Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:52 AM GMT

PDB ID	:	2J3N
Title	:	X-RAY STRUCTURE OF HUMAN THIOREDOXIN REDUCTASE 1
Authors	:	Fritz-Wolf, K.; Urig, S.; Becker, K.
Deposited on	:	2006-08-22
Resolution	:	2.80 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 (i) symbol.

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

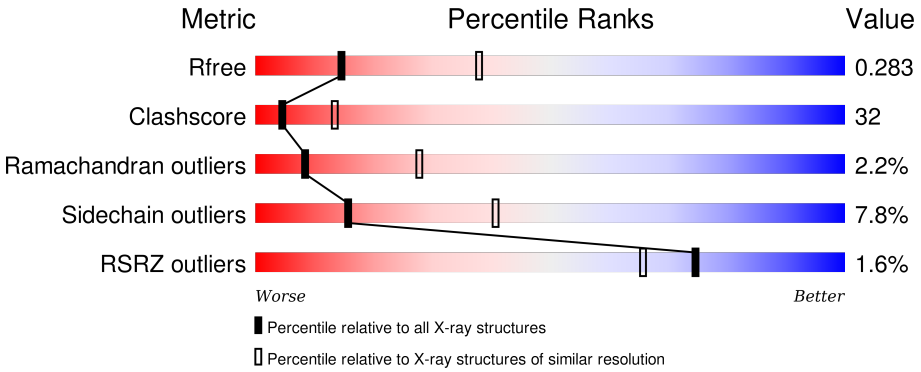
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	519	51% 37% 6% 6%
1	B	519	50% 39% 5% 6%
1	C	519	46% 41% 6% 6%
1	D	519	51% 37% 6% 5%
1	E	519	48% 39% 7% 6%

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Mol	Chain	Length	Quality of chain
1	F	519	2% 48% 40% 6% 6%

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	NAP	A	601	X	-	-	-
3	NAP	B	601	X	-	-	-
3	NAP	C	601	X	-	-	-
4	MPD	A	701	-	-	-	X
4	MPD	B	701	-	-	-	X
4	MPD	D	700	-	-	-	X

2 Entry composition (i)

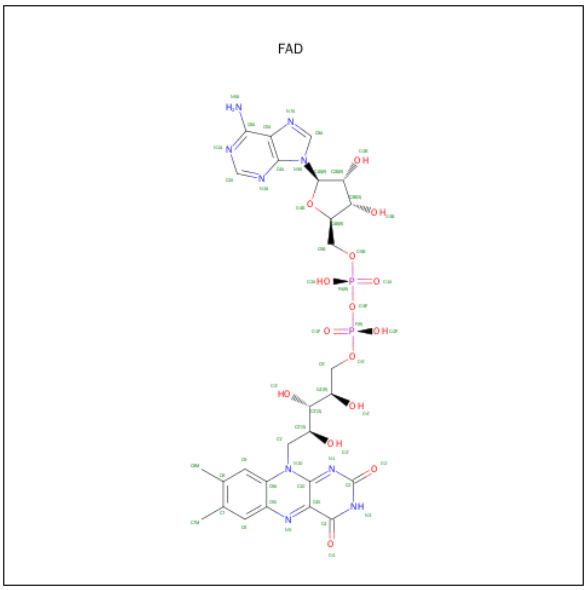
There are 5 unique types of molecules in this entry. The entry contains 23294 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THIOREDOXIN REDUCTASE 1.

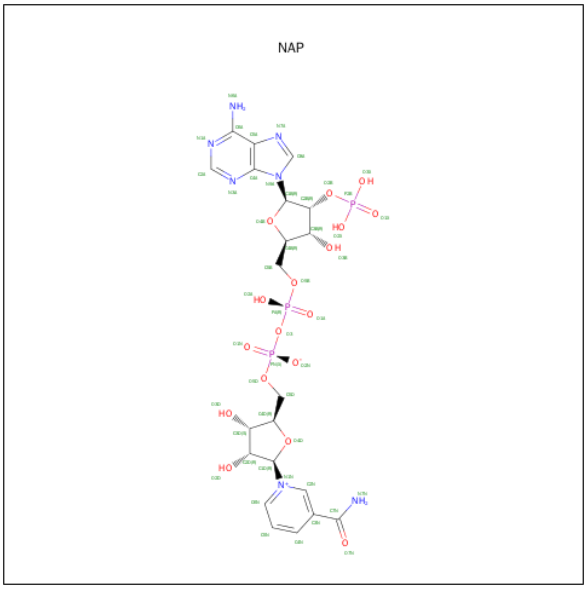
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	1
			3756	2387	642	708	19			
1	B	487	Total	C	N	O	S	0	0	1
			3760	2390	643	708	19			
1	C	490	Total	C	N	O	S	0	0	0
			3776	2397	645	713	21			
1	D	491	Total	C	N	O	S	0	0	0
			3785	2403	647	714	21			
1	E	490	Total	C	N	O	S	0	0	0
			3776	2397	645	713	21			
1	F	486	Total	C	N	O	S	0	0	1
			3751	2385	641	706	19			

- 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		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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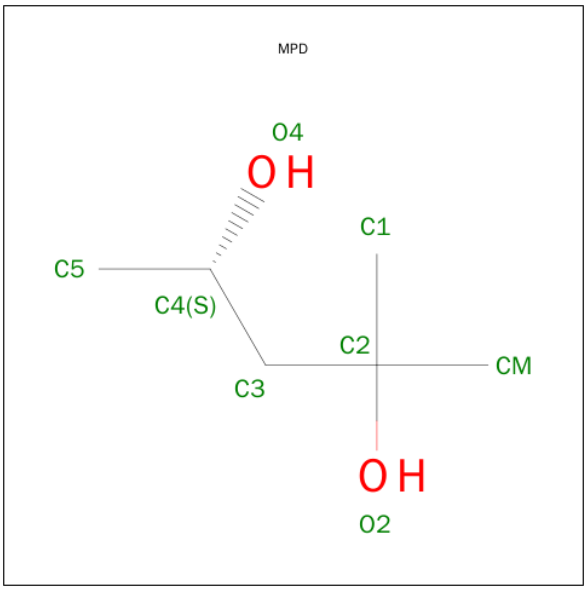
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	D	1	Total	C	O	0	0
			8	6	2		
4	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	B	9	Total	O	0	0
			9	9		
5	C	7	Total	O	0	0
			7	7		

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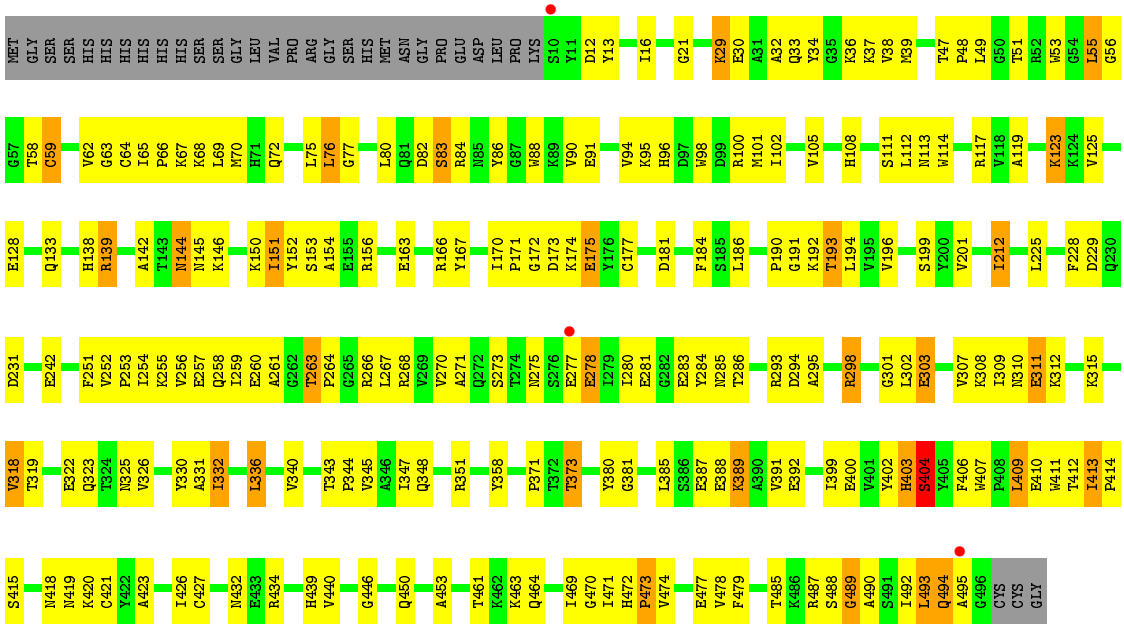
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	8	Total O 8 8	0	0
5	E	4	Total O 4 4	0	0
5	F	7	Total O 7 7	0	0

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 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.

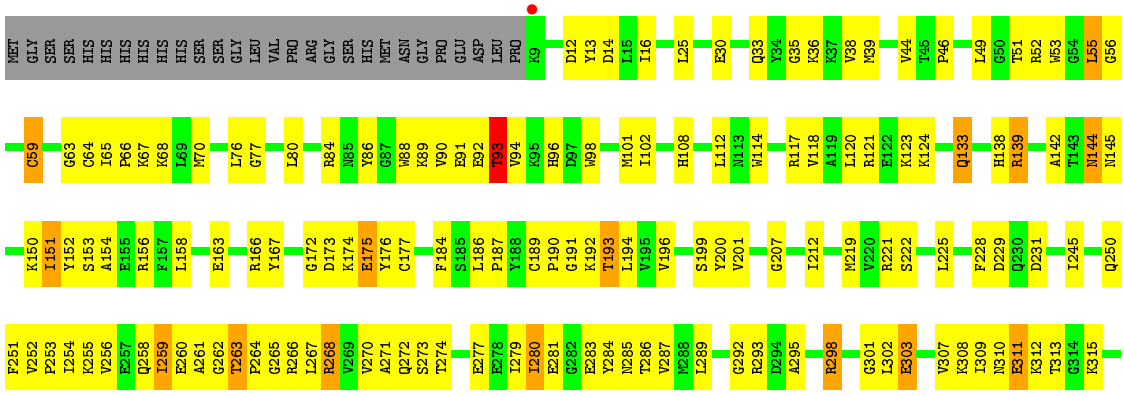
- Molecule 1: THIOREDOXIN REDUCTASE 1

Chain A:



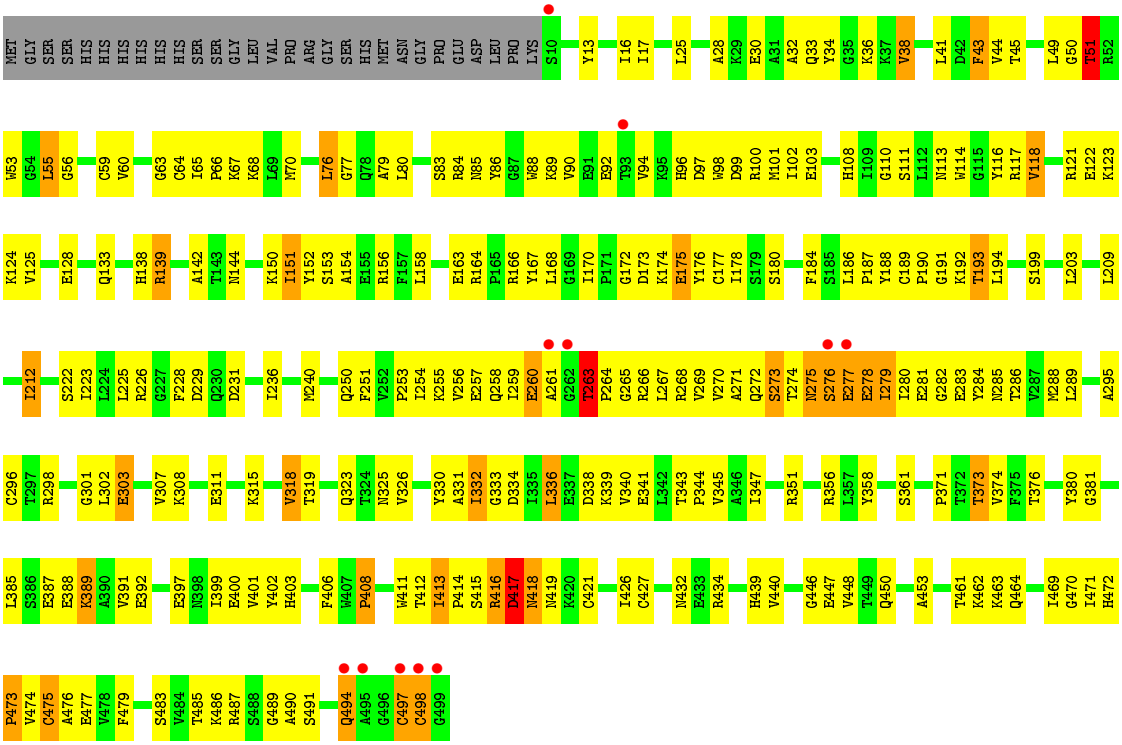
- Molecule 1: THIOREDOXIN REDUCTASE 1

Chain B:



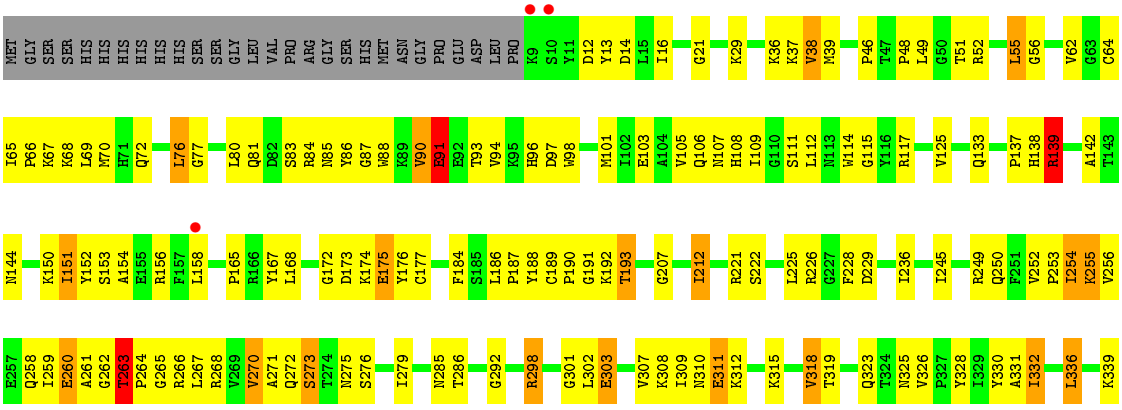
• Molecule 1: THIOREDOXIN REDUCTASE 1

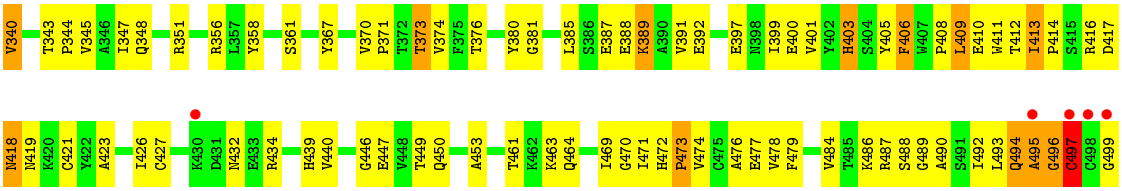
Chain C:



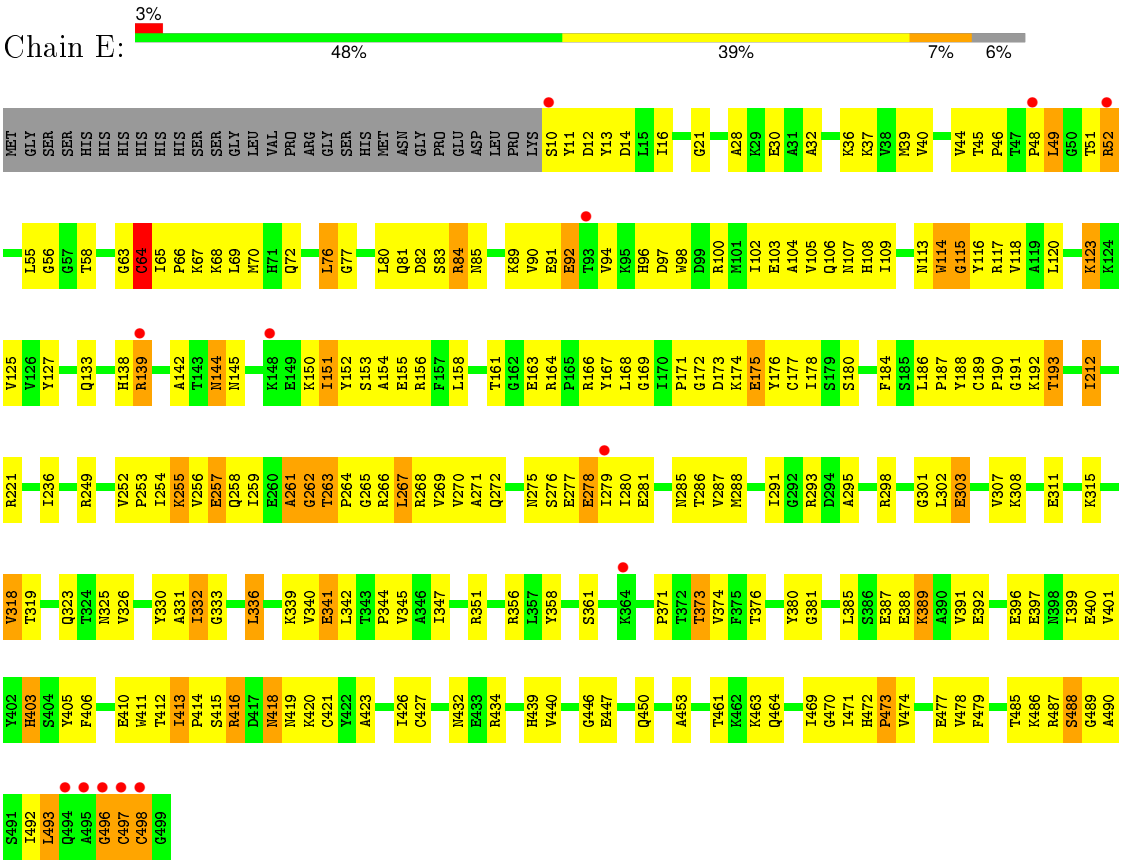
• Molecule 1: THIOREDOXIN REDUCTASE 1

Chain D:

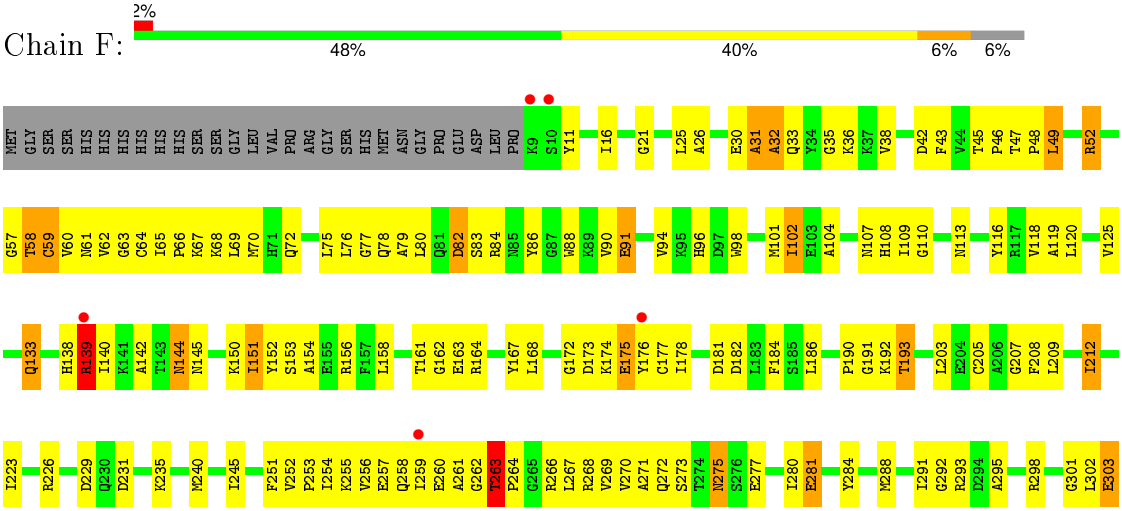


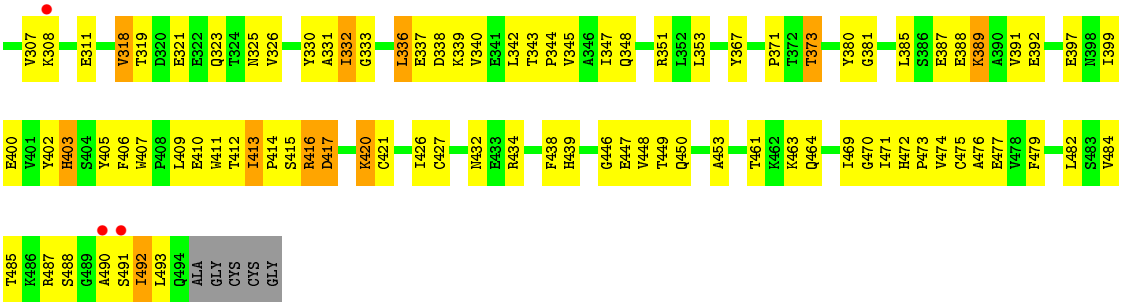


• Molecule 1: THIOREDOXIN REDUCTASE 1



• Molecule 1: THIOREDOXIN REDUCTASE 1




V307 K308 E311 V318 T319 D320 E321 E322 Q323 T324 N325 V326 Y330 A331 I332 G333 L336 E337 D338 K339 V340 E341 L342 T343 P344 V345 A346 I347 Q348 R351 L352 L353 Y367 P371 T372 T373 Y380 G381 L385 S386 E387 E388 K389 A390 V391 E392 E397 N398 I399
E400 V401 Y402 H403 S404 Y405 F406 W407 P408 L409 E410 W411 T412 I413 P414 S415 R416 D417 K420 C421 I426 C427 N432 E433 R434 F438 H439 G446 E447 V448 T449 Q450 A453 T461 K462 K463 Q464 I469 G470 I471 H472 P473 V474 C475 A476 E477 V478 F479 L482 S483 V484
T485 K486 R487 S488 G489 A490 S491 I492 L493 Q494 ALA GLY CYS CYS GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	144.63Å 90.64Å 166.60Å 90.00° 112.46° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 19.99 – 2.80	Depositor EDS
% Data completeness (in resolution range)	92.8 (15.00-2.80) 99.5 (19.99-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.249 , 0.287 0.249 , 0.283	Depositor DCC
R_{free} test set	4866 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	57.1	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 65.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 97692 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	23294	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: NAP, MPD, 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	0.44	0/3830	0.66	1/5187 (0.0%)
1	B	0.44	0/3834	0.66	1/5191 (0.0%)
1	C	0.43	0/3850	0.66	1/5211 (0.0%)
1	D	0.44	0/3859	0.79	4/5222 (0.1%)
1	E	0.41	0/3850	0.64	1/5211 (0.0%)
1	F	0.41	0/3825	0.65	2/5179 (0.0%)
All	All	0.43	0/23048	0.68	10/31201 (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	B	0	1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	139	ARG	NE-CZ-NH2	21.20	130.90	120.30
1	D	139	ARG	NE-CZ-NH1	-20.89	109.86	120.30
1	D	139	ARG	CD-NE-CZ	10.58	138.41	123.60
1	C	263	THR	C-N-CD	6.38	141.81	128.40
1	D	263	THR	C-N-CD	6.08	141.17	128.40
1	B	59	CYS	CA-CB-SG	5.95	124.72	114.00
1	F	263	THR	C-N-CD	5.80	140.59	128.40
1	A	59	CYS	CA-CB-SG	5.50	123.89	114.00
1	E	496	GLY	N-CA-C	5.33	126.42	113.10
1	F	139	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	13	TYR	Sidechain

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	A	3756	0	3764	247	0
1	B	3760	0	3772	261	0
1	C	3776	0	3780	273	0
1	D	3785	0	3793	254	0
1	E	3776	0	3778	325	0
1	F	3751	0	3764	279	0
2	A	53	0	31	4	0
2	B	53	0	31	1	0
2	C	53	0	31	0	0
2	D	53	0	31	5	0
2	E	53	0	31	4	0
2	F	53	0	31	10	0
3	A	48	0	24	1	0
3	B	48	0	24	6	0
3	C	48	0	24	1	0
3	D	48	0	25	4	0
3	E	48	0	25	1	0
3	F	48	0	25	1	0
4	A	8	0	14	2	0
4	B	16	0	28	5	0
4	D	8	0	14	3	0
4	F	8	0	14	5	0
5	A	9	0	0	2	0
5	B	9	0	0	3	0
5	C	7	0	0	1	0
5	D	8	0	0	3	0
5	E	4	0	0	2	0
5	F	7	0	0	2	0
All	All	23294	0	23054	1495	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (1495) 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:F:46:PRO:HG3	1:F:52:ARG:HE	1.15	1.10
1:E:80:LEU:HD23	1:F:80:LEU:HD23	1.34	1.10
1:B:199:SER:HB3	3:B:601:NAP:H52A	1.37	1.05
1:D:418:ASN:HD21	1:D:495:ALA:HB2	1.19	1.05
1:A:199:SER:HB3	3:A:601:NAP:H52A	1.39	1.04
1:E:84:ARG:HH11	1:E:84:ARG:HB2	1.20	1.01
1:E:336:LEU:HD23	1:E:339:LYS:HG3	1.41	1.00
1:E:84:ARG:HB2	1:E:84:ARG:NH1	1.77	1.00
1:B:86:TYR:CD1	1:B:413:ILE:HD11	1.97	0.99
1:E:106:GLN:HE22	1:E:109:ILE:HD12	1.28	0.99
1:A:259:ILE:HD11	1:A:268:ARG:HB2	1.44	0.99
1:F:163:GLU:HG2	1:F:295:ALA:HA	1.43	0.99
1:A:53:TRP:CZ3	1:A:62:VAL:HG11	1.98	0.98
1:E:106:GLN:NE2	1:E:109:ILE:HD12	1.78	0.97
1:C:199:SER:HB3	3:C:601:NAP:H52A	1.43	0.97
1:D:308:LYS:H	1:D:325:ASN:ND2	1.63	0.97
1:B:308:LYS:H	1:B:325:ASN:ND2	1.63	0.96
1:E:308:LYS:H	1:E:325:ASN:ND2	1.63	0.96
1:F:308:LYS:H	1:F:325:ASN:ND2	1.63	0.95
1:C:418:ASN:ND2	1:C:419:ASN:H	1.64	0.95
1:C:308:LYS:H	1:C:325:ASN:ND2	1.64	0.95
1:A:308:LYS:H	1:A:325:ASN:ND2	1.62	0.95
1:B:260:GLU:HB3	1:B:266:ARG:HG3	1.48	0.93
1:F:46:PRO:HG3	1:F:52:ARG:NE	1.82	0.93
1:D:308:LYS:H	1:D:325:ASN:HD21	0.94	0.93
1:E:418:ASN:HD22	1:E:419:ASN:H	1.16	0.93
1:A:308:LYS:N	1:A:325:ASN:HD21	1.67	0.92
1:C:271:ALA:HB3	1:C:280:ILE:HG13	1.52	0.92
1:D:418:ASN:ND2	1:D:495:ALA:HB2	1.83	0.92
1:E:308:LYS:N	1:E:325:ASN:HD21	1.67	0.92
1:C:308:LYS:N	1:C:325:ASN:HD21	1.68	0.92
1:B:308:LYS:N	1:B:325:ASN:HD21	1.68	0.92
1:C:471:ILE:HG21	1:D:373:THR:CG2	1.98	0.92
1:C:308:LYS:H	1:C:325:ASN:HD21	0.94	0.92
1:E:259:ILE:HD11	1:E:268:ARG:HB2	1.52	0.91
1:E:120:LEU:HD13	1:E:127:TYR:HB2	1.51	0.91
1:F:30:GLU:O	1:F:33:GLN:HB3	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:PRO:CG	1:F:52:ARG:HE	1.84	0.91
1:F:308:LYS:N	1:F:325:ASN:HD21	1.67	0.91
1:E:497:CYS:SG	1:E:498:CYS:N	2.44	0.91
1:D:308:LYS:N	1:D:325:ASN:HD21	1.67	0.90
1:F:308:LYS:H	1:F:325:ASN:HD21	0.94	0.90
1:F:340:VAL:HG13	1:F:345:VAL:HG21	1.53	0.90
1:E:308:LYS:HG2	1:E:325:ASN:HD22	1.37	0.90
1:D:255:LYS:HE2	1:D:270:VAL:HG21	1.53	0.89
1:D:418:ASN:HD22	1:D:419:ASN:H	1.20	0.89
1:B:308:LYS:H	1:B:325:ASN:HD21	0.93	0.89
1:A:308:LYS:H	1:A:325:ASN:HD21	0.92	0.88
1:C:418:ASN:HD22	1:C:419:ASN:H	1.17	0.88
1:E:308:LYS:H	1:E:325:ASN:HD21	0.91	0.88
1:F:308:LYS:HG2	1:F:325:ASN:HD22	1.36	0.88
1:C:110:GLY:HA2	1:C:113:ASN:HD22	1.38	0.88
1:E:90:VAL:HG22	1:F:94:VAL:HG21	1.54	0.88
1:A:471:ILE:HG21	1:B:373:THR:CG2	2.04	0.88
1:A:308:LYS:HG2	1:A:325:ASN:HD22	1.40	0.87
1:E:168:LEU:HD23	1:E:291:ILE:HD13	1.55	0.86
1:E:139:ARG:HG3	1:E:151:ILE:HD11	1.56	0.86
1:B:411:TRP:HZ3	1:B:421:CYS:SG	1.98	0.86
1:F:21:GLY:HA3	2:F:600:FAD:H51A	1.57	0.86
1:A:139:ARG:HG3	1:A:151:ILE:HD11	1.57	0.86
1:C:255:LYS:HE2	1:C:270:VAL:HG21	1.57	0.86
1:D:308:LYS:HG2	1:D:325:ASN:HD22	1.41	0.85
1:E:259:ILE:HD11	1:E:268:ARG:HH11	1.41	0.85
1:A:493:LEU:H	1:A:493:LEU:HD12	1.40	0.85
1:E:373:THR:CG2	1:F:471:ILE:HG21	2.05	0.85
1:F:176:TYR:HB3	1:F:267:LEU:HD21	1.58	0.85
1:B:308:LYS:HG2	1:B:325:ASN:HD22	1.41	0.84
1:E:80:LEU:HD13	1:E:94:VAL:HG11	1.59	0.84
1:C:497:CYS:SG	1:C:498:CYS:N	2.50	0.84
1:C:413:ILE:HG13	1:C:414:PRO:HD3	1.60	0.84
1:C:259:ILE:HD11	1:C:268:ARG:HB2	1.59	0.84
1:E:163:GLU:HG2	1:E:295:ALA:HA	1.60	0.83
1:D:139:ARG:HG2	1:D:151:ILE:HD11	1.58	0.83
1:E:413:ILE:HD12	1:F:104:ALA:HB1	1.61	0.83
1:F:139:ARG:HG3	1:F:151:ILE:HD11	1.59	0.83
1:B:139:ARG:HG3	1:B:151:ILE:HD11	1.59	0.82
1:C:85:ASN:HB3	1:C:413:ILE:HD12	1.62	0.82
1:C:139:ARG:HG3	1:C:151:ILE:HD11	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:TRP:CZ3	1:B:421:CYS:SG	2.73	0.81
1:C:268:ARG:HA	1:C:282:GLY:O	1.81	0.81
1:F:253:PRO:HA	1:F:271:ALA:HB2	1.62	0.81
1:E:259:ILE:HB	1:E:266:ARG:O	1.80	0.81
1:B:484:VAL:HG13	1:B:490:ALA:HB3	1.62	0.81
1:D:139:ARG:CG	1:D:151:ILE:HD11	2.11	0.81
1:C:497:CYS:HB2	1:D:112:LEU:HD23	1.64	0.80
1:E:485:THR:HB	5:E:2004:HOH:O	1.80	0.80
1:D:91:GLU:HG3	1:D:93:THR:H	1.47	0.80
1:C:373:THR:CG2	1:D:471:ILE:HG21	2.12	0.80
1:C:89:LYS:NZ	1:D:97:ASP:HB2	1.97	0.80
1:D:418:ASN:HD21	1:D:495:ALA:CB	1.92	0.79
1:C:254:ILE:HD13	1:C:272:GLN:HB2	1.64	0.79
1:C:450:GLN:HE22	1:D:470:GLY:HA2	1.47	0.79
1:A:80:LEU:HD23	1:B:80:LEU:HD23	1.63	0.79
1:C:308:LYS:HG2	1:C:325:ASN:HD22	1.45	0.79
1:A:254:ILE:HG23	1:A:271:ALA:HA	1.63	0.79
1:B:91:GLU:HB2	1:B:93:THR:HG22	1.65	0.79
1:E:471:ILE:HG21	1:F:373:THR:CG2	2.13	0.79
1:D:413:ILE:HG13	1:D:414:PRO:HD3	1.62	0.79
1:D:493:LEU:O	1:D:494:GLN:HG3	1.82	0.79
1:C:471:ILE:HG21	1:D:373:THR:HG23	1.65	0.78
1:D:254:ILE:HG12	1:D:271:ALA:HA	1.65	0.78
1:D:12:ASP:O	1:D:37:LYS:HE2	1.83	0.78
1:B:84:ARG:HH21	1:B:92:GLU:HG3	1.48	0.78
1:B:408:PRO:HD2	1:B:411:TRP:CE3	2.16	0.78
1:B:336:LEU:HB3	1:B:339:LYS:HG3	1.65	0.78
1:B:397:GLU:HA	1:B:487:ARG:NH2	1.97	0.78
1:B:163:GLU:HG2	1:B:295:ALA:HA	1.66	0.78
1:B:263:THR:OG1	1:B:264:PRO:HD2	1.82	0.78
1:E:84:ARG:CB	1:E:84:ARG:HH11	1.97	0.77
1:F:258:GLN:HE22	1:F:261:ALA:HB2	1.49	0.77
1:C:98:TRP:O	1:C:102:ILE:HG12	1.85	0.77
1:D:399:ILE:HD12	1:D:399:ILE:O	1.84	0.77
1:F:254:ILE:HG12	1:F:271:ALA:HA	1.65	0.77
1:E:263:THR:HB	1:E:264:PRO:HD3	1.66	0.76
1:E:418:ASN:ND2	1:E:419:ASN:H	1.84	0.76
1:A:488:SER:O	1:A:490:ALA:N	2.17	0.76
1:D:418:ASN:ND2	1:D:419:ASN:H	1.83	0.76
1:B:406:PHE:CZ	1:B:421:CYS:HB3	2.21	0.76
1:D:13:TYR:CE1	1:D:37:LYS:HE3	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:LYS:HG2	1:E:325:ASN:ND2	2.00	0.76
1:E:418:ASN:HD22	1:E:419:ASN:N	1.83	0.76
1:F:252:VAL:O	1:F:271:ALA:HB1	1.84	0.76
1:C:163:GLU:HG2	1:C:295:ALA:HA	1.66	0.76
1:E:253:PRO:HA	1:E:271:ALA:HB2	1.68	0.76
1:F:340:VAL:CG1	1:F:345:VAL:HG21	2.16	0.75
1:B:259:ILE:HG13	1:B:268:ARG:HB2	1.68	0.75
1:F:75:LEU:HB3	4:F:700:MPD:H51	1.69	0.75
1:A:470:GLY:HA2	1:B:450:GLN:HE22	1.52	0.75
1:F:308:LYS:HG2	1:F:325:ASN:ND2	2.00	0.75
1:C:258:GLN:HE22	1:C:261:ALA:HB2	1.51	0.75
1:B:25:LEU:HD22	1:B:120:LEU:HD11	1.69	0.74
1:A:293:ARG:HD3	5:A:2005:HOH:O	1.86	0.74
1:F:258:GLN:NE2	1:F:261:ALA:HB2	2.02	0.74
1:F:38:VAL:HG23	1:F:125:VAL:HG13	1.68	0.74
1:A:96:HIS:CD2	1:A:212:ILE:HG13	2.22	0.74
1:E:259:ILE:HD11	1:E:268:ARG:NH1	2.02	0.74
1:A:171:PRO:HB2	1:A:255:LYS:HG3	1.68	0.74
1:B:84:ARG:NH2	1:B:92:GLU:HG3	2.01	0.74
1:C:110:GLY:HA2	1:C:113:ASN:ND2	2.03	0.74
1:E:470:GLY:HA2	1:F:450:GLN:HE22	1.51	0.74
1:A:308:LYS:HG2	1:A:325:ASN:ND2	2.03	0.74
1:F:340:VAL:HG11	1:F:345:VAL:HG11	1.68	0.74
1:D:255:LYS:CE	1:D:270:VAL:HG21	2.18	0.74
1:C:278:GLU:HG2	1:C:279:ILE:H	1.51	0.74
1:A:258:GLN:HG3	1:A:260:GLU:O	1.88	0.74
1:C:38:VAL:HG22	1:C:125:VAL:HG13	1.70	0.74
1:F:163:GLU:HG2	1:F:295:ALA:CA	2.18	0.74
1:D:418:ASN:HD22	1:D:419:ASN:N	1.86	0.73
1:E:150:LYS:HD3	1:E:152:TYR:OH	1.88	0.73
1:B:262:GLY:O	1:B:263:THR:C	2.25	0.73
1:C:164:ARG:HG2	1:C:296:CYS:SG	2.28	0.73
1:A:13:TYR:HD1	1:A:37:LYS:HG2	1.52	0.73
1:E:98:TRP:CZ2	1:E:102:ILE:HD11	2.23	0.73
1:E:102:ILE:O	1:E:105:VAL:HG12	1.89	0.73
1:B:380:TYR:OH	1:B:439:HIS:HD2	1.72	0.73
1:A:450:GLN:HE22	1:B:470:GLY:HA2	1.53	0.73
1:A:88:TRP:CZ2	1:B:77:GLY:HA3	2.24	0.72
1:E:84:ARG:NH2	1:E:92:GLU:HA	2.03	0.72
1:B:86:TYR:CD1	1:B:413:ILE:CD1	2.71	0.72
1:E:440:VAL:HB	1:E:479:PHE:HZ	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:LYS:HB3	1:D:270:VAL:CG2	2.18	0.72
1:C:418:ASN:HD22	1:C:419:ASN:N	1.86	0.72
1:A:373:THR:CG2	1:B:471:ILE:HG21	2.20	0.72
1:F:255:LYS:HE2	1:F:257:GLU:HB3	1.70	0.72
1:B:418:ASN:HB2	4:B:701:MPD:HM2	1.70	0.72
1:E:493:LEU:HD12	1:E:493:LEU:N	2.04	0.72
1:A:47:THR:HG23	1:A:51:THR:O	1.89	0.72
1:B:86:TYR:CG	1:B:413:ILE:HD11	2.24	0.72
1:D:308:LYS:HG2	1:D:325:ASN:ND2	2.04	0.72
1:C:402:TYR:CD2	1:C:462:LYS:HE3	2.25	0.71
1:F:273:SER:OG	1:F:275:ASN:HB2	1.91	0.71
1:C:80:LEU:HD23	1:D:80:LEU:HD23	1.70	0.71
1:A:86:TYR:HE2	1:A:414:PRO:HG3	1.55	0.71
1:B:416:ARG:HH11	1:B:416:ARG:HG2	1.55	0.71
1:B:313:THR:OG1	1:B:315:LYS:HG2	1.90	0.71
1:B:259:ILE:HD11	1:B:268:ARG:HG3	1.72	0.71
1:E:106:GLN:HE21	1:E:106:GLN:HA	1.56	0.70
1:E:49:LEU:HD22	1:E:49:LEU:N	2.06	0.70
1:F:344:PRO:O	1:F:347:ILE:HG12	1.90	0.70
1:E:399:ILE:O	1:E:399:ILE:HD12	1.90	0.70
1:B:268:ARG:HH21	1:B:281:GLU:CD	1.94	0.70
1:E:344:PRO:O	1:E:347:ILE:HG12	1.91	0.70
1:B:308:LYS:HG2	1:B:325:ASN:ND2	2.06	0.70
1:D:46:PRO:HG3	1:D:52:ARG:CZ	2.22	0.70
1:B:344:PRO:O	1:B:347:ILE:HG12	1.92	0.70
1:C:418:ASN:ND2	1:C:419:ASN:N	2.39	0.70
1:B:260:GLU:HB3	1:B:266:ARG:CG	2.22	0.70
1:E:485:THR:O	1:E:488:SER:HB3	1.91	0.70
1:A:478:VAL:HG23	4:A:701:MPD:H51	1.72	0.70
1:A:29:LYS:HB2	1:A:29:LYS:NZ	2.07	0.70
1:C:469:ILE:HG21	1:D:345:VAL:HG12	1.73	0.70
1:E:193:THR:HB	1:E:286:THR:HB	1.73	0.69
1:D:315:LYS:HD2	1:D:336:LEU:O	1.92	0.69
1:E:254:ILE:HD11	1:E:270:VAL:HG12	1.75	0.69
1:E:164:ARG:O	1:E:293:ARG:HB3	1.92	0.69
1:F:49:LEU:N	1:F:49:LEU:HD22	2.07	0.69
1:B:419:ASN:HD21	1:B:494:GLN:C	1.96	0.69
1:B:133:GLN:NE2	5:B:2003:HOH:O	2.24	0.69
1:E:36:LYS:HE3	1:E:358:TYR:CD1	2.28	0.69
1:C:373:THR:HG23	1:D:471:ILE:HG21	1.75	0.69
1:A:399:ILE:HD12	1:A:399:ILE:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:470:GLY:HA2	1:D:450:GLN:HE22	1.56	0.69
1:D:260:GLU:OE2	1:D:266:ARG:HD3	1.92	0.69
1:E:106:GLN:HA	1:E:106:GLN:NE2	2.07	0.69
1:A:150:LYS:HD3	1:A:152:TYR:OH	1.93	0.69
1:C:308:LYS:HG2	1:C:325:ASN:ND2	2.07	0.69
1:A:267:LEU:HD12	1:A:267:LEU:N	2.07	0.68
1:E:450:GLN:HE22	1:F:470:GLY:HA2	1.58	0.68
1:D:292:GLY:HA2	3:D:601:NAP:O1A	1.92	0.68
1:A:258:GLN:NE2	1:A:261:ALA:HB2	2.07	0.68
1:C:413:ILE:HG13	1:C:414:PRO:CD	2.23	0.68
1:A:432:ASN:HD22	1:A:463:LYS:NZ	1.92	0.68
1:D:418:ASN:ND2	1:D:419:ASN:N	2.42	0.68
1:D:36:LYS:HE3	1:D:358:TYR:CD1	2.28	0.68
1:D:193:THR:HB	1:D:286:THR:HB	1.76	0.68
1:A:344:PRO:HG3	1:B:472:HIS:HB2	1.74	0.68
1:F:336:LEU:HD23	1:F:339:LYS:HG3	1.75	0.68
1:A:492:ILE:H	1:A:493:LEU:HD12	1.59	0.67
1:A:344:PRO:O	1:A:347:ILE:HG12	1.94	0.67
1:B:315:LYS:HE3	1:B:336:LEU:O	1.94	0.67
1:E:380:TYR:OH	1:E:439:HIS:HD2	1.76	0.67
1:F:339:LYS:HD2	1:F:367:TYR:CD2	2.30	0.67
1:A:471:ILE:HG21	1:B:373:THR:HG23	1.75	0.67
1:C:223:ILE:HG12	1:C:226:ARG:NH2	2.10	0.67
1:F:380:TYR:OH	1:F:439:HIS:HD2	1.77	0.67
1:E:80:LEU:HD23	1:F:80:LEU:CD2	2.21	0.67
1:C:89:LYS:HZ2	1:D:97:ASP:HB2	1.60	0.67
1:E:259:ILE:CD1	1:E:268:ARG:HB2	2.25	0.67
1:C:258:GLN:NE2	1:C:261:ALA:HB2	2.08	0.67
1:B:411:TRP:HZ3	1:B:421:CYS:HG	1.43	0.66
1:E:55:LEU:HD13	1:E:56:GLY:N	2.10	0.66
1:F:150:LYS:HD3	1:F:152:TYR:OH	1.95	0.66
1:B:293:ARG:HD3	5:B:2007:HOH:O	1.95	0.66
1:F:96:HIS:CD2	1:F:212:ILE:HG13	2.30	0.66
1:E:450:GLN:HE22	1:F:471:ILE:H	1.43	0.66
1:F:251:PHE:CE2	1:F:273:SER:HB2	2.30	0.66
1:B:397:GLU:HA	1:B:487:ARG:HH21	1.61	0.66
1:B:416:ARG:HD2	1:B:417:ASP:OD2	1.95	0.66
1:C:406:PHE:CZ	1:C:421:CYS:HB3	2.30	0.66
1:E:96:HIS:CD2	1:E:212:ILE:HG13	2.30	0.66
1:C:170:ILE:HB	1:C:254:ILE:O	1.95	0.66
1:D:150:LYS:HD3	1:D:152:TYR:OH	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:GLU:OE2	1:D:400:GLU:HA	1.94	0.66
1:A:315:LYS:HE3	1:A:336:LEU:O	1.95	0.66
1:E:315:LYS:HD2	1:E:336:LEU:O	1.96	0.66
1:E:103:GLU:HG2	1:E:107:ASN:HD21	1.61	0.66
1:B:339:LYS:HE2	1:B:339:LYS:HA	1.78	0.66
1:A:194:LEU:HD22	1:A:284:TYR:CE1	2.30	0.66
1:A:252:VAL:O	1:A:271:ALA:HB1	1.96	0.66
1:E:418:ASN:ND2	1:E:419:ASN:N	2.44	0.65
1:C:399:ILE:O	1:C:399:ILE:HD12	1.96	0.65
1:E:405:TYR:HE1	1:E:493:LEU:HG	1.61	0.65
1:A:29:LYS:HE3	1:A:119:ALA:HB1	1.78	0.65
1:E:272:GLN:CB	1:E:279:ILE:HG12	2.27	0.65
1:C:344:PRO:O	1:C:347:ILE:HG12	1.96	0.65
1:D:117:ARG:HH11	1:D:117:ARG:HA	1.61	0.65
1:E:373:THR:HB	1:E:381:GLY:HA2	1.79	0.65
1:F:417:ASP:OD1	1:F:420:LYS:HE3	1.96	0.65
1:C:432:ASN:HD22	1:C:463:LYS:NZ	1.93	0.65
1:E:401:VAL:HG11	1:E:486:LYS:HE3	1.78	0.65
1:A:139:ARG:CG	1:A:151:ILE:HD11	2.27	0.65
1:A:13:TYR:CD1	1:A:37:LYS:HG2	2.32	0.65
1:D:96:HIS:CD2	1:D:212:ILE:HG13	2.31	0.65
1:C:334:ASP:HA	1:C:341:GLU:HG3	1.78	0.65
1:A:469:ILE:HG21	1:B:345:VAL:HG12	1.79	0.65
1:D:344:PRO:O	1:D:347:ILE:HG12	1.96	0.65
1:C:259:ILE:HD11	1:C:268:ARG:CB	2.27	0.64
1:A:487:ARG:C	1:A:489:GLY:H	2.01	0.64
1:C:85:ASN:CB	1:C:413:ILE:HD12	2.27	0.64
1:C:150:LYS:HD3	1:C:152:TYR:OH	1.97	0.64
3:E:601:NAP:H6N	3:E:601:NAP:O2N	1.96	0.64
1:C:380:TYR:OH	1:C:439:HIS:HD2	1.81	0.64
1:D:172:GLY:HA2	1:D:175:GLU:CG	2.27	0.64
1:E:139:ARG:CG	1:E:151:ILE:HD11	2.26	0.64
1:F:84:ARG:HG2	1:F:90:VAL:HG12	1.78	0.64
1:C:474:VAL:HG21	1:D:446:GLY:HA3	1.78	0.64
1:D:432:ASN:HD22	1:D:463:LYS:NZ	1.96	0.64
1:B:260:GLU:CB	1:B:266:ARG:HG3	2.26	0.64
1:C:373:THR:HB	1:C:381:GLY:HA2	1.80	0.64
1:E:120:LEU:CD1	1:E:127:TYR:HB2	2.27	0.64
1:E:108:HIS:CD2	1:F:412:THR:HB	2.33	0.64
1:F:31:ALA:O	1:F:33:GLN:N	2.31	0.64
1:D:254:ILE:O	1:D:255:LYS:HB2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:GLU:O	1:E:164:ARG:HG2	1.98	0.64
1:B:432:ASN:HD22	1:B:463:LYS:NZ	1.95	0.64
1:E:104:ALA:HB1	1:F:413:ILE:HD12	1.78	0.64
1:A:95:LYS:HB2	1:B:89:LYS:HD2	1.80	0.64
1:B:373:THR:HB	1:B:381:GLY:HA2	1.80	0.64
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.79	0.64
1:C:123:LYS:O	1:C:124:LYS:HB2	1.96	0.64
1:A:76:LEU:HD23	1:B:86:TYR:CD2	2.32	0.64
1:A:173:ASP:OD1	1:A:174:LYS:N	2.31	0.64
1:F:302:LEU:HD22	1:F:307:VAL:HB	1.80	0.63
1:A:493:LEU:HD12	1:A:493:LEU:N	2.12	0.63
1:C:263:THR:OG1	1:C:264:PRO:CD	2.47	0.63
1:C:172:GLY:HA2	1:C:175:GLU:CG	2.29	0.63
1:E:336:LEU:HD23	1:E:339:LYS:CG	2.22	0.63
1:E:13:TYR:HD1	1:E:37:LYS:HG2	1.64	0.63
1:F:252:VAL:C	1:F:271:ALA:HB1	2.19	0.63
1:D:172:GLY:HA2	1:D:175:GLU:HG2	1.80	0.63
1:F:172:GLY:HA2	1:F:175:GLU:CG	2.29	0.63
1:F:484:VAL:HG13	1:F:490:ALA:HB3	1.80	0.63
1:E:336:LEU:HB3	1:E:339:LYS:HG2	1.79	0.63
1:F:173:ASP:OD1	1:F:174:LYS:N	2.32	0.63
1:E:52:ARG:HH11	1:E:52:ARG:HB2	1.64	0.63
1:B:86:TYR:CE1	1:B:413:ILE:CD1	2.82	0.63
1:F:269:VAL:O	1:F:281:GLU:HA	1.99	0.63
1:B:172:GLY:HA2	1:B:175:GLU:CG	2.28	0.63
1:E:172:GLY:HA2	1:E:175:GLU:CG	2.29	0.63
1:E:172:GLY:HA2	1:E:175:GLU:HG2	1.81	0.63
1:A:191:GLY:O	1:A:193:THR:HG22	1.98	0.63
1:A:461:THR:OG1	1:A:464:GLN:HG3	1.98	0.62
1:B:150:LYS:HD3	1:B:152:TYR:OH	1.99	0.62
1:B:96:HIS:CD2	1:B:212:ILE:HG13	2.35	0.62
1:E:397:GLU:HA	1:E:487:ARG:HH22	1.64	0.62
1:F:406:PHE:O	1:F:421:CYS:HB2	1.98	0.62
1:E:262:GLY:O	1:E:263:THR:C	2.38	0.62
1:C:163:GLU:O	1:C:164:ARG:HD2	1.99	0.62
1:F:25:LEU:HD22	1:F:120:LEU:HD11	1.81	0.62
1:E:261:ALA:O	1:E:262:GLY:O	2.17	0.62
1:F:403:HIS:CE1	1:F:492:ILE:HD13	2.35	0.62
1:D:38:VAL:HG22	1:D:125:VAL:HG13	1.80	0.62
1:F:427:CYS:HA	1:F:434:ARG:O	1.99	0.62
1:A:493:LEU:H	1:A:493:LEU:CD1	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:391:VAL:HG12	1:E:399:ILE:HD11	1.79	0.62
1:A:193:THR:HB	1:A:286:THR:HB	1.82	0.62
1:D:496:GLY:O	1:D:499:GLY:N	2.30	0.62
1:C:450:GLN:HE22	1:D:470:GLY:CA	2.12	0.62
1:F:172:GLY:HA2	1:F:175:GLU:HG2	1.82	0.62
1:D:380:TYR:OH	1:D:439:HIS:HD2	1.81	0.62
1:D:373:THR:HB	1:D:381:GLY:HA2	1.82	0.62
1:E:373:THR:HG22	1:F:471:ILE:HG21	1.80	0.62
1:B:272:GLN:HB2	1:B:279:ILE:HG12	1.81	0.62
1:D:13:TYR:CD1	1:D:37:LYS:HE3	2.35	0.62
1:D:336:LEU:HD23	1:D:339:LYS:HG3	1.81	0.62
1:E:401:VAL:HG22	1:E:426:ILE:HG12	1.81	0.62
1:C:263:THR:OG1	1:C:264:PRO:HD3	2.00	0.62
1:E:168:LEU:CD2	1:E:291:ILE:HD13	2.30	0.61
1:A:172:GLY:HA2	1:A:175:GLU:HG2	1.82	0.61
1:B:196:VAL:HB	1:B:289:LEU:HD23	1.81	0.61
1:C:167:TYR:CD2	1:C:289:LEU:HD12	2.34	0.61
1:E:267:LEU:N	1:E:267:LEU:HD12	2.15	0.61
1:E:470:GLY:CA	1:F:450:GLN:HE22	2.12	0.61
1:A:450:GLN:HE22	1:B:471:ILE:H	1.47	0.61
1:C:477:GLU:HA	1:D:450:GLN:HE21	1.65	0.61
1:E:474:VAL:HG12	1:F:447:GLU:OE1	2.00	0.61
1:D:302:LEU:HD22	1:D:307:VAL:HB	1.82	0.61
1:C:447:GLU:CD	1:D:474:VAL:HG13	2.21	0.61
1:D:13:TYR:O	1:D:154:ALA:HA	1.99	0.61
1:A:419:ASN:OD1	1:A:495:ALA:HB3	2.00	0.61
1:E:471:ILE:H	1:F:450:GLN:HE22	1.48	0.61
1:B:461:THR:OG1	1:B:464:GLN:HG3	2.01	0.61
1:D:250:GLN:HG2	1:D:275:ASN:ND2	2.15	0.61
1:F:256:VAL:HG13	1:F:256:VAL:O	2.01	0.61
1:B:172:GLY:HA2	1:B:175:GLU:HG2	1.81	0.61
1:A:380:TYR:OH	1:A:439:HIS:HD2	1.82	0.61
1:E:432:ASN:HD22	1:E:463:LYS:NZ	1.98	0.61
1:F:263:THR:OG1	1:F:264:PRO:CD	2.48	0.61
1:F:432:ASN:HD22	1:F:463:LYS:NZ	1.98	0.61
1:C:277:GLU:OE1	1:C:277:GLU:O	2.19	0.60
1:F:471:ILE:HA	5:F:2006:HOH:O	2.01	0.60
1:F:139:ARG:CG	1:F:151:ILE:HD11	2.30	0.60
1:F:373:THR:HB	1:F:381:GLY:HA2	1.82	0.60
1:C:251:PHE:CD2	1:C:273:SER:HA	2.36	0.60
1:E:13:TYR:HB3	1:E:37:LYS:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ASP:OD1	1:C:174:LYS:N	2.33	0.60
1:D:173:ASP:OD1	1:D:174:LYS:N	2.35	0.60
1:B:139:ARG:CG	1:B:151:ILE:HD11	2.27	0.60
1:B:92:GLU:C	1:B:94:VAL:H	2.04	0.60
1:D:259:ILE:HD11	1:D:268:ARG:HB2	1.82	0.60
1:C:172:GLY:HA2	1:C:175:GLU:HG2	1.82	0.60
1:F:226:ARG:HG3	1:F:226:ARG:HH11	1.66	0.60
1:E:89:LYS:O	1:F:94:VAL:HG13	2.01	0.60
1:C:139:ARG:CG	1:C:151:ILE:HD11	2.29	0.60
1:C:278:GLU:CG	1:C:279:ILE:H	2.14	0.60
1:E:344:PRO:HG3	1:F:472:HIS:HB2	1.82	0.60
1:A:88:TRP:CZ2	1:B:77:GLY:CA	2.84	0.60
1:D:411:TRP:C	1:D:414:PRO:HD2	2.22	0.60
1:C:250:GLN:HB3	1:C:274:THR:HB	1.84	0.60
1:B:302:LEU:HD22	1:B:307:VAL:HB	1.83	0.60
1:C:498:CYS:SG	1:D:29:LYS:NZ	2.75	0.60
1:A:21:GLY:HA3	2:A:600:FAD:H52A	1.83	0.60
1:A:166:ARG:HB2	1:A:294:ASP:OD2	2.01	0.60
1:B:427:CYS:HA	1:B:434:ARG:O	2.02	0.60
1:F:340:VAL:CG1	1:F:345:VAL:HG11	2.32	0.60
1:C:86:TYR:CE1	1:C:413:ILE:HG12	2.36	0.60
1:E:397:GLU:HA	1:E:487:ARG:NH2	2.17	0.60
1:A:242:GLU:OE2	1:A:420:LYS:NZ	2.35	0.60
1:C:13:TYR:O	1:C:154:ALA:HA	2.02	0.60
1:A:76:LEU:HD13	4:B:700:MPD:H51	1.82	0.60
1:E:472:HIS:ND1	1:E:473:PRO:HA	2.17	0.60
1:A:114:TRP:O	1:A:117:ARG:HB2	2.02	0.60
1:E:80:LEU:CD2	1:F:80:LEU:HD23	2.21	0.59
1:A:470:GLY:CA	1:B:450:GLN:HE22	2.14	0.59
1:B:91:GLU:HB2	1:B:93:THR:CG2	2.32	0.59
1:D:259:ILE:O	1:D:260:GLU:HB2	2.01	0.59
1:E:16:ILE:HG13	1:E:154:ALA:HB2	1.83	0.59
1:D:401:VAL:HG11	1:D:486:LYS:HD2	1.84	0.59
1:B:173:ASP:OD1	1:B:174:LYS:N	2.35	0.59
1:A:186:LEU:HD12	1:A:190:PRO:HG3	1.84	0.59
1:E:173:ASP:OD1	1:E:174:LYS:N	2.35	0.59
1:E:259:ILE:HD11	1:E:268:ARG:CB	2.31	0.59
1:C:432:ASN:HD22	1:C:463:LYS:HZ1	1.50	0.59
1:E:411:TRP:C	1:E:414:PRO:HD2	2.23	0.59
1:D:16:ILE:HG12	1:D:39:MET:HE2	1.83	0.59
1:A:201:VAL:HG22	2:A:600:FAD:HM73	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:403:HIS:NE2	1:F:492:ILE:HD13	2.17	0.59
1:A:172:GLY:HA2	1:A:175:GLU:CG	2.32	0.59
1:C:401:VAL:HG11	1:C:486:LYS:HD2	1.84	0.59
1:F:58:THR:HG22	1:F:59:CYS:N	2.17	0.59
1:D:16:ILE:HG13	1:D:154:ALA:HB2	1.84	0.59
1:E:474:VAL:HG13	1:F:447:GLU:CD	2.23	0.59
1:C:302:LEU:HD22	1:C:307:VAL:HB	1.85	0.59
1:E:191:GLY:O	1:E:193:THR:HG22	2.02	0.59
1:B:49:LEU:HD22	1:B:49:LEU:N	2.16	0.59
1:B:292:GLY:HA3	3:B:601:NAP:O2N	2.02	0.59
1:A:267:LEU:CD1	1:A:267:LEU:N	2.65	0.59
1:C:472:HIS:ND1	1:C:473:PRO:HA	2.18	0.59
1:A:263:THR:OG1	1:A:264:PRO:HD3	2.03	0.59
3:B:601:NAP:O1A	3:B:601:NAP:H52N	2.02	0.59
1:A:77:GLY:HA3	1:B:88:TRP:CZ2	2.37	0.59
1:F:16:ILE:HG13	1:F:154:ALA:HB2	1.84	0.59
1:A:192:LYS:HE2	1:A:284:TYR:CD2	2.38	0.59
1:D:344:PRO:HD3	2:D:600:FAD:O2	2.03	0.59
1:F:402:TYR:HB3	1:F:482:LEU:HB3	1.83	0.59
1:E:280:ILE:HD12	1:E:281:GLU:H	1.65	0.59
1:C:256:VAL:HG13	1:C:269:VAL:HG22	1.83	0.58
1:A:450:GLN:NE2	1:B:471:ILE:H	2.01	0.58
1:F:48:PRO:HG2	1:F:167:TYR:CE1	2.38	0.58
1:E:180:SER:HA	1:E:288:MET:CE	2.33	0.58
1:E:272:GLN:HB2	1:E:279:ILE:HG12	1.85	0.58
1:E:302:LEU:HD22	1:E:307:VAL:HB	1.84	0.58
1:F:397:GLU:HA	1:F:487:ARG:HH22	1.67	0.58
1:C:345:VAL:HG12	1:D:469:ILE:HG21	1.85	0.58
1:E:76:LEU:HD23	1:F:86:TYR:CD2	2.38	0.58
1:F:407:TRP:CZ2	1:F:412:THR:HA	2.38	0.58
1:B:319:THR:HG23	1:B:323:GLN:O	2.04	0.58
1:E:450:GLN:NE2	1:F:471:ILE:H	2.00	0.58
1:A:270:VAL:HG22	1:A:281:GLU:HB3	1.84	0.58
1:E:471:ILE:H	1:F:450:GLN:NE2	2.01	0.58
1:A:373:THR:HB	1:A:381:GLY:HA2	1.84	0.58
1:C:191:GLY:O	1:C:193:THR:HG22	2.04	0.58
1:E:123:LYS:NZ	1:E:123:LYS:HB2	2.17	0.58
1:F:484:VAL:HG13	1:F:490:ALA:CB	2.34	0.58
1:C:259:ILE:CD1	1:C:268:ARG:HB2	2.30	0.58
1:D:12:ASP:HB2	1:D:153:SER:H	1.68	0.58
1:E:70:MET:HE1	1:E:184:PHE:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:255:LYS:HB3	1:D:270:VAL:HG23	1.84	0.58
1:B:338:ASP:O	1:B:339:LYS:HE3	2.04	0.58
1:E:186:LEU:HD12	1:E:190:PRO:HG3	1.86	0.58
1:E:102:ILE:O	1:E:106:GLN:HG2	2.03	0.58
1:D:385:LEU:HD22	1:D:389:LYS:HG3	1.86	0.58
1:F:319:THR:HG23	1:F:323:GLN:O	2.03	0.58
1:D:70:MET:HE1	1:D:184:PHE:HA	1.84	0.58
1:B:91:GLU:CB	1:B:93:THR:HG22	2.32	0.58
1:E:263:THR:CB	1:E:264:PRO:HD3	2.32	0.58
1:A:450:GLN:HE22	1:B:470:GLY:CA	2.15	0.58
1:E:440:VAL:HB	1:E:479:PHE:CZ	2.37	0.58
1:E:275:ASN:OD1	1:E:276:SER:N	2.37	0.58
1:A:302:LEU:HD22	1:A:307:VAL:HB	1.86	0.58
1:B:254:ILE:HD11	1:B:270:VAL:HG12	1.85	0.58
1:D:427:CYS:HA	1:D:434:ARG:O	2.04	0.58
1:B:266:ARG:NH2	1:B:283:GLU:OE2	2.37	0.57
1:E:450:GLN:HE22	1:F:470:GLY:CA	2.16	0.57
1:C:194:LEU:HD22	1:C:284:TYR:CE1	2.38	0.57
1:A:70:MET:HE3	1:A:184:PHE:HD1	1.69	0.57
1:B:411:TRP:C	1:B:414:PRO:HD2	2.24	0.57
1:C:259:ILE:HG22	1:C:259:ILE:O	2.02	0.57
1:A:171:PRO:HB2	1:A:255:LYS:CG	2.34	0.57
1:A:446:GLY:HA3	1:B:474:VAL:HG21	1.86	0.57
1:D:339:LYS:HD2	1:D:367:TYR:CE2	2.39	0.57
1:D:117:ARG:HH11	1:D:117:ARG:CA	2.17	0.57
1:F:186:LEU:HD12	1:F:190:PRO:HG3	1.86	0.57
1:C:417:ASP:N	1:C:417:ASP:OD2	2.35	0.57
1:C:44:VAL:HG11	1:C:53:TRP:CE2	2.39	0.57
1:D:418:ASN:CG	1:D:495:ALA:HB2	2.24	0.57
1:A:194:LEU:HD22	1:A:284:TYR:HE1	1.68	0.57
1:B:401:VAL:HB	1:B:486:LYS:HG3	1.87	0.57
1:D:262:GLY:O	1:D:263:THR:C	2.42	0.57
1:F:413:ILE:HG23	1:F:414:PRO:HD3	1.84	0.57
1:D:81:GLN:OE1	1:D:84:ARG:NH2	2.32	0.57
1:B:396:GLU:OE2	1:B:487:ARG:NH2	2.37	0.57
1:C:461:THR:OG1	1:C:464:GLN:HG3	2.05	0.57
1:D:319:THR:HG23	1:D:323:GLN:O	2.05	0.57
1:B:46:PRO:HA	1:B:51:THR:O	2.04	0.57
1:E:413:ILE:HD12	1:F:104:ALA:CB	2.33	0.57
1:E:97:ASP:OD2	1:E:100:ARG:HB2	2.04	0.57
1:E:345:VAL:HG12	1:F:469:ILE:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ASN:CB	4:B:701:MPD:HM2	2.34	0.57
1:E:49:LEU:H	1:E:49:LEU:CD2	2.18	0.57
1:E:49:LEU:CD2	1:E:49:LEU:N	2.68	0.57
1:B:166:ARG:HG3	5:B:2006:HOH:O	2.05	0.57
1:E:178:ILE:O	1:E:288:MET:HA	2.05	0.57
1:C:427:CYS:HA	1:C:434:ARG:O	2.04	0.57
1:F:38:VAL:CG2	1:F:125:VAL:HG13	2.33	0.57
1:B:191:GLY:O	1:B:193:THR:HG22	2.05	0.56
1:E:413:ILE:HG23	1:E:414:PRO:HD3	1.87	0.56
1:E:478:VAL:HG13	1:E:479:PHE:N	2.20	0.56
1:C:278:GLU:O	1:C:279:ILE:HG13	2.05	0.56
1:E:163:GLU:HG2	1:E:295:ALA:CA	2.34	0.56
1:D:339:LYS:HD2	1:D:367:TYR:CD2	2.40	0.56
1:A:432:ASN:HD22	1:A:463:LYS:HZ1	1.52	0.56
1:E:474:VAL:CG1	1:F:447:GLU:CD	2.74	0.56
1:C:186:LEU:HD12	1:C:190:PRO:HG3	1.87	0.56
1:F:48:PRO:C	1:F:49:LEU:HD13	2.26	0.56
1:F:448:VAL:HG22	1:F:476:ALA:HB2	1.88	0.56
1:C:76:LEU:HD23	1:D:86:TYR:CD2	2.41	0.56
1:F:403:HIS:CD2	1:F:492:ILE:HG21	2.40	0.56
1:D:432:ASN:HD22	1:D:463:LYS:HZ1	1.54	0.56
1:B:272:GLN:HG2	1:B:273:SER:O	2.05	0.56
1:E:259:ILE:HG22	1:E:259:ILE:O	2.05	0.56
1:A:450:GLN:NE2	1:B:470:GLY:HA2	2.20	0.56
1:D:259:ILE:CD1	1:D:268:ARG:HB2	2.36	0.56
1:B:267:LEU:HD23	1:B:287:VAL:HG23	1.87	0.56
1:E:416:ARG:HH11	1:E:416:ARG:HG2	1.71	0.56
1:C:70:MET:HE1	1:C:184:PHE:HA	1.88	0.56
1:A:192:LYS:HE2	1:A:284:TYR:HD2	1.71	0.56
1:E:123:LYS:HZ3	1:E:123:LYS:HB2	1.71	0.56
1:F:82:ASP:CG	1:F:416:ARG:HH12	2.09	0.55
1:C:255:LYS:HB3	1:C:270:VAL:CG2	2.36	0.55
1:E:470:GLY:HA2	1:F:450:GLN:NE2	2.21	0.55
1:E:254:ILE:O	1:E:255:LYS:HB2	2.06	0.55
1:E:171:PRO:HB2	1:E:255:LYS:HG3	1.89	0.55
1:B:416:ARG:CD	1:B:417:ASP:OD2	2.54	0.55
1:F:266:ARG:C	1:F:267:LEU:HD12	2.26	0.55
1:E:262:GLY:O	1:E:263:THR:O	2.24	0.55
1:E:252:VAL:O	1:E:271:ALA:HB1	2.06	0.55
1:D:250:GLN:HG2	1:D:275:ASN:HD21	1.71	0.55
1:C:16:ILE:HG13	1:C:154:ALA:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:CYS:HB2	1:D:447:GLU:OE2	2.07	0.55
1:B:406:PHE:CE1	1:B:421:CYS:HB3	2.41	0.55
1:C:192:LYS:H	1:C:285:ASN:HD22	1.54	0.55
1:C:450:GLN:NE2	1:D:470:GLY:HA2	2.19	0.55
1:B:93:THR:O	1:B:93:THR:OG1	2.25	0.55
1:B:259:ILE:CG1	1:B:268:ARG:HB2	2.36	0.55
1:B:416:ARG:HG2	1:B:416:ARG:NH1	2.20	0.55
1:C:319:THR:HG23	1:C:323:GLN:O	2.06	0.55
1:E:410:GLU:OE2	1:F:68:LYS:HE2	2.06	0.55
1:E:427:CYS:HA	1:E:434:ARG:O	2.07	0.55
1:E:319:THR:HG23	1:E:323:GLN:O	2.06	0.55
1:E:55:LEU:O	1:E:113:ASN:ND2	2.40	0.55
1:C:273:SER:HB2	1:C:278:GLU:HB3	1.89	0.55
1:C:278:GLU:HG2	1:C:279:ILE:N	2.20	0.55
1:F:263:THR:OG1	1:F:264:PRO:HD3	2.07	0.55
1:F:411:TRP:CZ3	1:F:421:CYS:SG	2.99	0.55
1:A:427:CYS:HA	1:A:434:ARG:O	2.06	0.55
1:F:235:LYS:NZ	1:F:405:TYR:OH	2.40	0.55
1:C:50:GLY:O	1:C:51:THR:C	2.45	0.55
1:E:49:LEU:H	1:E:49:LEU:HD22	1.72	0.55
1:A:123:LYS:HB2	1:A:123:LYS:NZ	2.21	0.55
1:E:272:GLN:HB3	1:E:279:ILE:HG12	1.89	0.55
1:F:461:THR:OG1	1:F:464:GLN:HG3	2.06	0.55
1:A:477:GLU:HA	1:B:450:GLN:HE21	1.71	0.55
1:F:57:GLY:HA2	2:F:600:FAD:H3B	1.89	0.55
1:F:151:ILE:HD13	1:F:152:TYR:N	2.22	0.55
1:E:472:HIS:HB2	1:F:344:PRO:HG3	1.87	0.55
1:E:279:ILE:HG22	1:E:280:ILE:N	2.21	0.55
1:D:343:THR:OG1	2:D:600:FAD:H2'	2.07	0.55
1:C:388:GLU:O	1:C:391:VAL:HG22	2.07	0.55
1:F:191:GLY:O	1:F:193:THR:HG22	2.07	0.55
1:B:186:LEU:HD12	1:B:190:PRO:HG3	1.87	0.55
1:F:266:ARG:O	1:F:267:LEU:HD12	2.07	0.54
1:C:497:CYS:HB3	1:D:115:GLY:HA3	1.88	0.54
1:F:226:ARG:HG3	1:F:226:ARG:NH1	2.21	0.54
1:C:408:PRO:HG3	1:C:475:CYS:SG	2.48	0.54
1:B:30:GLU:O	1:B:33:GLN:HB3	2.07	0.54
1:D:48:PRO:HG2	1:D:167:TYR:CE1	2.42	0.54
1:A:112:LEU:O	1:A:113:ASN:C	2.45	0.54
1:C:470:GLY:CA	1:D:450:GLN:HE22	2.20	0.54
1:B:263:THR:OG1	1:B:264:PRO:CD	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HG13	1:A:154:ALA:HB2	1.89	0.54
1:B:12:ASP:HB2	1:B:153:SER:O	2.07	0.54
1:C:450:GLN:HE22	1:D:471:ILE:H	1.56	0.54
1:F:167:TYR:CE2	1:F:174:LYS:HA	2.43	0.54
1:B:487:ARG:O	1:B:487:ARG:HG2	2.08	0.54
1:D:259:ILE:HG22	1:D:259:ILE:O	2.08	0.54
1:C:472:HIS:HB2	1:D:344:PRO:HG3	1.88	0.54
1:E:461:THR:OG1	1:E:464:GLN:HG3	2.07	0.54
1:E:192:LYS:H	1:E:285:ASN:HD22	1.53	0.54
1:C:448:VAL:HG22	1:C:476:ALA:HB2	1.89	0.54
1:A:319:THR:HG23	1:A:323:GLN:O	2.08	0.54
1:A:450:GLN:HE22	1:B:471:ILE:N	2.05	0.54
1:E:151:ILE:HD13	1:E:152:TYR:N	2.23	0.54
1:D:191:GLY:O	1:D:193:THR:HG22	2.08	0.54
1:D:400:GLU:OE1	1:D:487:ARG:HD2	2.08	0.54
1:F:25:LEU:HD13	1:F:116:TYR:CD1	2.43	0.54
1:C:86:TYR:CD2	1:C:413:ILE:HD11	2.43	0.54
1:C:259:ILE:HD12	1:C:283:GLU:OE1	2.08	0.54
1:A:254:ILE:HG12	1:A:270:VAL:O	2.07	0.54
1:C:447:GLU:CD	1:D:474:VAL:CG1	2.75	0.54
1:F:262:GLY:O	1:F:263:THR:O	2.26	0.54
1:E:32:ALA:HB2	1:E:125:VAL:HG22	1.90	0.54
1:A:170:ILE:HD12	1:A:255:LYS:HA	1.89	0.54
1:D:156:ARG:HG3	1:D:156:ARG:HH11	1.72	0.54
1:D:273:SER:OG	1:D:276:SER:HB3	2.08	0.54
1:E:105:VAL:HG13	1:E:106:GLN:N	2.23	0.54
1:D:472:HIS:ND1	1:D:473:PRO:HA	2.23	0.54
1:E:403:HIS:CD2	1:E:492:ILE:HG21	2.43	0.54
1:A:36:LYS:HE3	1:A:358:TYR:CD1	2.43	0.54
1:C:450:GLN:NE2	1:D:471:ILE:H	2.07	0.53
1:B:70:MET:HE3	1:B:184:PHE:HD1	1.73	0.53
1:A:260:GLU:HB2	1:A:266:ARG:HB2	1.91	0.53
1:F:42:ASP:OD1	2:F:600:FAD:H1B	2.08	0.53
1:A:388:GLU:O	1:A:391:VAL:HG22	2.08	0.53
1:E:387:GLU:OE2	1:E:486:LYS:NZ	2.41	0.53
1:A:263:THR:OG1	1:A:264:PRO:CD	2.57	0.53
1:C:259:ILE:O	1:C:260:GLU:HB2	2.07	0.53
1:F:253:PRO:HA	1:F:271:ALA:CB	2.36	0.53
1:B:336:LEU:HD23	1:B:339:LYS:HG3	1.91	0.53
1:E:493:LEU:CD1	1:E:493:LEU:N	2.70	0.53
1:C:263:THR:O	1:C:265:GLY:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:387:GLU:OE2	1:C:486:LYS:NZ	2.41	0.53
1:B:156:ARG:HH11	1:B:156:ARG:HG3	1.73	0.53
1:E:11:TYR:CZ	1:E:155:GLU:HA	2.43	0.53
1:E:85:ASN:C	1:E:413:ILE:HD11	2.29	0.53
1:F:49:LEU:H	1:F:49:LEU:HD22	1.74	0.53
1:F:84:ARG:CG	1:F:90:VAL:HG12	2.37	0.53
1:B:86:TYR:CE1	1:B:413:ILE:HD13	2.44	0.53
1:E:55:LEU:HD13	1:E:56:GLY:H	1.73	0.53
1:C:139:ARG:NH1	5:C:2003:HOH:O	2.41	0.53
1:F:49:LEU:HD11	1:F:174:LYS:O	2.08	0.53
1:E:12:ASP:HB2	1:E:153:SER:O	2.08	0.53
1:C:86:TYR:CD2	1:D:76:LEU:HD23	2.42	0.53
1:F:151:ILE:HD13	1:F:151:ILE:C	2.29	0.53
1:A:400:GLU:OE1	1:A:487:ARG:NH1	2.42	0.53
1:C:412:THR:HG21	1:D:108:HIS:CE1	2.43	0.53
1:A:254:ILE:HG12	1:A:270:VAL:HG12	1.89	0.53
1:E:278:GLU:HG2	1:E:279:ILE:N	2.24	0.53
1:D:488:SER:O	1:D:490:ALA:N	2.41	0.53
1:E:450:GLN:HE22	1:F:471:ILE:N	2.07	0.53
1:D:413:ILE:HG13	1:D:414:PRO:CD	2.35	0.53
1:A:347:ILE:O	1:A:351:ARG:HG3	2.09	0.53
1:B:325:ASN:OD1	1:B:326:VAL:HG23	2.09	0.52
1:F:162:GLY:HA3	2:F:600:FAD:O1A	2.08	0.52
1:E:450:GLN:HE21	1:F:477:GLU:HA	1.74	0.52
1:A:400:GLU:HA	1:A:400:GLU:OE2	2.08	0.52
1:A:318:VAL:HG13	1:A:319:THR:O	2.09	0.52
1:D:186:LEU:HD12	1:D:190:PRO:HG3	1.90	0.52
1:D:423:ALA:HB1	1:D:479:PHE:CZ	2.44	0.52
1:B:388:GLU:O	1:B:391:VAL:HG22	2.09	0.52
1:A:76:LEU:CD2	1:B:86:TYR:CD2	2.92	0.52
1:B:373:THR:HG21	1:B:446:GLY:HA2	1.89	0.52
1:C:86:TYR:CZ	1:C:413:ILE:HG12	2.45	0.52
1:E:280:ILE:HG13	1:E:281:GLU:N	2.25	0.52
1:C:347:ILE:O	1:C:351:ARG:HG3	2.10	0.52
1:D:496:GLY:O	1:D:497:CYS:C	2.46	0.52
1:A:263:THR:CB	1:A:264:PRO:HD3	2.39	0.52
1:D:388:GLU:O	1:D:391:VAL:HG22	2.08	0.52
1:B:35:GLY:O	1:B:36:LYS:C	2.47	0.52
1:A:53:TRP:HH2	1:A:181:ASP:CG	2.13	0.52
1:D:139:ARG:HG3	1:D:151:ILE:HD11	1.88	0.52
1:D:91:GLU:HG3	1:D:93:THR:N	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:373:THR:HG23	1:F:471:ILE:HG21	1.86	0.52
1:F:272:GLN:HE21	1:F:277:GLU:HA	1.75	0.52
1:F:110:GLY:HA2	1:F:113:ASN:HD22	1.75	0.52
1:C:471:ILE:CG2	1:D:373:THR:HG23	2.36	0.52
1:A:404:SER:HA	1:A:492:ILE:HD12	1.92	0.52
1:C:258:GLN:HE21	1:C:260:GLU:C	2.12	0.52
1:C:373:THR:HG21	1:C:446:GLY:HA2	1.91	0.52
1:D:106:GLN:HA	1:D:109:ILE:HD12	1.92	0.52
1:B:262:GLY:O	1:B:263:THR:O	2.27	0.52
1:D:292:GLY:HA3	3:D:601:NAP:O2A	2.10	0.52
1:E:356:ARG:HG2	1:E:361:SER:O	2.08	0.52
1:B:251:PHE:CE2	1:B:280:ILE:HD12	2.44	0.52
1:F:325:ASN:OD1	1:F:326:VAL:HG23	2.10	0.52
1:C:151:ILE:HD13	1:C:151:ILE:C	2.30	0.52
1:A:385:LEU:HD22	1:A:389:LYS:HG3	1.91	0.52
1:D:461:THR:OG1	1:D:464:GLN:HG3	2.09	0.52
1:C:192:LYS:N	1:C:285:ASN:HD22	2.08	0.52
1:D:340:VAL:HG11	1:D:370:VAL:HG21	1.92	0.52
1:D:348:GLN:NE2	1:D:351:ARG:HH12	2.08	0.52
1:F:21:GLY:CA	2:F:600:FAD:H51A	2.36	0.52
1:C:194:LEU:HB2	1:C:284:TYR:CE1	2.45	0.52
1:E:388:GLU:O	1:E:391:VAL:HG22	2.10	0.52
1:A:472:HIS:ND1	1:A:473:PRO:HA	2.25	0.52
1:D:221:ARG:HH21	3:D:601:NAP:P2B	2.33	0.52
1:A:32:ALA:O	1:A:34:TYR:N	2.43	0.52
1:B:493:LEU:N	1:B:493:LEU:HD12	2.25	0.52
1:D:408:PRO:O	1:D:409:LEU:C	2.49	0.51
1:E:263:THR:CB	1:E:264:PRO:CD	2.87	0.51
1:E:98:TRP:CE2	1:E:102:ILE:HD11	2.45	0.51
1:C:255:LYS:HE3	1:C:257:GLU:HG3	1.91	0.51
1:C:255:LYS:HB3	1:C:270:VAL:HG21	1.92	0.51
1:E:85:ASN:O	1:E:413:ILE:HD11	2.09	0.51
1:A:123:LYS:HZ2	1:A:123:LYS:HB2	1.75	0.51
1:F:25:LEU:CD2	1:F:120:LEU:HD11	2.41	0.51
1:E:114:TRP:O	1:E:117:ARG:N	2.43	0.51
1:A:348:GLN:HG3	1:B:469:ILE:HD12	1.92	0.51
1:E:30:GLU:HG3	1:E:351:ARG:HA	1.92	0.51
1:B:114:TRP:CE2	1:B:117:ARG:NH2	2.74	0.51
1:E:291:ILE:HG13	1:E:291:ILE:O	2.10	0.51
1:F:343:THR:OG1	2:F:600:FAD:H2'	2.10	0.51
1:C:254:ILE:CD1	1:C:272:GLN:HB2	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:VAL:HG13	1:E:345:VAL:HG21	1.92	0.51
1:E:115:GLY:O	1:E:118:VAL:HB	2.10	0.51
1:E:104:ALA:CB	1:F:413:ILE:HD12	2.41	0.51
1:A:470:GLY:HA2	1:B:450:GLN:NE2	2.23	0.51
1:A:29:LYS:HD2	1:A:123:LYS:HZ2	1.75	0.51
1:C:344:PRO:HG3	1:D:472:HIS:HB2	1.92	0.51
1:E:169:GLY:N	1:E:173:ASP:OD2	2.44	0.51
1:A:411:TRP:CZ3	1:A:421:CYS:SG	3.03	0.51
1:C:318:VAL:HG13	1:C:319:THR:O	2.11	0.51
1:E:256:VAL:HG23	1:E:269:VAL:HG22	1.91	0.51
1:F:271:ALA:O	1:F:280:ILE:HG12	2.11	0.51
1:F:474:VAL:HG12	1:F:475:CYS:N	2.26	0.51
1:A:273:SER:OG	1:A:275:ASN:N	2.44	0.51
1:E:84:ARG:HH21	1:E:92:GLU:HA	1.74	0.51
1:C:151:ILE:HD13	1:C:152:TYR:N	2.25	0.51
1:D:85:ASN:HB2	1:D:413:ILE:CD1	2.41	0.51
1:C:173:ASP:O	1:C:177:CYS:HB2	2.10	0.51
1:A:146:LYS:HE2	1:C:187:PRO:O	2.11	0.51
1:C:258:GLN:HE21	1:C:261:ALA:N	2.09	0.51
1:C:222:SER:OG	1:C:226:ARG:NH2	2.43	0.51
1:A:487:ARG:C	1:A:489:GLY:N	2.65	0.51
1:A:151:ILE:HD13	1:A:151:ILE:C	2.31	0.50
1:C:98:TRP:NE1	1:C:102:ILE:HG13	2.25	0.50
1:B:416:ARG:HD2	1:B:417:ASP:CG	2.31	0.50
1:D:318:VAL:HG13	1:D:319:THR:O	2.11	0.50
1:A:156:ARG:HD3	1:A:330:TYR:HE2	1.76	0.50
1:D:325:ASN:OD1	1:D:326:VAL:HG23	2.10	0.50
1:C:325:ASN:OD1	1:C:326:VAL:HG23	2.12	0.50
1:E:474:VAL:CG1	1:F:447:GLU:OE1	2.59	0.50
1:A:471:ILE:H	1:B:450:GLN:HE22	1.58	0.50
1:E:151:ILE:C	1:E:151:ILE:HD13	2.32	0.50
1:A:201:VAL:HG13	2:A:600:FAD:HM73	1.92	0.50
1:E:46:PRO:HG3	1:E:52:ARG:CZ	2.41	0.50
1:E:385:LEU:HD22	1:E:389:LYS:HG3	1.93	0.50
1:E:164:ARG:NH1	1:E:164:ARG:HG3	2.27	0.50
1:E:48:PRO:HB2	1:E:49:LEU:HD22	1.93	0.50
1:D:348:GLN:NE2	1:D:351:ARG:NH1	2.58	0.50
4:D:700:MPD:H11	4:D:700:MPD:O4	2.12	0.50
1:F:156:ARG:HH11	1:F:156:ARG:HG3	1.77	0.50
1:E:168:LEU:HD21	1:E:291:ILE:HG21	1.93	0.50
1:D:13:TYR:HA	1:D:37:LYS:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:GLU:OE1	1:D:474:VAL:HG12	2.12	0.50
1:E:318:VAL:HG13	1:E:319:THR:O	2.12	0.50
1:E:28:ALA:HB2	1:E:40:VAL:CG2	2.42	0.50
1:D:418:ASN:OD1	1:D:495:ALA:HB2	2.12	0.50
1:E:471:ILE:N	1:F:450:GLN:HE22	2.09	0.50
1:B:418:ASN:ND2	1:B:419:ASN:H	2.09	0.50
1:B:432:ASN:HD22	1:B:463:LYS:HZ1	1.58	0.50
1:D:168:LEU:HD13	1:D:253:PRO:HB2	1.93	0.50
1:A:128:GLU:CD	1:C:100:ARG:HH12	2.15	0.50
1:A:325:ASN:OD1	1:A:326:VAL:HG23	2.11	0.50
1:A:94:VAL:HG11	1:B:90:VAL:HG22	1.94	0.50
1:B:340:VAL:HG13	1:B:345:VAL:HG21	1.94	0.50
1:A:266:ARG:C	1:A:267:LEU:HD12	2.32	0.50
1:E:266:ARG:HB2	1:E:266:ARG:HH11	1.76	0.50
1:C:259:ILE:O	1:C:260:GLU:CB	2.59	0.50
1:C:259:ILE:HD11	1:C:268:ARG:HD2	1.93	0.50
1:D:151:ILE:HD13	1:D:152:TYR:N	2.26	0.50
1:D:387:GLU:HA	1:D:426:ILE:HD13	1.93	0.50
1:B:55:LEU:HD23	1:B:56:GLY:H	1.76	0.50
1:A:53:TRP:CH2	1:A:62:VAL:HG11	2.45	0.49
1:B:176:TYR:CE1	1:B:258:GLN:HB2	2.47	0.49
4:A:701:MPD:O4	4:A:701:MPD:HM1	2.12	0.49
1:E:114:TRP:O	1:E:116:TYR:N	2.44	0.49
1:B:387:GLU:HA	1:B:426:ILE:HD13	1.93	0.49
1:D:374:VAL:HG12	1:D:376:THR:HG23	1.94	0.49
1:D:373:THR:HG21	1:D:446:GLY:HA2	1.93	0.49
1:F:251:PHE:CZ	1:F:273:SER:HB2	2.46	0.49
1:E:387:GLU:HA	1:E:426:ILE:HD13	1.93	0.49
1:A:32:ALA:C	1:A:34:TYR:H	2.16	0.49
1:B:151:ILE:HD13	1:B:152:TYR:N	2.27	0.49
1:D:406:PHE:CZ	1:D:421:CYS:HB3	2.47	0.49
1:E:400:GLU:OE1	1:E:487:ARG:HD2	2.13	0.49
1:E:487:ARG:O	1:E:489:GLY:N	2.46	0.49
1:E:167:TYR:CE2	1:E:174:LYS:HA	2.47	0.49
1:F:318:VAL:HG13	1:F:319:THR:O	2.13	0.49
1:B:46:PRO:HG3	1:B:52:ARG:HB3	1.95	0.49
1:C:331:ALA:O	1:C:332:ILE:HD12	2.13	0.49
1:D:356:ARG:HG2	1:D:361:SER:O	2.13	0.49
1:F:331:ALA:O	1:F:332:ILE:HD12	2.13	0.49
1:C:400:GLU:OE1	1:C:487:ARG:NH1	2.45	0.49
1:C:259:ILE:HG22	1:C:266:ARG:HH21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:254:ILE:HG12	1:E:271:ALA:HA	1.95	0.49
1:C:402:TYR:CE2	1:C:462:LYS:HE3	2.47	0.49
1:E:96:HIS:HB2	1:F:88:TRP:CZ3	2.48	0.49
1:E:432:ASN:HD22	1:E:463:LYS:HZ1	1.60	0.49
1:F:263:THR:CB	1:F:264:PRO:HD3	2.43	0.49
1:B:167:TYR:CE2	1:B:174:LYS:HG2	2.48	0.49
1:B:194:LEU:HB2	1:B:284:TYR:CE2	2.47	0.49
1:B:200:TYR:CD2	1:B:201:VAL:N	2.80	0.49
1:B:258:GLN:O	1:B:258:GLN:CG	2.60	0.49
1:E:389:LYS:HD3	1:E:389:LYS:O	2.12	0.49
1:B:16:ILE:HG13	1:B:154:ALA:HB2	1.94	0.49
1:E:373:THR:HG21	1:E:446:GLY:HA2	1.95	0.49
1:D:173:ASP:O	1:D:177:CYS:HB2	2.12	0.49
1:B:193:THR:HB	1:B:286:THR:HB	1.95	0.49
1:E:301:GLY:HA2	1:E:303:GLU:OE2	2.13	0.49
1:A:253:PRO:HA	1:A:271:ALA:HB2	1.95	0.49
1:D:85:ASN:HB2	1:D:413:ILE:HD12	1.94	0.49
1:E:396:GLU:OE2	1:E:487:ARG:NH2	2.46	0.49
1:E:123:LYS:HG3	1:E:123:LYS:O	2.13	0.49
1:A:32:ALA:C	1:A:34:TYR:N	2.67	0.49
1:F:388:GLU:O	1:F:391:VAL:HG22	2.12	0.49
1:E:82:ASP:O	1:E:83:SER:C	2.51	0.49
1:B:408:PRO:O	1:B:411:TRP:N	2.37	0.49
1:D:255:LYS:HB3	1:D:270:VAL:HG21	1.95	0.49
1:E:410:GLU:OE2	1:F:68:LYS:NZ	2.46	0.49
1:F:110:GLY:HA2	1:F:113:ASN:ND2	2.27	0.49
1:B:55:LEU:CD2	1:B:56:GLY:N	2.76	0.49
1:C:84:ARG:HE	1:C:90:VAL:HG23	1.78	0.49
1:F:178:ILE:O	1:F:288:MET:HA	2.12	0.49
4:F:700:MPD:H11	4:F:700:MPD:O4	2.13	0.48
1:C:76:LEU:CD2	1:D:86:TYR:CD2	2.95	0.48
1:A:29:LYS:HB2	1:A:29:LYS:HZ3	1.75	0.48
1:F:98:TRP:CZ2	1:F:102:ILE:HD11	2.48	0.48
1:E:469:ILE:HG21	1:F:345:VAL:HG12	1.95	0.48
1:C:194:LEU:HB2	1:C:284:TYR:CD1	2.49	0.48
1:E:280:ILE:CD1	1:E:281:GLU:H	2.26	0.48
1:C:188:TYR:CB	1:C:263:THR:HB	2.43	0.48
1:F:491:SER:OG	1:F:492:ILE:N	2.46	0.48
1:B:30:GLU:HG2	1:B:351:ARG:HG2	1.94	0.48
1:B:114:TRP:O	1:B:118:VAL:HG23	2.13	0.48
1:E:447:GLU:OE1	1:F:474:VAL:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:GLY:O	1:B:66:PRO:HG2	2.13	0.48
1:C:283:GLU:O	1:C:283:GLU:HG3	2.12	0.48
1:A:171:PRO:HB2	1:A:255:LYS:HD2	1.95	0.48
1:F:173:ASP:O	1:F:177:CYS:HB2	2.13	0.48
1:C:88:TRP:CZ3	1:D:96:HIS:HB2	2.49	0.48
1:B:253:PRO:HA	1:B:271:ALA:HB2	1.94	0.48
1:D:188:TYR:HB2	1:D:264:PRO:HD3	1.95	0.48
1:A:163:GLU:HG2	1:A:295:ALA:HA	1.95	0.48
1:E:266:ARG:CB	1:E:266:ARG:NH1	2.76	0.48
1:A:471:ILE:HB	1:A:474:VAL:HG21	1.94	0.48
1:C:259:ILE:CG1	1:C:268:ARG:HB2	2.44	0.48
1:E:471:ILE:HG21	1:F:373:THR:HG23	1.90	0.48
1:D:86:TYR:CE1	1:D:413:ILE:HG12	2.49	0.48
1:F:339:LYS:HD2	1:F:367:TYR:CE2	2.48	0.48
1:B:391:VAL:CG2	1:B:392:GLU:N	2.76	0.48
1:C:108:HIS:CE1	1:D:412:THR:HG21	2.48	0.48
1:D:476:ALA:O	1:D:478:VAL:N	2.47	0.48
1:D:212:ILE:HA	1:D:212:ILE:HD12	1.70	0.48
1:D:403:HIS:CE1	1:D:492:ILE:HD13	2.48	0.48
1:A:251:PHE:CD2	1:A:280:ILE:HD11	2.49	0.48
1:B:44:VAL:HG21	1:B:53:TRP:CD1	2.48	0.48
1:A:65:ILE:HB	1:A:66:PRO:CD	2.44	0.48
1:C:70:MET:HE3	1:C:184:PHE:HD1	1.78	0.48
1:D:64:CYS:SG	2:D:600:FAD:C10	3.02	0.48
1:B:403:HIS:H	1:B:403:HIS:CD2	2.32	0.48
1:D:65:ILE:HB	1:D:66:PRO:CD	2.43	0.48
1:F:477:GLU:O	1:F:477:GLU:HG3	2.14	0.48
1:F:78:GLN:NE2	1:F:82:ASP:OD1	2.42	0.48
1:C:391:VAL:CG2	1:C:392:GLU:N	2.77	0.48
1:E:192:LYS:N	1:E:285:ASN:HD22	2.11	0.48
1:E:114:TRP:O	1:E:115:GLY:C	2.51	0.48
1:B:200:TYR:CE2	1:B:201:VAL:HG23	2.48	0.48
1:F:389:LYS:HD3	1:F:389:LYS:O	2.14	0.48
1:E:156:ARG:HH11	1:E:156:ARG:HG3	1.78	0.48
1:E:150:LYS:HD3	1:E:152:TYR:CZ	2.48	0.48
1:F:58:THR:O	1:F:59:CYS:C	2.52	0.48
1:A:150:LYS:HD3	1:A:152:TYR:CZ	2.48	0.48
1:F:176:TYR:HB3	1:F:267:LEU:CD2	2.35	0.48
1:D:151:ILE:C	1:D:151:ILE:HD13	2.34	0.48
1:D:263:THR:OG1	1:D:264:PRO:CD	2.62	0.48
1:D:156:ARG:HG3	1:D:156:ARG:NH1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:LEU:HD22	1:F:240:MET:SD	2.54	0.48
1:B:385:LEU:HD22	1:B:389:LYS:HG3	1.95	0.48
1:C:49:LEU:N	1:C:49:LEU:HD22	2.28	0.48
1:A:471:ILE:H	1:B:450:GLN:NE2	2.11	0.48
1:B:400:GLU:OE1	1:B:487:ARG:HD2	2.14	0.48
1:F:257:GLU:OE2	1:F:268:ARG:NH1	2.47	0.48
1:E:52:ARG:HB2	1:E:52:ARG:NH1	2.29	0.48
1:B:423:ALA:HB1	1:B:479:PHE:CZ	2.49	0.48
1:E:98:TRP:O	1:E:102:ILE:HG12	2.14	0.48
1:B:151:ILE:C	1:B:151:ILE:HD13	2.34	0.48
1:D:340:VAL:O	1:D:340:VAL:HG22	2.13	0.48
1:D:385:LEU:HD22	1:D:389:LYS:CG	2.44	0.48
1:F:385:LEU:HD22	1:F:389:LYS:HG3	1.95	0.48
1:A:98:TRP:CZ2	1:A:102:ILE:HD11	2.49	0.48
1:E:69:LEU:CD1	1:E:105:VAL:HG23	2.44	0.47
1:E:106:GLN:HE21	1:E:106:GLN:CA	2.19	0.47
1:C:471:ILE:HD13	1:D:373:THR:HG22	1.96	0.47
1:F:58:THR:O	1:F:60:VAL:N	2.47	0.47
1:C:272:GLN:HA	1:C:279:ILE:HG12	1.95	0.47
1:C:101:MET:HG3	1:D:86:TYR:O	2.14	0.47
1:E:478:VAL:CG1	1:E:479:PHE:N	2.77	0.47
1:E:138:HIS:O	1:E:153:SER:HA	2.14	0.47
1:C:412:THR:O	1:C:415:SER:N	2.47	0.47
1:F:156:ARG:HD3	1:F:330:TYR:HE2	1.79	0.47
1:A:108:HIS:CD2	1:B:412:THR:HB	2.49	0.47
1:E:469:ILE:HD12	1:F:348:GLN:HG3	1.95	0.47
1:C:263:THR:CB	1:C:264:PRO:HD3	2.44	0.47
1:F:403:HIS:CD2	1:F:492:ILE:HD13	2.49	0.47
1:B:401:VAL:O	1:B:485:THR:HA	2.13	0.47
1:D:222:SER:OG	1:D:226:ARG:NH2	2.47	0.47
1:B:192:LYS:H	1:B:285:ASN:HD22	1.61	0.47
1:F:411:TRP:C	1:F:414:PRO:HD2	2.35	0.47
1:F:270:VAL:HG13	1:F:280:ILE:O	2.15	0.47
1:F:484:VAL:HG11	1:F:491:SER:O	2.13	0.47
1:B:389:LYS:O	1:B:389:LYS:HD3	2.15	0.47
1:A:55:LEU:CD2	1:A:56:GLY:H	2.26	0.47
1:E:325:ASN:OD1	1:E:326:VAL:HG23	2.14	0.47
1:A:151:ILE:HD13	1:A:152:TYR:N	2.29	0.47
1:C:70:MET:HG2	1:C:101:MET:CE	2.45	0.47
1:F:351:ARG:HD3	5:F:2005:HOH:O	2.13	0.47
1:F:70:MET:HG2	1:F:101:MET:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:TYR:CE1	1:B:413:ILE:HD11	2.41	0.47
1:E:166:ARG:HG2	1:E:291:ILE:HD11	1.97	0.47
1:C:258:GLN:C	1:C:260:GLU:H	2.18	0.47
1:A:391:VAL:CG2	1:A:392:GLU:N	2.78	0.47
1:E:265:GLY:O	1:E:285:ASN:HA	2.14	0.47
1:F:79:ALA:HB2	4:F:700:MPD:HM2	1.97	0.47
1:A:259:ILE:HB	1:A:266:ARG:O	2.14	0.47
1:C:450:GLN:HE21	1:D:477:GLU:HA	1.79	0.47
1:B:318:VAL:HG13	1:B:319:THR:O	2.13	0.47
1:F:474:VAL:HG12	1:F:475:CYS:H	1.79	0.47
1:B:403:HIS:HB2	1:B:422:TYR:CE1	2.49	0.47
1:E:58:THR:O	1:E:63:GLY:N	2.48	0.47
1:D:150:LYS:HD3	1:D:152:TYR:CZ	2.50	0.47
1:D:90:VAL:CG2	1:D:91:GLU:N	2.77	0.47
1:B:262:GLY:O	1:B:265:GLY:N	2.47	0.47
1:B:258:GLN:O	1:B:259:ILE:C	2.52	0.47
1:E:287:VAL:HG12	1:E:287:VAL:O	2.14	0.47
1:E:256:VAL:C	1:E:257:GLU:HG2	2.34	0.47
1:C:100:ARG:O	1:C:103:GLU:HB3	2.14	0.47
1:F:70:MET:HE3	1:F:184:PHE:HD1	1.79	0.47
1:D:55:LEU:HD22	1:D:56:GLY:N	2.29	0.47
1:C:96:HIS:HA	1:D:87:GLY:O	2.15	0.47
1:C:168:LEU:HD13	1:C:253:PRO:HB2	1.96	0.47
1:E:90:VAL:HG21	1:F:80:LEU:CD2	2.45	0.47
1:A:170:ILE:HB	1:A:254:ILE:O	2.14	0.47
1:A:29:LYS:CE	1:A:119:ALA:HB1	2.44	0.47
1:D:21:GLY:HA3	2:D:600:FAD:H52A	1.96	0.47
1:E:396:GLU:O	1:E:487:ARG:NH2	2.48	0.47
1:B:30:GLU:HG3	1:B:351:ARG:HA	1.96	0.47
1:E:336:LEU:HB3	1:E:339:LYS:CG	2.44	0.47
1:C:79:ALA:HB2	4:D:700:MPD:HM2	1.96	0.47
1:C:97:ASP:OD1	1:C:99:ASP:HB2	2.15	0.47
1:C:389:LYS:NZ	1:C:389:LYS:HB2	2.30	0.47
1:B:301:GLY:HA2	1:B:303:GLU:OE2	2.15	0.47
1:B:123:LYS:O	1:B:124:LYS:HB2	2.13	0.47
1:F:31:ALA:O	1:F:32:ALA:C	2.54	0.47
1:C:70:MET:SD	1:C:101:MET:HE1	2.55	0.47
1:B:55:LEU:CD2	1:B:56:GLY:H	2.28	0.47
1:C:485:THR:C	1:C:487:ARG:H	2.17	0.47
1:C:225:LEU:HB3	1:C:228:PHE:CD2	2.50	0.47
1:F:412:THR:O	1:F:415:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:ILE:HD11	1:C:270:VAL:HG12	1.97	0.46
1:E:254:ILE:H	1:E:271:ALA:HA	1.78	0.46
1:E:279:ILE:CG2	1:E:280:ILE:N	2.78	0.46
1:F:223:ILE:HG12	1:F:226:ARG:NH2	2.30	0.46
1:E:70:MET:HE3	1:E:184:PHE:HD1	1.80	0.46
1:D:262:GLY:O	1:D:263:THR:O	2.32	0.46
1:F:67:LYS:HD2	1:F:68:LYS:N	2.30	0.46
1:F:387:GLU:HA	1:F:426:ILE:HD13	1.97	0.46
1:F:399:ILE:C	1:F:399:ILE:HD12	2.35	0.46
1:B:292:GLY:CA	3:B:601:NAP:O2N	2.63	0.46
1:C:259:ILE:HD11	1:C:268:ARG:CG	2.44	0.46
1:D:212:ILE:HG23	1:D:212:ILE:O	2.15	0.46
1:A:173:ASP:O	1:A:177:CYS:HB2	2.15	0.46
1:E:400:GLU:OE2	1:E:400:GLU:HA	2.16	0.46
1:A:389:LYS:HD3	1:A:389:LYS:O	2.15	0.46
1:C:32:ALA:O	1:C:34:TYR:N	2.48	0.46
1:E:106:GLN:CA	1:E:106:GLN:NE2	2.73	0.46
1:F:57:GLY:HA3	2:F:600:FAD:H52A	1.96	0.46
1:B:419:ASN:HD21	1:B:495:ALA:N	2.12	0.46
1:C:401:VAL:HB	1:C:486:LYS:HB2	1.98	0.46
1:F:82:ASP:OD2	1:F:416:ARG:NH1	2.47	0.46
1:C:440:VAL:HB	1:C:479:PHE:HZ	1.80	0.46
1:D:62:VAL:HG23	1:D:62:VAL:O	2.16	0.46
1:F:168:LEU:HD23	1:F:291:ILE:HD13	1.97	0.46
1:A:101:MET:HB2	1:B:86:TYR:O	2.16	0.46
1:E:105:VAL:CG1	1:E:106:GLN:N	2.79	0.46
1:C:477:GLU:HA	1:D:450:GLN:NE2	2.30	0.46
1:A:474:VAL:HG12	1:B:447:GLU:CD	2.36	0.46
1:C:77:GLY:HA2	1:C:80:LEU:HD12	1.97	0.46
1:A:30:GLU:OE1	1:A:34:TYR:HE2	1.99	0.46
1:E:98:TRP:NE1	1:E:102:ILE:HG13	2.30	0.46
1:C:92:GLU:OE2	1:E:150:LYS:CE	2.63	0.46
1:F:66:PRO:HB3	1:F:109:ILE:HD11	1.96	0.46
1:B:25:LEU:CD2	1:B:120:LEU:HD11	2.43	0.46
1:E:12:ASP:O	1:E:37:LYS:CE	2.64	0.46
1:E:46:PRO:HG3	1:E:52:ARG:NH2	2.30	0.46
1:B:156:ARG:NH1	1:B:156:ARG:HG3	2.30	0.46
1:B:55:LEU:HD22	1:B:56:GLY:N	2.31	0.46
1:C:471:ILE:HG21	1:D:373:THR:HG22	1.90	0.46
1:E:164:ARG:HG3	1:E:164:ARG:HH11	1.80	0.46
1:B:92:GLU:C	1:B:94:VAL:N	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:SER:O	1:D:86:TYR:N	2.48	0.46
1:A:212:ILE:HD12	1:A:212:ILE:HA	1.66	0.46
1:D:440:VAL:HB	1:D:479:PHE:CZ	2.51	0.46
1:A:138:HIS:O	1:A:153:SER:HA	2.15	0.46
1:C:260:GLU:HG2	1:C:261:ALA:O	2.16	0.46
1:A:77:GLY:HA2	1:A:80:LEU:HD12	1.97	0.46
1:E:477:GLU:HA	1:F:450:GLN:HE21	1.81	0.46
1:D:406:PHE:CE1	1:D:421:CYS:HB3	2.51	0.46
1:E:256:VAL:HG22	1:E:257:GLU:N	2.30	0.46
1:A:156:ARG:HH11	1:A:156:ARG:HG3	1.81	0.46
1:A:108:HIS:NE2	1:B:412:THR:HB	2.31	0.46
1:A:423:ALA:HB1	1:A:479:PHE:CZ	2.51	0.46
1:A:387:GLU:HA	1:A:426:ILE:HD13	1.96	0.46
1:D:331:ALA:O	1:D:332:ILE:HD12	2.16	0.46
1:E:77:GLY:HA2	1:E:80:LEU:HD12	1.97	0.46
1:A:53:TRP:CZ3	1:A:62:VAL:CG1	2.86	0.46
1:F:62:VAL:HG23	1:F:62:VAL:O	2.16	0.46
1:A:70:MET:HE1	1:A:184:PHE:HA	1.98	0.46
1:A:69:LEU:HD12	1:A:105:VAL:HG13	1.97	0.46
1:E:176:TYR:CE1	1:E:258:GLN:HB2	2.50	0.46
1:A:471:ILE:CG2	1:B:373:THR:HG23	2.44	0.46
1:C:101:MET:HE2	1:C:102:ILE:HD13	1.98	0.46
1:E:280:ILE:CG1	1:E:281:GLU:N	2.79	0.46
1:B:98:TRP:CE2	1:B:190:PRO:HD3	2.50	0.46
1:F:70:MET:HG2	1:F:101:MET:CE	2.45	0.46
1:C:385:LEU:HD22	1:C:389:LYS:HG3	1.97	0.46
1:E:331:ALA:O	1:E:332:ILE:HD12	2.16	0.46
1:B:221:ARG:HD3	3:B:601:NAP:C2A	2.46	0.46
1:B:222:SER:OG	3:B:601:NAP:O3X	2.26	0.46
1:B:266:ARG:NE	1:B:283:GLU:OE2	2.49	0.46
1:F:26:ALA:O	1:F:30:GLU:HB2	2.16	0.46
1:B:36:LYS:HD2	1:B:358:TYR:CD1	2.51	0.46
1:D:416:ARG:HG2	1:D:416:ARG:HH11	1.81	0.46
1:F:138:HIS:O	1:F:153:SER:HA	2.16	0.46
1:E:44:VAL:HG22	2:E:600:FAD:O2B	2.16	0.45
1:C:387:GLU:HA	1:C:426:ILE:HD13	1.98	0.45
1:D:98:TRP:CE2	1:D:190:PRO:HD3	2.52	0.45
1:C:180:SER:HA	1:C:288:MET:CE	2.46	0.45
1:F:340:VAL:HG13	1:F:345:VAL:CG2	2.37	0.45
1:B:263:THR:CB	1:B:264:PRO:CD	2.94	0.45
1:E:253:PRO:HA	1:E:271:ALA:CB	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:186:LEU:HA	1:E:187:PRO:HD3	1.82	0.45
1:F:78:GLN:NE2	1:F:416:ARG:NH1	2.64	0.45
1:A:345:VAL:HG12	1:B:469:ILE:HG21	1.98	0.45
1:B:408:PRO:O	1:B:409:LEU:C	2.53	0.45
1:E:106:GLN:C	1:E:108:HIS:H	2.19	0.45
1:E:72:GLN:CD	1:F:410:GLU:HG3	2.37	0.45
1:D:411:TRP:CZ3	1:D:421:CYS:SG	3.10	0.45
1:D:138:HIS:O	1:D:153:SER:HA	2.16	0.45
4:B:701:MPD:HM1	4:B:701:MPD:O4	2.17	0.45
1:A:344:PRO:HD3	2:A:600:FAD:O2	2.17	0.45
1:E:65:ILE:HB	1:E:66:PRO:CD	2.46	0.45
1:A:82:ASP:O	1:A:84:ARG:N	2.50	0.45
1:C:176:TYR:CE1	1:C:258:GLN:OE1	2.70	0.45
1:C:450:GLN:HE22	1:D:471:ILE:N	2.15	0.45
1:A:29:LYS:HD2	1:A:123:LYS:NZ	2.31	0.45
1:E:267:LEU:H	1:E:267:LEU:HD12	1.81	0.45
1:B:166:ARG:HG2	1:B:167:TYR:N	2.31	0.45
1:A:277:GLU:O	1:A:278:GLU:C	2.54	0.45
1:D:484:VAL:O	1:D:484:VAL:HG12	2.16	0.45
1:C:65:ILE:HB	1:C:66:PRO:CD	2.47	0.45
1:E:120:LEU:HD22	1:E:125:VAL:CG1	2.46	0.45
1:E:21:GLY:HA3	2:E:600:FAD:O2A	2.16	0.45
1:A:283:GLU:O	1:A:284:TYR:CD2	2.69	0.45
1:C:32:ALA:C	1:C:34:TYR:H	2.20	0.45
1:E:90:VAL:HG21	1:F:80:LEU:HD21	1.97	0.45
1:C:277:GLU:O	1:C:278:GLU:O	2.35	0.45
1:E:450:GLN:NE2	1:F:470:GLY:HA2	2.26	0.45
1:C:142:ALA:HB3	1:C:152:TYR:HE1	1.81	0.45
1:F:373:THR:HG21	1:F:446:GLY:HA2	1.97	0.45
1:E:161:THR:O	2:E:600:FAD:H8A	2.17	0.45
1:F:488:SER:C	1:F:490:ALA:H	2.20	0.45
1:B:138:HIS:O	1:B:153:SER:HA	2.17	0.45
1:F:158:LEU:HD11	1:F:332:ILE:HB	1.98	0.45
1:B:65:ILE:HB	1:B:66:PRO:CD	2.46	0.45
1:F:192:LYS:HE2	1:F:284:TYR:CD2	2.52	0.45
1:A:38:VAL:HG13	1:A:125:VAL:HG22	1.97	0.45
1:E:81:GLN:O	1:E:84:ARG:HB3	2.16	0.45
1:F:412:THR:OG1	1:F:413:ILE:N	2.50	0.45
1:C:86:TYR:O	1:D:101:MET:HG3	2.17	0.45
1:D:403:HIS:ND1	1:D:486:LYS:HE3	2.32	0.45
1:C:340:VAL:HG22	1:C:340:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:340:VAL:HG13	1:E:345:VAL:HG11	1.98	0.45
1:F:156:ARG:NH1	1:F:156:ARG:HG3	2.32	0.45
1:B:389:LYS:HB2	1:B:389:LYS:NZ	2.32	0.45
1:C:389:LYS:HD3	1:C:389:LYS:O	2.16	0.45
1:D:301:GLY:HA2	1:D:303:GLU:OE2	2.17	0.45
1:F:292:GLY:HA3	3:F:601:NAP:O1A	2.16	0.45
1:E:412:THR:HG21	1:F:108:HIS:CE1	2.51	0.45
1:A:403:HIS:CE1	1:A:492:ILE:CD1	3.00	0.45
1:E:252:VAL:C	1:E:271:ALA:HB1	2.37	0.45
1:A:373:THR:HG23	1:B:471:ILE:HG21	1.96	0.45
1:C:166:ARG:HG2	1:C:167:TYR:N	2.32	0.45
1:C:121:ARG:HG2	1:C:122:GLU:N	2.30	0.45
1:C:94:VAL:HG12	1:D:88:TRP:HE3	1.80	0.45
1:B:374:VAL:HG12	1:B:376:THR:HG23	1.97	0.45
1:F:65:ILE:HB	1:F:66:PRO:CD	2.47	0.45
1:F:150:LYS:HD3	1:F:152:TYR:CZ	2.51	0.45
1:E:173:ASP:O	1:E:177:CYS:HB2	2.17	0.45
1:D:192:LYS:H	1:D:285:ASN:HD22	1.64	0.45
1:E:156:ARG:HD3	1:E:330:TYR:HE2	1.81	0.45
1:C:114:TRP:O	1:C:117:ARG:N	2.49	0.45
1:A:301:GLY:HA2	1:A:303:GLU:OE2	2.16	0.45
1:A:53:TRP:CE3	1:A:62:VAL:HG11	2.48	0.45
1:F:33:GLN:NE2	1:F:33:GLN:O	2.50	0.45
1:D:46:PRO:CG	1:D:52:ARG:CZ	2.93	0.45
1:E:191:GLY:O	1:E:193:THR:CG2	2.65	0.45
1:F:212:ILE:HD12	1:F:212:ILE:HA	1.64	0.45
1:B:391:VAL:HG23	1:B:392:GLU:N	2.32	0.45
1:E:371:PRO:HB3	1:E:453:ALA:HB2	1.99	0.45
1:B:207:GLY:HA2	1:B:245:ILE:HD11	1.98	0.45
1:F:308:LYS:N	1:F:325:ASN:ND2	2.44	0.44
1:F:31:ALA:C	1:F:33:GLN:N	2.71	0.44
1:F:57:GLY:HA2	2:F:600:FAD:C3B	2.47	0.44
1:E:391:VAL:CG2	1:E:392:GLU:N	2.80	0.44
1:D:265:GLY:O	1:D:285:ASN:OD1	2.35	0.44
1:F:303:GLU:H	1:F:303:GLU:CD	2.20	0.44
1:E:266:ARG:CB	1:E:266:ARG:HH11	2.30	0.44
1:A:139:ARG:NH1	5:A:2002:HOH:O	2.50	0.44
1:E:485:THR:OG1	1:E:488:SER:CB	2.65	0.44
1:E:106:GLN:C	1:E:108:HIS:N	2.70	0.44
1:D:408:PRO:O	1:D:410:GLU:N	2.51	0.44
1:E:392:GLU:HG2	1:E:392:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:90:VAL:O	1:F:91:GLU:C	2.55	0.44
1:B:310:ASN:O	1:B:312:LYS:N	2.50	0.44
1:B:356:ARG:HG2	1:B:361:SER:O	2.16	0.44
1:B:67:LYS:HD2	1:B:68:LYS:N	2.32	0.44
1:E:106:GLN:HE22	1:E:109:ILE:CD1	2.13	0.44
1:C:92:GLU:OE2	1:E:150:LYS:HE2	2.17	0.44
1:F:58:THR:HG23	1:F:62:VAL:HG23	1.99	0.44
1:D:413:ILE:HD12	1:D:413:ILE:C	2.38	0.44
1:A:413:ILE:C	1:A:415:SER:N	2.71	0.44
1:A:343:THR:HB	1:A:344:PRO:HD3	2.00	0.44
1:B:59:CYS:HA	1:B:63:GLY:HA3	1.99	0.44
1:B:403:HIS:HD2	1:B:403:HIS:H	1.64	0.44
1:C:138:HIS:O	1:C:153:SER:HA	2.17	0.44
1:C:25:LEU:HD13	1:C:116:TYR:CD1	2.51	0.44
1:E:69:LEU:HD22	1:F:413:ILE:CG2	2.47	0.44
1:C:477:GLU:CA	1:D:450:GLN:HE21	2.30	0.44
1:C:258:GLN:HE21	1:C:261:ALA:CA	2.31	0.44
1:D:476:ALA:C	1:D:478:VAL:N	2.71	0.44
1:C:163:GLU:OE1	1:C:334:ASP:HB3	2.18	0.44
1:A:86:TYR:CE2	1:A:414:PRO:HG3	2.44	0.44
1:F:47:THR:HG21	1:F:181:ASP:HB3	1.99	0.44
1:C:178:ILE:O	1:C:288:MET:HA	2.17	0.44
1:D:252:VAL:O	1:D:271:ALA:HB1	2.18	0.44
1:F:57:GLY:O	1:F:58:THR:O	2.35	0.44
1:E:221:ARG:HG3	1:E:252:VAL:CG2	2.48	0.44
1:A:373:THR:HG21	1:A:446:GLY:HA2	1.99	0.44
1:A:391:VAL:HG23	1:A:392:GLU:N	2.33	0.44
1:A:191:GLY:O	1:A:193:THR:CG2	2.66	0.44
1:F:432:ASN:HD22	1:F:463:LYS:HZ3	1.63	0.44
1:B:186:LEU:HA	1:B:187:PRO:HD3	1.83	0.44
1:D:391:VAL:CG2	1:D:392:GLU:N	2.80	0.44
1:C:114:TRP:O	1:C:118:VAL:HG23	2.18	0.44
1:A:310:ASN:O	1:A:312:LYS:N	2.50	0.44
1:A:471:ILE:HG21	1:B:373:THR:HG22	1.94	0.44
1:C:373:THR:HG21	1:C:446:GLY:CA	2.47	0.44
1:B:94:VAL:O	1:B:94:VAL:HG23	2.16	0.44
1:F:49:LEU:CD2	1:F:49:LEU:N	2.78	0.44
1:D:105:VAL:HG12	1:D:106:GLN:N	2.32	0.44
1:B:144:ASN:CG	1:B:145:ASN:N	2.71	0.44
1:D:228:PHE:O	1:D:229:ASP:C	2.55	0.44
1:A:100:ARG:HH11	1:A:100:ARG:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:THR:HG22	1:E:52:ARG:N	2.32	0.44
1:C:193:THR:HB	1:C:286:THR:HB	1.99	0.44
1:B:389:LYS:HB2	1:B:389:LYS:HZ3	1.82	0.44
1:C:259:ILE:HG22	1:C:266:ARG:NH2	2.33	0.44
1:E:277:GLU:O	1:E:278:GLU:C	2.56	0.44
1:E:16:ILE:HG12	1:E:39:MET:HE2	2.00	0.44
1:D:389:LYS:NZ	1:D:389:LYS:HB2	2.32	0.44
1:D:262:GLY:O	1:D:265:GLY:N	2.51	0.44
1:E:340:VAL:CG1	1:E:345:VAL:HG11	2.48	0.44
1:F:391:VAL:CG2	1:F:392:GLU:N	2.80	0.44
1:F:205:CYS:HA	1:F:208:PHE:CE2	2.53	0.44
1:D:249:ARG:NH1	5:D:2004:HOH:O	2.51	0.44
1:F:58:THR:O	1:F:61:ASN:N	2.51	0.43
1:C:255:LYS:HE3	1:C:257:GLU:CG	2.48	0.43
1:C:150:LYS:HD3	1:C:152:TYR:CZ	2.52	0.43
1:A:196:VAL:HG21	1:A:253:PRO:HG2	2.00	0.43
1:D:117:ARG:NH1	1:D:117:ARG:HB3	2.33	0.43
1:B:156:ARG:HD3	1:B:330:TYR:HE2	1.82	0.43
1:A:49:LEU:N	1:A:49:LEU:HD22	2.33	0.43
1:C:36:LYS:HE3	1:C:358:TYR:CD1	2.53	0.43
1:C:43:PHE:CD2	1:C:43:PHE:C	2.91	0.43
1:F:86:TYR:CE2	1:F:414:PRO:HG3	2.53	0.43
1:F:293:ARG:CZ	2:F:600:FAD:HM81	2.48	0.43
1:C:278:GLU:CG	1:C:279:ILE:N	2.78	0.43
1:B:333:GLY:O	1:B:336:LEU:HB2	2.18	0.43
1:E:405:TYR:CE1	1:E:493:LEU:HG	2.48	0.43
1:F:167:TYR:CD2	1:F:174:LYS:HG2	2.53	0.43
1:B:36:LYS:HG3	1:B:358:TYR:CG	2.53	0.43
1:C:32:ALA:C	1:C:34:TYR:N	2.72	0.43
1:F:301:GLY:HA2	1:F:303:GLU:OE2	2.18	0.43
1:F:371:PRO:HB3	1:F:453:ALA:HB2	2.00	0.43
1:C:494:GLN:HB3	1:C:494:GLN:HE21	1.60	0.43
1:B:408:PRO:HG2	1:B:411:TRP:CZ3	2.53	0.43
1:B:339:LYS:CE	1:B:339:LYS:HA	2.46	0.43
1:F:116:TYR:C	1:F:118:VAL:N	2.70	0.43
1:C:392:GLU:O	1:C:392:GLU:HG2	2.18	0.43
1:D:225:LEU:HB3	1:D:228:PHE:CD2	2.53	0.43
1:D:51:THR:HA	5:D:2001:HOH:O	2.17	0.43
1:C:275:ASN:CG	1:C:276:SER:H	2.21	0.43
1:A:407:TRP:CD1	1:A:418:ASN:HA	2.53	0.43
1:F:176:TYR:CE1	1:F:258:GLN:OE1	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:LYS:HE2	1:C:284:TYR:CD2	2.53	0.43
1:E:485:THR:OG1	1:E:488:SER:HB2	2.19	0.43
1:B:91:GLU:HB3	1:B:92:GLU:H	1.62	0.43
1:C:447:GLU:OE1	1:D:474:VAL:CG1	2.66	0.43
1:B:101:MET:O	1:B:102:ILE:C	2.56	0.43
1:D:310:ASN:O	1:D:312:LYS:N	2.51	0.43
1:D:258:GLN:NE2	1:D:261:ALA:HB2	2.32	0.43
1:A:144:ASN:CG	1:A:145:ASN:N	2.72	0.43
1:B:413:ILE:N	1:B:414:PRO:CD	2.82	0.43
1:B:373:THR:HG21	1:B:446:GLY:CA	2.48	0.43
1:A:29:LYS:HB2	1:A:29:LYS:HZ2	1.80	0.43
1:E:212:ILE:O	1:E:212:ILE:HG23	2.18	0.43
1:C:88:TRP:HE3	1:D:94:VAL:HG12	1.83	0.43
1:E:13:TYR:CD1	1:E:37:LYS:HG2	2.48	0.43
1:B:173:ASP:O	1:B:177:CYS:HB2	2.19	0.43
1:D:263:THR:O	1:D:264:PRO:C	2.50	0.43
1:A:146:LYS:HE3	1:C:187:PRO:HB3	2.01	0.43
1:E:158:LEU:HD11	1:E:332:ILE:HB	2.01	0.43
1:A:38:VAL:CG2	1:A:39:MET:N	2.81	0.43
1:B:331:ALA:O	1:B:332:ILE:HD12	2.18	0.43
1:E:67:LYS:HD2	1:E:68:LYS:N	2.33	0.43
1:C:156:ARG:HD3	1:C:330:TYR:HE2	1.82	0.43
1:C:85:ASN:CB	1:C:413:ILE:CD1	2.96	0.43
1:B:77:GLY:HA2	1:B:80:LEU:HD12	2.00	0.43
1:D:64:CYS:SG	2:D:600:FAD:C4X	3.06	0.43
1:C:44:VAL:CG1	1:C:53:TRP:CE2	3.01	0.43
1:E:256:VAL:HG22	1:E:257:GLU:H	1.82	0.43
1:A:371:PRO:HB3	1:A:453:ALA:HB2	1.99	0.43
1:C:315:LYS:HD2	1:C:336:LEU:O	2.19	0.43
1:F:411:TRP:HZ3	1:F:421:CYS:SG	2.42	0.43
1:B:336:LEU:CB	1:B:339:LYS:HG3	2.43	0.43
1:E:399:ILE:HA	1:E:427:CYS:O	2.18	0.43
1:A:487:ARG:O	1:A:489:GLY:N	2.43	0.43
1:D:262:GLY:O	1:D:265:GLY:CA	2.67	0.43
1:E:410:GLU:OE2	1:F:68:LYS:CE	2.65	0.43
1:E:389:LYS:NZ	1:E:389:LYS:HB2	2.33	0.43
1:E:156:ARG:NH1	1:E:156:ARG:HG3	2.33	0.43
1:E:420:LYS:HA	1:E:420:LYS:HD3	1.69	0.43
1:F:77:GLY:HA2	1:F:80:LEU:HD12	2.00	0.43
1:C:411:TRP:C	1:C:414:PRO:HD2	2.39	0.43
1:C:269:VAL:N	1:C:282:GLY:O	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LYS:HE2	1:A:257:GLU:HG2	2.01	0.43
1:D:413:ILE:N	1:D:414:PRO:CD	2.82	0.43
1:E:236:ILE:HD11	1:E:380:TYR:CB	2.49	0.43
1:B:432:ASN:HD22	1:B:463:LYS:HZ3	1.65	0.43
1:D:262:GLY:O	1:D:264:PRO:C	2.57	0.43
1:E:10:SER:OG	1:E:11:TYR:N	2.49	0.43
1:D:186:LEU:HA	1:D:187:PRO:HD3	1.84	0.43
1:D:165:PRO:HG3	5:D:2005:HOH:O	2.18	0.43
1:A:67:LYS:HD2	1:A:68:LYS:N	2.33	0.43
1:D:371:PRO:HB3	1:D:453:ALA:HB2	2.01	0.43
1:C:67:LYS:HD2	1:C:68:LYS:N	2.34	0.43
1:E:413:ILE:C	1:E:415:SER:N	2.73	0.43
1:B:344:PRO:HD3	2:B:600:FAD:O2	2.19	0.43
1:E:14:ASP:CG	1:E:36:LYS:HD2	2.39	0.43
1:A:59:CYS:SG	1:B:472:HIS:CD2	3.12	0.43
1:E:13:TYR:O	1:E:154:ALA:HA	2.19	0.43
1:F:432:ASN:HD22	1:F:463:LYS:HZ1	1.64	0.43
1:C:391:VAL:HG23	1:C:392:GLU:N	2.32	0.43
1:E:341:GLU:CD	1:E:341:GLU:H	2.22	0.43
1:A:298:ARG:HG2	1:A:298:ARG:H	1.51	0.43
1:A:53:TRP:CE3	1:A:62:VAL:CG1	3.02	0.43
1:D:449:THR:O	1:D:450:GLN:C	2.57	0.43
1:F:144:ASN:CG	1:F:145:ASN:N	2.72	0.43
1:D:298:ARG:H	1:D:298:ARG:HG2	1.51	0.43
1:E:98:TRP:C	1:E:98:TRP:CD1	2.91	0.42
1:F:342:LEU:O	1:F:345:VAL:HG22	2.19	0.42
1:A:403:HIS:CE1	1:A:492:ILE:HD13	2.53	0.42
1:E:471:ILE:HG21	1:F:373:THR:HG22	1.99	0.42
1:D:389:LYS:HD3	1:D:389:LYS:O	2.19	0.42
1:C:416:ARG:O	1:C:417:ASP:C	2.58	0.42
1:A:69:LEU:O	1:A:72:GLN:HB3	2.19	0.42
1:E:374:VAL:HG12	1:E:376:THR:HG23	2.01	0.42
1:F:337:GLU:HG2	1:F:338:ASP:OD2	2.18	0.42
1:A:229:ASP:OD1	1:A:231:ASP:HB3	2.19	0.42
1:F:272:GLN:HG2	1:F:273:SER:H	1.85	0.42
1:E:488:SER:C	1:E:490:ALA:H	2.23	0.42
1:D:93:THR:HG22	1:D:93:THR:O	2.20	0.42
1:B:258:GLN:HE21	1:B:261:ALA:HA	1.84	0.42
1:C:343:THR:HB	1:C:344:PRO:HD3	2.01	0.42
1:D:55:LEU:CD2	1:D:56:GLY:N	2.82	0.42
1:A:228:PHE:O	1:A:229:ASP:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ASP:O	1:C:339:LYS:HD3	2.18	0.42
1:E:249:ARG:NH1	5:E:2001:HOH:O	2.50	0.42
1:C:59:CYS:HA	1:C:63:GLY:HA3	2.00	0.42
1:C:471:ILE:H	1:D:450:GLN:HE22	1.68	0.42
1:D:397:GLU:HA	1:D:487:ARG:NH2	2.34	0.42
1:B:273:SER:OG	1:B:274:THR:N	2.52	0.42
1:E:267:LEU:CD1	1:E:267:LEU:N	2.82	0.42
1:C:340:VAL:CG2	1:C:340:VAL:O	2.67	0.42
1:F:389:LYS:NZ	1:F:389:LYS:HB2	2.34	0.42
1:A:55:LEU:HD22	1:A:56:GLY:N	2.35	0.42
1:A:82:ASP:O	1:A:83:SER:C	2.57	0.42
1:C:176:TYR:HB3	1:C:267:LEU:HD21	2.02	0.42
1:D:406:PHE:CD1	1:D:406:PHE:N	2.88	0.42
1:B:339:LYS:HD3	1:B:367:TYR:CE2	2.54	0.42
1:F:333:GLY:O	1:F:336:LEU:HB2	2.20	0.42
1:C:186:LEU:HA	1:C:187:PRO:HD3	1.83	0.42
1:A:406:PHE:O	1:A:421:CYS:HB2	2.19	0.42
1:C:156:ARG:HH11	1:C:156:ARG:HG3	1.83	0.42
1:A:412:THR:HB	1:B:108:HIS:CD2	2.53	0.42
1:E:423:ALA:HB1	1:E:479:PHE:CE1	2.54	0.42
1:E:116:TYR:O	1:E:117:ARG:C	2.57	0.42
1:C:96:HIS:CE1	1:C:212:ILE:HD11	2.54	0.42
1:C:333:GLY:O	1:C:336:LEU:HB2	2.18	0.42
1:A:225:LEU:HB3	1:A:228:PHE:CD2	2.54	0.42
1:C:371:PRO:HB3	1:C:453:ALA:HB2	2.01	0.42
1:F:229:ASP:OD1	1:F:231:ASP:HB3	2.20	0.42
1:D:256:VAL:O	1:D:256:VAL:HG13	2.19	0.42
1:E:266:ARG:NH1	1:E:266:ARG:HB3	2.34	0.42
1:A:142:ALA:HB3	1:A:152:TYR:HE1	1.85	0.42
1:F:142:ALA:HB3	1:F:152:TYR:HE1	1.85	0.42
1:B:337:GLU:O	1:B:339:LYS:HG2	2.20	0.42
1:A:212:ILE:HG23	1:A:212:ILE:O	2.18	0.42
1:E:277:GLU:O	1:E:278:GLU:O	2.38	0.42
1:C:188:TYR:CG	1:C:263:THR:HB	2.54	0.42
1:D:263:THR:O	1:D:265:GLY:N	2.53	0.42
1:D:158:LEU:HD11	1:D:332:ILE:HB	2.01	0.42
1:B:229:ASP:OD1	1:B:231:ASP:HB3	2.19	0.42
1:F:80:LEU:O	1:F:83:SER:OG	2.35	0.42
1:E:69:LEU:O	1:E:72:GLN:HB3	2.19	0.42
4:F:700:MPD:HM2	4:F:700:MPD:H4	1.89	0.42
1:E:142:ALA:HB3	1:E:152:TYR:HE1	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ALA:HB3	1:B:152:TYR:HE1	1.85	0.42
1:D:77:GLY:HA2	1:D:80:LEU:HD12	2.00	0.42
1:E:344:PRO:HD3	2:E:600:FAD:O2	2.19	0.42
1:A:391:VAL:HG12	1:A:399:ILE:HD11	2.01	0.42
1:A:194:LEU:HB2	1:A:284:TYR:CD1	2.55	0.42
1:C:30:GLU:HG3	1:C:351:ARG:HA	2.01	0.42
1:C:123:LYS:O	1:C:124:LYS:CB	2.62	0.42
1:B:212:ILE:HA	1:B:212:ILE:HD12	1.76	0.42
1:B:392:GLU:HG2	1:B:392:GLU:O	2.18	0.42
1:A:389:LYS:NZ	1:A:389:LYS:HB2	2.34	0.42
1:D:225:LEU:HB3	1:D:228:PHE:HD2	1.85	0.42
1:C:301:GLY:HA2	1:C:303:GLU:OE2	2.20	0.42
1:A:75:LEU:HB3	4:B:700:MPD:H53	2.02	0.42
1:E:76:LEU:CD2	1:F:86:TYR:CD2	3.03	0.42
1:E:373:THR:HG21	1:E:446:GLY:CA	2.49	0.42
1:D:142:ALA:HB3	1:D:152:TYR:HE1	1.85	0.42
1:B:219:MET:SD	1:B:253:PRO:HD3	2.60	0.42
1:A:273:SER:HG	1:A:275:ASN:H	1.65	0.42
1:A:12:ASP:HB2	1:A:153:SER:O	2.20	0.42
1:C:41:LEU:HD23	1:C:128:GLU:HB3	2.00	0.42
1:F:164:ARG:O	1:F:293:ARG:HB3	2.19	0.42
1:F:161:THR:O	2:F:600:FAD:H8A	2.20	0.42
1:F:209:LEU:O	1:F:212:ILE:HG22	2.19	0.42
1:D:405:TYR:CD1	1:D:492:ILE:HG13	2.55	0.42
1:C:340:VAL:HG22	1:C:345:VAL:HG11	2.01	0.42
1:B:70:MET:HG2	1:B:101:MET:HE3	2.01	0.42
1:A:98:TRP:NE1	1:A:102:ILE:HG13	2.34	0.42
1:C:55:LEU:HD22	1:C:56:GLY:N	2.35	0.42
1:E:98:TRP:HB3	1:E:189:CYS:HB2	2.02	0.42
1:B:163:GLU:OE1	1:B:334:ASP:HB3	2.19	0.42
1:A:410:GLU:O	1:A:414:PRO:HG2	2.20	0.42
1:D:191:GLY:O	1:D:193:THR:CG2	2.67	0.42
1:C:17:ILE:HD12	1:C:28:ALA:HB2	2.02	0.42
1:B:38:VAL:CG2	1:B:39:MET:N	2.83	0.42
1:A:58:THR:O	1:A:63:GLY:N	2.52	0.42
1:B:309:ILE:O	1:B:311:GLU:N	2.53	0.42
1:F:410:GLU:O	1:F:414:PRO:HG2	2.20	0.41
1:A:477:GLU:HA	1:B:450:GLN:NE2	2.35	0.41
1:E:188:TYR:HD2	1:E:264:PRO:HG3	1.85	0.41
1:A:84:ARG:HD2	1:A:90:VAL:O	2.20	0.41
1:A:48:PRO:HG2	1:A:167:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:GLY:HA2	1:F:245:ILE:HD11	2.02	0.41
1:F:400:GLU:OE2	1:F:400:GLU:HA	2.20	0.41
1:E:55:LEU:HD23	1:E:127:TYR:CZ	2.55	0.41
1:F:36:LYS:O	1:F:38:VAL:HG13	2.20	0.41
1:F:167:TYR:CE2	1:F:174:LYS:HG2	2.55	0.41
1:F:397:GLU:HA	1:F:487:ARG:NH2	2.33	0.41
1:D:391:VAL:HG23	1:D:392:GLU:N	2.34	0.41
1:D:303:GLU:H	1:D:303:GLU:CD	2.23	0.41
1:D:69:LEU:O	1:D:72:GLN:HB3	2.20	0.41
1:B:298:ARG:HG2	1:B:298:ARG:H	1.50	0.41
1:A:402:TYR:CD2	1:A:485:THR:HG22	2.55	0.41
1:E:333:GLY:O	1:E:336:LEU:HB2	2.20	0.41
1:E:72:GLN:CD	1:F:410:GLU:CG	2.88	0.41
1:F:61:ASN:HA	1:F:109:ILE:HD13	2.02	0.41
1:C:413:ILE:N	1:C:414:PRO:CD	2.83	0.41
1:D:408:PRO:O	1:D:411:TRP:N	2.39	0.41
1:D:16:ILE:HG23	1:D:39:MET:HE3	2.02	0.41
1:C:236:ILE:HD11	1:C:380:TYR:HB2	2.02	0.41
1:B:189:CYS:HA	1:B:190:PRO:HD3	1.93	0.41
1:B:303:GLU:CD	1:B:303:GLU:H	2.22	0.41
1:A:48:PRO:HB2	1:A:49:LEU:HD22	2.01	0.41
1:B:225:LEU:HB3	1:B:228:PHE:CD2	2.55	0.41
1:E:103:GLU:O	1:E:104:ALA:C	2.58	0.41
1:A:471:ILE:N	1:B:450:GLN:HE22	2.18	0.41
1:F:260:GLU:H	1:F:266:ARG:HB2	1.85	0.41
1:A:192:LYS:HB3	1:A:285:ASN:HD22	1.84	0.41
1:F:191:GLY:O	1:F:193:THR:CG2	2.67	0.41
1:D:374:VAL:CG1	1:D:376:THR:HG23	2.51	0.41
1:C:487:ARG:C	1:C:489:GLY:N	2.73	0.41
1:B:108:HIS:CE1	1:B:112:LEU:HD11	2.55	0.41
1:A:309:ILE:O	1:A:311:GLU:N	2.53	0.41
1:E:286:THR:HG22	1:E:287:VAL:N	2.34	0.41
1:B:267:LEU:HD23	1:B:287:VAL:CG2	2.50	0.41
1:D:273:SER:CB	1:D:276:SER:HB3	2.51	0.41
1:A:348:GLN:HG3	1:B:469:ILE:CD1	2.50	0.41
1:E:303:GLU:CD	1:E:303:GLU:H	2.22	0.41
1:F:391:VAL:HG23	1:F:392:GLU:N	2.34	0.41
1:E:64:CYS:O	1:E:67:LYS:HB3	2.19	0.41
1:F:69:LEU:O	1:F:72:GLN:HB3	2.19	0.41
1:A:494:GLN:HE21	1:A:494:GLN:HB3	1.63	0.41
1:C:267:LEU:HD13	1:C:285:ASN:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLN:O	1:B:258:GLN:HG2	2.21	0.41
1:A:86:TYR:CD2	1:A:413:ILE:HD11	2.55	0.41
1:F:118:VAL:O	1:F:119:ALA:C	2.59	0.41
1:F:263:THR:CB	1:F:264:PRO:CD	2.98	0.41
1:A:69:LEU:CD1	1:A:105:VAL:HG13	2.50	0.41
1:B:158:LEU:HD11	1:B:332:ILE:HB	2.02	0.41
1:D:207:GLY:HA2	1:D:245:ILE:HD11	2.03	0.41
1:C:229:ASP:OD1	1:C:231:ASP:HB3	2.21	0.41
1:A:94:VAL:HG13	1:B:89:LYS:O	2.20	0.41
1:A:86:TYR:HE2	1:A:414:PRO:CG	2.29	0.41
1:A:392:GLU:HG2	1:A:392:GLU:O	2.21	0.41
1:D:272:GLN:HA	1:D:279:ILE:HA	2.02	0.41
1:A:440:VAL:O	1:A:440:VAL:HG13	2.20	0.41
1:F:251:PHE:CE2	1:F:280:ILE:HG23	2.56	0.41
1:F:47:THR:O	1:F:49:LEU:N	2.54	0.41
1:D:292:GLY:HA2	3:D:601:NAP:PA	2.61	0.41
1:B:472:HIS:HA	1:B:473:PRO:HA	1.92	0.41
1:E:236:ILE:HD11	1:E:380:TYR:HB2	2.03	0.41
1:F:485:THR:O	1:F:488:SER:O	2.39	0.41
1:B:49:LEU:N	1:B:49:LEU:CD2	2.84	0.41
1:A:318:VAL:CG1	1:A:322:GLU:HA	2.51	0.41
1:D:156:ARG:HD3	1:D:330:TYR:HE2	1.86	0.41
1:F:438:PHE:CE2	1:F:479:PHE:CE1	3.09	0.41
1:A:409:LEU:HD12	1:A:409:LEU:O	2.21	0.41
1:A:259:ILE:CD1	1:A:268:ARG:HB2	2.31	0.41
1:A:252:VAL:C	1:A:271:ALA:HB1	2.40	0.41
1:A:13:TYR:O	1:A:154:ALA:HA	2.21	0.41
1:A:446:GLY:CA	1:B:474:VAL:HG21	2.50	0.41
1:D:340:VAL:O	1:D:345:VAL:HG21	2.20	0.41
1:C:236:ILE:HD11	1:C:380:TYR:CB	2.50	0.41
1:E:12:ASP:OD1	1:E:153:SER:OG	2.37	0.41
1:D:236:ILE:HD11	1:D:380:TYR:CB	2.51	0.41
1:B:318:VAL:CG1	1:B:322:GLU:HA	2.51	0.41
1:F:319:THR:C	1:F:321:GLU:H	2.25	0.41
1:D:440:VAL:HB	1:D:479:PHE:HZ	1.85	0.41
1:A:385:LEU:HD22	1:A:389:LYS:CG	2.51	0.41
1:C:397:GLU:HA	1:C:487:ARG:HH22	1.86	0.41
1:C:440:VAL:HG13	1:C:440:VAL:O	2.21	0.41
1:C:303:GLU:CD	1:C:303:GLU:H	2.23	0.41
1:C:56:GLY:O	1:C:60:VAL:HG23	2.21	0.41
1:F:43:PHE:HE2	1:F:45:THR:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LYS:HG2	1:B:256:VAL:N	2.35	0.41
1:D:103:GLU:O	1:D:107:ASN:HB2	2.21	0.41
1:D:309:ILE:O	1:D:311:GLU:N	2.54	0.41
1:C:209:LEU:HA	1:C:209:LEU:HD23	1.94	0.41
1:E:84:ARG:HH22	1:E:91:GLU:C	2.24	0.41
1:A:471:ILE:HD13	1:B:373:THR:HG22	2.01	0.41
1:D:114:TRP:O	1:D:117:ARG:HB2	2.21	0.41
1:B:172:GLY:CA	1:B:175:GLU:HG2	2.51	0.41
1:D:405:TYR:CE1	1:D:492:ILE:HG13	2.56	0.41
1:E:123:LYS:NZ	1:E:123:LYS:CB	2.83	0.41
1:A:156:ARG:NH1	1:A:156:ARG:HG3	2.35	0.41
1:A:98:TRP:CD1	1:A:98:TRP:C	2.93	0.41
1:A:55:LEU:HD23	1:A:56:GLY:H	1.86	0.41
1:D:373:THR:HG21	1:D:446:GLY:CA	2.52	0.40
1:F:373:THR:HG21	1:F:446:GLY:CA	2.52	0.40
1:F:49:LEU:HD23	1:F:182:ASP:OD2	2.20	0.40
1:B:250:GLN:O	1:B:273:SER:HA	2.21	0.40
1:C:186:LEU:HD23	1:C:186:LEU:HA	1.95	0.40
1:F:133:GLN:O	1:F:140:ILE:HG13	2.21	0.40
1:D:137:PRO:HA	1:D:328:TYR:OH	2.21	0.40
1:E:144:ASN:CG	1:E:145:ASN:N	2.73	0.40
1:E:76:LEU:CD1	4:F:700:MPD:HM3	2.50	0.40
1:C:255:LYS:O	1:C:270:VAL:N	2.39	0.40
1:E:340:VAL:O	1:E:340:VAL:HG13	2.22	0.40
1:E:342:LEU:O	1:E:345:VAL:HG22	2.21	0.40
1:C:189:CYS:HA	1:C:190:PRO:HD3	1.91	0.40
1:E:447:GLU:CD	1:F:474:VAL:CG1	2.90	0.40
1:C:158:LEU:HD11	1:C:332:ILE:HB	2.03	0.40
1:E:406:PHE:O	1:E:421:CYS:HB2	2.22	0.40
1:B:413:ILE:HG12	1:B:414:PRO:HD3	2.02	0.40
1:F:270:VAL:HA	1:F:280:ILE:O	2.21	0.40
1:F:449:THR:O	1:F:450:GLN:C	2.60	0.40
1:A:446:GLY:C	1:B:474:VAL:HG21	2.41	0.40
1:F:47:THR:C	1:F:49:LEU:N	2.74	0.40
1:B:191:GLY:O	1:B:193:THR:CG2	2.67	0.40
1:E:447:GLU:CD	1:F:474:VAL:HG12	2.42	0.40
1:F:392:GLU:HG2	1:F:392:GLU:O	2.20	0.40
1:F:385:LEU:HD22	1:F:389:LYS:CG	2.51	0.40
1:F:203:LEU:HA	1:F:203:LEU:HD23	1.93	0.40
1:B:67:LYS:C	1:B:67:LYS:HD2	2.41	0.40
1:D:176:TYR:CE1	1:D:258:GLN:HB2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:LEU:HD22	1:C:240:MET:SD	2.61	0.40
1:C:374:VAL:HG12	1:C:376:THR:HG23	2.03	0.40
1:C:356:ARG:HG2	1:C:361:SER:O	2.22	0.40
1:F:63:GLY:O	1:F:66:PRO:HG2	2.21	0.40
1:D:476:ALA:O	1:D:477:GLU:C	2.59	0.40
1:A:80:LEU:HD21	1:B:90:VAL:HG21	2.03	0.40
1:C:399:ILE:O	1:C:399:ILE:CD1	2.68	0.40
1:B:342:LEU:O	1:B:345:VAL:HG22	2.22	0.40
1:B:212:ILE:HG23	1:B:212:ILE:O	2.20	0.40
1:D:263:THR:HB	1:D:264:PRO:HD3	2.03	0.40
1:D:189:CYS:HA	1:D:190:PRO:HD3	1.91	0.40
1:F:332:ILE:HD13	1:F:353:LEU:HD22	2.04	0.40
1:A:55:LEU:CD2	1:A:56:GLY:N	2.85	0.40
1:F:164:ARG:HA	1:F:164:ARG:HD2	1.89	0.40
1:E:391:VAL:HG23	1:E:392:GLU:N	2.36	0.40
1:B:271:ALA:O	1:B:279:ILE:HG23	2.22	0.40
4:D:700:MPD:C1	4:D:700:MPD:O4	2.69	0.40
1:A:100:ARG:HG3	1:A:100:ARG:NH1	2.37	0.40
1:C:43:PHE:HD2	1:C:43:PHE:C	2.25	0.40
1:C:156:ARG:NH1	1:C:156:ARG:HG3	2.36	0.40
1:A:331:ALA:O	1:A:332:ILE:HD12	2.21	0.40
1:D:67:LYS:HD2	1:D:68:LYS:N	2.36	0.40
1:F:409:LEU:O	1:F:409:LEU:HG	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/519 (93%)	426 (88%)	51 (10%)	8 (2%)	12	38
1	B	485/519 (93%)	419 (86%)	60 (12%)	6 (1%)	16	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	488/519 (94%)	425 (87%)	51 (10%)	12 (2%)	7	24
1	D	489/519 (94%)	424 (87%)	51 (10%)	14 (3%)	6	19
1	E	488/519 (94%)	421 (86%)	54 (11%)	13 (3%)	6	21
1	F	484/519 (93%)	417 (86%)	55 (11%)	12 (2%)	7	24
All	All	2919/3114 (94%)	2532 (87%)	322 (11%)	65 (2%)	8	28

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	489	GLY
1	B	263	THR
1	C	263	THR
1	C	276	SER
1	C	278	GLU
1	C	417	ASP
1	D	263	THR
1	D	497	CYS
1	E	261	ALA
1	E	262	GLY
1	E	263	THR
1	E	278	GLU
1	F	58	THR
1	F	59	CYS
1	F	263	THR
1	A	311	GLU
1	B	311	GLU
1	C	51	THR
1	C	260	GLU
1	C	311	GLU
1	D	260	GLU
1	D	273	SER
1	D	311	GLU
1	D	489	GLY
1	D	495	ALA
1	E	115	GLY
1	E	311	GLU
1	E	341	GLU
1	E	488	SER
1	E	496	GLY
1	F	32	ALA
1	F	259	ILE

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Mol	Chain	Res	Type
1	F	311	GLU
1	F	417	ASP
1	F	492	ILE
1	A	33	GLN
1	A	83	SER
1	A	278	GLU
1	B	476	ALA
1	C	33	GLN
1	D	91	GLU
1	D	255	LYS
1	D	494	GLN
1	D	496	GLY
1	E	64	CYS
1	E	114	TRP
1	A	404	SER
1	B	93	THR
1	C	490	ALA
1	D	409	LEU
1	F	275	ASN
1	A	263	THR
1	C	273	SER
1	C	275	ASN
1	D	417	ASP
1	F	31	ALA
1	B	259	ILE
1	E	255	LYS
1	F	35	GLY
1	A	473	PRO
1	B	473	PRO
1	C	473	PRO
1	D	473	PRO
1	F	473	PRO
1	E	473	PRO

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	399/426 (94%)	370 (93%)	29 (7%)	17	44
1	B	400/426 (94%)	372 (93%)	28 (7%)	19	47
1	C	401/426 (94%)	362 (90%)	39 (10%)	10	29
1	D	402/426 (94%)	371 (92%)	31 (8%)	16	41
1	E	401/426 (94%)	370 (92%)	31 (8%)	16	41
1	F	399/426 (94%)	370 (93%)	29 (7%)	17	44
All	All	2402/2556 (94%)	2215 (92%)	187 (8%)	16	41

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	55	LEU
1	A	64	CYS
1	A	76	LEU
1	A	91	GLU
1	A	111	SER
1	A	123	LYS
1	A	133	GLN
1	A	139	ARG
1	A	144	ASN
1	A	151	ILE
1	A	175	GLU
1	A	193	THR
1	A	212	ILE
1	A	256	VAL
1	A	298	ARG
1	A	303	GLU
1	A	318	VAL
1	A	332	ILE
1	A	336	LEU
1	A	340	VAL
1	A	373	THR
1	A	389	LYS
1	A	403	HIS
1	A	404	SER
1	A	409	LEU
1	A	413	ILE
1	A	493	LEU
1	A	494	GLN
1	B	14	ASP

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Mol	Chain	Res	Type
1	B	55	LEU
1	B	64	CYS
1	B	76	LEU
1	B	93	THR
1	B	121	ARG
1	B	133	GLN
1	B	139	ARG
1	B	144	ASN
1	B	151	ILE
1	B	175	GLU
1	B	193	THR
1	B	252	VAL
1	B	268	ARG
1	B	277	GLU
1	B	280	ILE
1	B	298	ARG
1	B	303	GLU
1	B	318	VAL
1	B	332	ILE
1	B	336	LEU
1	B	373	THR
1	B	389	LYS
1	B	403	HIS
1	B	413	ILE
1	B	416	ARG
1	B	474	VAL
1	B	483	SER
1	C	38	VAL
1	C	43	PHE
1	C	45	THR
1	C	51	THR
1	C	55	LEU
1	C	64	CYS
1	C	76	LEU
1	C	83	SER
1	C	111	SER
1	C	118	VAL
1	C	133	GLN
1	C	139	ARG
1	C	144	ASN
1	C	151	ILE
1	C	175	GLU

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Mol	Chain	Res	Type
1	C	193	THR
1	C	212	ILE
1	C	277	GLU
1	C	279	ILE
1	C	281	GLU
1	C	298	ARG
1	C	303	GLU
1	C	318	VAL
1	C	332	ILE
1	C	336	LEU
1	C	373	THR
1	C	389	LYS
1	C	403	HIS
1	C	408	PRO
1	C	413	ILE
1	C	416	ARG
1	C	417	ASP
1	C	418	ASN
1	C	475	CYS
1	C	483	SER
1	C	491	SER
1	C	494	GLN
1	C	497	CYS
1	C	498	CYS
1	D	14	ASP
1	D	38	VAL
1	D	49	LEU
1	D	55	LEU
1	D	76	LEU
1	D	90	VAL
1	D	91	GLU
1	D	111	SER
1	D	133	GLN
1	D	139	ARG
1	D	144	ASN
1	D	151	ILE
1	D	175	GLU
1	D	193	THR
1	D	212	ILE
1	D	254	ILE
1	D	267	LEU
1	D	270	VAL

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Mol	Chain	Res	Type
1	D	298	ARG
1	D	303	GLU
1	D	318	VAL
1	D	332	ILE
1	D	336	LEU
1	D	340	VAL
1	D	373	THR
1	D	389	LYS
1	D	403	HIS
1	D	406	PHE
1	D	413	ILE
1	D	418	ASN
1	D	497	CYS
1	E	45	THR
1	E	49	LEU
1	E	52	ARG
1	E	64	CYS
1	E	76	LEU
1	E	84	ARG
1	E	92	GLU
1	E	123	LYS
1	E	133	GLN
1	E	139	ARG
1	E	144	ASN
1	E	151	ILE
1	E	175	GLU
1	E	193	THR
1	E	212	ILE
1	E	257	GLU
1	E	267	LEU
1	E	298	ARG
1	E	303	GLU
1	E	318	VAL
1	E	332	ILE
1	E	336	LEU
1	E	373	THR
1	E	389	LYS
1	E	403	HIS
1	E	413	ILE
1	E	416	ARG
1	E	418	ASN
1	E	493	LEU

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Mol	Chain	Res	Type
1	E	497	CYS
1	E	498	CYS
1	F	11	TYR
1	F	49	LEU
1	F	52	ARG
1	F	64	CYS
1	F	76	LEU
1	F	82	ASP
1	F	91	GLU
1	F	102	ILE
1	F	107	ASN
1	F	133	GLN
1	F	139	ARG
1	F	144	ASN
1	F	151	ILE
1	F	175	GLU
1	F	193	THR
1	F	212	ILE
1	F	281	GLU
1	F	298	ARG
1	F	303	GLU
1	F	318	VAL
1	F	332	ILE
1	F	336	LEU
1	F	373	THR
1	F	389	LYS
1	F	403	HIS
1	F	413	ILE
1	F	416	ARG
1	F	420	LYS
1	F	493	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (91) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	HIS
1	A	106	GLN
1	A	113	ASN
1	A	129	ASN
1	A	133	GLN
1	A	138	HIS
1	A	250	GLN

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Mol	Chain	Res	Type
1	A	258	GLN
1	A	285	ASN
1	A	325	ASN
1	A	432	ASN
1	A	439	HIS
1	A	450	GLN
1	A	494	GLN
1	B	78	GLN
1	B	85	ASN
1	B	96	HIS
1	B	108	HIS
1	B	113	ASN
1	B	129	ASN
1	B	133	GLN
1	B	250	GLN
1	B	258	GLN
1	B	285	ASN
1	B	325	ASN
1	B	418	ASN
1	B	419	ASN
1	B	432	ASN
1	B	439	HIS
1	B	450	GLN
1	B	472	HIS
1	B	494	GLN
1	C	96	HIS
1	C	106	GLN
1	C	107	ASN
1	C	113	ASN
1	C	129	ASN
1	C	133	GLN
1	C	258	GLN
1	C	285	ASN
1	C	325	ASN
1	C	348	GLN
1	C	418	ASN
1	C	432	ASN
1	C	439	HIS
1	C	450	GLN
1	C	494	GLN
1	D	96	HIS
1	D	108	HIS

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Mol	Chain	Res	Type
1	D	113	ASN
1	D	129	ASN
1	D	133	GLN
1	D	138	HIS
1	D	258	GLN
1	D	275	ASN
1	D	285	ASN
1	D	325	ASN
1	D	348	GLN
1	D	418	ASN
1	D	432	ASN
1	D	439	HIS
1	D	450	GLN
1	E	96	HIS
1	E	106	GLN
1	E	107	ASN
1	E	129	ASN
1	E	133	GLN
1	E	138	HIS
1	E	250	GLN
1	E	258	GLN
1	E	285	ASN
1	E	325	ASN
1	E	418	ASN
1	E	428	ASN
1	E	432	ASN
1	E	439	HIS
1	E	450	GLN
1	F	96	HIS
1	F	106	GLN
1	F	113	ASN
1	F	129	ASN
1	F	133	GLN
1	F	258	GLN
1	F	272	GLN
1	F	285	ASN
1	F	325	ASN
1	F	348	GLN
1	F	428	ASN
1	F	432	ASN
1	F	439	HIS
1	F	450	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

17 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	1.78	8 (16%)	54,89,89	2.50	9 (16%)
3	NAP	A	601	-	42,52,52	1.62	6 (14%)	54,80,80	2.90	9 (16%)
4	MPD	A	701	-	6,7,7	0.33	0	7,10,10	0.56	0
2	FAD	B	600	-	48,58,58	1.76	9 (18%)	54,89,89	2.56	11 (20%)
3	NAP	B	601	-	42,52,52	1.50	7 (16%)	54,80,80	2.64	9 (16%)
4	MPD	B	700	-	6,7,7	0.34	0	7,10,10	0.59	0
4	MPD	B	701	-	6,7,7	0.37	0	7,10,10	0.51	0
2	FAD	C	600	-	48,58,58	1.90	7 (14%)	54,89,89	2.52	10 (18%)
3	NAP	C	601	-	42,52,52	1.58	6 (14%)	54,80,80	2.83	9 (16%)
2	FAD	D	600	-	48,58,58	2.23	10 (20%)	54,89,89	2.54	11 (20%)
3	NAP	D	601	-	42,52,52	1.83	9 (21%)	54,80,80	1.25	4 (7%)
4	MPD	D	700	-	6,7,7	0.35	0	7,10,10	0.50	0
2	FAD	E	600	-	48,58,58	1.82	11 (22%)	54,89,89	2.55	8 (14%)
3	NAP	E	601	-	42,52,52	1.52	6 (14%)	54,80,80	1.29	6 (11%)
2	FAD	F	600	-	48,58,58	1.70	8 (16%)	54,89,89	2.58	11 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAP	F	601	-	42,52,52	1.28	4 (9%)	54,80,80	1.29	6 (11%)
4	MPD	F	700	-	6,7,7	0.41	0	7,10,10	0.58	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	-	-	0/30/50/50	0/6/6/6
3	NAP	A	601	-	1/1/12/12	0/27/67/67	0/5/5/5
4	MPD	A	701	-	-	0/5/5/5	0/0/0/0
2	FAD	B	600	-	-	0/30/50/50	0/6/6/6
3	NAP	B	601	-	1/1/12/12	0/27/67/67	0/5/5/5
4	MPD	B	700	-	-	0/5/5/5	0/0/0/0
4	MPD	B	701	-	-	0/5/5/5	0/0/0/0
2	FAD	C	600	-	-	0/30/50/50	0/6/6/6
3	NAP	C	601	-	1/1/12/12	0/27/67/67	0/5/5/5
2	FAD	D	600	-	-	0/30/50/50	0/6/6/6
3	NAP	D	601	-	-	0/27/67/67	0/5/5/5
4	MPD	D	700	-	-	0/5/5/5	0/0/0/0
2	FAD	E	600	-	-	0/30/50/50	0/6/6/6
3	NAP	E	601	-	-	0/27/67/67	0/5/5/5
2	FAD	F	600	-	-	0/30/50/50	0/6/6/6
3	NAP	F	601	-	-	0/27/67/67	0/5/5/5
4	MPD	F	700	-	-	0/5/5/5	0/0/0/0

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	NAP	C3B-C2B	-3.13	1.46	1.53
3	B	601	NAP	C3B-C2B	-2.48	1.47	1.53
2	A	600	FAD	C5A-C4A	-2.06	1.35	1.40
3	D	601	NAP	C2N-C3N	2.00	1.42	1.39
2	B	600	FAD	O4B-C1B	2.00	1.43	1.41
2	D	600	FAD	C9A-C5X	2.05	1.46	1.42
2	D	600	FAD	C2A-N3A	2.10	1.35	1.32
2	E	600	FAD	C10-N10	2.10	1.41	1.39
3	D	601	NAP	C2A-N1A	2.21	1.38	1.33
2	F	600	FAD	C2A-N3A	2.22	1.36	1.32
2	B	600	FAD	C4X-C10	2.24	1.45	1.41
3	E	601	NAP	C4A-N3A	2.27	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	FAD	C6-C5X	2.28	1.45	1.41
2	E	600	FAD	C2A-N3A	2.29	1.36	1.32
3	B	601	NAP	O4B-C1B	2.31	1.44	1.41
3	B	601	NAP	C2A-N3A	2.38	1.36	1.32
2	A	600	FAD	C9-C8	2.39	1.44	1.37
2	F	600	FAD	C5X-N5	2.39	1.39	1.35
2	A	600	FAD	C5X-N5	2.44	1.39	1.35
2	B	600	FAD	C5X-N5	2.47	1.39	1.35
3	A	601	NAP	C4A-N3A	2.51	1.39	1.35
2	E	600	FAD	C10-N1	2.54	1.39	1.35
2	D	600	FAD	C9-C8	2.59	1.44	1.37
2	E	600	FAD	C9-C8	2.62	1.45	1.37
3	D	601	NAP	C4A-N3A	2.64	1.39	1.35
3	A	601	NAP	C2A-N3A	2.65	1.36	1.32
3	B	601	NAP	C4A-N3A	2.65	1.39	1.35
2	E	600	FAD	C4X-C10	2.66	1.46	1.41
2	E	600	FAD	O4B-C1B	2.67	1.44	1.41
3	C	601	NAP	O4B-C1B	2.67	1.44	1.41
2	E	600	FAD	C5X-N5	2.68	1.39	1.35
2	B	600	FAD	C9-C8	2.75	1.45	1.37
3	E	601	NAP	C2A-N3A	2.84	1.37	1.32
2	D	600	FAD	C4X-C10	2.88	1.46	1.41
2	F	600	FAD	C9-C8	2.90	1.45	1.37
3	F	601	NAP	C4A-N3A	2.96	1.40	1.35
3	E	601	NAP	C6N-N1N	2.98	1.43	1.35
3	D	601	NAP	C2A-N3A	2.99	1.37	1.32
2	B	600	FAD	C10-N10	3.01	1.42	1.39
3	C	601	NAP	C4A-N3A	3.03	1.40	1.35
2	C	600	FAD	C9-C8	3.06	1.46	1.37
3	D	601	NAP	C6N-N1N	3.09	1.43	1.35
3	D	601	NAP	C3N-C7N	3.13	1.55	1.50
3	F	601	NAP	C2A-N3A	3.14	1.37	1.32
3	B	601	NAP	C6N-N1N	3.16	1.43	1.35
2	F	600	FAD	C4A-N3A	3.17	1.40	1.35
3	E	601	NAP	C4N-C3N	3.18	1.44	1.39
2	E	600	FAD	C4A-N3A	3.20	1.40	1.35
2	A	600	FAD	C4A-N3A	3.29	1.40	1.35
3	F	601	NAP	C6N-N1N	3.29	1.44	1.35
3	C	601	NAP	C6N-N1N	3.31	1.44	1.35
3	A	601	NAP	C6N-N1N	3.33	1.44	1.35
3	C	601	NAP	C2A-N3A	3.33	1.38	1.32
3	F	601	NAP	C4N-C3N	3.35	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	601	NAP	O4B-C4B	3.37	1.52	1.45
2	C	600	FAD	C4A-N3A	3.37	1.40	1.35
2	C	600	FAD	C4-N3	3.41	1.39	1.33
3	A	601	NAP	C4N-C3N	3.42	1.45	1.39
3	B	601	NAP	C4N-C3N	3.52	1.45	1.39
2	B	600	FAD	C4-N3	3.55	1.39	1.33
2	F	600	FAD	O4B-C1B	3.58	1.45	1.41
3	D	601	NAP	O4B-C4B	3.58	1.53	1.45
3	C	601	NAP	C4N-C3N	3.62	1.45	1.39
2	A	600	FAD	C9A-N10	3.68	1.43	1.38
2	D	600	FAD	C4-N3	3.70	1.40	1.33
2	D	600	FAD	C4A-N3A	3.72	1.41	1.35
3	D	601	NAP	C4N-C3N	3.77	1.45	1.39
2	D	600	FAD	C5X-N5	3.78	1.41	1.35
2	F	600	FAD	C4-N3	3.81	1.40	1.33
2	E	600	FAD	C4-N3	3.85	1.40	1.33
2	B	600	FAD	C4A-N3A	3.91	1.41	1.35
2	C	600	FAD	C1'-N10	4.14	1.52	1.48
2	A	600	FAD	C4-N3	4.24	1.41	1.33
3	B	601	NAP	O4B-C4B	4.55	1.55	1.45
2	F	600	FAD	C4X-N5	4.69	1.40	1.33
2	B	600	FAD	C9A-N10	4.74	1.45	1.38
2	B	600	FAD	C4X-N5	5.17	1.41	1.33
3	C	601	NAP	O4B-C4B	5.18	1.57	1.45
2	F	600	FAD	C9A-N10	5.24	1.46	1.38
2	A	600	FAD	O4B-C1B	5.25	1.47	1.41
3	E	601	NAP	O4B-C1B	5.40	1.48	1.41
2	E	600	FAD	C4X-N5	5.46	1.41	1.33
2	E	600	FAD	C9A-N10	5.47	1.46	1.38
2	A	600	FAD	C4X-N5	5.62	1.42	1.33
3	A	601	NAP	O4B-C4B	5.77	1.58	1.45
2	C	600	FAD	C4X-N5	5.91	1.42	1.33
2	D	600	FAD	C9A-N10	5.97	1.47	1.38
3	D	601	NAP	O4B-C1B	6.46	1.49	1.41
2	C	600	FAD	C9A-N10	6.50	1.47	1.38
2	D	600	FAD	C4X-N5	6.58	1.43	1.33
2	D	600	FAD	O4B-C1B	7.48	1.50	1.41

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	600	FAD	O3P-PA-O5B	-7.92	81.93	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	NAP	O4B-C4B-C5B	-7.91	81.03	109.32
3	B	601	NAP	O4B-C4B-C5B	-7.24	83.43	109.32
3	C	601	NAP	O4B-C4B-C5B	-7.19	83.59	109.32
2	B	600	FAD	O3P-PA-O5B	-7.04	84.27	102.94
2	C	600	FAD	O3P-PA-O5B	-6.86	84.72	102.94
2	D	600	FAD	O3P-PA-O5B	-6.84	84.79	102.94
3	C	601	NAP	O4B-C1B-C2B	-6.73	94.42	106.60
2	A	600	FAD	O3P-PA-O5B	-6.65	85.28	102.94
2	F	600	FAD	O2A-PA-O3P	-6.54	75.42	105.09
3	A	601	NAP	O4B-C4B-C3B	-6.35	92.35	105.15
2	A	600	FAD	C4X-C4-N3	-6.33	114.93	123.59
2	D	600	FAD	O2A-PA-O3P	-6.30	76.49	105.09
2	A	600	FAD	O2A-PA-O3P	-6.30	76.52	105.09
2	B	600	FAD	C4X-C4-N3	-6.26	115.02	123.59
2	C	600	FAD	O2A-PA-O3P	-6.22	76.88	105.09
3	A	601	NAP	O4B-C1B-C2B	-6.02	95.71	106.60
2	F	600	FAD	C4X-C4-N3	-5.93	115.48	123.59
2	F	600	FAD	O3P-PA-O5B	-5.84	87.44	102.94
2	D	600	FAD	C4X-C4-N3	-5.76	115.72	123.59
2	B	600	FAD	O2A-PA-O3P	-5.73	79.11	105.09
2	C	600	FAD	C4X-C4-N3	-5.71	115.79	123.59
3	C	601	NAP	C3B-C2B-C1B	-5.64	91.83	102.73
2	E	600	FAD	O2A-PA-O3P	-5.62	79.61	105.09
2	E	600	FAD	C4X-C4-N3	-5.60	115.93	123.59
3	C	601	NAP	O4B-C4B-C3B	-5.58	93.89	105.15
3	B	601	NAP	O4B-C1B-C2B	-5.19	97.22	106.60
3	B	601	NAP	O4B-C4B-C3B	-4.79	95.49	105.15
3	A	601	NAP	N3A-C2A-N1A	-4.77	125.24	128.89
2	F	600	FAD	C4B-O4B-C1B	-4.47	104.81	109.72
3	A	601	NAP	C3B-C2B-C1B	-4.29	94.42	102.73
3	C	601	NAP	N3A-C2A-N1A	-4.16	125.71	128.89
3	F	601	NAP	N3A-C2A-N1A	-4.05	125.79	128.89
3	B	601	NAP	N3A-C2A-N1A	-4.04	125.80	128.89
3	E	601	NAP	N3A-C2A-N1A	-3.87	125.93	128.89
3	C	601	NAP	O5B-C5B-C4B	-3.85	94.93	109.12
3	D	601	NAP	N3A-C2A-N1A	-3.71	126.06	128.89
3	A	601	NAP	O5B-C5B-C4B	-3.09	97.73	109.12
3	D	601	NAP	O4B-C1B-C2B	-3.06	101.07	106.60
3	B	601	NAP	C3B-C2B-C1B	-2.94	97.03	102.73
3	E	601	NAP	O4B-C4B-C5B	-2.86	99.11	109.32
3	F	601	NAP	O4B-C1B-N9A	-2.84	102.15	108.10
3	B	601	NAP	O5B-C5B-C4B	-2.51	99.87	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	601	NAP	O4B-C1B-C2B	-2.37	102.32	106.60
3	E	601	NAP	O4B-C4B-C3B	-2.14	100.84	105.15
3	E	601	NAP	O4B-C1B-C2B	-2.08	102.84	106.60
2	D	600	FAD	O4B-C1B-N9A	2.01	112.30	108.10
2	D	600	FAD	C5X-C9A-N10	2.01	119.15	117.62
3	F	601	NAP	O2A-PA-O1A	2.03	123.56	112.53
2	C	600	FAD	O2B-C2B-C3B	2.08	118.59	111.83
2	E	600	FAD	C5X-C9A-N10	2.09	119.21	117.62
3	B	601	NAP	C2A-N1A-C6A	2.10	122.52	118.77
3	F	601	NAP	C2A-N1A-C6A	2.12	122.56	118.77
2	C	600	FAD	O4B-C1B-N9A	2.12	112.55	108.10
3	F	601	NAP	C4A-C5A-N7A	2.13	111.44	109.48
2	A	600	FAD	C2B-C1B-N9A	2.13	117.55	114.29
3	A	601	NAP	C2A-N1A-C6A	2.16	122.63	118.77
3	C	601	NAP	C2A-N1A-C6A	2.17	122.64	118.77
3	B	601	NAP	O2B-C2B-C1B	2.18	118.54	110.02
3	D	601	NAP	O2B-C2B-C1B	2.20	118.59	110.02
2	B	600	FAD	C1'-N10-C9A	2.20	121.33	118.86
3	E	601	NAP	C2A-N1A-C6A	2.23	122.74	118.77
2	B	600	FAD	O2B-C2B-C3B	2.26	119.18	111.83
2	B	600	FAD	C4A-C5A-N7A	2.33	111.62	109.48
2	F	600	FAD	C1'-N10-C9A	2.33	121.48	118.86
2	D	600	FAD	O2B-C2B-C3B	2.36	119.51	111.83
3	D	601	NAP	C4A-C5A-N7A	2.56	111.83	109.48
3	E	601	NAP	O3-PA-O5B	2.57	109.76	102.94
2	D	600	FAD	O5B-C5B-C4B	2.58	118.63	109.12
3	A	601	NAP	O2B-C2B-C1B	2.64	120.31	110.02
2	A	600	FAD	O3P-P-O5'	2.77	110.28	102.94
2	C	600	FAD	C1'-N10-C9A	2.80	122.00	118.86
2	F	600	FAD	O4B-C1B-N9A	2.81	113.98	108.10
3	C	601	NAP	O2B-C2B-C1B	3.06	121.97	110.02
2	F	600	FAD	O5B-C5B-C4B	3.09	120.51	109.12
2	B	600	FAD	O3P-P-O5'	3.11	111.19	102.94
2	B	600	FAD	O5B-C5B-C4B	3.16	120.77	109.12
2	A	600	FAD	O5B-C5B-C4B	3.20	120.90	109.12
2	C	600	FAD	O3P-P-O5'	3.23	111.50	102.94
2	B	600	FAD	O2A-PA-O1A	3.50	131.48	112.53
2	D	600	FAD	O2A-PA-O1A	3.54	131.72	112.53
2	F	600	FAD	O2A-PA-O1A	3.55	131.78	112.53
2	F	600	FAD	P-O3P-PA	3.55	142.71	132.73
2	E	600	FAD	O2A-PA-O1A	3.57	131.86	112.53
2	C	600	FAD	O2A-PA-O1A	3.63	132.19	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	FAD	O2A-PA-O1A	3.66	132.34	112.53
2	F	600	FAD	O4B-C4B-C5B	3.71	122.59	109.32
2	D	600	FAD	O3P-P-O5'	3.94	113.40	102.94
2	E	600	FAD	O3P-P-O5'	4.14	113.93	102.94
2	A	600	FAD	P-O3P-PA	4.93	146.58	132.73
2	C	600	FAD	P-O3P-PA	4.96	146.66	132.73
2	E	600	FAD	P-O3P-PA	5.03	146.85	132.73
2	B	600	FAD	P-O3P-PA	5.27	147.52	132.73
2	D	600	FAD	P-O3P-PA	5.67	148.64	132.73
2	A	600	FAD	C4-N3-C2	10.58	124.39	115.25
2	D	600	FAD	C4-N3-C2	10.98	124.74	115.25
2	C	600	FAD	C4-N3-C2	11.01	124.77	115.25
2	F	600	FAD	C4-N3-C2	11.16	124.89	115.25
2	E	600	FAD	C4-N3-C2	11.18	124.91	115.25
2	B	600	FAD	C4-N3-C2	11.36	125.07	115.25
3	C	601	NAP	C5B-C4B-C3B	13.54	168.96	115.21
3	B	601	NAP	C5B-C4B-C3B	13.68	169.49	115.21
3	A	601	NAP	C5B-C4B-C3B	14.29	171.93	115.21

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	601	NAP	C4B
3	A	601	NAP	C4B
3	C	601	NAP	C4B

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	FAD	4	0
3	A	601	NAP	1	0
4	A	701	MPD	2	0
2	B	600	FAD	1	0
3	B	601	NAP	6	0
4	B	700	MPD	2	0
4	B	701	MPD	3	0
3	C	601	NAP	1	0
2	D	600	FAD	5	0
3	D	601	NAP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	700	MPD	3	0
2	E	600	FAD	4	0
3	E	601	NAP	1	0
2	F	600	FAD	10	0
3	F	601	NAP	1	0
4	F	700	MPD	5	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	487/519 (93%)	-0.18	3 (0%)	90	86	25, 51, 70, 83	0
1	B	487/519 (93%)	-0.22	4 (0%)	87	81	26, 51, 69, 93	0
1	C	490/519 (94%)	-0.09	11 (2%)	65	54	31, 55, 75, 102	0
1	D	491/519 (94%)	-0.14	8 (1%)	74	66	26, 52, 73, 107	0
1	E	490/519 (94%)	-0.00	13 (2%)	58	45	32, 59, 82, 105	0
1	F	486/519 (93%)	-0.08	8 (1%)	74	66	29, 57, 77, 91	0
All	All	2931/3114 (94%)	-0.12	47 (1%)	74	66	25, 54, 75, 107	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	499	GLY	4.6
1	B	495	ALA	4.1
1	E	498	CYS	4.0
1	C	498	CYS	4.0
1	E	496	GLY	4.0
1	A	10	SER	3.9
1	E	497	CYS	3.8
1	E	495	ALA	3.6
1	D	9	LYS	3.6
1	F	491	SER	3.6
1	F	490	ALA	3.5
1	D	495	ALA	3.5
1	F	9	LYS	3.4
1	B	9	LYS	3.4
1	E	52	ARG	3.3
1	B	494	GLN	3.1
1	F	10	SER	3.0
1	A	495	ALA	2.9
1	E	148	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	499	GLY	2.9
1	C	10	SER	2.7
1	C	494	GLN	2.7
1	C	261	ALA	2.6
1	C	277	GLU	2.6
1	C	262	GLY	2.6
1	C	495	ALA	2.6
1	D	10	SER	2.5
1	C	497	CYS	2.5
1	F	259	ILE	2.5
1	C	276	SER	2.4
1	D	498	CYS	2.3
1	B	493	LEU	2.3
1	E	10	SER	2.3
1	F	308	LYS	2.3
1	F	139	ARG	2.2
1	E	93	THR	2.2
1	E	139	ARG	2.2
1	E	494	GLN	2.1
1	D	158	LEU	2.1
1	D	497	CYS	2.1
1	E	364	LYS	2.1
1	E	279	ILE	2.1
1	F	176	TYR	2.1
1	D	430	LYS	2.0
1	C	93	THR	2.0
1	A	277	GLU	2.0
1	E	48	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	MPD	A	701	8/8	0.86	0.41	8.81	76,78,79,79	0
4	MPD	D	700	8/8	0.92	0.20	2.43	39,41,43,43	0
4	MPD	B	701	8/8	0.85	0.29	2.38	58,60,61,62	0
3	NAP	E	601	48/48	0.84	0.25	0.99	73,104,121,121	0
2	FAD	F	600	53/53	0.94	0.21	0.80	52,60,62,64	0
3	NAP	B	601	48/48	0.88	0.21	0.50	63,86,104,105	0
2	FAD	E	600	53/53	0.94	0.20	0.49	54,59,83,84	0
3	NAP	A	601	48/48	0.90	0.20	0.46	68,86,102,104	0
4	MPD	B	700	8/8	0.94	0.18	0.45	34,38,39,44	0
4	MPD	F	700	8/8	0.94	0.17	0.40	34,35,37,37	0
3	NAP	F	601	48/48	0.81	0.21	0.26	83,108,119,120	0
3	NAP	C	601	48/48	0.87	0.22	0.18	80,95,101,102	0
3	NAP	D	601	48/48	0.89	0.20	-0.02	26,68,87,87	0
2	FAD	B	600	53/53	0.95	0.16	-0.13	35,45,50,52	0
2	FAD	D	600	53/53	0.94	0.16	-0.22	25,49,70,70	0
2	FAD	C	600	53/53	0.96	0.15	-0.45	20,40,61,62	0
2	FAD	A	600	53/53	0.96	0.15	-0.63	25,35,44,47	0

6.5 Other polymers (i)

There are no such residues in this entry.