198:LYS:C	2.19	0.63
1:B:35:HIS:ND1	1:B:35:HIS:O	2.32	0.63
1:B:332:VAL:CG2	1:B:441:LEU:HD13	2.28	0.62
1:A:403:LYS:HG2	1:A:434:TYR:CZ	2.35	0.62
1:B:340:THR:HG22	1:B:429:TYR:HB3	1.80	0.62
1:A:281:SER:HA	1:A:295:GLU:O	2.00	0.62
1:B:310:LYS:HD2	1:B:310:LYS:C	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:CG1	1:A:109:LEU:HD13	2.30	0.61
1:B:326:ILE:HD12	1:B:328:GLU:N	2.15	0.61
1:A:332:VAL:HG23	1:A:441:LEU:HD13	1.80	0.61
1:B:171:PRO:HG3	1:B:358:PRO:HG3	1.81	0.61
1:A:340:THR:HG22	1:A:429:TYR:HB3	1.82	0.61
1:B:281:SER:HA	1:B:295:GLU:O	2.00	0.61
1:A:334:LEU:HD22	1:A:438:ALA:CB	2.30	0.61
1:B:360:LYS:O	1:B:363:GLN:HG2	2.01	0.61
1:A:100:ILE:CD1	1:A:109:LEU:HD13	2.31	0.61
1:A:57:GLN:HG3	1:A:62:TRP:CH2	2.36	0.61
1:B:403:LYS:HG2	1:B:434:TYR:CZ	2.37	0.60
1:B:334:LEU:HD22	1:B:438:ALA:HB2	1.83	0.60
1:B:253:LEU:HA	5:B:636:HOH:O	2.01	0.60
1:A:16:VAL:HG13	1:A:299:ALA:HB3	1.85	0.59
1:A:410:LYS:CE	1:A:427:PRO:HD2	2.31	0.59
1:A:356:LEU:HD11	4:A:603:TON:H31	1.82	0.59
1:A:316:LYS:HG3	1:A:317:ARG:N	2.15	0.59
1:B:57:GLN:HG3	1:B:58:ASP:OD1	2.03	0.59
1:A:326:ILE:O	1:A:326:ILE:HD12	2.02	0.59
1:B:183:SER:O	1:B:184:LEU:HD12	2.02	0.59
1:A:209:ARG:NH1	1:A:209:ARG:HG2	2.16	0.59
1:B:131:LEU:O	1:B:134:PRO:HD2	2.03	0.58
1:A:70:THR:HG22	1:A:71:GLU:N	2.18	0.58
1:B:109:LEU:HD12	1:B:110:PRO:HD2	1.84	0.58
1:B:283:ILE:HD12	1:B:283:ILE:N	2.18	0.58
1:B:106:PRO:HG2	1:B:350:LEU:HD11	1.84	0.58
1:A:198:LYS:C	1:A:198:LYS:HD3	2.23	0.58
1:A:66:ALA:HA	2:A:600:FAD:N5	2.19	0.58
1:B:340:THR:O	1:B:340:THR:HG23	2.03	0.58
1:B:79:LEU:HD12	1:B:479:LEU:HD21	1.86	0.57
1:A:266:GLU:CB	1:A:283:ILE:HD13	2.34	0.57
1:A:332:VAL:CG2	1:A:441:LEU:HD13	2.35	0.57
1:B:49:GLY:CA	5:B:651:HOH:O	2.52	0.57
1:A:398:ASN:HD22	1:A:401:LEU:HD22	1.70	0.57
1:A:19:ILE:O	1:A:303:THR:HB	2.05	0.57
1:B:66:ALA:HA	2:B:610:FAD:N5	2.20	0.57
1:A:334:LEU:HD22	1:A:438:ALA:HB2	1.85	0.57
1:B:459:ASN:O	1:B:461:PRO:HD3	2.05	0.57
1:A:334:LEU:HD23	1:A:334:LEU:C	2.26	0.56
1:A:170:ASP:HB3	1:A:171:PRO:HD3	1.87	0.56
1:B:39:VAL:HG12	1:B:40:THR:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:LYS:C	1:A:310:LYS:HD2	2.25	0.56
1:A:79:LEU:HD12	1:A:479:LEU:HD21	1.87	0.56
1:B:398:ASN:ND2	1:B:401:LEU:HD22	2.21	0.56
1:B:295:GLU:HB3	5:B:624:HOH:O	2.04	0.56
1:B:464:PHE:CD2	1:B:488:LEU:HD23	2.40	0.55
1:A:183:SER:O	1:A:184:LEU:HD12	2.06	0.55
1:B:70:THR:HG22	1:B:71:GLU:N	2.21	0.55
1:B:102:ARG:HD3	1:B:167:TYR:CE2	2.41	0.55
1:B:244:THR:HG22	5:B:629:HOH:O	2.07	0.55
1:B:23:VAL:HG13	1:B:24:SER:N	2.21	0.55
1:A:69:MSE:HE2	1:A:242:MSE:SE	2.57	0.55
1:B:368:THR:HG23	1:B:416:ASP:OD1	2.07	0.55
1:B:372:LEU:HD22	1:B:377:MSE:HE1	1.89	0.55
1:A:346:VAL:HG21	1:A:387:TYR:HD1	1.72	0.54
1:B:302:MSE:HB3	1:B:465:TYR:HA	1.89	0.54
1:B:123:SER:O	1:B:127:LYS:HG3	2.07	0.54
1:B:13:ALA:HB3	5:B:616:HOH:O	2.08	0.54
1:B:323:LEU:HB2	1:B:326:ILE:CG2	2.37	0.54
1:B:133:GLU:N	1:B:134:PRO:CD	2.70	0.54
1:B:102:ARG:C	1:B:104:GLY:H	2.09	0.54
1:B:353:PHE:O	1:B:377:MSE:HE2	2.07	0.54
1:A:368:THR:HG23	1:A:416:ASP:OD1	2.07	0.54
1:A:86:ARG:HH11	1:A:89:GLN:HE22	1.54	0.54
1:B:49:GLY:HA2	1:B:246:THR:HG21	1.90	0.54
1:A:96:ASN:CG	1:A:96:ASN:O	2.46	0.54
1:A:71:GLU:O	1:A:71:GLU:HG3	2.08	0.54
1:B:398:ASN:ND2	1:B:401:LEU:HB2	2.23	0.54
1:B:445:ASN:C	1:B:445:ASN:HD22	2.10	0.54
1:A:103:ASN:C	1:A:103:ASN:OD1	2.46	0.54
1:A:427:PRO:C	1:A:429:TYR:H	2.11	0.53
1:A:419:GLN:HG2	5:A:655:HOH:O	2.08	0.53
1:A:325:PHE:N	1:A:325:PHE:CD2	2.75	0.53
1:A:346:VAL:HG12	1:A:349:PRO:HG3	1.89	0.53
1:A:283:ILE:N	1:A:283:ILE:HD12	2.23	0.53
1:B:14:LYS:HD2	1:B:298:ASP:OD2	2.07	0.53
1:B:427:PRO:C	1:B:429:TYR:H	2.11	0.53
1:B:309:VAL:O	1:B:312:MSE:HB2	2.08	0.53
1:A:251:LYS:CA	1:A:251:LYS:HE2	2.38	0.53
1:A:73:GLU:HB2	1:A:76:VAL:HG23	1.91	0.53
1:A:411:GLU:CB	5:A:650:HOH:O	2.54	0.53
1:B:346:VAL:HG21	1:B:387:TYR:CD1	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:GLU:CB	1:B:283:ILE:HD13	2.39	0.52
1:B:372:LEU:HB3	1:B:377:MSE:HE1	1.91	0.52
1:A:95:GLN:NE2	1:A:97:LYS:HD2	2.24	0.52
1:A:171:PRO:HG3	1:A:358:PRO:HG3	1.92	0.52
1:B:334:LEU:HD23	1:B:334:LEU:C	2.30	0.52
1:B:48:ALA:O	1:B:49:GLY:C	2.48	0.52
1:A:294:GLU:HG2	1:A:295:GLU:N	2.24	0.52
1:B:170:ASP:HB3	1:B:171:PRO:HD3	1.91	0.52
1:B:169:ILE:C	1:B:169:ILE:HD12	2.30	0.52
1:B:346:VAL:HG12	1:B:349:PRO:HG3	1.91	0.52
1:A:15:ARG:HD2	5:A:613:HOH:O	2.10	0.52
1:B:383:PRO:O	1:B:386:VAL:HG12	2.09	0.52
1:B:386:VAL:HG22	1:B:387:TYR:N	2.24	0.52
1:A:79:LEU:HD12	1:A:479:LEU:HD11	1.91	0.52
1:A:294:GLU:O	1:A:295:GLU:HG3	2.09	0.51
1:A:168:LEU:O	1:A:171:PRO:HD2	2.09	0.51
1:B:119:SER:HB3	5:B:659:HOH:O	2.09	0.51
1:B:254:ARG:O	1:B:257:GLU:HB2	2.10	0.51
1:A:104:GLY:O	1:A:105:THR:HG23	2.09	0.51
1:B:473:LEU:H	1:B:473:LEU:HD12	1.76	0.51
1:A:134:PRO:HB3	1:A:205:LEU:HD13	1.92	0.51
1:A:253:LEU:HB3	1:A:257:GLU:HB3	1.93	0.51
1:B:340:THR:O	1:B:340:THR:CG2	2.58	0.51
1:A:48:ALA:O	1:A:49:GLY:C	2.48	0.51
1:B:372:LEU:HB3	1:B:377:MSE:CE	2.41	0.51
1:A:420:LEU:HD23	5:A:655:HOH:O	2.10	0.51
1:A:372:LEU:HB3	1:A:377:MSE:CE	2.41	0.50
1:B:327:PRO:O	1:B:328:GLU:C	2.49	0.50
1:A:39:VAL:HG12	1:A:40:THR:N	2.25	0.50
1:B:15:ARG:HB3	1:B:297:PHE:CD2	2.46	0.50
1:B:341:PHE:O	1:B:386:VAL:HG23	2.10	0.50
1:A:340:THR:O	1:A:340:THR:HG23	2.10	0.50
1:B:347:LYS:C	1:B:349:PRO:HD3	2.32	0.50
1:A:323:LEU:HA	1:A:325:PHE:HE2	1.74	0.50
1:A:114:ILE:HD11	1:B:208:ILE:HG22	1.94	0.50
1:A:169:ILE:C	1:A:169:ILE:HD12	2.32	0.50
1:A:269:CYS:HB3	1:A:280:TRP:CD2	2.46	0.50
1:A:51:LYS:HB2	2:A:600:FAD:O4'	2.12	0.50
1:B:69:MSE:HE3	1:B:236:PHE:CE1	2.47	0.50
1:A:113:PRO:HB3	5:A:678:HOH:O	2.12	0.50
1:B:347:LYS:O	1:B:349:PRO:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLU:N	1:A:134:PRO:CD	2.75	0.49
1:A:445:ASN:C	1:A:445:ASN:HD22	2.13	0.49
1:B:155:PHE:CD1	1:B:186:MSE:HG2	2.48	0.49
1:B:438:ALA:HB1	2:B:610:FAD:HM83	1.94	0.49
1:B:340:THR:CG2	1:B:428:THR:HG22	2.42	0.49
1:A:62:TRP:HE1	1:A:64:GLU:HG2	1.77	0.49
1:A:454:ASP:O	1:A:458:LYS:HG3	2.12	0.49
1:B:88:LYS:HD3	5:B:654:HOH:O	2.11	0.49
1:A:407:THR:O	5:A:650:HOH:O	2.20	0.49
1:A:26:LEU:HB3	1:A:249:ILE:HG21	1.93	0.49
1:B:69:MSE:HE2	1:B:242:MSE:CE	2.40	0.49
1:B:410:LYS:CE	1:B:427:PRO:HD2	2.42	0.49
1:A:100:ILE:HG13	1:A:109:LEU:HD13	1.95	0.48
1:A:316:LYS:HG2	1:A:319:ASN:O	2.13	0.48
1:B:66:ALA:O	1:B:242:MSE:HG3	2.14	0.48
1:B:496:VAL:O	1:B:496:VAL:HG12	2.13	0.48
1:B:294:GLU:O	1:B:295:GLU:HG3	2.13	0.48
1:B:86:ARG:HH11	1:B:89:GLN:HE22	1.61	0.48
1:A:316:LYS:HE2	1:A:321:PHE:CD1	2.46	0.48
1:B:282:ILE:O	1:B:294:GLU:HA	2.13	0.48
1:B:110:PRO:HG2	1:B:116:LEU:HD12	1.95	0.48
1:B:164:VAL:O	1:B:168:LEU:HB2	2.13	0.48
1:A:151:SER:HA	1:A:184:LEU:O	2.13	0.48
1:A:104:GLY:N	1:A:361:GLU:OE1	2.47	0.48
1:A:52:LEU:HD23	1:A:66:ALA:HB3	1.95	0.48
1:B:96:ASN:CG	1:B:96:ASN:O	2.51	0.48
1:B:68:THR:OG1	1:B:235:SER:HB2	2.14	0.48
1:B:69:MSE:CG	1:B:70:THR:N	2.75	0.47
1:A:340:THR:CG2	1:A:428:THR:HG22	2.44	0.47
1:A:253:LEU:CD2	1:A:257:GLU:HG2	2.39	0.47
1:B:62:TRP:HE1	1:B:64:GLU:HG2	1.78	0.47
1:A:411:GLU:CG	5:A:650:HOH:O	2.62	0.47
1:A:54:SER:H	1:A:243:GLN:HB2	1.79	0.47
1:B:22:GLY:HA2	1:B:50:GLY:HA3	1.97	0.47
1:A:202:SER:OG	1:A:205:LEU:HB2	2.14	0.47
1:B:15:ARG:HG2	1:B:15:ARG:HH11	1.79	0.47
1:B:270:SER:OG	1:B:279:SER:HB3	2.14	0.47
1:B:294:GLU:HG2	1:B:295:GLU:N	2.30	0.47
1:B:19:ILE:O	1:B:303:THR:HB	2.15	0.47
1:A:302:MSE:HB3	1:A:465:TYR:HA	1.96	0.47
1:A:427:PRO:O	1:A:429:TYR:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ILE:O	1:A:294:GLU:HA	2.15	0.47
1:B:323:LEU:HA	5:B:619:HOH:O	2.14	0.47
1:A:393:VAL:HG12	1:A:394:GLY:N	2.30	0.47
1:A:187:HIS:ND1	1:A:194:TRP:CD1	2.83	0.47
1:A:316:LYS:CG	1:A:317:ARG:N	2.76	0.47
1:A:259:ARG:NH1	1:A:295:GLU:OE2	2.48	0.46
1:B:371:THR:HB	1:B:391:THR:OG1	2.14	0.46
1:A:306:LEU:H	1:A:469:HIS:CE1	2.33	0.46
1:B:172:PHE:HA	4:B:605:TON:H32	1.98	0.46
1:B:202:SER:OG	1:B:205:LEU:HB2	2.15	0.46
1:A:316:LYS:CG	1:A:317:ARG:H	2.15	0.46
1:B:268:SER:HB2	1:B:281:SER:OG	2.16	0.46
1:B:23:VAL:CG1	1:B:24:SER:N	2.78	0.46
1:A:103:ASN:HA	1:A:364:HIS:CD2	2.51	0.46
1:A:33:LYS:HD2	1:A:253:LEU:HD23	1.98	0.46
1:B:445:ASN:C	1:B:445:ASN:ND2	2.68	0.46
1:B:242:MSE:HE2	1:B:475:VAL:HG21	1.98	0.46
1:B:52:LEU:CD2	1:B:66:ALA:HB3	2.46	0.46
1:A:340:THR:O	1:A:340:THR:CG2	2.64	0.46
1:A:372:LEU:HB3	1:A:377:MSE:HE1	1.98	0.46
1:B:155:PHE:HD2	1:B:156:PHE:N	2.14	0.46
1:B:70:THR:CG2	1:B:71:GLU:N	2.78	0.46
1:B:408:GLU:O	1:B:412:ILE:HG12	2.15	0.46
1:B:339:THR:HB	1:B:427:PRO:HB3	1.97	0.46
1:B:427:PRO:O	1:B:428:THR:HB	2.16	0.45
1:A:168:LEU:C	1:A:171:PRO:HD2	2.37	0.45
1:A:52:LEU:CD2	1:A:66:ALA:HB3	2.47	0.45
1:A:310:LYS:HD2	1:A:311:SER:N	2.31	0.45
1:B:321:PHE:CZ	1:B:459:ASN:ND2	2.84	0.45
1:A:448:SER:HA	1:A:451:ASP:OD2	2.16	0.45
1:B:168:LEU:O	1:B:171:PRO:HD2	2.16	0.45
1:B:151:SER:HA	1:B:184:LEU:O	2.17	0.45
1:A:69:MSE:CG	1:A:70:THR:N	2.78	0.45
1:B:64:GLU:O	1:B:336:VAL:HG21	2.16	0.45
1:B:102:ARG:C	1:B:104:GLY:N	2.70	0.45
1:A:445:ASN:ND2	1:A:445:ASN:C	2.70	0.45
1:B:487:ASP:HA	1:B:490:ILE:HB	1.98	0.45
1:B:326:ILE:HD12	1:B:328:GLU:H	1.82	0.45
1:A:33:LYS:C	1:A:35:HIS:H	2.19	0.45
1:A:310:LYS:CG	1:A:311:SER:N	2.80	0.45
1:A:35:HIS:CG	1:A:35:HIS:O	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LYS:HA	1:B:423:ALA:N	2.31	0.44
1:A:496:VAL:O	1:A:497:SER:HB2	2.18	0.44
1:A:340:THR:CG2	1:A:429:TYR:HB3	2.48	0.44
1:B:362:GLN:C	1:B:364:HIS:H	2.20	0.44
1:B:418:LYS:O	1:B:422:GLY:N	2.49	0.44
1:B:39:VAL:CG1	1:B:40:THR:N	2.81	0.44
1:B:393:VAL:HG12	1:B:394:GLY:N	2.33	0.44
1:A:316:LYS:HD2	1:A:319:ASN:ND2	2.33	0.44
1:A:398:ASN:ND2	1:A:401:LEU:HD22	2.30	0.44
1:A:362:GLN:C	1:A:364:HIS:H	2.21	0.44
1:A:70:THR:CG2	1:A:71:GLU:N	2.80	0.44
1:A:276:ALA:O	1:A:277:ILE:C	2.54	0.44
1:B:14:LYS:HG2	1:B:37:LEU:HD22	1.99	0.44
1:B:417:LEU:HD23	1:B:417:LEU:HA	1.79	0.44
1:A:100:ILE:O	1:A:107:VAL:HG12	2.18	0.44
1:B:294:GLU:CG	1:B:295:GLU:N	2.81	0.44
1:A:48:ALA:HB2	1:A:258:LEU:HD21	1.99	0.43
1:A:474:SER:O	1:A:475:VAL:C	2.56	0.43
1:A:269:CYS:HB3	1:A:280:TRP:CE3	2.54	0.43
1:B:86:ARG:NH2	5:B:653:HOH:O	2.51	0.43
1:B:269:CYS:HB3	1:B:280:TRP:CE3	2.53	0.43
1:A:339:THR:HB	1:A:427:PRO:HB3	1.99	0.43
1:A:59:GLY:O	1:A:383:PRO:HD3	2.18	0.43
1:A:172:PHE:HA	4:A:603:TON:H32	2.00	0.43
1:A:326:ILE:CG1	1:A:326:ILE:O	2.66	0.43
1:A:322:LEU:O	1:A:325:PHE:HE2	2.01	0.43
1:A:57:GLN:O	1:A:59:GLY:N	2.52	0.43
1:B:115:ASP:O	1:B:119:SER:HB3	2.18	0.43
1:A:294:GLU:CG	1:A:295:GLU:N	2.80	0.43
1:A:209:ARG:NH1	1:B:114:ILE:HD12	2.33	0.43
1:B:459:ASN:O	1:B:461:PRO:CD	2.67	0.43
1:A:408:GLU:O	1:A:412:ILE:HG12	2.18	0.43
1:B:69:MSE:CE	1:B:242:MSE:HE1	2.45	0.43
1:A:280:TRP:O	1:A:296:SER:HA	2.19	0.43
1:A:78:PHE:C	1:A:78:PHE:CD1	2.92	0.43
1:A:236:PHE:C	1:A:236:PHE:CD1	2.92	0.43
1:B:73:GLU:HB2	1:B:76:VAL:HG23	2.00	0.42
1:A:133:GLU:OE1	1:A:204:ILE:HB	2.18	0.42
1:A:202:SER:CB	5:A:659:HOH:O	2.65	0.42
1:A:242:MSE:HE2	1:A:475:VAL:HG21	2.01	0.42
1:B:427:PRO:O	1:B:429:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ALA:O	1:B:49:GLY:O	2.36	0.42
1:A:310:LYS:HG3	1:A:311:SER:N	2.34	0.42
1:B:323:LEU:HB2	1:B:326:ILE:HG23	2.01	0.42
1:B:69:MSE:HE2	1:B:242:MSE:SE	2.70	0.42
1:A:374:SER:HB2	1:A:388:LEU:O	2.20	0.42
1:B:168:LEU:HA	1:B:168:LEU:HD23	1.80	0.42
1:B:420:LEU:C	1:B:421:LEU:HD23	2.40	0.42
1:B:88:LYS:O	1:B:238:PHE:HA	2.20	0.42
1:A:79:LEU:CD1	1:A:479:LEU:HD21	2.50	0.42
1:B:112:ASN:HA	1:B:113:PRO:HD3	1.93	0.42
1:B:479:LEU:C	1:B:479:LEU:HD23	2.40	0.42
1:A:486:ALA:O	1:A:490:ILE:HG13	2.20	0.42
1:B:307:CYS:HB3	1:B:331:TYR:CE1	2.55	0.41
1:A:355:VAL:HG23	1:A:373:PHE:CZ	2.55	0.41
1:A:391:THR:HG21	1:A:413:VAL:HG22	2.01	0.41
1:B:99:TYR:HB2	1:B:355:VAL:HG22	2.01	0.41
1:A:162:LYS:NZ	1:A:166:ASP:OD1	2.44	0.41
1:A:309:VAL:O	1:A:312:MSE:HB2	2.20	0.41
1:B:36:GLY:O	1:B:37:LEU:C	2.59	0.41
1:B:186:MSE:HE3	1:B:190:PHE:HB2	2.03	0.41
1:A:336:VAL:HG22	1:A:392:PHE:CE2	2.55	0.41
1:A:22:GLY:HA2	1:A:50:GLY:HA3	2.02	0.41
1:B:494:GLU:C	1:B:496:VAL:N	2.73	0.41
1:A:131:LEU:O	1:A:134:PRO:HD2	2.21	0.41
1:B:280:TRP:O	1:B:296:SER:HA	2.21	0.41
1:A:116:LEU:HD12	1:A:116:LEU:HA	1.93	0.41
1:A:52:LEU:HD22	1:A:242:MSE:HB3	2.01	0.41
1:A:326:ILE:HG22	5:A:609:HOH:O	2.21	0.41
1:B:464:PHE:HD2	1:B:488:LEU:HD23	1.82	0.41
1:A:378:PHE:HB2	1:A:381:ARG:HG3	2.02	0.41
1:A:417:LEU:HA	1:A:417:LEU:HD23	1.82	0.41
1:B:206:GLY:O	1:B:209:ARG:N	2.53	0.41
1:B:260:LEU:C	1:B:262:SER:H	2.23	0.41
1:A:441:LEU:HD12	1:A:441:LEU:HA	1.71	0.41
1:A:164:VAL:O	1:A:168:LEU:HB2	2.20	0.41
1:B:378:PHE:HB2	1:B:381:ARG:HG3	2.01	0.41
1:B:49:GLY:C	5:B:651:HOH:O	2.55	0.41
1:B:202:SER:O	1:B:203:VAL:C	2.59	0.41
1:B:95:GLN:O	1:B:352:GLY:HA2	2.20	0.41
1:B:466:ALA:HB2	1:B:485:ALA:HB2	2.03	0.41
1:B:333:PRO:O	1:B:334:LEU:HB3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:THR:CG2	1:B:429:TYR:HB3	2.49	0.40
1:B:441:LEU:HA	1:B:441:LEU:HD12	1.75	0.40
1:B:102:ARG:HD3	1:B:167:TYR:CD2	2.55	0.40
1:B:119:SER:CB	5:B:659:HOH:O	2.68	0.40
1:B:205:LEU:HA	1:B:205:LEU:HD12	1.84	0.40
1:B:148:SER:N	1:B:194:TRP:HH2	2.18	0.40
1:A:57:GLN:HG3	1:A:62:TRP:CZ3	2.56	0.40
1:A:326:ILE:CD1	1:A:326:ILE:O	2.68	0.40
1:B:375:SER:O	1:B:379:PRO:HA	2.20	0.40
1:A:88:LYS:O	1:A:238:PHE:HA	2.21	0.40
1:A:303:THR:O	1:A:303:THR:CG2	2.69	0.40
1:A:269:CYS:HA	1:A:279:SER:O	2.21	0.40
1:B:20:GLY:HA2	2:B:610:FAD:H1B	2.02	0.40
1:A:306:LEU:HA	1:A:306:LEU:HD12	1.70	0.40
1:B:168:LEU:C	1:B:171:PRO:HD2	2.42	0.40
1:A:168:LEU:HA	1:A:168:LEU:HD23	1.89	0.40
1:A:99:TYR:HB2	1:A:355:VAL:HG22	2.03	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	459/504 (91%)	391 (85%)	50 (11%)	18 (4%)	4 15
1	B	459/504 (91%)	373 (81%)	60 (13%)	26 (6%)	2 6
All	All	918/1008 (91%)	764 (83%)	110 (12%)	44 (5%)	3 10

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	ASP

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Mol	Chain	Res	Type
1	A	210	SER
1	A	211	LYS
1	A	272	THR
1	A	275	SER
1	A	276	ALA
1	A	496	VAL
1	B	114	ILE
1	B	150	GLU
1	B	275	SER
1	B	276	ALA
1	B	287	PRO
1	B	320	PRO
1	B	323	LEU
1	B	328	GLU
1	A	316	LYS
1	A	317	ARG
1	B	37	LEU
1	B	49	GLY
1	B	210	SER
1	B	272	THR
1	B	278	ASP
1	A	212	LEU
1	A	229	LYS
1	A	427	PRO
1	B	203	VAL
1	B	254	ARG
1	B	322	LEU
1	B	459	ASN
1	A	155	PHE
1	A	288	HIS
1	B	113	PRO
1	B	316	LYS
1	A	278	ASP
1	B	277	ILE
1	B	317	ARG
1	B	327	PRO
1	A	228	ASN
1	B	325	PHE
1	B	427	PRO
1	B	445	ASN
1	A	277	ILE
1	A	49	GLY

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Mol	Chain	Res	Type
1	B	467	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	362/423 (86%)	341 (94%)	21 (6%)	25	58
1	B	362/423 (86%)	338 (93%)	24 (7%)	21	51
All	All	724/846 (86%)	679 (94%)	45 (6%)	23	55

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	58	ASP
1	A	69	MSE
1	A	102	ARG
1	A	113	PRO
1	A	120	ASN
1	A	137	TRP
1	A	158	ARG
1	A	180	ASP
1	A	209	ARG
1	A	246	THR
1	A	257	GLU
1	A	310	LYS
1	A	319	ASN
1	A	323	LEU
1	A	325	PHE
1	A	334	LEU
1	A	371	THR
1	A	445	ASN
1	A	446	TYR
1	A	473	LEU
1	B	45	GLU

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Mol	Chain	Res	Type
1	B	58	ASP
1	B	69	MSE
1	B	102	ARG
1	B	105	THR
1	B	114	ILE
1	B	115	ASP
1	B	126	SER
1	B	137	TRP
1	B	169	ILE
1	B	180	ASP
1	B	182	ASP
1	B	246	THR
1	B	257	GLU
1	B	310	LYS
1	B	319	ASN
1	B	323	LEU
1	B	334	LEU
1	B	371	THR
1	B	445	ASN
1	B	446	TYR
1	B	460	LEU
1	B	473	LEU
1	B	493	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	89	GLN
1	A	95	GLN
1	A	149	HIS
1	A	157	GLN
1	A	319	ASN
1	A	398	ASN
1	A	445	ASN
1	A	469	HIS
1	B	89	GLN
1	B	398	ASN
1	B	445	ASN
1	B	459	ASN
1	B	469	HIS

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

6 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	-	48,58,58	1.50	6 (12%)	54,89,89	2.01	8 (14%)
3	OMN	A	601	-	20,23,23	2.68	5 (25%)	25,36,36	1.79	6 (24%)
4	TON	A	603	-	21,21,21	1.87	8 (38%)	29,29,29	1.07	1 (3%)
3	OMN	B	604	-	20,23,23	2.66	6 (30%)	25,36,36	1.84	7 (28%)
4	TON	B	605	-	21,21,21	1.88	5 (23%)	29,29,29	1.02	0
2	FAD	B	610	-	48,58,58	1.40	6 (12%)	54,89,89	2.11	7 (12%)

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	-	-	0/30/50/50	0/6/6/6
3	OMN	A	601	-	-	0/8/14/14	0/2/2/2
4	TON	A	603	-	-	0/19/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMN	B	604	-	-	0/8/14/14	0/2/2/2
4	TON	B	605	-	-	0/19/19/19	0/1/1/1
2	FAD	B	610	-	-	0/30/50/50	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	OMN	N2-N1	-2.28	1.35	1.37
3	B	604	OMN	C1-N1	-2.09	1.44	1.46
3	B	604	OMN	N2-N1	-2.05	1.35	1.37
4	A	603	TON	C6-C9	2.00	1.61	1.54
4	A	603	TON	C14-C15	2.02	1.42	1.38
4	B	605	TON	C6-C9	2.03	1.61	1.54
4	A	603	TON	C17-C16	2.05	1.42	1.38
2	A	600	FAD	C1'-N10	2.08	1.50	1.48
3	A	601	OMN	C4-C3	2.10	1.42	1.39
4	A	603	TON	C16-C15	2.16	1.43	1.38
2	A	600	FAD	C2A-N1A	2.18	1.38	1.33
3	B	604	OMN	C4-C3	2.22	1.42	1.39
4	B	605	TON	C14-C13	2.28	1.42	1.38
4	A	603	TON	O1-C15	2.33	1.43	1.37
2	B	610	FAD	C5X-N5	2.34	1.39	1.35
2	B	610	FAD	C2A-N3A	2.36	1.36	1.32
4	A	603	TON	C13-C18	2.44	1.43	1.39
2	B	610	FAD	C2A-N1A	2.62	1.38	1.33
2	A	600	FAD	C4-N3	2.84	1.38	1.33
2	B	610	FAD	C4-N3	2.96	1.38	1.33
4	B	605	TON	C13-C18	3.02	1.44	1.39
4	B	605	TON	C17-C18	3.07	1.44	1.39
3	A	601	OMN	C5-C4	3.08	1.54	1.50
2	A	600	FAD	C5X-N5	3.18	1.40	1.35
4	A	603	TON	C17-C18	3.46	1.44	1.39
4	A	603	TON	C5-C18	3.78	1.59	1.53
2	B	610	FAD	C9A-N10	3.83	1.44	1.38
3	B	604	OMN	C6-C12	3.88	1.44	1.38
4	B	605	TON	C5-C18	3.94	1.60	1.53
2	A	600	FAD	C9A-N10	4.23	1.44	1.38
2	B	610	FAD	C4X-N5	4.32	1.40	1.33
2	A	600	FAD	C4X-N5	5.11	1.41	1.33
3	A	601	OMN	C6-C12	5.33	1.45	1.38
3	B	604	OMN	C5-C4	5.42	1.56	1.50
3	B	604	OMN	C2-N2	7.99	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	OMN	C2-N2	8.69	1.42	1.35

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	610	FAD	C4X-C4-N3	-4.88	116.92	123.59
2	B	610	FAD	N3A-C2A-N1A	-4.61	125.36	128.89
2	A	600	FAD	C4X-C4-N3	-4.35	117.64	123.59
2	A	600	FAD	N3A-C2A-N1A	-4.16	125.71	128.89
3	A	601	OMN	C4-N1-N2	-4.11	107.27	112.10
3	A	601	OMN	C11-C12-C6	-3.83	119.42	124.24
2	B	610	FAD	C4B-O4B-C1B	-3.77	105.58	109.72
3	B	604	OMN	C4-N1-N2	-3.76	107.68	112.10
3	B	604	OMN	C11-C12-C6	-3.72	119.56	124.24
2	A	600	FAD	C4-C4X-C10	-3.09	117.96	119.94
2	B	610	FAD	C4X-C10-N10	-2.69	118.93	120.52
2	A	600	FAD	C4B-O4B-C1B	-2.60	106.86	109.72
3	B	604	OMN	BR1-C3-C4	2.00	129.44	127.10
2	A	600	FAD	C4-C4X-N5	2.02	121.17	118.72
4	A	603	TON	C13-C14-C15	2.14	122.44	119.74
2	B	610	FAD	C1'-N10-C9A	2.23	121.37	118.86
3	B	604	OMN	F4-C12-C6	2.24	122.13	118.80
3	A	601	OMN	F4-C12-C6	2.33	122.26	118.80
3	B	604	OMN	C1-N1-N2	2.65	122.45	118.05
2	A	600	FAD	C1'-N10-C9A	2.79	121.99	118.86
3	A	601	OMN	C10-C11-C12	2.83	120.27	118.57
3	A	601	OMN	C1-N1-N2	2.98	123.02	118.05
3	B	604	OMN	C7-C6-C12	3.16	119.03	115.95
2	A	600	FAD	C4X-N5-C5X	3.37	120.64	116.76
3	A	601	OMN	C7-C6-C12	3.44	119.30	115.95
2	B	610	FAD	C4X-N5-C5X	3.81	121.14	116.76
3	B	604	OMN	C10-C11-C12	4.02	120.98	118.57
2	A	600	FAD	C4-N3-C2	10.28	124.13	115.25
2	B	610	FAD	C4-N3-C2	10.68	124.48	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	2	0
4	A	603	TON	2	0
4	B	605	TON	1	0
2	B	610	FAD	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	A	455/504 (90%)	0.11	21 (4%)	36	30	41, 63, 89, 99	25 (5%)
1	B	448/504 (88%)	0.16	28 (6%)	23	17	41, 68, 96, 100	47 (10%)
All	All	903/1008 (89%)	0.14	49 (5%)	29	23	41, 65, 94, 100	72 (7%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	SER	13.4
1	A	227	ALA	12.0
1	B	271	CYS	11.2
1	A	225	THR	9.2
1	A	224	LYS	8.3
1	A	226	SER	7.3
1	A	272	THR	6.0
1	B	224	LYS	5.8
1	A	291	GLN	5.4
1	B	276	ALA	5.3
1	B	270	SER	4.4
1	A	287	PRO	4.3
1	B	149	HIS	4.2
1	B	495	SER	4.0
1	A	270	SER	4.0
1	B	287	PRO	3.7
1	A	228	ASN	3.7
1	B	225	THR	3.5
1	B	227	ALA	3.4
1	A	294	GLU	3.4
1	A	290	ARG	3.3
1	B	497	SER	3.2
1	B	289	LYS	3.0
1	B	496	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	271	CYS	3.0
1	A	274	ASP	3.0
1	A	230	LYS	3.0
1	A	273	GLU	2.9
1	B	148	SER	2.8
1	A	288	HIS	2.8
1	A	319	ASN	2.7
1	A	497	SER	2.6
1	B	468	ASN	2.6
1	B	467	GLY	2.5
1	B	13	ALA	2.5
1	B	261	ASN	2.4
1	A	148	SER	2.4
1	A	293	GLU	2.4
1	B	320	PRO	2.3
1	B	323	LEU	2.3
1	B	72	SER	2.3
1	B	198	LYS	2.2
1	B	363	GLN	2.2
1	B	315	ALA	2.1
1	B	232	GLN	2.1
1	B	137	TRP	2.1
1	B	213	SER	2.1
1	B	233	ARG	2.1
1	B	379	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
4	TON	B	605	21/21	0.80	0.29	2.01	83,86,90,91	0
4	TON	A	603	21/21	0.78	0.28	1.54	78,85,93,93	0
3	OMN	B	604	22/22	0.97	0.15	-0.34	61,63,66,73	0
2	FAD	B	610	53/53	0.95	0.16	-0.54	49,63,72,73	0
2	FAD	A	600	53/53	0.96	0.15	-0.76	27,42,50,51	0
3	OMN	A	601	22/22	0.97	0.14	-0.93	52,58,60,70	0

6.5 Other polymers (i)

There are no such residues in this entry.