



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2017 – 01:30 AM EDT

PDB ID : 2ZZC
Title : Crystal structure of NADP(H):human thioredoxin reductase I
Authors : Lo, Y.C.; Ko, T.P.; Wang, A.H.J.
Deposited on : unknown
Resolution : 2.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

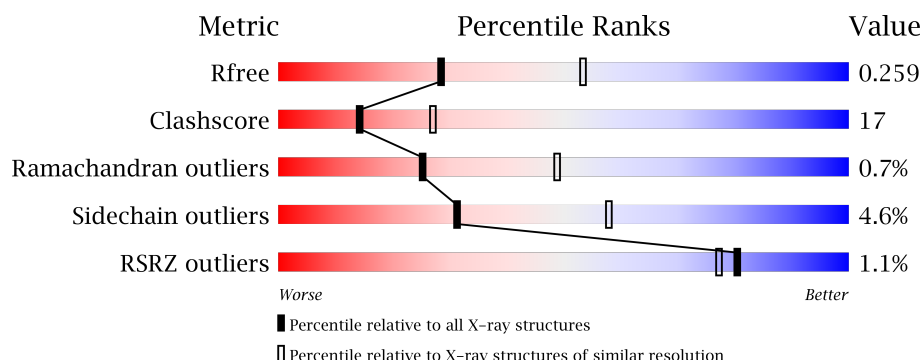
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	513	<div> <div> <div>0.1%</div> <div>60%</div> <div>32%</div> <div>5%</div> </div> </div>
1	B	513	<div> <div>69%</div> <div>24%</div> <div>6%</div> </div>
1	C	513	<div> <div>2%</div> <div>60%</div> <div>31%</div> <div>5%</div> </div>
1	D	513	<div> <div>0.1%</div> <div>64%</div> <div>27%</div> <div>6%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16283 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, cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	485	Total	C	N	O	S	0	0	0
			3750	2384	640	707	19			
1	B	484	Total	C	N	O	S	0	0	0
			3741	2379	638	705	19			
1	C	485	Total	C	N	O	S	0	0	0
			3750	2384	640	707	19			
1	D	484	Total	C	N	O	S	0	0	0
			3741	2379	638	705	19			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q16881
A	-12	ALA	-	EXPRESSION TAG	UNP Q16881
A	-11	HIS	-	EXPRESSION TAG	UNP Q16881
A	-10	HIS	-	EXPRESSION TAG	UNP Q16881
A	-9	HIS	-	EXPRESSION TAG	UNP Q16881
A	-8	HIS	-	EXPRESSION TAG	UNP Q16881
A	-7	HIS	-	EXPRESSION TAG	UNP Q16881
A	-6	HIS	-	EXPRESSION TAG	UNP Q16881
A	-5	VAL	-	EXPRESSION TAG	UNP Q16881
A	-4	ASP	-	EXPRESSION TAG	UNP Q16881
A	-3	ASP	-	EXPRESSION TAG	UNP Q16881
A	-2	ASP	-	EXPRESSION TAG	UNP Q16881
A	-1	ASP	-	EXPRESSION TAG	UNP Q16881
A	498	CYS	U	SEE REMARK 999	UNP Q16881
B	-13	MET	-	EXPRESSION TAG	UNP Q16881
B	-12	ALA	-	EXPRESSION TAG	UNP Q16881
B	-11	HIS	-	EXPRESSION TAG	UNP Q16881
B	-10	HIS	-	EXPRESSION TAG	UNP Q16881
B	-9	HIS	-	EXPRESSION TAG	UNP Q16881
B	-8	HIS	-	EXPRESSION TAG	UNP Q16881
B	-7	HIS	-	EXPRESSION TAG	UNP Q16881

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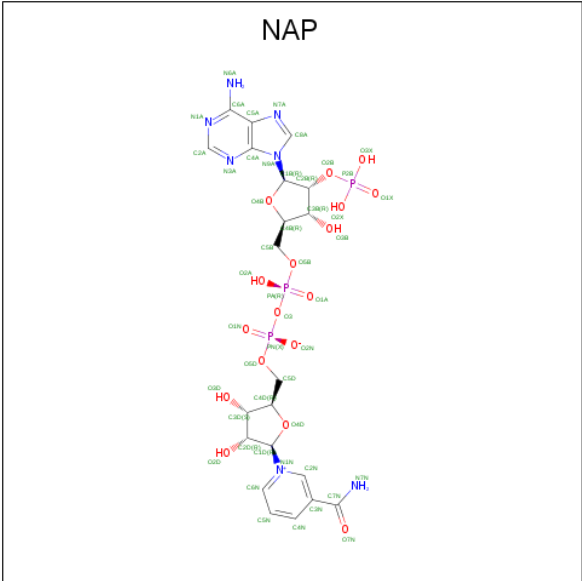
Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	EXPRESSION TAG	UNP Q16881
B	-5	VAL	-	EXPRESSION TAG	UNP Q16881
B	-4	ASP	-	EXPRESSION TAG	UNP Q16881
B	-3	ASP	-	EXPRESSION TAG	UNP Q16881
B	-2	ASP	-	EXPRESSION TAG	UNP Q16881
B	-1	ASP	-	EXPRESSION TAG	UNP Q16881
B	498	CYS	U	SEE REMARK 999	UNP Q16881
C	-13	MET	-	EXPRESSION TAG	UNP Q16881
C	-12	ALA	-	EXPRESSION TAG	UNP Q16881
C	-11	HIS	-	EXPRESSION TAG	UNP Q16881
C	-10	HIS	-	EXPRESSION TAG	UNP Q16881
C	-9	HIS	-	EXPRESSION TAG	UNP Q16881
C	-8	HIS	-	EXPRESSION TAG	UNP Q16881
C	-7	HIS	-	EXPRESSION TAG	UNP Q16881
C	-6	HIS	-	EXPRESSION TAG	UNP Q16881
C	-5	VAL	-	EXPRESSION TAG	UNP Q16881
C	-4	ASP	-	EXPRESSION TAG	UNP Q16881
C	-3	ASP	-	EXPRESSION TAG	UNP Q16881
C	-2	ASP	-	EXPRESSION TAG	UNP Q16881
C	-1	ASP	-	EXPRESSION TAG	UNP Q16881
C	498	CYS	U	SEE REMARK 999	UNP Q16881
D	-13	MET	-	EXPRESSION TAG	UNP Q16881
D	-12	ALA	-	EXPRESSION TAG	UNP Q16881
D	-11	HIS	-	EXPRESSION TAG	UNP Q16881
D	-10	HIS	-	EXPRESSION TAG	UNP Q16881
D	-9	HIS	-	EXPRESSION TAG	UNP Q16881
D	-8	HIS	-	EXPRESSION TAG	UNP Q16881
D	-7	HIS	-	EXPRESSION TAG	UNP Q16881
D	-6	HIS	-	EXPRESSION TAG	UNP Q16881
D	-5	VAL	-	EXPRESSION TAG	UNP Q16881
D	-4	ASP	-	EXPRESSION TAG	UNP Q16881
D	-3	ASP	-	EXPRESSION TAG	UNP Q16881
D	-2	ASP	-	EXPRESSION TAG	UNP Q16881
D	-1	ASP	-	EXPRESSION TAG	UNP Q16881
D	498	CYS	U	SEE REMARK 999	UNP Q16881

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



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		

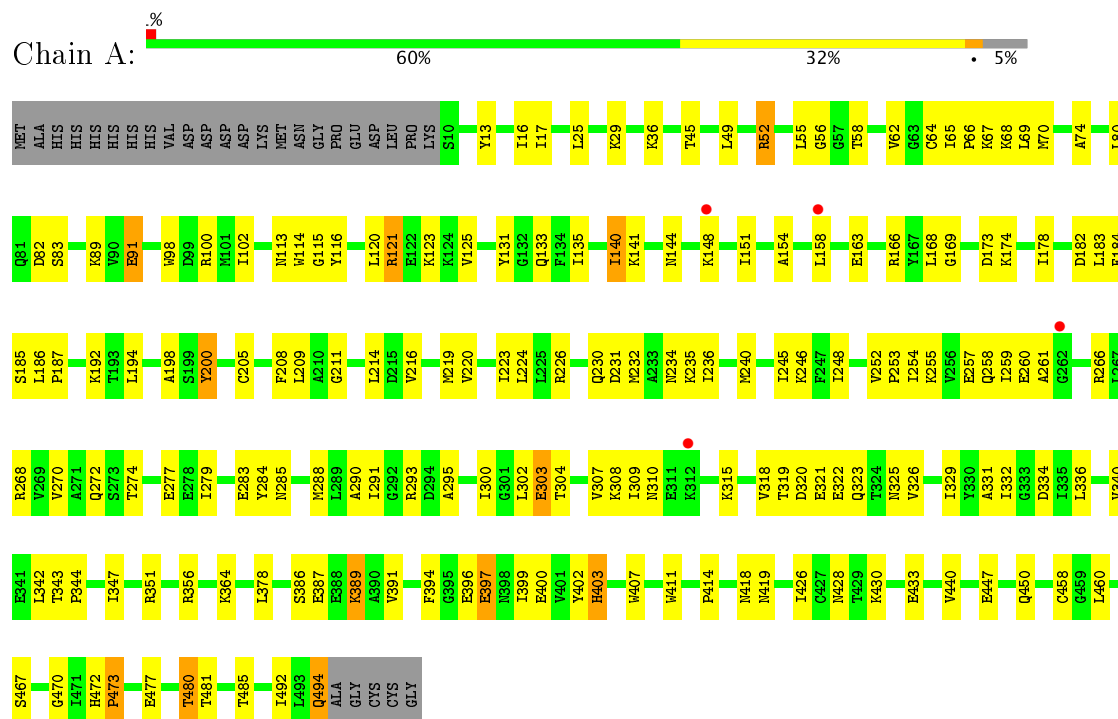
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	246	Total	O	0	0
			246	246		
4	B	260	Total	O	0	0
			260	260		
4	C	184	Total	O	0	0
			184	184		
4	D	207	Total	O	0	0
			207	207		

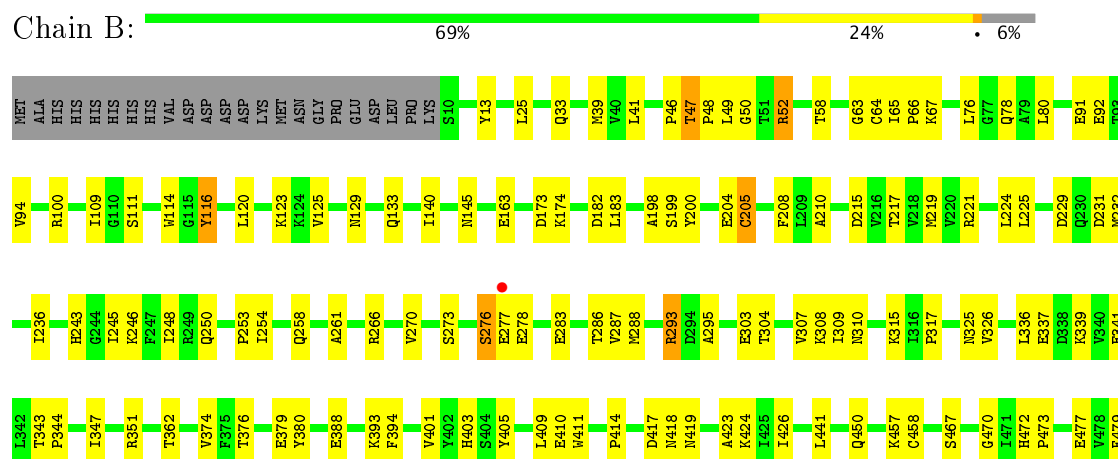
3 Residue-property plots

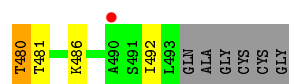
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Thioredoxin reductase 1, cytoplasmic

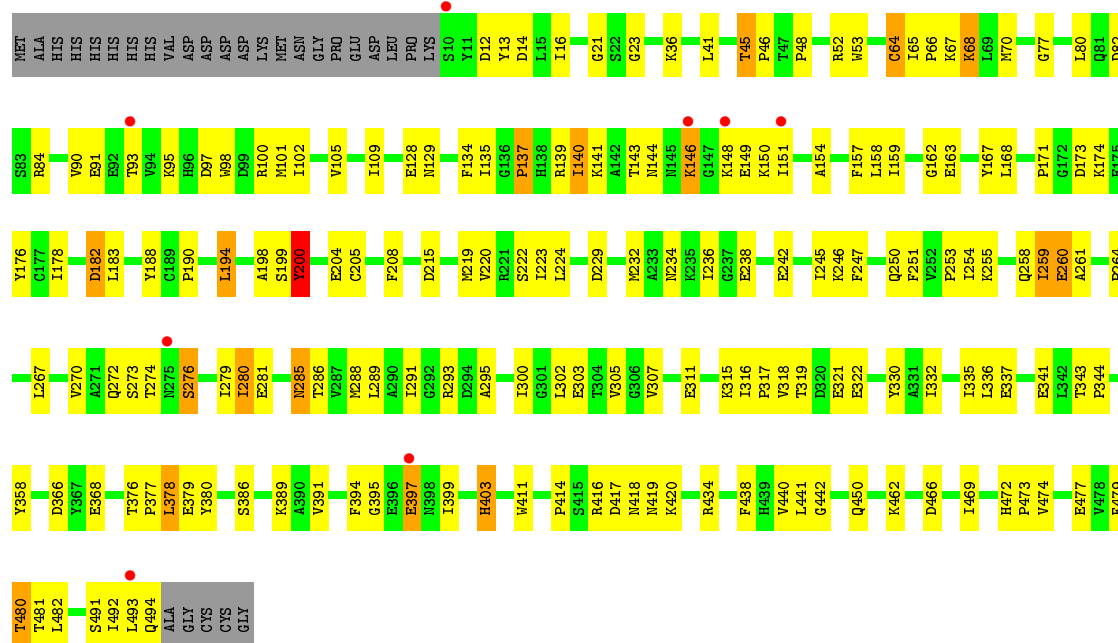


- Molecule 1: Thioredoxin reductase 1, cytoplasmic

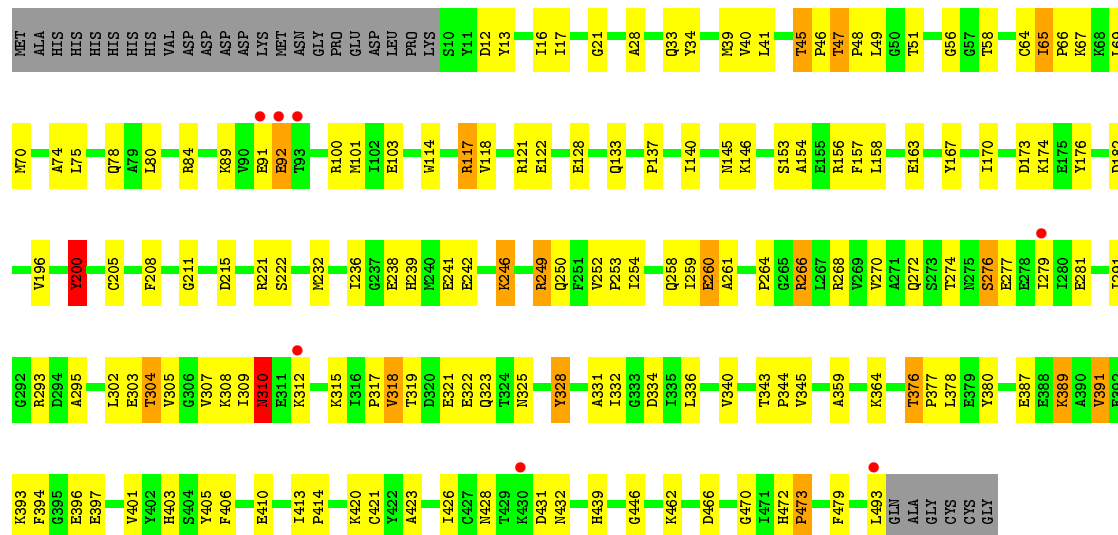




- Molecule 1: Thioredoxin reductase 1, cytoplasmic



- Molecule 1: Thioredoxin reductase 1, cytoplasmic



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	120.86Å 135.17Å 346.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.3 (30.00-2.60) 94.3 (29.92-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.61Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.211 , 0.260 0.210 , 0.259	Depositor DCC
R_{free} test set	4147 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16283	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, 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	0.94	2/3824 (0.1%)	0.96	4/5178 (0.1%)
1	B	0.97	2/3815 (0.1%)	0.95	2/5166 (0.0%)
1	C	0.89	1/3824 (0.0%)	0.91	4/5178 (0.1%)
1	D	0.93	2/3815 (0.1%)	0.94	2/5166 (0.0%)
All	All	0.93	7/15278 (0.0%)	0.94	12/20688 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	3
All	All	0	5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	GLU	CG-CD	6.97	1.62	1.51
1	D	103	GLU	CG-CD	6.89	1.62	1.51
1	B	114	TRP	CB-CG	-6.17	1.39	1.50
1	D	397	GLU	CG-CD	5.87	1.60	1.51
1	C	53	TRP	CB-CG	-5.44	1.40	1.50
1	B	205	CYS	CB-SG	5.12	1.91	1.82
1	A	91	GLU	CB-CG	5.02	1.61	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	194	LEU	CA-CB-CG	-5.94	101.64	115.30
1	C	182	ASP	CB-CG-OD2	5.74	123.46	118.30
1	B	293	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	A	82	ASP	CB-CG-OD1	5.67	123.40	118.30
1	D	310	ASN	N-CA-C	-5.61	95.84	111.00
1	C	378	LEU	N-CA-C	-5.56	95.99	111.00
1	C	182	ASP	CB-CG-OD1	-5.38	113.45	118.30
1	A	100	ARG	NE-CZ-NH2	5.33	122.96	120.30
1	B	310	ASN	N-CA-C	-5.29	96.73	111.00
1	D	65	ILE	C-N-CD	5.22	139.37	128.40
1	A	248	ILE	N-CA-C	-5.04	97.40	111.00
1	A	293	ARG	NE-CZ-NH1	-5.03	117.78	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	116	TYR	Sidechain
1	C	200	TYR	Sidechain
1	D	200	TYR	Sidechain
1	D	328	TYR	Sidechain
1	D	405	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3750	0	3759	151	0
1	B	3741	0	3751	110	0
1	C	3750	0	3759	167	0
1	D	3741	0	3751	134	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	2	0
3	A	48	0	25	3	0
3	B	48	0	25	4	0
3	C	48	0	25	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	48	0	25	3	0
4	A	246	0	0	5	0
4	B	260	0	0	7	0
4	C	184	0	0	5	0
4	D	207	0	0	1	0
All	All	16283	0	15244	534	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 17.

All (534) 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:B:308:LYS:N	1:B:325:ASN:HD21	1.43	1.17
1:C:419:ASN:ND2	1:C:494:GLN:HB2	1.62	1.13
1:D:302:LEU:HD22	1:D:307:VAL:HG21	1.27	1.12
1:B:308:LYS:H	1:B:325:ASN:ND2	1.48	1.09
1:C:183:LEU:HD22	1:C:288:MET:HE1	1.37	1.06
1:C:258:GLN:HE22	1:C:261:ALA:HB2	1.18	1.05
1:C:419:ASN:HD21	1:C:494:GLN:CB	1.69	1.05
1:C:311:GLU:OE2	4:C:702:HOH:O	1.77	1.01
1:D:39:MET:HE2	1:D:128:GLU:HG3	1.42	1.01
1:A:49:LEU:HD11	4:A:559:HOH:O	1.61	0.99
1:A:80:LEU:HD23	1:B:80:LEU:HD23	1.44	0.99
1:B:66:PRO:HG3	1:B:109:ILE:HD11	1.41	0.97
1:C:254:ILE:HD11	1:C:270:VAL:HG12	1.47	0.96
1:B:480:THR:HG22	1:B:481:THR:HG23	1.48	0.95
1:D:302:LEU:HD22	1:D:307:VAL:CG2	1.97	0.94
1:D:303:GLU:HG2	1:D:304:THR:N	1.84	0.93
1:C:493:LEU:O	1:C:493:LEU:HD12	1.70	0.92
1:D:39:MET:CE	1:D:128:GLU:HG3	1.99	0.92
1:A:36:LYS:HE2	1:A:36:LYS:HA	1.52	0.92
1:C:285:ASN:HD22	1:C:285:ASN:N	1.68	0.92
1:C:258:GLN:NE2	1:C:261:ALA:HB2	1.86	0.91
1:D:303:GLU:HG2	1:D:304:THR:H	1.38	0.89
1:D:84:ARG:NH1	1:D:92:GLU:HA	1.86	0.88
1:C:419:ASN:HD21	1:C:494:GLN:HB2	0.77	0.88
1:C:302:LEU:HD22	1:C:307:VAL:HB	1.56	0.88
1:C:318:VAL:HG11	1:C:322:GLU:HA	1.55	0.87
1:A:163:GLU:HG2	1:A:295:ALA:HA	1.56	0.85
1:D:47:THR:HG22	1:D:49:LEU:H	1.38	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ASP:OD1	1:C:174:LYS:N	2.09	0.85
1:C:199:SER:OG	1:C:200:TYR:N	2.11	0.79
1:C:68:LYS:HE3	1:D:410:GLU:OE2	1.83	0.79
1:C:183:LEU:HD22	1:C:288:MET:CE	2.12	0.79
1:C:397:GLU:H	1:C:397:GLU:CD	1.84	0.78
1:C:258:GLN:HE21	1:C:261:ALA:N	1.81	0.78
1:C:254:ILE:CD1	1:C:270:VAL:HG12	2.14	0.77
1:C:254:ILE:HD11	1:C:270:VAL:CG1	2.14	0.77
1:A:121:ARG:HH11	1:A:121:ARG:CG	1.98	0.77
1:A:480:THR:HG22	1:A:481:THR:HG23	1.66	0.77
1:D:238:GLU:O	1:D:242:GLU:HG3	1.84	0.77
1:C:158:LEU:HD11	1:C:332:ILE:HG12	1.68	0.75
1:D:47:THR:HG22	1:D:49:LEU:N	2.00	0.75
1:C:168:LEU:HD23	1:C:291:ILE:HD13	1.69	0.74
1:B:100:ARG:HG2	1:B:100:ARG:HH21	1.51	0.74
1:A:70:MET:HE1	1:A:184:PHE:HD1	1.52	0.74
1:D:117:ARG:HG2	1:D:117:ARG:HH21	1.52	0.73
1:D:259:ILE:HD11	1:D:268:ARG:HB2	1.70	0.73
1:D:200:TYR:HB3	3:D:901:NAP:C5N	2.19	0.73
1:D:17:ILE:HG12	1:D:158:LEU:HD23	1.69	0.72
1:D:84:ARG:HH11	1:D:92:GLU:HA	1.52	0.72
1:A:67:LYS:C	1:A:67:LYS:HD2	2.09	0.72
1:B:215:ASP:OD1	1:B:246:LYS:NZ	2.23	0.72
1:C:67:LYS:HD2	1:C:67:LYS:C	2.10	0.72
1:B:258:GLN:OE1	1:B:261:ALA:HB2	1.90	0.72
1:A:200:TYR:HB3	3:A:901:NAP:C5N	2.20	0.71
1:B:200:TYR:HB3	3:B:901:NAP:C5N	2.20	0.71
1:C:394:PHE:HB2	1:C:399:ILE:HD11	1.73	0.71
1:B:405:TYR:CD1	1:B:492:ILE:HD13	2.25	0.70
1:C:41:LEU:HD23	1:C:128:GLU:HB2	1.73	0.70
1:A:173:ASP:OD1	1:A:174:LYS:N	2.25	0.70
1:C:16:ILE:HB	1:C:157:PHE:CE2	2.25	0.70
1:A:254:ILE:HD11	1:A:270:VAL:HG12	1.73	0.70
1:A:121:ARG:HH11	1:A:121:ARG:HG3	1.57	0.70
1:C:36:LYS:HE2	1:C:358:TYR:CD1	2.27	0.69
1:D:47:THR:CG2	1:D:49:LEU:H	2.05	0.69
1:A:266:ARG:NH1	1:A:283:GLU:OE1	2.22	0.69
1:B:250:GLN:HE22	1:D:222:SER:HB2	1.56	0.69
1:C:378:LEU:HD11	1:C:442:GLY:HA2	1.75	0.68
1:A:120:LEU:HD22	1:A:125:VAL:HG11	1.74	0.68
1:C:200:TYR:HB3	3:C:901:NAP:C5N	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:CYS:HA	1:D:208:PHE:CE2	2.28	0.68
1:A:36:LYS:HE2	1:A:36:LYS:CA	2.22	0.68
1:C:80:LEU:HD23	1:D:80:LEU:HD23	1.76	0.68
1:A:98:TRP:NE1	1:A:102:ILE:HG13	2.08	0.68
1:D:315:LYS:HE3	1:D:336:LEU:O	1.92	0.67
1:C:146:LYS:HE3	1:C:148:LYS:HE2	1.76	0.67
1:C:259:ILE:O	1:C:259:ILE:HG22	1.94	0.67
1:D:302:LEU:HB3	1:D:307:VAL:HG23	1.75	0.67
1:D:47:THR:HG21	1:D:182:ASP:OD1	1.94	0.67
1:A:70:MET:CE	1:A:184:PHE:HD1	2.07	0.67
1:C:474:VAL:O	1:C:477:GLU:HG2	1.95	0.67
1:A:194:LEU:HD22	1:A:284:TYR:CE1	2.29	0.66
1:A:80:LEU:HD23	1:B:80:LEU:CD2	2.23	0.66
1:C:254:ILE:CG1	1:C:270:VAL:HG12	2.24	0.66
1:B:315:LYS:HB2	1:B:337:GLU:HB2	1.76	0.66
1:C:70:MET:HG2	1:C:101:MET:HE3	1.77	0.66
1:C:168:LEU:CD2	1:C:291:ILE:HD13	2.25	0.66
1:B:205:CYS:HA	1:B:208:PHE:CE2	2.30	0.66
1:C:258:GLN:NE2	1:C:261:ALA:CB	2.56	0.66
1:C:238:GLU:O	1:C:242:GLU:HG3	1.94	0.66
1:A:121:ARG:NH1	1:A:121:ARG:HG3	2.09	0.66
1:A:319:THR:HG23	1:A:323:GLN:O	1.96	0.66
1:C:198:ALA:HB2	1:C:220:VAL:HG13	1.78	0.66
1:C:379:GLU:O	1:C:441:LEU:HD12	1.96	0.66
1:B:393:LYS:HD3	1:B:394:PHE:CE1	2.30	0.65
1:D:428:ASN:ND2	1:D:431:ASP:HB3	2.10	0.65
1:C:480:THR:HG22	1:C:481:THR:HG23	1.79	0.65
1:D:176:TYR:CE1	1:D:258:GLN:HB2	2.31	0.65
1:A:205:CYS:HA	1:A:208:PHE:CE2	2.32	0.65
1:C:258:GLN:NE2	1:C:261:ALA:CA	2.60	0.64
1:B:219:MET:SD	1:B:253:PRO:HD3	2.37	0.64
1:D:117:ARG:HG2	1:D:117:ARG:NH2	2.13	0.64
1:A:315:LYS:HD2	1:A:336:LEU:O	1.98	0.64
1:A:480:THR:CG2	1:A:481:THR:HG23	2.28	0.64
1:A:340:VAL:CG1	1:A:342:LEU:HD12	2.28	0.64
1:C:105:VAL:O	1:C:109:ILE:HG13	1.98	0.64
1:A:192:LYS:H	1:A:285:ASN:HD22	1.43	0.64
1:D:272:GLN:HB2	1:D:279:ILE:HD13	1.80	0.63
1:A:400:GLU:HA	1:A:400:GLU:OE2	1.97	0.63
1:D:258:GLN:NE2	1:D:261:ALA:HA	2.14	0.63
1:D:462:LYS:HD2	1:D:466:ASP:OD1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HD11	1:A:226:ARG:HB2	1.81	0.63
1:A:477:GLU:O	1:A:480:THR:HB	1.99	0.63
1:B:47:THR:HG21	1:B:182:ASP:OD1	1.99	0.62
1:B:47:THR:HG23	1:B:48:PRO:HD2	1.81	0.62
1:A:308:LYS:N	1:A:325:ASN:OD1	2.27	0.62
1:D:242:GLU:OE2	1:D:420:LYS:NZ	2.23	0.62
1:C:318:VAL:CG1	1:C:322:GLU:HA	2.27	0.62
1:A:472:HIS:ND1	1:A:473:PRO:HA	2.14	0.62
1:B:325:ASN:OD1	1:B:326:VAL:HG23	1.99	0.62
1:B:374:VAL:HG12	1:B:376:THR:HG23	1.81	0.62
1:C:141:LYS:HD3	1:C:149:GLU:OE2	1.99	0.62
1:A:318:VAL:HG23	1:A:323:GLN:C	2.21	0.61
1:C:171:PRO:CG	1:C:255:LYS:HD2	2.30	0.61
1:D:100:ARG:HG2	1:D:100:ARG:NH2	2.14	0.61
1:B:91:GLU:OE2	4:B:660:HOH:O	2.16	0.61
1:C:254:ILE:HG12	1:C:270:VAL:O	2.00	0.61
1:C:322:GLU:HG2	1:C:332:ILE:HG22	1.83	0.61
1:A:186:LEU:HD12	1:A:187:PRO:HD2	1.80	0.61
1:A:387:GLU:O	1:A:391:VAL:HG23	2.01	0.60
1:C:315:LYS:HD2	1:C:336:LEU:O	2.01	0.60
1:A:17:ILE:HG12	1:A:158:LEU:HD23	1.83	0.60
1:C:293:ARG:HG2	1:C:293:ARG:HH11	1.67	0.60
1:D:413:ILE:HB	1:D:414:PRO:HD3	1.83	0.60
1:A:209:LEU:HB3	1:A:214:LEU:HD12	1.84	0.59
1:A:80:LEU:CD2	1:B:80:LEU:HD23	2.26	0.59
1:C:163:GLU:HG2	1:C:295:ALA:HA	1.83	0.59
1:A:303:GLU:OE1	1:A:304:THR:HG23	2.02	0.59
1:D:305:VAL:CG2	1:D:328:TYR:OH	2.51	0.58
1:D:258:GLN:NE2	1:D:261:ALA:CA	2.66	0.58
1:D:254:ILE:HD11	1:D:270:VAL:HG12	1.83	0.58
1:D:387:GLU:O	1:D:391:VAL:HG12	2.03	0.58
1:C:178:ILE:HB	1:C:182:ASP:HB2	1.86	0.58
1:C:293:ARG:HG2	1:C:293:ARG:NH1	2.17	0.58
1:A:325:ASN:ND2	1:A:326:VAL:HG23	2.18	0.58
1:A:419:ASN:OD1	1:A:494:GLN:HB2	2.03	0.58
1:A:168:LEU:HD21	3:A:901:NAP:N6A	2.19	0.58
1:B:100:ARG:NH2	1:B:100:ARG:HG2	2.19	0.57
1:B:245:ILE:HD12	1:B:245:ILE:H	1.68	0.57
1:B:401:VAL:HG11	1:B:486:LYS:HD2	1.86	0.57
1:A:318:VAL:CG2	1:A:322:GLU:C	2.73	0.57
1:A:183:LEU:O	1:A:183:LEU:HD12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:TYR:CE1	1:B:492:ILE:HD13	2.39	0.57
1:C:98:TRP:NE1	1:C:102:ILE:HG13	2.20	0.57
1:C:378:LEU:CD2	1:C:441:LEU:HG	2.35	0.57
1:D:270:VAL:HG22	1:D:281:GLU:HG2	1.87	0.57
1:D:272:GLN:OE1	1:D:279:ILE:HD11	2.04	0.57
1:C:36:LYS:HE2	1:C:358:TYR:HD1	1.70	0.57
1:A:394:PHE:HD2	1:A:430:LYS:HE2	1.70	0.57
1:D:156:ARG:HG3	1:D:156:ARG:HH11	1.70	0.57
1:A:351:ARG:HD3	4:A:723:HOH:O	2.05	0.57
1:B:92:GLU:HG2	1:B:92:GLU:O	2.05	0.57
1:C:234:ASN:O	1:C:238:GLU:HG3	2.05	0.57
1:C:137:PRO:O	1:C:139:ARG:HG3	2.04	0.56
1:C:250:GLN:HB3	1:C:274:THR:HG22	1.87	0.56
1:D:334:ASP:OD2	2:D:900:FAD:H5'1	2.05	0.56
1:A:234:ASN:ND2	4:A:699:HOH:O	2.37	0.56
1:D:41:LEU:HD23	1:D:128:GLU:HB2	1.88	0.56
1:A:343:THR:HB	1:A:344:PRO:HD3	1.87	0.56
1:C:417:ASP:HB3	1:C:420:LYS:HG3	1.87	0.56
1:B:424:LYS:HE3	1:B:426:ILE:HD11	1.87	0.56
1:D:309:ILE:HG13	1:D:310:ASN:N	2.20	0.56
1:D:91:GLU:HG2	1:D:92:GLU:N	2.21	0.56
1:A:472:HIS:HD1	1:A:473:PRO:HA	1.71	0.56
1:A:259:ILE:HG21	1:A:266:ARG:NH2	2.21	0.56
1:A:158:LEU:HD11	1:A:332:ILE:HG12	1.87	0.56
1:D:16:ILE:HD12	1:D:157:PHE:CZ	2.41	0.56
1:A:344:PRO:HG3	1:B:472:HIS:HB2	1.87	0.56
1:D:140:ILE:HG21	1:D:157:PHE:HE2	1.69	0.56
1:A:140:ILE:HG12	1:A:141:LYS:N	2.21	0.55
1:B:343:THR:HB	1:B:344:PRO:HD3	1.88	0.55
1:A:391:VAL:HG13	1:A:396:GLU:HA	1.86	0.55
1:C:173:ASP:HB2	1:C:289:LEU:HD11	1.88	0.55
1:B:173:ASP:OD1	1:B:174:LYS:N	2.37	0.55
1:B:405:TYR:HD1	1:B:492:ILE:HD13	1.72	0.55
1:C:70:MET:HG2	1:C:101:MET:CE	2.36	0.55
1:C:245:ILE:HG22	1:C:247:PHE:CE2	2.42	0.55
1:C:285:ASN:ND2	1:C:285:ASN:N	2.43	0.55
1:C:477:GLU:O	1:C:480:THR:HB	2.07	0.55
1:D:319:THR:HG23	1:D:323:GLN:O	2.07	0.55
1:D:428:ASN:ND2	1:D:431:ASP:CB	2.70	0.55
1:D:133:GLN:O	1:D:140:ILE:HG13	2.08	0.54
1:A:258:GLN:OE1	1:A:261:ALA:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ILE:CD1	1:D:268:ARG:HB2	2.36	0.54
1:A:319:THR:C	1:A:321:GLU:H	2.10	0.54
1:B:308:LYS:HB2	1:B:325:ASN:HD22	1.72	0.54
1:B:133:GLN:O	1:B:140:ILE:HG13	2.08	0.54
1:D:423:ALA:HB1	1:D:479:PHE:CZ	2.43	0.54
1:A:318:VAL:HG21	1:A:322:GLU:C	2.29	0.53
1:B:308:LYS:HE2	1:B:325:ASN:HD22	1.72	0.53
1:C:259:ILE:O	1:C:260:GLU:CB	2.56	0.53
1:C:319:THR:C	1:C:321:GLU:H	2.11	0.53
1:B:47:THR:HG22	1:B:49:LEU:H	1.72	0.53
1:C:258:GLN:HE21	1:C:261:ALA:CA	2.21	0.53
1:A:428:ASN:OD1	1:A:430:LYS:HG2	2.08	0.53
1:B:273:SER:OG	1:B:278:GLU:HG2	2.08	0.53
1:A:340:VAL:HG12	1:A:342:LEU:HD12	1.89	0.53
1:A:236:ILE:O	1:A:240:MET:HG3	2.09	0.53
1:A:391:VAL:HG13	1:A:396:GLU:CA	2.39	0.53
1:D:17:ILE:HB	1:D:40:VAL:HG22	1.89	0.53
1:A:325:ASN:HD21	1:A:326:VAL:HG23	1.74	0.53
1:A:178:ILE:HB	1:A:182:ASP:HB2	1.89	0.53
1:A:255:LYS:HE3	1:A:257:GLU:HB3	1.91	0.53
1:A:13:TYR:O	1:A:154:ALA:HA	2.08	0.53
1:B:293:ARG:HD3	3:B:901:NAP:H51N	1.90	0.53
1:B:379:GLU:O	1:B:441:LEU:HD12	2.09	0.53
1:C:302:LEU:HD22	1:C:307:VAL:CB	2.35	0.53
1:C:95:LYS:CB	1:D:89:LYS:HE3	2.39	0.52
1:D:34:TYR:CE2	1:D:359:ALA:HB2	2.45	0.52
1:D:293:ARG:HD3	3:D:901:NAP:H51N	1.90	0.52
1:C:366:ASP:C	1:C:366:ASP:OD1	2.48	0.52
1:B:308:LYS:HB2	1:B:325:ASN:ND2	2.24	0.52
1:D:241:GLU:CD	1:D:249:ARG:HH22	2.13	0.52
1:D:272:GLN:HB2	1:D:279:ILE:CD1	2.39	0.52
1:B:217:THR:HG21	1:B:248:ILE:HD12	1.92	0.52
1:C:322:GLU:O	1:C:330:TYR:HB3	2.10	0.52
1:C:450:GLN:OE1	1:D:470:GLY:HA2	2.09	0.52
1:D:258:GLN:HE21	1:D:261:ALA:HA	1.73	0.52
1:C:134:PHE:CD1	1:C:305:VAL:HG11	2.45	0.52
1:C:84:ARG:HG2	1:C:90:VAL:HG23	1.91	0.52
1:C:90:VAL:HG11	1:D:80:LEU:CD2	2.40	0.52
1:C:343:THR:HB	1:C:344:PRO:HD3	1.92	0.52
1:B:33:GLN:HE21	1:B:123:LYS:NZ	2.09	0.51
1:C:480:THR:CG2	1:C:481:THR:HG23	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:ILE:HD11	1:A:226:ARG:CB	2.39	0.51
1:D:100:ARG:HH21	1:D:100:ARG:HG2	1.74	0.51
1:C:258:GLN:HG2	1:C:260:GLU:H	1.75	0.50
1:C:462:LYS:HD2	1:C:462:LYS:O	2.11	0.50
1:D:309:ILE:HA	1:D:317:PRO:HD2	1.93	0.50
1:D:389:LYS:HD3	1:D:389:LYS:N	2.25	0.50
1:A:29:LYS:HG2	1:A:123:LYS:HG3	1.93	0.50
1:C:135:ILE:HD13	1:C:151:ILE:HD12	1.94	0.50
1:B:315:LYS:HE3	1:B:336:LEU:O	2.10	0.50
1:D:114:TRP:HZ3	1:D:117:ARG:HH11	1.58	0.50
1:D:276:SER:OG	1:D:277:GLU:N	2.44	0.50
1:A:472:HIS:HB2	1:B:344:PRO:HG3	1.94	0.50
1:C:140:ILE:HG21	1:C:157:PHE:CE2	2.47	0.50
1:C:198:ALA:CB	1:C:220:VAL:HG13	2.41	0.50
1:C:259:ILE:CG2	1:C:259:ILE:O	2.60	0.50
1:A:318:VAL:HG22	1:A:319:THR:N	2.27	0.50
1:D:322:GLU:HG2	1:D:332:ILE:HG22	1.94	0.50
1:A:394:PHE:CD2	1:A:430:LYS:HE2	2.46	0.50
1:B:410:GLU:H	1:B:410:GLU:CD	2.15	0.50
1:C:23:GLY:HA3	1:C:332:ILE:HD12	1.94	0.50
1:A:331:ALA:C	1:A:336:LEU:HD21	2.31	0.50
1:A:274:THR:CG2	1:A:274:THR:O	2.60	0.49
1:A:447:GLU:OE1	1:A:447:GLU:HA	2.13	0.49
1:B:307:VAL:HA	1:B:325:ASN:OD1	2.12	0.49
1:C:215:ASP:OD1	1:C:246:LYS:NZ	2.41	0.49
1:D:70:MET:HG2	1:D:101:MET:CE	2.41	0.49
1:A:309:ILE:HG13	1:A:310:ASN:N	2.27	0.49
1:B:198:ALA:HB1	1:B:224:LEU:HD22	1.93	0.49
1:B:245:ILE:HD12	1:B:245:ILE:N	2.27	0.49
1:C:440:VAL:HG13	1:C:440:VAL:O	2.13	0.49
1:D:236:ILE:HD11	1:D:380:TYR:HB2	1.95	0.49
1:C:251:PHE:CE1	1:C:280:ILE:HD12	2.48	0.49
1:C:318:VAL:CG1	1:C:319:THR:N	2.76	0.49
1:D:406:PHE:CZ	1:D:421:CYS:HB3	2.48	0.49
1:B:47:THR:O	1:B:50:GLY:N	2.37	0.49
1:D:343:THR:HB	1:D:344:PRO:HD3	1.95	0.49
1:A:318:VAL:HG23	1:A:323:GLN:O	2.13	0.49
1:B:200:TYR:CD2	3:B:901:NAP:H3D	2.47	0.49
1:A:356:ARG:NH1	1:A:364:LYS:HA	2.28	0.48
1:B:339:LYS:CE	4:B:783:HOH:O	2.60	0.48
1:C:143:THR:HG23	1:C:149:GLU:HG2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:GLU:OE1	1:D:266:ARG:NH2	2.46	0.48
1:A:214:LEU:O	1:A:216:VAL:HG23	2.13	0.48
1:B:405:TYR:CE1	1:B:492:ILE:CD1	2.96	0.48
1:B:46:PRO:HB3	1:B:52:ARG:NH1	2.28	0.48
1:B:65:ILE:HG22	1:B:66:PRO:N	2.28	0.48
1:D:75:LEU:O	1:D:78:GLN:HB3	2.14	0.48
1:C:258:GLN:HE21	1:C:260:GLU:C	2.16	0.48
1:D:12:ASP:HB2	1:D:153:SER:O	2.13	0.48
1:A:135:ILE:CD1	1:A:151:ILE:HD13	2.42	0.48
1:A:198:ALA:HB1	1:A:224:LEU:HD23	1.95	0.48
1:B:418:ASN:OD1	1:B:419:ASN:ND2	2.47	0.48
1:C:97:ASP:OD1	4:C:561:HOH:O	2.20	0.48
1:C:90:VAL:HG11	1:D:80:LEU:HD21	1.95	0.48
1:A:55:LEU:O	1:A:113:ASN:OD1	2.32	0.48
1:C:95:LYS:HB3	1:D:89:LYS:HE3	1.96	0.48
1:A:450:GLN:OE1	1:B:470:GLY:HA2	2.14	0.48
1:C:13:TYR:O	1:C:154:ALA:HA	2.14	0.48
1:C:67:LYS:HD2	1:C:68:LYS:N	2.29	0.48
1:A:272:GLN:HB2	1:A:279:ILE:HG12	1.95	0.48
1:C:198:ALA:HB1	1:C:224:LEU:CD2	2.43	0.48
1:B:308:LYS:CB	1:B:325:ASN:ND2	2.76	0.48
1:C:149:GLU:O	1:C:150:LYS:HG3	2.14	0.48
1:C:272:GLN:HB2	1:C:279:ILE:HD13	1.94	0.48
1:D:173:ASP:OD1	1:D:174:LYS:N	2.40	0.47
1:C:171:PRO:HG3	1:C:255:LYS:HD2	1.94	0.47
1:C:397:GLU:OE2	1:C:397:GLU:N	2.43	0.47
1:C:493:LEU:CD1	1:C:493:LEU:O	2.52	0.47
1:C:91:GLU:HG3	1:C:93:THR:H	1.78	0.47
1:D:258:GLN:HE22	1:D:261:ALA:HB2	1.79	0.47
1:D:74:ALA:HB1	1:D:211:GLY:HA3	1.97	0.47
1:B:47:THR:HG22	1:B:49:LEU:N	2.30	0.47
1:C:474:VAL:HG11	1:D:446:GLY:HA3	1.96	0.47
1:A:25:LEU:HD13	1:A:116:TYR:CD1	2.49	0.47
1:D:302:LEU:HB3	1:D:307:VAL:CG2	2.42	0.47
1:C:167:TYR:CE2	1:C:174:LYS:HA	2.50	0.47
1:D:167:TYR:CE2	1:D:174:LYS:HA	2.50	0.47
1:D:21:GLY:HA2	1:D:56:GLY:O	2.13	0.47
1:D:232:MET:HE2	1:D:439:HIS:HB3	1.96	0.47
1:A:98:TRP:CZ2	1:A:102:ILE:HD11	2.49	0.47
1:A:232:MET:O	1:A:236:ILE:HG13	2.14	0.47
1:A:343:THR:O	1:A:347:ILE:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:SER:OG	1:C:223:ILE:N	2.44	0.47
1:D:118:VAL:O	1:D:122:GLU:HG3	2.14	0.47
1:A:302:LEU:HD13	1:A:307:VAL:HG12	1.97	0.47
1:A:55:LEU:HD12	1:A:56:GLY:H	1.79	0.47
1:A:192:LYS:N	1:A:285:ASN:HD22	2.12	0.47
1:C:135:ILE:HD11	1:C:139:ARG:NH1	2.29	0.47
1:C:229:ASP:OD1	1:C:232:MET:HG2	2.15	0.47
1:D:340:VAL:HB	1:D:345:VAL:HG21	1.97	0.47
1:C:171:PRO:HG2	1:C:255:LYS:HD2	1.97	0.46
1:C:419:ASN:ND2	1:C:494:GLN:HE21	2.12	0.46
1:D:258:GLN:NE2	1:D:261:ALA:HB2	2.30	0.46
1:D:65:ILE:HG22	1:D:66:PRO:N	2.30	0.46
1:A:52:ARG:HG3	1:A:52:ARG:NH1	2.30	0.46
1:B:200:TYR:HD2	3:B:901:NAP:H3D	1.81	0.46
1:C:200:TYR:HB3	3:C:901:NAP:C4N	2.45	0.46
1:A:246:LYS:HE2	4:A:738:HOH:O	2.15	0.46
1:A:403:HIS:CE1	1:A:492:ILE:HD13	2.51	0.46
1:B:477:GLU:O	1:B:480:THR:HB	2.15	0.46
1:C:46:PRO:HG3	1:C:52:ARG:HG2	1.96	0.46
1:A:121:ARG:HH11	1:A:121:ARG:HG2	1.79	0.46
1:B:145:ASN:HB2	4:B:746:HOH:O	2.16	0.46
1:B:266:ARG:NH1	1:B:283:GLU:OE1	2.47	0.46
1:D:196:VAL:HG21	1:D:253:PRO:HG2	1.97	0.46
1:A:230:GLN:O	1:A:234:ASN:ND2	2.48	0.46
1:C:418:ASN:OD1	1:C:419:ASN:N	2.49	0.46
1:B:76:LEU:HA	1:B:76:LEU:HD23	1.60	0.46
1:C:302:LEU:CD2	1:C:307:VAL:HB	2.35	0.46
1:B:308:LYS:H	1:B:325:ASN:HD21	0.66	0.45
1:C:259:ILE:O	1:C:260:GLU:HB2	2.15	0.45
1:D:215:ASP:OD1	1:D:246:LYS:HE2	2.16	0.45
1:A:120:LEU:HD22	1:A:125:VAL:CG1	2.44	0.45
1:A:386:SER:OG	1:A:389:LYS:HB2	2.17	0.45
1:A:407:TRP:CD1	1:A:418:ASN:HA	2.52	0.45
1:B:236:ILE:HD11	1:B:380:TYR:HB2	1.98	0.45
1:D:196:VAL:HG12	1:D:291:ILE:CG2	2.46	0.45
1:B:163:GLU:HG2	1:B:295:ALA:HA	1.98	0.45
1:B:303:GLU:HG2	1:B:304:THR:N	2.30	0.45
1:A:458:CYS:CB	1:B:458:CYS:HB3	2.46	0.45
1:D:308:LYS:N	1:D:325:ASN:OD1	2.41	0.45
1:A:307:VAL:HA	1:A:325:ASN:OD1	2.15	0.45
1:D:13:TYR:O	1:D:154:ALA:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ARG:O	1:D:250:GLN:HA	2.16	0.45
1:A:268:ARG:NH2	4:A:619:HOH:O	2.49	0.45
1:B:347:ILE:O	1:B:351:ARG:HG3	2.16	0.45
1:A:186:LEU:HA	1:A:187:PRO:HD2	1.80	0.45
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.81	0.45
1:A:166:ARG:HB3	1:A:291:ILE:HD12	1.97	0.45
1:C:21:GLY:HA3	2:C:900:FAD:O5B	2.17	0.45
1:C:462:LYS:HE2	1:C:466:ASP:OD2	2.17	0.45
1:A:303:GLU:H	1:A:303:GLU:CD	2.19	0.45
1:A:440:VAL:O	1:A:440:VAL:HG13	2.17	0.45
1:B:120:LEU:HD22	1:B:125:VAL:HG11	1.99	0.45
1:B:13:TYR:CE2	1:B:39:MET:HB2	2.52	0.45
1:D:114:TRP:HZ3	1:D:117:ARG:NH1	2.13	0.45
1:D:140:ILE:HG21	1:D:157:PHE:CE2	2.49	0.45
1:D:266:ARG:HG2	1:D:266:ARG:HH11	1.81	0.45
1:D:303:GLU:CG	1:D:304:THR:N	2.68	0.45
1:C:251:PHE:CZ	1:C:280:ILE:HD12	2.52	0.45
1:C:440:VAL:HB	1:C:479:PHE:HZ	1.82	0.45
1:C:67:LYS:HE2	1:C:67:LYS:HB3	1.73	0.45
1:A:168:LEU:CD2	3:A:901:NAP:N6A	2.79	0.44
1:B:351:ARG:HD2	4:B:539:HOH:O	2.17	0.44
1:A:467:SER:OG	1:B:457:LYS:HD2	2.17	0.44
1:A:67:LYS:HD2	1:A:68:LYS:N	2.33	0.44
1:C:219:MET:SD	1:C:253:PRO:HG3	2.58	0.44
1:C:411:TRP:O	1:C:414:PRO:HD2	2.17	0.44
1:C:494:GLN:HG3	1:C:494:GLN:O	2.17	0.44
1:A:300:ILE:HD11	1:A:302:LEU:HD21	1.99	0.44
1:C:344:PRO:HG3	1:D:472:HIS:HB2	1.99	0.44
1:C:391:VAL:O	1:C:395:GLY:N	2.41	0.44
1:C:82:ASP:OD2	1:C:416:ARG:NH1	2.36	0.44
1:A:163:GLU:HG2	1:A:295:ALA:CA	2.39	0.44
1:B:325:ASN:OD1	1:B:326:VAL:N	2.50	0.44
1:A:351:ARG:HE	1:A:351:ARG:HB3	1.36	0.44
1:B:411:TRP:O	1:B:414:PRO:HG2	2.18	0.44
1:C:97:ASP:OD2	1:C:100:ARG:HB2	2.18	0.44
1:C:188:TYR:CE1	1:C:264:PRO:HB3	2.53	0.44
1:D:376:THR:O	1:D:377:PRO:C	2.56	0.44
1:A:141:LYS:HE3	1:A:141:LYS:HB3	1.69	0.44
1:A:318:VAL:CG2	1:A:323:GLN:N	2.80	0.44
1:A:470:GLY:HA2	1:B:450:GLN:OE1	2.18	0.44
1:C:417:ASP:HB3	1:C:420:LYS:CG	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ARG:CG	1:D:117:ARG:HH21	2.28	0.44
1:D:322:GLU:HB3	1:D:331:ALA:O	2.18	0.44
1:A:321:GLU:O	1:A:322:GLU:HB2	2.17	0.43
1:C:194:LEU:HA	1:C:194:LEU:HD12	1.67	0.43
1:C:318:VAL:HG12	1:C:319:THR:O	2.18	0.43
1:C:162:GLY:O	1:C:335:ILE:HG22	2.18	0.43
1:C:95:LYS:HB2	1:D:89:LYS:HE3	2.00	0.43
1:D:156:ARG:NH1	1:D:156:ARG:HG3	2.33	0.43
1:A:300:ILE:HG13	1:A:302:LEU:HG	2.00	0.43
1:A:402:TYR:CE2	1:A:485:THR:HG22	2.53	0.43
1:A:83:SER:HA	1:B:76:LEU:HD13	2.01	0.43
1:C:199:SER:O	1:C:200:TYR:C	2.57	0.43
1:C:65:ILE:HB	1:C:66:PRO:CD	2.48	0.43
1:A:303:GLU:OE1	1:A:304:THR:CG2	2.67	0.43
1:A:49:LEU:HD12	1:A:49:LEU:H	1.83	0.43
1:B:254:ILE:CG1	1:B:270:VAL:HG12	2.47	0.43
1:B:199:SER:HA	1:B:225:LEU:HD23	1.99	0.43
1:C:236:ILE:HD11	1:C:380:TYR:CD2	2.53	0.43
1:D:428:ASN:HD21	1:D:431:ASP:HB2	1.83	0.43
1:A:133:GLN:NE2	1:A:141:LYS:NZ	2.67	0.43
1:B:67:LYS:HD3	1:B:204:GLU:OE1	2.18	0.43
1:C:273:SER:OG	1:C:276:SER:N	2.46	0.43
1:B:339:LYS:NZ	4:B:783:HOH:O	2.45	0.43
1:C:188:TYR:C	1:C:188:TYR:CD1	2.92	0.43
1:C:394:PHE:HB2	1:C:399:ILE:CD1	2.46	0.43
1:C:163:GLU:HG2	1:C:295:ALA:CA	2.49	0.43
1:C:258:GLN:NE2	1:C:261:ALA:N	2.57	0.43
1:C:378:LEU:HD12	1:C:378:LEU:HA	1.72	0.43
1:D:176:TYR:CD1	1:D:258:GLN:HB2	2.53	0.43
1:A:231:ASP:O	1:A:235:LYS:HG3	2.19	0.43
1:D:39:MET:HE1	1:D:128:GLU:HG3	1.94	0.43
1:A:472:HIS:CE1	1:A:473:PRO:HB3	2.54	0.43
1:B:423:ALA:HB1	1:B:479:PHE:CE1	2.53	0.43
1:B:47:THR:HG23	1:B:48:PRO:CD	2.49	0.43
1:C:472:HIS:HB2	1:D:344:PRO:HG3	2.00	0.43
1:D:254:ILE:HD11	1:D:270:VAL:CG1	2.49	0.43
1:B:470:GLY:H	1:B:480:THR:HG21	1.85	0.42
1:C:190:PRO:O	1:C:286:THR:OG1	2.32	0.42
1:A:58:THR:HG23	1:A:62:VAL:HG23	2.01	0.42
1:B:47:THR:O	1:B:48:PRO:C	2.58	0.42
1:C:176:TYR:HB3	1:C:267:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:LYS:HE2	1:D:394:PHE:CZ	2.54	0.42
1:D:252:VAL:HG13	3:D:901:NAP:N1A	2.34	0.42
1:D:472:HIS:HA	1:D:473:PRO:HA	1.81	0.42
1:A:144:ASN:HD21	1:A:148:LYS:HB2	1.83	0.42
1:B:210:ALA:CB	1:B:245:ILE:HD11	2.50	0.42
1:A:98:TRP:HE1	1:A:102:ILE:HG13	1.84	0.42
1:A:240:MET:HE2	1:A:245:ILE:HD13	2.01	0.42
1:B:25:LEU:HD13	1:B:116:TYR:CD1	2.54	0.42
1:B:229:ASP:OD1	1:B:232:MET:HG2	2.20	0.42
1:B:411:TRP:CE3	1:B:417:ASP:HB2	2.55	0.42
1:A:418:ASN:ND2	1:A:419:ASN:H	2.17	0.42
1:B:215:ASP:CG	1:B:246:LYS:HZ1	2.19	0.42
1:C:198:ALA:HB1	1:C:224:LEU:HD23	2.00	0.42
1:C:68:LYS:HE2	1:D:473:PRO:O	2.20	0.42
1:D:65:ILE:O	1:D:69:LEU:HG	2.19	0.42
1:A:219:MET:SD	1:A:253:PRO:HD3	2.59	0.42
1:B:100:ARG:NH2	1:B:100:ARG:CG	2.83	0.42
1:C:366:ASP:OD1	1:C:368:GLU:N	2.45	0.42
1:D:302:LEU:CD2	1:D:307:VAL:CG2	2.85	0.42
1:A:397:GLU:CD	1:A:397:GLU:H	2.23	0.42
1:A:411:TRP:C	1:A:414:PRO:HD2	2.39	0.42
1:A:52:ARG:HG3	1:A:52:ARG:HH11	1.85	0.42
1:B:100:ARG:NH2	4:B:602:HOH:O	2.53	0.42
1:B:405:TYR:HE1	1:B:492:ILE:CD1	2.32	0.42
1:A:288:MET:CE	1:A:290:ALA:HB2	2.49	0.42
1:A:458:CYS:HB3	1:B:458:CYS:HB3	2.02	0.42
1:D:146:LYS:O	1:D:146:LYS:HE2	2.20	0.42
1:D:163:GLU:HG2	1:D:295:ALA:HA	2.02	0.42
1:A:307:VAL:HG21	1:A:329:ILE:HG21	2.01	0.41
1:A:91:GLU:H	1:A:91:GLU:CD	2.23	0.41
1:C:45:THR:HG23	4:C:813:HOH:O	2.19	0.41
1:D:170:ILE:O	1:D:170:ILE:HG13	2.19	0.41
1:B:243:HIS:CD2	4:B:625:HOH:O	2.72	0.41
1:C:386:SER:H	1:C:389:LYS:HE2	1.85	0.41
1:C:438:PHE:CE2	1:C:479:PHE:CE1	3.08	0.41
1:D:318:VAL:HG22	1:D:323:GLN:N	2.35	0.41
1:B:286:THR:HG22	1:B:287:VAL:N	2.36	0.41
1:C:377:PRO:HD2	4:C:569:HOH:O	2.19	0.41
1:D:137:PRO:HA	1:D:305:VAL:HG23	2.01	0.41
1:D:47:THR:HB	1:D:51:THR:H	1.85	0.41
1:A:131:TYR:C	1:A:131:TYR:CD2	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ARG:O	1:B:250:GLN:HA	2.21	0.41
1:C:134:PHE:N	1:C:300:ILE:O	2.52	0.41
1:C:67:LYS:HD3	1:C:204:GLU:OE1	2.21	0.41
1:B:58:THR:O	1:B:63:GLY:N	2.53	0.41
1:C:341:GLU:HB2	3:C:901:NAP:O2D	2.19	0.41
1:C:77:GLY:HA2	1:C:80:LEU:HD12	2.03	0.41
1:B:309:ILE:HA	1:B:317:PRO:HD2	2.02	0.41
1:C:321:GLU:O	1:C:322:GLU:HB2	2.20	0.41
1:D:67:LYS:HB3	1:D:67:LYS:HE2	1.81	0.41
1:C:205:CYS:HA	1:C:208:PHE:CE2	2.56	0.41
1:C:482:LEU:HB2	4:C:878:HOH:O	2.21	0.41
1:D:310:ASN:OD1	1:D:312:LYS:HB3	2.20	0.41
1:A:133:GLN:CD	1:A:141:LYS:HZ2	2.24	0.41
1:A:169:GLY:N	1:A:173:ASP:OD2	2.50	0.41
1:D:239:HIS:CE1	1:D:378:LEU:HB2	2.56	0.41
1:C:403:HIS:CE1	1:C:492:ILE:HD13	2.55	0.41
1:D:318:VAL:HG22	1:D:322:GLU:C	2.41	0.41
1:D:319:THR:C	1:D:321:GLU:H	2.23	0.41
1:D:446:GLY:N	4:D:551:HOH:O	2.36	0.41
1:B:229:ASP:OD1	1:B:231:ASP:HB3	2.20	0.41
1:A:89:LYS:O	1:B:94:VAL:HG13	2.20	0.41
1:C:251:PHE:CD2	1:C:273:SER:HA	2.56	0.41
1:C:258:GLN:C	1:C:260:GLU:H	2.24	0.41
1:D:401:VAL:HG22	1:D:426:ILE:HG13	2.02	0.41
1:A:315:LYS:HE3	1:A:334:ASP:O	2.21	0.41
1:A:70:MET:SD	1:A:208:PHE:CE1	3.14	0.41
1:B:276:SER:OG	1:B:277:GLU:N	2.53	0.41
1:C:315:LYS:O	1:C:317:PRO:HD3	2.21	0.41
1:D:45:THR:HA	1:D:46:PRO:HD3	1.71	0.41
1:A:114:TRP:O	1:A:115:GLY:C	2.59	0.40
1:A:318:VAL:HG21	1:A:322:GLU:HA	2.02	0.40
1:A:460:LEU:HD12	1:B:458:CYS:SG	2.62	0.40
1:B:183:LEU:HD22	1:B:288:MET:SD	2.61	0.40
1:A:69:LEU:HD21	1:B:409:LEU:HG	2.03	0.40
1:C:159:ILE:HD12	1:C:316:ILE:HD13	2.03	0.40
1:C:469:ILE:HG22	1:D:344:PRO:HB2	2.02	0.40
1:D:493:LEU:HD12	1:D:493:LEU:H	1.87	0.40
1:A:198:ALA:CB	1:A:220:VAL:HG13	2.51	0.40
1:B:198:ALA:HB1	1:B:224:LEU:CD2	2.51	0.40
1:D:16:ILE:HG13	1:D:154:ALA:HB2	2.02	0.40
1:D:332:ILE:HA	1:D:336:LEU:HD11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ALA:HB1	1:A:211:GLY:HA3	2.03	0.40
1:A:378:LEU:HA	1:A:378:LEU:HD12	1.80	0.40
1:B:229:ASP:HA	1:B:388:GLU:OE1	2.21	0.40
1:B:217:THR:CG2	1:B:248:ILE:HD12	2.51	0.40
1:B:258:GLN:OE1	1:B:261:ALA:CB	2.67	0.40
1:B:41:LEU:HD23	1:B:41:LEU:HA	1.86	0.40
1:C:315:LYS:HB3	1:C:337:GLU:HB2	2.03	0.40
1:C:67:LYS:CD	1:C:67:LYS:C	2.82	0.40
1:A:399:ILE:HG23	1:A:426:ILE:HG23	2.04	0.40
1:A:65:ILE:HB	1:A:66:PRO:CD	2.52	0.40
1:A:67:LYS:HE2	1:A:67:LYS:HB3	1.84	0.40
1:D:58:THR:OG1	2:D:900:FAD:O2A	2.18	0.40
1:D:100:ARG:HH21	1:D:100:ARG:CG	2.33	0.40
1:D:28:ALA:HB2	1:D:40:VAL:HG21	2.04	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	483/513 (94%)	446 (92%)	33 (7%)	4 (1%)	22	44
1	B	482/513 (94%)	455 (94%)	26 (5%)	1 (0%)	51	76
1	C	483/513 (94%)	443 (92%)	34 (7%)	6 (1%)	15	32
1	D	482/513 (94%)	443 (92%)	36 (8%)	3 (1%)	28	53
All	All	1930/2052 (94%)	1787 (93%)	129 (7%)	14 (1%)	25	49

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	260	GLU

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Mol	Chain	Res	Type
1	A	200	TYR
1	C	200	TYR
1	D	260	GLU
1	A	260	GLU
1	A	320	ASP
1	D	200	TYR
1	B	473	PRO
1	C	64	CYS
1	C	137	PRO
1	C	259	ILE
1	A	473	PRO
1	C	473	PRO
1	D	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	399/422 (94%)	383 (96%)	16 (4%)	36	64
1	B	398/422 (94%)	386 (97%)	12 (3%)	46	74
1	C	399/422 (94%)	378 (95%)	21 (5%)	26	50
1	D	398/422 (94%)	373 (94%)	25 (6%)	21	42
All	All	1594/1688 (94%)	1520 (95%)	74 (5%)	31	58

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ILE
1	A	45	THR
1	A	52	ARG
1	A	64	CYS
1	A	121	ARG
1	A	140	ILE
1	A	185	SER
1	A	252	VAL

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Mol	Chain	Res	Type
1	A	277	GLU
1	A	303	GLU
1	A	389	LYS
1	A	397	GLU
1	A	403	HIS
1	A	433	GLU
1	A	480	THR
1	A	494	GLN
1	B	47	THR
1	B	52	ARG
1	B	64	CYS
1	B	78	GLN
1	B	111	SER
1	B	129	ASN
1	B	276	SER
1	B	341	GLU
1	B	362	THR
1	B	403	HIS
1	B	467	SER
1	B	480	THR
1	C	12	ASP
1	C	14	ASP
1	C	45	THR
1	C	48	PRO
1	C	64	CYS
1	C	68	LYS
1	C	129	ASN
1	C	140	ILE
1	C	144	ASN
1	C	146	LYS
1	C	276	SER
1	C	280	ILE
1	C	281	GLU
1	C	285	ASN
1	C	303	GLU
1	C	376	THR
1	C	397	GLU
1	C	403	HIS
1	C	434	ARG
1	C	480	THR
1	C	491	SER
1	D	33	GLN

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Mol	Chain	Res	Type
1	D	45	THR
1	D	47	THR
1	D	48	PRO
1	D	64	CYS
1	D	92	GLU
1	D	117	ARG
1	D	121	ARG
1	D	145	ASN
1	D	246	LYS
1	D	249	ARG
1	D	264	PRO
1	D	266	ARG
1	D	274	THR
1	D	276	SER
1	D	304	THR
1	D	310	ASN
1	D	318	VAL
1	D	364	LYS
1	D	376	THR
1	D	389	LYS
1	D	391	VAL
1	D	396	GLU
1	D	403	HIS
1	D	432	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	A	113	ASN
1	A	129	ASN
1	A	133	GLN
1	A	234	ASN
1	A	285	ASN
1	A	418	ASN
1	B	33	GLN
1	B	107	ASN
1	B	113	ASN
1	B	129	ASN
1	B	145	ASN
1	B	250	GLN
1	B	419	ASN

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Mol	Chain	Res	Type
1	B	432	ASN
1	C	85	ASN
1	C	113	ASN
1	C	129	ASN
1	C	145	ASN
1	C	258	GLN
1	C	272	GLN
1	C	285	ASN
1	C	419	ASN
1	C	494	GLN
1	D	81	GLN
1	D	129	ASN
1	D	145	ASN
1	D	250	GLN
1	D	258	GLN
1	D	355	GLN
1	D	419	ASN
1	D	428	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	900	-	51,58,58	1.69	7 (13%)	54,89,89	2.36	11 (20%)
3	NAP	A	901	-	44,52,52	1.47	6 (13%)	51,80,80	1.20	3 (5%)
2	FAD	B	900	-	51,58,58	1.69	10 (19%)	54,89,89	2.19	11 (20%)
3	NAP	B	901	-	44,52,52	1.41	6 (13%)	51,80,80	1.27	2 (3%)
2	FAD	C	900	-	51,58,58	1.86	10 (19%)	54,89,89	2.37	11 (20%)
3	NAP	C	901	-	44,52,52	1.61	7 (15%)	51,80,80	1.29	3 (5%)
2	FAD	D	900	-	51,58,58	1.77	7 (13%)	54,89,89	2.20	11 (20%)
3	NAP	D	901	-	44,52,52	1.38	7 (15%)	51,80,80	1.28	4 (7%)

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	900	-	-	0/28/50/50	0/6/6/6
3	NAP	A	901	-	-	0/27/67/67	0/5/5/5
2	FAD	B	900	-	-	0/28/50/50	0/6/6/6
3	NAP	B	901	-	-	0/27/67/67	0/5/5/5
2	FAD	C	900	-	-	0/28/50/50	0/6/6/6
3	NAP	C	901	-	-	0/27/67/67	0/5/5/5
2	FAD	D	900	-	-	0/28/50/50	0/6/6/6
3	NAP	D	901	-	-	0/27/67/67	0/5/5/5

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	FAD	C8A-N7A	-3.58	1.28	1.34
2	C	900	FAD	C8A-N7A	-3.54	1.28	1.34
2	A	900	FAD	C8A-N7A	-3.29	1.28	1.34
2	D	900	FAD	C8A-N7A	-3.20	1.28	1.34
2	B	900	FAD	C2-N3	-3.07	1.32	1.38
2	A	900	FAD	O4-C4	-2.93	1.17	1.24
2	D	900	FAD	C2B-C1B	-2.74	1.49	1.53
2	B	900	FAD	C2B-C1B	-2.68	1.49	1.53
2	C	900	FAD	C2B-C1B	-2.33	1.49	1.53
2	B	900	FAD	P-O1P	-2.30	1.42	1.50
2	C	900	FAD	C2-N1	-2.23	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	FAD	C4-N3	2.03	1.36	1.33
3	A	901	NAP	C3N-C7N	2.12	1.53	1.50
2	D	900	FAD	C4-N3	2.16	1.37	1.33
3	D	901	NAP	C3N-C7N	2.17	1.53	1.50
3	D	901	NAP	O3B-C3B	2.36	1.48	1.43
2	B	900	FAD	C10-N1	2.41	1.36	1.33
3	B	901	NAP	O3B-C3B	2.45	1.48	1.43
2	C	900	FAD	C1'-N10	2.45	1.50	1.48
3	A	901	NAP	P2B-O2B	2.48	1.63	1.59
3	D	901	NAP	C2A-N3A	2.48	1.36	1.32
2	B	900	FAD	C6-C5X	2.57	1.45	1.41
2	B	900	FAD	C4X-C10	2.61	1.45	1.41
3	C	901	NAP	C3N-C7N	2.63	1.54	1.50
2	C	900	FAD	C4-N3	2.64	1.37	1.33
2	A	900	FAD	C4-C4X	2.69	1.46	1.41
3	A	901	NAP	C2A-N3A	2.70	1.36	1.32
3	D	901	NAP	C6N-N1N	2.81	1.42	1.35
2	B	900	FAD	C4-N3	2.97	1.38	1.33
3	C	901	NAP	C2A-N3A	3.04	1.37	1.32
3	B	901	NAP	C3N-C7N	3.06	1.55	1.50
3	D	901	NAP	C4A-N3A	3.10	1.40	1.35
3	B	901	NAP	C4N-C3N	3.19	1.44	1.39
3	B	901	NAP	C2A-N3A	3.23	1.37	1.32
3	D	901	NAP	C4N-C3N	3.23	1.44	1.39
3	B	901	NAP	C6N-N1N	3.24	1.43	1.35
3	C	901	NAP	C6N-N1N	3.25	1.43	1.35
2	C	900	FAD	C10-N1	3.28	1.37	1.33
3	D	901	NAP	O4B-C1B	3.40	1.46	1.41
3	A	901	NAP	C6N-N1N	3.57	1.44	1.35
3	C	901	NAP	C4N-C3N	3.77	1.45	1.39
3	C	901	NAP	C4A-N3A	4.05	1.41	1.35
2	A	900	FAD	O4B-C1B	4.07	1.46	1.41
3	B	901	NAP	O4B-C1B	4.18	1.47	1.41
3	C	901	NAP	P2B-O2B	4.18	1.66	1.59
3	A	901	NAP	C4N-C3N	4.20	1.46	1.39
3	C	901	NAP	O4B-C1B	4.21	1.47	1.41
2	D	900	FAD	O4B-C1B	4.24	1.47	1.41
2	C	900	FAD	C4-C4X	4.43	1.49	1.41
2	D	900	FAD	C4-C4X	4.49	1.49	1.41
2	C	900	FAD	O4B-C1B	4.63	1.47	1.41
2	A	900	FAD	C9A-N10	4.74	1.45	1.38
2	B	900	FAD	C4-C4X	4.78	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	901	NAP	O4B-C1B	4.78	1.47	1.41
2	D	900	FAD	C4X-C10	4.86	1.49	1.41
2	C	900	FAD	C4X-C10	4.97	1.49	1.41
2	B	900	FAD	O4B-C1B	5.01	1.48	1.41
2	C	900	FAD	C9A-N10	5.15	1.45	1.38
2	D	900	FAD	C9A-N10	5.67	1.46	1.38
2	A	900	FAD	C4X-C10	6.05	1.51	1.41

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	FAD	N3A-C2A-N1A	-8.74	121.25	128.86
2	A	900	FAD	N3A-C2A-N1A	-8.71	121.27	128.86
2	B	900	FAD	N3A-C2A-N1A	-8.28	121.65	128.86
2	D	900	FAD	N3A-C2A-N1A	-6.76	122.97	128.86
3	C	901	NAP	N3A-C2A-N1A	-5.18	124.35	128.86
2	C	900	FAD	C4-C4X-C10	-5.09	115.84	119.96
3	B	901	NAP	N3A-C2A-N1A	-4.84	124.64	128.86
3	D	901	NAP	N3A-C2A-N1A	-4.79	124.69	128.86
3	A	901	NAP	N3A-C2A-N1A	-4.69	124.77	128.86
2	D	900	FAD	C4X-C4-N3	-4.25	117.44	123.48
2	A	900	FAD	C4-C4X-C10	-4.19	116.57	119.96
2	D	900	FAD	C4-C4X-C10	-4.16	116.60	119.96
2	A	900	FAD	C4X-C4-N3	-3.95	117.86	123.48
2	C	900	FAD	C4B-O4B-C1B	-3.93	105.58	109.77
2	B	900	FAD	C4X-C4-N3	-3.87	117.98	123.48
2	C	900	FAD	C4X-C4-N3	-3.78	118.10	123.48
2	A	900	FAD	C4X-C10-N10	-3.70	117.95	120.52
2	B	900	FAD	C4X-C10-N10	-3.30	118.23	120.52
2	A	900	FAD	C4B-O4B-C1B	-3.03	106.55	109.77
2	D	900	FAD	C4X-C10-N10	-2.65	118.68	120.52
2	A	900	FAD	C4A-C5A-N7A	-2.62	106.88	109.41
2	C	900	FAD	C4X-C10-N10	-2.58	118.73	120.52
2	D	900	FAD	C4A-C5A-N7A	-2.55	106.95	109.41
3	B	901	NAP	O3B-C3B-C4B	-2.55	103.65	111.09
2	B	900	FAD	C4B-O4B-C1B	-2.46	107.16	109.77
2	B	900	FAD	C4-C4X-C10	-2.45	117.98	119.96
2	C	900	FAD	C4A-C5A-N7A	-2.23	107.25	109.41
2	D	900	FAD	C4B-O4B-C1B	-2.15	107.48	109.77
3	D	901	NAP	C4B-O4B-C1B	-2.11	107.52	109.77
3	D	901	NAP	O4D-C4D-C3D	-2.01	101.17	105.17
3	A	901	NAP	O3D-C3D-C4D	2.03	117.02	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	901	NAP	C4A-C5A-N7A	2.03	111.37	109.41
2	B	900	FAD	C1'-N10-C10	2.04	120.60	118.50
2	B	900	FAD	C1'-N10-C9A	2.18	120.34	118.35
3	C	901	NAP	C2A-N1A-C6A	2.26	122.72	118.77
3	A	901	NAP	C2A-N1A-C6A	2.31	122.81	118.77
3	D	901	NAP	C2A-N1A-C6A	2.35	122.88	118.77
2	B	900	FAD	C5X-C9A-N10	2.35	119.40	117.66
2	D	900	FAD	C5X-C9A-N10	2.43	119.46	117.66
2	A	900	FAD	C5X-C9A-N10	2.65	119.62	117.66
2	C	900	FAD	C5X-C9A-N10	2.84	119.77	117.66
2	B	900	FAD	C4-C4X-N5	2.91	121.88	118.68
2	A	900	FAD	C4-C4X-N5	3.21	122.20	118.68
2	A	900	FAD	C1'-N10-C9A	3.63	121.67	118.35
2	C	900	FAD	C4-C4X-N5	3.85	122.90	118.68
2	D	900	FAD	C4-C4X-N5	4.04	123.11	118.68
2	C	900	FAD	C1'-N10-C9A	4.66	122.61	118.35
2	D	900	FAD	C1'-N10-C9A	4.73	122.68	118.35
2	C	900	FAD	C4X-N5-C5X	4.89	121.92	116.76
2	A	900	FAD	C4X-N5-C5X	5.04	122.09	116.76
2	D	900	FAD	C4X-N5-C5X	5.53	122.60	116.76
2	B	900	FAD	C4X-N5-C5X	6.66	123.79	116.76
2	B	900	FAD	C4-N3-C2	6.81	121.12	115.16
2	D	900	FAD	C4-N3-C2	7.52	121.73	115.16
2	C	900	FAD	C4-N3-C2	8.13	122.27	115.16
2	A	900	FAD	C4-N3-C2	8.67	122.75	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	NAP	3	0
3	B	901	NAP	4	0
2	C	900	FAD	1	0
3	C	901	NAP	3	0
2	D	900	FAD	2	0
3	D	901	NAP	3	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, 95th 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	485/513 (94%)	-0.31	4 (0%) 86 83	26, 50, 70, 84	0
1	B	484/513 (94%)	-0.51	2 (0%) 92 91	28, 44, 63, 87	0
1	C	485/513 (94%)	-0.25	8 (1%) 72 67	34, 53, 74, 94	0
1	D	484/513 (94%)	-0.38	7 (1%) 75 71	28, 49, 70, 89	0
All	All	1938/2052 (94%)	-0.36	21 (1%) 80 77	26, 49, 71, 94	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	493	LEU	3.8
1	C	275	ASN	3.2
1	D	92	GLU	3.1
1	C	10	SER	2.8
1	D	279	ILE	2.7
1	D	312	LYS	2.5
1	C	493	LEU	2.5
1	A	262	GLY	2.5
1	A	158	LEU	2.5
1	C	397	GLU	2.4
1	D	93	THR	2.3
1	C	148	LYS	2.3
1	C	146	LYS	2.3
1	D	91	GLU	2.2
1	A	148	LYS	2.2
1	A	312	LYS	2.2
1	D	430	LYS	2.1
1	B	490	ALA	2.1
1	B	277	GLU	2.1
1	C	151	ILE	2.0
1	C	93	THR	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, 95th 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
2	FAD	C	900	53/53	0.96	0.16	0.17	38,48,65,66	0
2	FAD	A	900	53/53	0.96	0.17	0.12	42,50,68,68	0
2	FAD	B	900	53/53	0.98	0.12	-0.27	30,37,43,43	0
2	FAD	D	900	53/53	0.97	0.12	-0.63	30,42,49,51	0
3	NAP	B	901	48/48	0.97	0.12	-0.63	45,53,63,64	0
3	NAP	D	901	48/48	0.97	0.12	-0.70	51,60,83,85	0
3	NAP	C	901	48/48	0.94	0.13	-0.82	61,72,86,87	0
3	NAP	A	901	48/48	0.96	0.13	-0.98	49,64,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.