



Full wwPDB X-ray Structure Validation Report

Nov 7, 2014 – 07:18 PM EST

PDB ID : 2ONO
Title : Arg475Gln Mutant of Mitochondrial Aldehyde Dehydrogenase, apo form,
pseudo-merohedrally twinned
Authors : Larson, H.N.; Hurley, T.D.
Deposited on : 2007-01-24
Resolution : 2.15 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

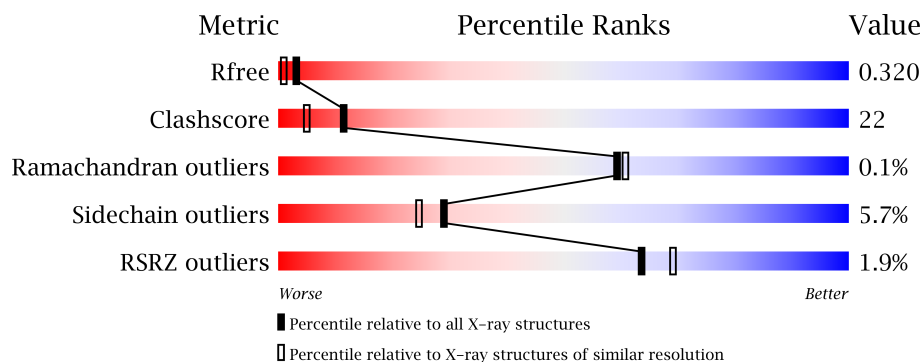
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24103
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24103

1 Overall quality at a glance

The reported resolution of this entry is 2.15 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}	66092	1094 (2.18-2.14)
Clashscore	79885	1299 (2.18-2.14)
Ramachandran outliers	78287	1272 (2.18-2.14)
Sidechain outliers	78261	1272 (2.18-2.14)
RSRZ outliers	66119	1094 (2.18-2.14)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	500	
1	B	500	
1	C	500	
1	D	500	
1	E	500	
1	F	500	
1	G	500	
1	H	500	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 31388 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Aldehyde dehydrogenase.

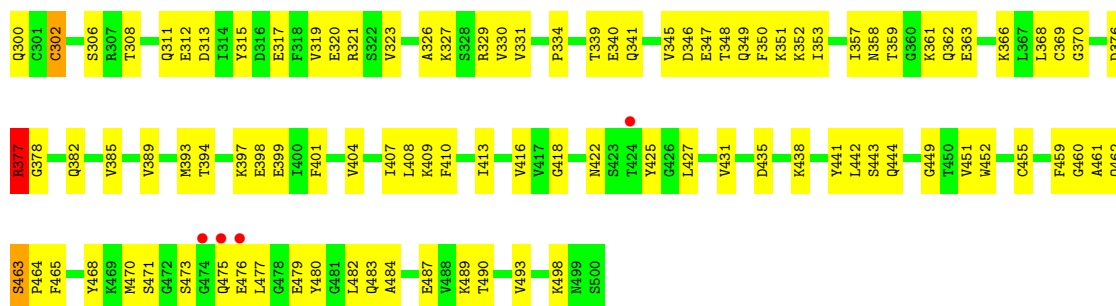
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	B	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	C	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	D	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	E	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	F	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	G	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			
1	H	494	Total	C	N	O	S	0	0	0
			3796	2414	646	718	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	475	GLN	ARG	ENGINEERED	UNP P05091
B	475	GLN	ARG	ENGINEERED	UNP P05091
C	475	GLN	ARG	ENGINEERED	UNP P05091
D	475	GLN	ARG	ENGINEERED	UNP P05091
E	475	GLN	ARG	ENGINEERED	UNP P05091
F	475	GLN	ARG	ENGINEERED	UNP P05091
G	475	GLN	ARG	ENGINEERED	UNP P05091
H	475	GLN	ARG	ENGINEERED	UNP P05091

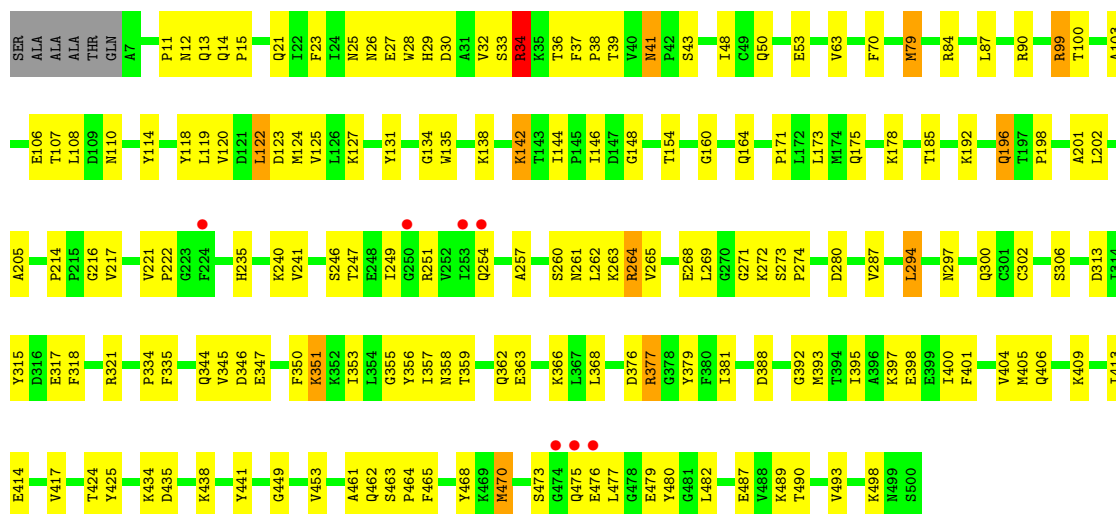
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	134	Total 134	O 134	0	0
2	B	131	Total 131	O 131	0	0
2	C	145	Total 145	O 145	0	0
2	D	133	Total 133	O 133	0	0
2	E	140	Total 140	O 140	0	0
2	F	114	Total 114	O 114	0	0
2	G	118	Total 118	O 118	0	0
2	H	105	Total 105	O 105	0	0



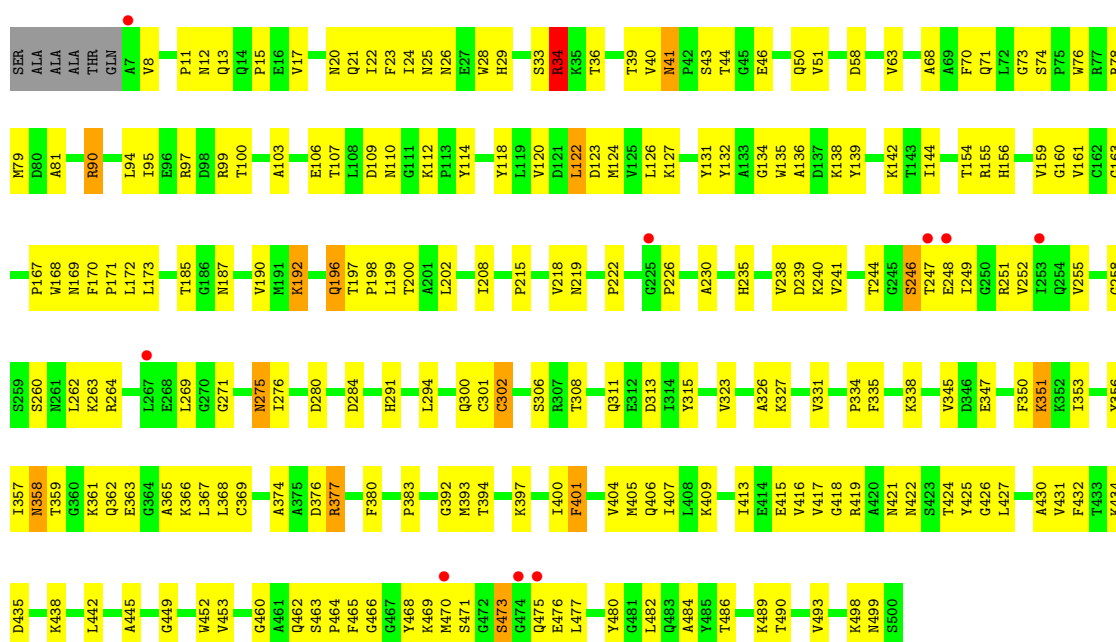
• Molecule 1: Aldehyde dehydrogenase

Chain C:



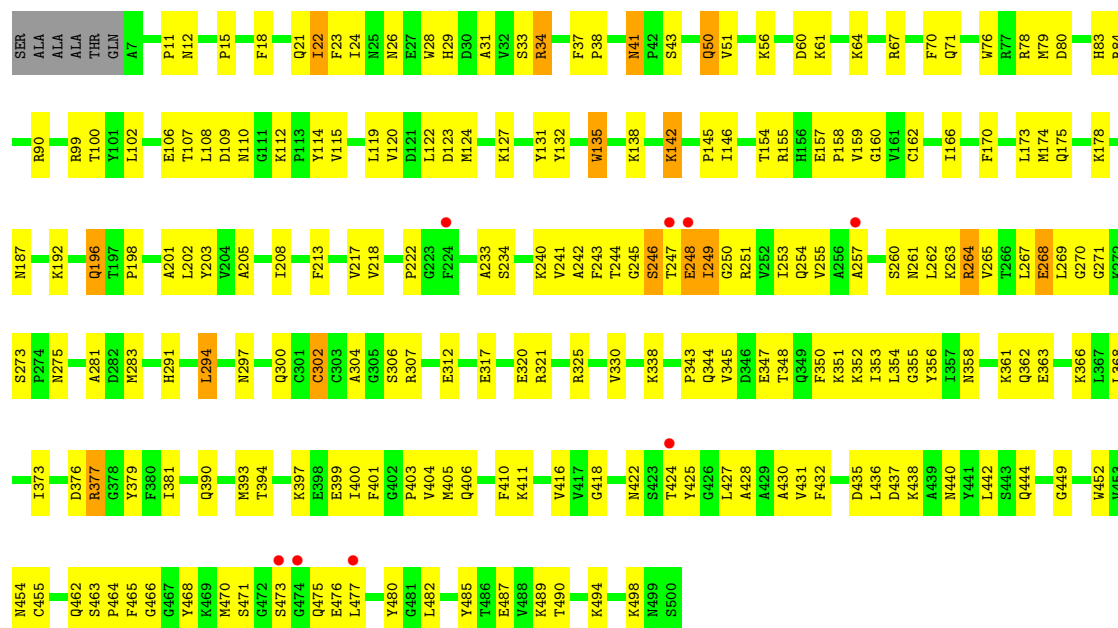
• Molecule 1: Aldehyde dehydrogenase

Chain D:



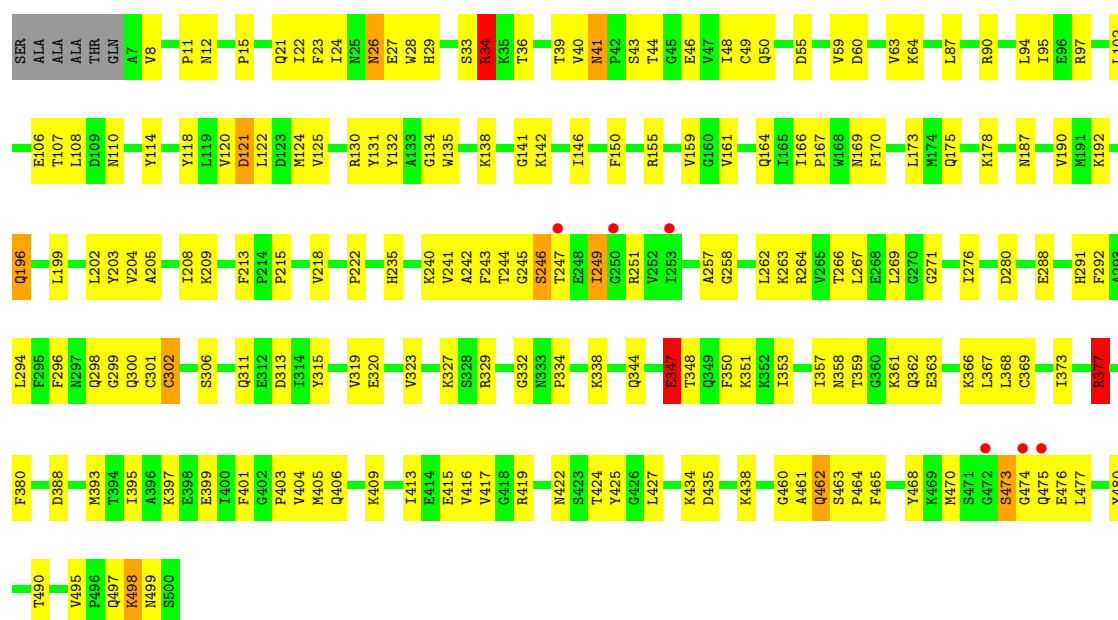
• Molecule 1: Aldehyde dehydrogenase

Chain E:



• Molecule 1: Aldehyde dehydrogenase

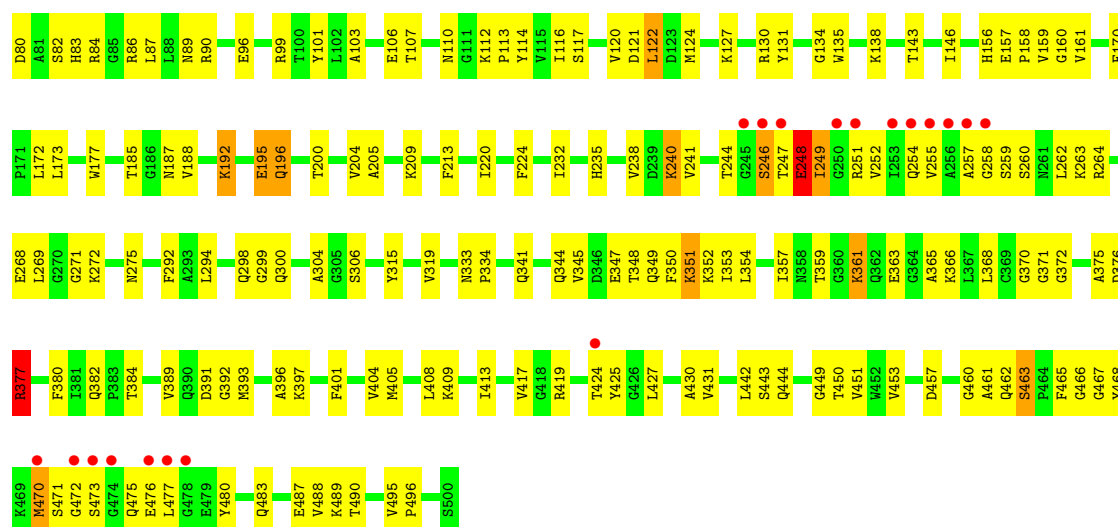
Chain F:



• Molecule 1: Aldehyde dehydrogenase

Chain G:





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.47Å 175.85Å 101.46Å 90.00° 94.79° 90.00°	Depositor
Resolution (Å)	10.00 – 2.15 24.89 – 2.15	Depositor EDS
% Data completeness (in resolution range)	92.5 (10.00-2.15) 96.5 (24.89-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.22 (at 2.15Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.251 , 0.314 0.266 , 0.320	Depositor DCC
R_{free} test set	9369 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	18.8	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 32.1	EDS
Estimated twinning fraction	0.467 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 186984 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	31388	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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	0.38	3/3880 (0.1%)	0.87	10/5265 (0.2%)
1	B	0.28	0/3880	0.67	7/5265 (0.1%)
1	C	0.36	2/3880 (0.1%)	0.95	10/5265 (0.2%)
1	D	0.29	0/3880	0.67	6/5265 (0.1%)
1	E	0.36	2/3880 (0.1%)	1.01	11/5265 (0.2%)
1	F	0.30	0/3880	0.68	8/5265 (0.2%)
1	G	0.33	2/3880 (0.1%)	0.81	8/5265 (0.2%)
1	H	0.31	1/3880 (0.0%)	0.68	7/5265 (0.1%)
All	All	0.33	10/31040 (0.0%)	0.80	67/42120 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	248	GLU	CD-OE1	10.60	1.37	1.25
1	G	361	LYS	CD-CE	9.20	1.74	1.51
1	A	115	VAL	CB-CG1	9.17	1.72	1.52
1	C	268	GLU	CG-CD	8.86	1.65	1.51
1	C	268	GLU	CD-OE2	8.37	1.34	1.25
1	H	409	LYS	CD-CE	7.90	1.71	1.51
1	A	288	GLU	CD-OE2	6.80	1.33	1.25
1	A	115	VAL	CB-CG2	6.43	1.66	1.52
1	E	248	GLU	CD-OE2	5.55	1.31	1.25
1	G	361	LYS	CE-NZ	5.09	1.61	1.49

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	90	ARG	CD-NE-CZ	37.79	176.51	123.60
1	E	99	ARG	NE-CZ-NH1	27.66	134.13	120.30
1	C	34	ARG	NE-CZ-NH1	27.45	134.03	120.30
1	A	90	ARG	CD-NE-CZ	26.80	161.12	123.60
1	E	99	ARG	NE-CZ-NH2	-25.64	107.48	120.30
1	G	377	ARG	NE-CZ-NH2	24.20	132.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	ARG	NE-CZ-NH2	-23.04	108.78	120.30
1	C	377	ARG	NE-CZ-NH2	21.15	130.87	120.30
1	A	90	ARG	NE-CZ-NH1	20.30	130.45	120.30
1	C	377	ARG	NE-CZ-NH1	-19.36	110.62	120.30
1	C	377	ARG	CD-NE-CZ	19.16	150.43	123.60
1	G	377	ARG	NE-CZ-NH1	-18.65	110.97	120.30
1	A	90	ARG	NE-CZ-NH2	-18.32	111.14	120.30
1	G	377	ARG	CD-NE-CZ	17.97	148.75	123.60
1	C	34	ARG	CD-NE-CZ	16.17	146.24	123.60
1	F	377	ARG	NE-CZ-NH1	13.05	126.82	120.30
1	E	99	ARG	CD-NE-CZ	11.73	140.03	123.60
1	E	90	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	A	377	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	B	377	ARG	CD-NE-CZ	9.98	137.57	123.60
1	G	34	ARG	CD-NE-CZ	9.91	137.48	123.60
1	H	377	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	D	377	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	H	377	ARG	CD-NE-CZ	9.13	136.38	123.60
1	E	377	ARG	NE-CZ-NH1	9.04	124.82	120.30
1	C	90	ARG	NE-CZ-NH2	9.01	124.81	120.30
1	E	377	ARG	CD-NE-CZ	8.94	136.11	123.60
1	H	90	ARG	NE-CZ-NH2	8.72	124.66	120.30
1	D	90	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	B	90	ARG	NE-CZ-NH2	8.49	124.55	120.30
1	F	90	ARG	NE-CZ-NH2	8.46	124.53	120.30
1	E	90	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	D	377	ARG	CD-NE-CZ	8.11	134.95	123.60
1	D	34	ARG	NE-CZ-NH2	8.09	124.35	120.30
1	B	377	ARG	NE-CZ-NH1	8.09	124.35	120.30
1	B	34	ARG	NE-CZ-NH2	8.04	124.32	120.30
1	A	320	GLU	CA-CB-CG	7.68	130.29	113.40
1	G	90	ARG	NE-CZ-NH2	7.53	124.07	120.30
1	A	34	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	275	ASN	CB-CG-OD1	7.33	136.26	121.60
1	F	377	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	H	34	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	E	34	ARG	NE-CZ-NH2	6.92	123.76	120.30
1	A	377	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	F	90	ARG	CD-NE-CZ	6.64	132.89	123.60
1	C	90	ARG	CD-NE-CZ	6.52	132.73	123.60
1	B	90	ARG	CD-NE-CZ	6.48	132.67	123.60
1	H	90	ARG	CD-NE-CZ	6.32	132.45	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	90	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	A	377	ARG	CD-NE-CZ	6.12	132.16	123.60
1	B	377	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	E	377	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	F	377	ARG	CD-NE-CZ	5.93	131.91	123.60
1	F	34	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	D	90	ARG	CD-NE-CZ	5.75	131.65	123.60
1	H	377	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	G	90	ARG	CD-NE-CZ	5.61	131.45	123.60
1	F	34	ARG	CD-NE-CZ	5.49	131.29	123.60
1	D	377	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	G	361	LYS	CD-CE-NZ	-5.37	99.35	111.70
1	B	34	ARG	CD-NE-CZ	5.34	131.08	123.60
1	G	248	GLU	CA-CB-CG	5.32	125.11	113.40
1	F	347	GLU	CA-CB-CG	5.28	125.01	113.40
1	C	90	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	E	34	ARG	CD-NE-CZ	5.13	130.78	123.60
1	A	275	ASN	CB-CG-ND2	-5.11	104.44	116.70
1	C	99	ARG	NE-CZ-NH2	5.06	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3796	0	3740	221	0
1	B	3796	0	3740	171	0
1	C	3796	0	3740	140	0
1	D	3796	0	3740	182	0
1	E	3796	0	3740	191	0
1	F	3796	0	3740	171	0
1	G	3796	0	3740	182	0
1	H	3796	0	3740	173	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	134	0	0	27	0
2	B	131	0	0	9	0
2	C	145	0	0	10	0
2	D	133	0	0	11	0
2	E	140	0	0	13	0
2	F	114	0	0	11	0
2	G	118	0	0	18	0
2	H	105	0	0	18	0
All	All	31388	0	29920	1330	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (1330) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:249:ILE:CG1	1:D:249:ILE:CD1	1.83	1.52
1:E:424:THR:HG22	1:E:470:MET:HB2	1.20	1.11
1:A:262:LEU:HD21	1:B:251:ARG:HG2	1.41	1.02
1:E:424:THR:HG21	1:E:470:MET:SD	2.02	0.99
1:H:247:THR:HA	1:H:269:LEU:HD22	1.45	0.99
1:D:247:THR:HG23	1:D:269:LEU:HD13	1.46	0.97
1:E:424:THR:HG22	1:E:470:MET:CB	1.95	0.97
1:A:196:GLN:HE21	1:A:196:GLN:H	1.09	0.97
1:C:461:ALA:HA	1:C:477:LEU:HD22	1.45	0.95
1:A:272:LYS:HE3	1:A:306:SER:HB2	1.46	0.95
1:F:26:ASN:HB3	1:F:209:LYS:HD2	1.49	0.95
1:H:247:THR:HG23	1:H:269:LEU:HD13	1.47	0.95
1:G:196:GLN:HE21	1:G:196:GLN:H	1.16	0.92
1:C:424:THR:HG22	1:C:470:MET:HB2	1.51	0.92
1:D:196:GLN:HE21	1:D:196:GLN:H	1.16	0.92
1:A:461:ALA:HA	1:A:477:LEU:HD22	1.53	0.90
1:F:461:ALA:HA	1:F:477:LEU:HD22	1.53	0.89
1:E:424:THR:CG2	1:E:470:MET:SD	2.61	0.88
1:G:248:GLU:HG2	1:G:249:ILE:HD13	1.56	0.88
1:F:124:MET:HE3	1:F:173:LEU:HD22	1.55	0.87
1:G:41:ASN:HD22	1:G:43:SER:H	1.16	0.87
1:G:475:GLN:OE1	1:G:480:TYR:HB3	1.75	0.86
1:C:124:MET:HE3	1:C:173:LEU:HD22	1.56	0.86
1:H:298:GLN:HG3	1:H:341:GLN:HG3	1.60	0.84
1:G:258:GLY:HA3	1:H:254:GLN:HG2	1.60	0.83
1:E:247:THR:HG23	1:E:269:LEU:HD13	1.58	0.83
1:F:247:THR:HA	1:F:269:LEU:HD22	1.61	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:360:GLY:HA2	2:A:9084:HOH:O	1.78	0.82
1:C:453:VAL:HB	1:D:493:VAL:HG13	1.61	0.82
1:G:255:VAL:HG22	1:H:255:VAL:HG13	1.60	0.82
1:D:124:MET:HE3	1:D:173:LEU:HD22	1.60	0.81
1:E:247:THR:HA	1:E:269:LEU:HD22	1.60	0.81
1:E:124:MET:HE3	1:E:173:LEU:HD22	1.63	0.81
1:F:196:GLN:H	1:F:196:GLN:HE21	1.30	0.80
1:C:393:MET:O	1:C:397:LYS:HG3	1.82	0.79
1:H:276:ILE:HD12	1:H:446:LEU:HD11	1.64	0.79
1:A:90:ARG:HH21	1:A:94:LEU:HD21	1.47	0.79
1:G:294:LEU:HD12	1:G:306:SER:HA	1.64	0.79
1:H:294:LEU:HD12	1:H:306:SER:HA	1.63	0.79
1:A:336:ASP:HB3	1:A:339:THR:OG1	1.83	0.78
1:E:41:ASN:HD22	1:E:43:SER:H	1.31	0.78
1:D:249:ILE:CB	1:D:249:ILE:CD1	2.61	0.78
1:H:32:VAL:HG11	1:H:57:GLU:OE2	1.84	0.78
1:D:21:GLN:HB3	1:D:29:HIS:O	1.84	0.77
1:E:247:THR:HA	1:E:269:LEU:HB3	1.66	0.77
1:D:294:LEU:HD12	1:D:306:SER:HA	1.65	0.77
1:C:359:THR:O	1:C:363:GLU:HG3	1.85	0.77
1:A:41:ASN:HD22	1:A:43:SER:H	1.33	0.77
1:F:266:THR:O	1:F:267:LEU:HD23	1.85	0.77
1:B:329:ARG:HE	1:B:341:GLN:HB2	1.49	0.77
1:H:300:GLN:HE22	1:H:345:VAL:H	1.32	0.77
1:G:77:ARG:HD2	2:G:8877:HOH:O	1.85	0.76
1:H:238:VAL:O	1:H:263:LYS:HE3	1.85	0.76
1:D:172:LEU:HD21	1:D:200:THR:HB	1.65	0.76
1:C:351:LYS:HB3	1:E:38:PRO:HG2	1.67	0.76
1:A:350:PHE:O	1:A:354:LEU:HG	1.86	0.76
1:A:40:VAL:HG13	1:A:46:GLU:O	1.86	0.76
1:E:120:VAL:HG12	1:E:124:MET:HE2	1.68	0.76
1:G:424:THR:HG22	1:G:470:MET:HB2	1.68	0.76
1:G:157:GLU:OE2	1:G:489:LYS:HD2	1.85	0.76
1:H:196:GLN:HE21	1:H:196:GLN:H	1.33	0.76
1:E:22:ILE:HD13	1:E:222:PRO:HD2	1.66	0.76
1:G:393:MET:O	1:G:397:LYS:HG3	1.85	0.76
1:D:12:ASN:O	1:D:15:PRO:HD3	1.86	0.76
1:F:240:LYS:NZ	1:F:242:ALA:HB2	2.01	0.76
1:E:436:LEU:HB3	2:H:8628:HOH:O	1.86	0.75
1:F:393:MET:O	1:F:397:LYS:HG3	1.85	0.75
1:G:257:ALA:HB1	1:G:263:LYS:HG3	1.69	0.75
1:H:22:ILE:HG12	1:H:222:PRO:HD2	1.69	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:317:GLU:O	1:C:321:ARG:HG3	1.87	0.74
1:H:244:THR:HG23	1:H:268:GLU:HB2	1.66	0.74
1:A:172:LEU:HD21	1:A:200:THR:HB	1.67	0.74
1:A:235:HIS:HB3	1:A:238:VAL:HG23	1.68	0.74
1:E:449:GLY:HA3	1:E:466:GLY:O	1.87	0.74
1:G:294:LEU:HD22	1:G:405:MET:HB2	1.70	0.74
1:E:475:GLN:OE1	1:E:480:TYR:HB3	1.88	0.74
1:F:298:GLN:HB2	1:F:300:GLN:HE21	1.53	0.74
1:G:359:THR:O	1:G:363:GLU:HG3	1.87	0.73
1:B:60:ASP:O	1:B:64:LYS:HG3	1.89	0.73
1:A:244:THR:HG23	1:A:268:GLU:O	1.88	0.73
1:E:244:THR:HG23	1:E:268:GLU:HB3	1.69	0.73
1:E:317:GLU:O	1:E:321:ARG:HG3	1.89	0.73
1:F:247:THR:HA	1:F:269:LEU:HB3	1.71	0.73
1:F:257:ALA:HB1	1:F:263:LYS:HG3	1.71	0.73
1:A:196:GLN:HE21	1:A:196:GLN:N	1.87	0.73
1:A:32:VAL:HG11	1:A:57:GLU:OE2	1.89	0.72
1:B:240:LYS:HE3	1:B:484:ALA:O	1.89	0.72
1:C:413:ILE:O	1:C:417:VAL:HG23	1.89	0.72
1:E:300:GLN:HE22	1:E:345:VAL:H	1.36	0.72
1:H:120:VAL:HG12	1:H:124:MET:HE2	1.71	0.72
1:B:194:ALA:HB3	1:B:197:THR:OG1	1.90	0.72
1:H:100:THR:HG22	2:H:9608:HOH:O	1.88	0.72
1:D:40:VAL:HG13	1:D:46:GLU:O	1.90	0.72
1:E:12:ASN:O	1:E:15:PRO:HD3	1.88	0.72
1:G:262:LEU:HD22	1:H:254:GLN:OE1	1.89	0.72
1:G:489:LYS:HB2	1:H:468:TYR:OH	1.89	0.72
1:E:41:ASN:HD21	1:E:43:SER:HB2	1.54	0.72
1:H:185:THR:HG23	1:H:482:LEU:HD22	1.72	0.72
1:G:366:LYS:HE2	1:G:368:LEU:HD21	1.71	0.71
1:G:41:ASN:ND2	1:G:43:SER:H	1.88	0.71
1:C:353:ILE:O	1:C:357:ILE:HG13	1.91	0.71
1:D:300:GLN:HE22	1:D:345:VAL:H	1.37	0.71
1:D:156:HIS:HB3	1:D:486:THR:HG21	1.73	0.71
1:B:313:ASP:HB3	2:B:9435:HOH:O	1.91	0.71
1:B:257:ALA:HB1	1:B:263:LYS:HG3	1.71	0.71
1:F:247:THR:HG23	1:F:269:LEU:HD13	1.72	0.71
1:F:366:LYS:HD3	1:F:388:ASP:OD2	1.90	0.71
1:F:22:ILE:HG12	1:F:222:PRO:HD2	1.73	0.70
1:A:238:VAL:HB	1:A:263:LYS:HE2	1.72	0.70
1:B:159:VAL:HG23	2:B:9130:HOH:O	1.90	0.70
1:H:359:THR:O	1:H:363:GLU:HG3	1.92	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:294:LEU:HD12	1:B:306:SER:HA	1.74	0.70
1:A:142:LYS:HD2	1:B:480:TYR:OH	1.91	0.70
1:B:44:THR:HB	1:B:377:ARG:NH2	2.07	0.70
1:D:359:THR:O	1:D:363:GLU:HG3	1.92	0.70
1:G:41:ASN:HD21	1:G:43:SER:HB2	1.57	0.70
1:A:41:ASN:ND2	1:A:43:SER:H	1.88	0.70
1:B:393:MET:O	1:B:397:LYS:HG3	1.92	0.70
1:F:134:GLY:O	1:F:138:LYS:HD2	1.92	0.69
1:F:12:ASN:O	1:F:15:PRO:HD3	1.91	0.69
1:D:246:SER:OG	1:D:249:ILE:HD12	1.92	0.69
1:B:358:ASN:O	1:B:362:GLN:HG2	1.92	0.69
1:B:86:ARG:HD3	2:D:9167:HOH:O	1.92	0.69
1:F:190:VAL:HG23	2:F:8853:HOH:O	1.92	0.69
1:H:257:ALA:HB1	1:H:263:LYS:HG3	1.75	0.69
1:A:294:LEU:HD22	1:A:405:MET:HB2	1.74	0.69
1:G:117:SER:O	1:G:121:ASP:HB2	1.92	0.69
1:B:121:ASP:O	1:B:125:VAL:HG23	1.93	0.69
1:G:196:GLN:HE21	1:G:196:GLN:N	1.89	0.69
1:A:425:TYR:O	1:A:469:LYS:HD2	1.93	0.68
1:B:378:GLY:HA2	2:B:8708:HOH:O	1.93	0.68
1:E:424:THR:CG2	1:E:470:MET:CG	2.71	0.68
1:A:317:GLU:O	1:A:321:ARG:HG3	1.92	0.68
1:A:330:VAL:HG23	1:A:340:GLU:OE2	1.93	0.68
1:A:109:ASP:OD2	1:A:197:THR:HA	1.92	0.68
1:B:244:THR:HG23	1:B:268:GLU:HB2	1.75	0.68
1:D:413:ILE:O	1:D:417:VAL:HG23	1.94	0.68
1:E:196:GLN:HE21	1:E:196:GLN:H	1.41	0.68
1:D:235:HIS:HB3	1:D:238:VAL:HG23	1.75	0.68
1:F:298:GLN:HE21	1:F:300:GLN:HE21	1.40	0.68
1:B:315:TYR:O	1:B:319:VAL:HG23	1.94	0.68
1:D:358:ASN:O	1:D:362:GLN:HG2	1.93	0.68
1:G:258:GLY:CA	1:H:254:GLN:HG2	2.23	0.68
1:H:468:TYR:O	1:H:471:SER:HB2	1.94	0.68
1:G:26:ASN:HB3	1:G:209:LYS:HD2	1.76	0.68
1:C:241:VAL:HG12	1:C:265:VAL:HG22	1.77	0.67
1:C:294:LEU:HD12	1:C:306:SER:HA	1.74	0.67
1:G:124:MET:HE3	1:G:173:LEU:HD22	1.76	0.67
1:B:196:GLN:H	1:B:196:GLN:NE2	1.92	0.67
1:H:46:GLU:HB2	2:H:8788:HOH:O	1.93	0.67
1:A:185:THR:HG23	1:A:482:LEU:HD22	1.75	0.67
1:G:177:TRP:NE1	1:G:477:LEU:HD21	2.09	0.67
1:H:426:GLY:O	1:H:468:TYR:HB2	1.94	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:196:GLN:H	1:B:196:GLN:HE21	1.41	0.67
1:H:312:GLU:OE1	1:H:411:LYS:HG3	1.95	0.67
1:C:280:ASP:O	1:C:434:LYS:HD2	1.94	0.67
1:E:366:LYS:HD3	1:E:368:LEU:HD21	1.77	0.67
1:H:358:ASN:O	1:H:362:GLN:HG2	1.94	0.67
1:A:303:CYS:HG	1:A:459:PHE:HZ	1.40	0.67
1:G:120:VAL:HG12	1:G:124:MET:HE2	1.77	0.67
1:H:111:GLY:O	1:H:343:PRO:HD2	1.95	0.67
1:C:464:PRO:HG2	1:D:490:THR:OG1	1.95	0.67
1:C:38:PRO:HG2	1:E:351:LYS:HB3	1.75	0.67
1:E:60:ASP:O	1:E:64:LYS:HG3	1.95	0.67
1:F:59:VAL:O	1:F:63:VAL:HG23	1.94	0.67
1:E:490:THR:OG1	1:F:464:PRO:HG2	1.95	0.67
1:G:12:ASN:O	1:G:15:PRO:HD3	1.95	0.67
1:A:251:ARG:HG2	1:B:262:LEU:HD21	1.77	0.66
1:C:300:GLN:HE22	1:C:345:VAL:H	1.43	0.66
1:G:77:ARG:HA	2:G:8877:HOH:O	1.95	0.66
1:E:261:ASN:HA	1:F:251:ARG:HH22	1.59	0.66
1:G:463:SER:HB3	2:G:9569:HOH:O	1.95	0.66
1:H:245:GLY:O	1:H:269:LEU:HA	1.95	0.66
1:A:206:ASN:O	1:A:209:LYS:HB3	1.96	0.66
1:G:350:PHE:O	1:G:354:LEU:HG	1.95	0.66
1:G:361:LYS:HG2	2:G:9353:HOH:O	1.95	0.66
1:E:247:THR:HG23	1:E:269:LEU:CD1	2.25	0.66
1:G:470:MET:SD	1:H:262:LEU:HD12	2.36	0.66
1:H:461:ALA:HA	1:H:477:LEU:HD22	1.77	0.66
1:F:280:ASP:O	1:F:434:LYS:HG3	1.94	0.66
1:D:284:ASP:HB2	2:D:9470:HOH:O	1.96	0.66
1:E:294:LEU:HD12	1:E:306:SER:HA	1.78	0.66
1:A:32:VAL:HG23	1:A:58:ASP:OD1	1.96	0.66
1:D:109:ASP:OD2	1:D:197:THR:HA	1.96	0.66
1:C:462:GLN:O	1:D:144:ILE:HG21	1.96	0.65
1:G:244:THR:OG1	1:G:268:GLU:HB2	1.95	0.65
1:A:15:PRO:HD2	1:A:108:LEU:HD13	1.77	0.65
1:C:103:ALA:HB2	1:C:122:LEU:HD13	1.79	0.65
1:G:361:LYS:HA	2:G:9353:HOH:O	1.95	0.65
1:A:36:THR:OG1	1:A:50:GLN:HG3	1.96	0.65
1:A:146:ILE:HG22	2:A:8700:HOH:O	1.97	0.65
1:C:134:GLY:O	1:C:138:LYS:HD2	1.96	0.65
1:E:251:ARG:HA	1:F:262:LEU:HD21	1.79	0.65
1:G:195:GLU:HA	2:G:8776:HOH:O	1.97	0.65
1:D:306:SER:O	1:D:406:GLN:HB2	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:68:ALA:HA	1:B:71:GLN:HG2	1.79	0.65
1:D:155:ARG:HD3	1:D:489:LYS:HD2	1.78	0.64
1:E:347:GLU:O	1:E:351:LYS:HG3	1.97	0.64
1:F:358:ASN:O	1:F:362:GLN:HG2	1.96	0.64
1:G:247:THR:HA	1:G:269:LEU:HD22	1.78	0.64
1:G:431:VAL:HG21	1:G:442:LEU:HB3	1.79	0.64
1:F:161:VAL:HG13	2:F:8853:HOH:O	1.97	0.64
1:F:315:TYR:O	1:F:319:VAL:HG23	1.98	0.64
1:H:106:GLU:OE2	1:H:200:THR:HG21	1.97	0.64
1:H:196:GLN:H	1:H:196:GLN:NE2	1.95	0.64
1:C:13:GLN:NE2	1:C:335:PHE:HB3	2.13	0.64
1:A:55:ASP:O	1:A:59:VAL:HG23	1.98	0.64
1:B:271:GLY:HA2	1:B:425:TYR:CG	2.33	0.64
1:D:134:GLY:O	1:D:138:LYS:HD2	1.97	0.64
1:A:393:MET:O	1:A:397:LYS:HG3	1.97	0.64
1:H:37:PHE:HD2	1:H:53:GLU:HB2	1.63	0.64
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.33	0.64
1:E:247:THR:CA	1:E:269:LEU:HB3	2.27	0.64
1:H:356:TYR:CG	1:H:400:ILE:HG12	2.33	0.63
1:H:408:LEU:HB3	2:H:8635:HOH:O	1.97	0.63
1:D:155:ARG:HB2	1:D:489:LYS:HB3	1.80	0.63
1:G:315:TYR:CG	1:G:409:LYS:HE2	2.33	0.63
1:G:391:ASP:OD2	1:G:419:ARG:HG2	1.98	0.63
1:G:156:HIS:CD2	1:G:488:VAL:HG22	2.33	0.63
1:E:424:THR:CG2	1:E:470:MET:CE	2.76	0.63
1:G:365:ALA:HB2	1:G:393:MET:SD	2.38	0.63
1:G:47:VAL:HG13	2:G:8768:HOH:O	1.97	0.63
1:E:344:GLN:HG3	1:E:353:ILE:HD12	1.79	0.63
1:G:32:VAL:HG23	1:G:58:ASP:OD1	1.98	0.63
1:A:480:TYR:OH	1:B:142:LYS:HG3	1.98	0.63
1:E:424:THR:CG2	1:E:470:MET:CB	2.73	0.63
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.33	0.63
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.33	0.63
1:A:24:ILE:HG22	1:A:25:ASN:OD1	1.99	0.62
1:C:50:GLN:HG2	1:E:358:ASN:OD1	1.99	0.62
1:H:418:GLY:HA3	2:H:8803:HOH:O	1.98	0.62
1:A:350:PHE:CZ	1:A:373:ILE:HD13	2.35	0.62
1:E:464:PRO:HA	1:E:476:GLU:O	1.99	0.62
1:G:348:THR:O	1:G:352:LYS:HB2	2.00	0.62
1:E:112:LYS:HE2	1:E:297:ASN:OD1	1.99	0.62
1:B:59:VAL:O	1:B:63:VAL:HG23	1.98	0.62
1:F:353:ILE:O	1:F:357:ILE:HG13	2.00	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:424:THR:HG23	1:E:470:MET:CE	2.29	0.62
1:H:87:LEU:HB3	1:H:213:PHE:CZ	2.34	0.62
1:C:315:TYR:CD1	1:C:409:LYS:HE2	2.34	0.62
1:F:44:THR:HA	1:F:377:ARG:HD3	1.80	0.62
1:G:461:ALA:HA	1:G:477:LEU:HD22	1.82	0.62
1:F:413:ILE:O	1:F:417:VAL:HG23	1.99	0.62
1:E:424:THR:CG2	1:E:470:MET:HB2	2.12	0.62
1:E:175:GLN:HE22	1:E:201:ALA:HA	1.64	0.62
1:F:23:PHE:CZ	1:F:26:ASN:HA	2.34	0.62
1:F:359:THR:O	1:F:363:GLU:HG3	2.00	0.62
1:G:248:GLU:O	1:G:252:VAL:HG23	2.00	0.62
1:H:12:ASN:O	1:H:15:PRO:HD3	2.00	0.62
1:C:475:GLN:OE1	1:C:480:TYR:HB3	1.99	0.61
1:E:241:VAL:HG13	1:E:265:VAL:HG13	1.82	0.61
1:E:41:ASN:ND2	1:E:43:SER:HB2	2.16	0.61
1:F:460:GLY:O	1:F:477:LEU:HD13	2.00	0.61
1:B:347:GLU:O	1:B:351:LYS:HG3	1.99	0.61
1:D:95:ILE:HG22	1:D:126:LEU:HD21	1.82	0.61
1:D:23:PHE:HB2	1:D:28:TRP:CZ3	2.36	0.61
1:A:424:THR:HG21	1:A:470:MET:HE3	1.82	0.61
1:C:120:VAL:HG12	1:C:124:MET:HE2	1.82	0.61
1:A:271:GLY:O	1:A:399:GLU:HB2	2.01	0.61
1:D:366:LYS:HD3	1:D:368:LEU:HD21	1.82	0.61
1:H:41:ASN:HD22	1:H:43:SER:H	1.47	0.61
1:B:203:TYR:HB2	2:B:8930:HOH:O	2.00	0.61
1:E:31:ALA:HA	2:E:8812:HOH:O	2.01	0.61
1:C:30:ASP:HB2	1:C:34:ARG:NH2	2.16	0.61
1:D:435:ASP:HB3	1:D:438:LYS:HB2	1.81	0.60
1:F:422:ASN:HB3	2:F:9339:HOH:O	2.01	0.60
1:G:375:ALA:HB3	1:G:380:PHE:HB2	1.82	0.60
1:A:23:PHE:CZ	1:A:26:ASN:HA	2.36	0.60
1:A:70:PHE:CD1	1:A:77:ARG:HD3	2.36	0.60
1:D:11:PRO:HB3	1:D:114:TYR:CE1	2.36	0.60
1:D:99:ARG:HG3	1:D:122:LEU:HD22	1.82	0.60
1:E:23:PHE:CZ	1:E:26:ASN:HA	2.36	0.60
1:A:237:ASP:HA	2:A:9067:HOH:O	2.01	0.60
1:H:393:MET:O	1:H:397:LYS:HG3	2.02	0.60
1:E:246:SER:HG	1:E:249:ILE:H	1.49	0.60
1:H:429:ALA:HB1	1:H:446:LEU:HD13	1.84	0.60
1:B:464:PRO:HG3	1:B:480:TYR:CE1	2.37	0.60
1:C:489:LYS:HB2	1:D:468:TYR:OH	2.01	0.60
1:F:298:GLN:HE21	1:F:300:GLN:NE2	1.99	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:347:GLU:HA	1:B:350:PHE:HB3	1.83	0.60
1:C:251:ARG:HG2	1:D:262:LEU:HD11	1.82	0.60
1:C:196:GLN:H	1:C:196:GLN:HE21	1.48	0.60
1:F:8:VAL:HG13	1:F:118:TYR:CD2	2.36	0.60
1:B:12:ASN:O	1:B:15:PRO:HD3	2.01	0.60
1:B:94:LEU:HD13	1:B:210:GLU:OE2	2.01	0.60
1:D:294:LEU:HD13	1:D:405:MET:HA	1.83	0.60
1:F:11:PRO:HB3	1:F:114:TYR:CE1	2.36	0.60
1:F:294:LEU:O	1:F:299:GLY:HA2	2.02	0.60
1:G:468:TYR:O	1:G:471:SER:HB2	2.02	0.60
1:H:107:THR:HG23	1:H:334:PRO:HB2	1.83	0.60
1:A:424:THR:HG22	1:A:470:MET:HB2	1.84	0.59
1:E:294:LEU:HD22	1:E:405:MET:HB2	1.83	0.59
1:E:435:ASP:OD1	1:E:438:LYS:HG3	2.01	0.59
1:F:298:GLN:HB2	1:F:300:GLN:NE2	2.15	0.59
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.37	0.59
1:G:36:THR:OG1	1:G:50:GLN:HG3	2.02	0.59
1:A:45:GLY:HA3	2:A:9090:HOH:O	2.01	0.59
1:G:205:ALA:HB2	1:G:220:ILE:HD12	1.84	0.59
1:H:244:THR:OG1	1:H:268:GLU:HG3	2.02	0.59
1:C:388:ASP:HA	2:C:8979:HOH:O	2.02	0.59
1:F:347:GLU:O	1:F:351:LYS:HG3	2.01	0.59
1:E:146:ILE:HG13	1:F:460:GLY:HA3	1.84	0.59
1:C:247:THR:HA	1:C:269:LEU:HB3	1.84	0.59
1:C:135:TRP:CZ2	1:C:479:GLU:HB2	2.38	0.59
1:D:468:TYR:O	1:D:471:SER:HB2	2.02	0.59
1:E:11:PRO:HB3	1:E:114:TYR:CZ	2.37	0.59
1:B:331:VAL:HG13	1:B:341:GLN:O	2.03	0.59
1:B:461:ALA:O	1:B:477:LEU:HB3	2.01	0.59
1:A:109:ASP:OD2	1:A:198:PRO:HD2	2.03	0.59
1:F:209:LYS:HD3	2:F:8843:HOH:O	2.02	0.59
1:G:413:ILE:O	1:G:417:VAL:HG23	2.03	0.59
1:B:418:GLY:O	1:B:422:ASN:HB2	2.03	0.59
1:C:11:PRO:HB3	1:C:114:TYR:CZ	2.38	0.59
1:A:21:GLN:OE1	1:A:28:TRP:HB3	2.03	0.58
1:A:155:ARG:CZ	1:B:444:GLN:HG3	2.33	0.58
1:F:311:GLN:OE1	1:F:313:ASP:HB2	2.02	0.58
1:B:348:THR:O	1:B:352:LYS:HB2	2.04	0.58
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.38	0.58
1:C:261:ASN:HD21	1:C:263:LYS:HE3	1.68	0.58
1:C:247:THR:HG23	1:C:269:LEU:CB	2.33	0.58
1:E:240:LYS:NZ	1:E:242:ALA:HB2	2.18	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:39:THR:HG23	1:A:48:ILE:HB	1.85	0.58
1:D:196:GLN:HE21	1:D:196:GLN:N	1.95	0.58
1:G:205:ALA:HB2	1:G:220:ILE:CD1	2.34	0.58
1:G:31:ALA:O	1:G:34:ARG:NE	2.37	0.58
1:A:366:LYS:HE2	1:A:368:LEU:HD21	1.84	0.58
1:A:76:TRP:O	1:A:79:MET:HB3	2.04	0.58
1:F:497:GLN:HG2	1:F:499:ASN:ND2	2.19	0.58
1:E:115:VAL:HG13	1:E:119:LEU:HD12	1.86	0.58
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.39	0.58
1:H:269:LEU:HD12	1:H:472:GLY:N	2.19	0.58
1:E:41:ASN:ND2	1:E:43:SER:H	2.01	0.58
1:A:200:THR:O	1:A:204:VAL:HG23	2.03	0.58
1:B:300:GLN:HE22	1:B:345:VAL:H	1.52	0.58
1:A:116:ILE:HG22	1:A:121:ASP:OD2	2.04	0.57
1:B:135:TRP:CZ2	1:B:479:GLU:HB2	2.39	0.57
1:D:280:ASP:O	1:D:434:LYS:HG3	2.03	0.57
1:A:241:VAL:HG12	1:A:265:VAL:HG22	1.86	0.57
1:F:294:LEU:HD11	1:F:404:VAL:O	2.04	0.57
1:H:300:GLN:HE22	1:H:345:VAL:N	2.01	0.57
1:A:363:GLU:HB2	2:A:9084:HOH:O	2.03	0.57
1:D:291:HIS:HE1	1:D:326:ALA:HA	1.69	0.57
1:E:294:LEU:HD11	1:E:404:VAL:O	2.04	0.57
1:A:366:LYS:HG2	1:A:368:LEU:HD21	1.85	0.57
1:A:149:ASP:HA	1:A:498:LYS:HB2	1.85	0.57
1:C:34:ARG:HD2	1:C:34:ARG:N	2.18	0.57
1:D:449:GLY:HA3	1:D:466:GLY:O	2.05	0.57
1:G:11:PRO:HB3	1:G:114:TYR:CE1	2.39	0.57
1:C:106:GLU:O	1:C:110:ASN:HB3	2.03	0.57
1:D:68:ALA:HA	1:D:71:GLN:HG2	1.87	0.57
1:E:109:ASP:OD2	1:E:198:PRO:HD2	2.04	0.57
1:F:292:PHE:CD2	1:F:296:PHE:HB2	2.40	0.57
1:G:41:ASN:ND2	1:G:43:SER:HB2	2.18	0.57
1:G:146:ILE:HG13	1:H:460:GLY:HA3	1.85	0.57
1:B:366:LYS:HG2	1:B:368:LEU:HD21	1.85	0.57
1:A:20:ASN:HA	1:A:202:LEU:HD12	1.87	0.57
1:A:363:GLU:CG	2:A:9084:HOH:O	2.51	0.57
1:A:8:VAL:HG21	1:A:115:VAL:HG22	1.85	0.57
1:A:146:ILE:HG13	1:B:460:GLY:HA3	1.87	0.57
1:G:304:ALA:HA	2:G:9554:HOH:O	2.04	0.57
1:H:477:LEU:HD21	2:H:8838:HOH:O	2.05	0.57
1:C:12:ASN:O	1:C:15:PRO:HD3	2.04	0.57
1:D:44:THR:HB	1:D:46:GLU:HG2	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:86:ARG:HG3	2:G:9545:HOH:O	2.04	0.57
1:A:366:LYS:HG2	1:A:368:LEU:CD2	2.35	0.57
1:G:468:TYR:OH	1:H:489:LYS:HB2	2.04	0.57
1:C:39:THR:HG23	1:C:48:ILE:HB	1.87	0.57
1:D:262:LEU:HB3	2:D:9469:HOH:O	2.05	0.57
1:E:275:ASN:ND2	1:E:430:ALA:HB3	2.20	0.57
1:F:41:ASN:HD22	1:F:43:SER:H	1.51	0.57
2:E:8837:HOH:O	1:H:436:LEU:HB2	2.04	0.57
1:A:12:ASN:O	1:A:15:PRO:HD3	2.04	0.56
1:A:37:PHE:HD2	1:A:53:GLU:HB2	1.70	0.56
1:E:234:SER:HA	1:E:260:SER:HB3	1.87	0.56
1:F:142:LYS:NZ	2:F:8849:HOH:O	2.37	0.56
1:A:117:SER:O	1:A:122:LEU:HD12	2.05	0.56
1:A:424:THR:CG2	1:A:470:MET:CE	2.83	0.56
1:F:245:GLY:O	1:F:269:LEU:HA	2.04	0.56
1:H:329:ARG:HA	1:H:340:GLU:OE2	2.05	0.56
1:D:392:GLY:O	1:D:397:LYS:HE2	2.05	0.56
1:F:167:PRO:HD3	1:F:244:THR:HB	1.85	0.56
1:F:240:LYS:HZ3	1:F:242:ALA:HB2	1.70	0.56
1:B:201:ALA:HB2	2:B:8940:HOH:O	2.04	0.56
1:D:246:SER:HG	1:D:248:GLU:HB3	1.69	0.56
1:G:131:TYR:CZ	1:G:462:GLN:HA	2.40	0.56
1:H:394:THR:HG23	1:H:398:GLU:HG3	1.88	0.56
1:A:424:THR:HG23	1:A:470:MET:HE2	1.88	0.56
1:C:30:ASP:HB2	1:C:34:ARG:HH21	1.70	0.56
1:E:464:PRO:HG2	1:F:490:THR:OG1	2.05	0.56
1:H:476:GLU:O	1:H:477:LEU:HB2	2.05	0.56
1:E:358:ASN:O	1:E:362:GLN:HG2	2.05	0.56
1:A:22:ILE:CD1	1:A:221:VAL:HG13	2.36	0.56
1:A:63:VAL:HG11	1:A:235:HIS:CE1	2.41	0.56
1:E:102:LEU:HD21	1:E:203:TYR:HD2	1.70	0.56
1:G:127:LYS:HE2	2:H:9549:HOH:O	2.05	0.56
1:G:315:TYR:CD1	1:G:409:LYS:HE2	2.40	0.56
1:G:156:HIS:HD2	1:G:488:VAL:HG22	1.69	0.56
1:A:131:TYR:CZ	1:A:462:GLN:HA	2.41	0.56
1:B:16:GLU:HB3	1:B:18:PHE:CZ	2.41	0.56
1:D:418:GLY:O	1:D:422:ASN:HB2	2.06	0.56
1:A:302:CYS:HB2	1:A:427:LEU:CD2	2.35	0.56
1:F:196:GLN:HE21	1:F:196:GLN:N	2.00	0.56
1:G:70:PHE:CZ	1:G:160:GLY:HA2	2.40	0.56
1:A:13:GLN:HG2	1:A:335:PHE:CG	2.41	0.56
1:D:276:ILE:HG23	1:D:416:VAL:HG21	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:132:TYR:OH	1:E:477:LEU:HA	2.06	0.56
1:E:61:LYS:HD2	2:E:9482:HOH:O	2.05	0.56
1:G:294:LEU:CD1	1:G:405:MET:HA	2.36	0.56
1:H:294:LEU:CD1	1:H:306:SER:HA	2.34	0.56
1:A:405:MET:CE	1:A:407:ILE:HD11	2.36	0.55
1:A:271:GLY:HA2	1:A:425:TYR:CG	2.41	0.55
1:D:36:THR:OG1	1:D:50:GLN:HG3	2.05	0.55
1:E:22:ILE:CD1	1:E:222:PRO:HD2	2.35	0.55
1:F:63:VAL:HG11	1:F:235:HIS:CE1	2.41	0.55
1:G:16:GLU:HB3	1:G:18:PHE:CZ	2.41	0.55
1:A:11:PRO:HB3	1:A:114:TYR:CE1	2.41	0.55
1:C:392:GLY:O	1:C:397:LYS:HE2	2.06	0.55
1:E:251:ARG:HB3	1:F:258:GLY:O	2.06	0.55
1:H:240:LYS:HD2	1:H:264:ARG:HB3	1.88	0.55
1:A:124:MET:HE3	1:A:173:LEU:HD22	1.88	0.55
1:C:123:ASP:O	1:C:127:LYS:HG3	2.05	0.55
1:C:36:THR:OG1	1:C:50:GLN:HG3	2.06	0.55
1:A:424:THR:HG21	1:A:470:MET:CE	2.36	0.55
1:B:366:LYS:HG2	1:B:368:LEU:CD2	2.35	0.55
1:D:196:GLN:H	1:D:196:GLN:NE2	1.96	0.55
1:D:172:LEU:CD2	1:D:200:THR:HB	2.36	0.55
1:F:344:GLN:OE1	1:F:403:PRO:HD3	2.06	0.55
1:G:11:PRO:HB3	1:G:114:TYR:CD1	2.40	0.55
1:G:134:GLY:O	1:G:138:LYS:HD2	2.06	0.55
1:A:195:GLU:HG2	1:A:196:GLN:NE2	2.20	0.55
1:A:489:LYS:HB2	1:B:468:TYR:OH	2.06	0.55
1:B:131:TYR:CZ	1:B:462:GLN:HA	2.41	0.55
1:F:240:LYS:HZ1	1:F:242:ALA:HB2	1.70	0.55
1:G:292:PHE:CE1	1:G:457:ASP:HB2	2.41	0.55
1:G:427:LEU:HD11	1:G:465:PHE:CZ	2.42	0.55
1:E:350:PHE:O	1:E:354:LEU:HG	2.07	0.55
1:H:461:ALA:O	1:H:477:LEU:HD22	2.06	0.55
1:H:477:LEU:HD11	2:H:8838:HOH:O	2.05	0.55
1:C:241:VAL:CG1	1:C:265:VAL:HG22	2.37	0.55
1:D:271:GLY:HA2	1:D:425:TYR:CG	2.42	0.55
1:E:248:GLU:O	1:E:251:ARG:HG3	2.07	0.55
1:F:495:VAL:HA	2:H:8766:HOH:O	2.06	0.55
1:G:172:LEU:HG	1:G:200:THR:HB	1.89	0.55
1:A:271:GLY:HA2	1:A:425:TYR:CD2	2.41	0.55
1:B:113:PRO:HB2	1:B:116:ILE:HG12	1.88	0.55
1:B:294:LEU:HD11	1:B:404:VAL:O	2.07	0.55
1:G:106:GLU:O	1:G:110:ASN:HB3	2.07	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:255:VAL:CG2	1:H:255:VAL:HG13	2.36	0.55
1:B:32:VAL:HG21	1:B:57:GLU:HB3	1.89	0.55
1:B:90:ARG:CZ	1:B:94:LEU:HD21	2.37	0.55
1:C:404:VAL:HG12	1:C:406:GLN:OE1	2.06	0.55
1:E:107:THR:HG23	1:E:112:LYS:O	2.07	0.55
1:G:192:LYS:HB2	1:G:232:ILE:CD1	2.37	0.55
1:B:461:ALA:HA	1:B:477:LEU:HD22	1.89	0.55
1:C:63:VAL:HG11	1:C:235:HIS:CE1	2.42	0.55
1:E:254:GLN:OE1	1:F:262:LEU:HD22	2.07	0.55
1:E:300:GLN:HE22	1:E:345:VAL:N	2.05	0.55
1:C:395:ILE:HD12	1:C:406:GLN:HG3	1.88	0.54
1:E:390:GLN:HG2	1:E:393:MET:CE	2.37	0.54
1:H:109:ASP:OD2	1:H:199:LEU:HG	2.07	0.54
1:C:351:LYS:HB3	1:E:38:PRO:CG	2.35	0.54
1:D:120:VAL:HG12	1:D:124:MET:CE	2.38	0.54
1:G:443:SER:HA	1:G:451:VAL:HG11	1.89	0.54
1:A:8:VAL:HG13	1:A:118:TYR:CD2	2.43	0.54
1:B:95:ILE:HG22	1:B:126:LEU:HD21	1.90	0.54
1:B:317:GLU:O	1:B:321:ARG:HG3	2.07	0.54
1:D:258:GLY:HA2	1:D:262:LEU:HD23	1.88	0.54
1:D:311:GLN:OE1	1:D:313:ASP:HB2	2.06	0.54
1:G:292:PHE:HE1	1:G:457:ASP:HB2	1.73	0.54
1:G:372:GLY:O	1:G:382:GLN:HG3	2.07	0.54
1:G:255:VAL:HG13	1:H:255:VAL:HG22	1.89	0.54
1:A:22:ILE:HD13	1:A:221:VAL:HG13	1.89	0.54
1:A:146:ILE:CG1	1:B:460:GLY:HA3	2.38	0.54
1:B:82:SER:HB3	2:B:9159:HOH:O	2.08	0.54
1:D:424:THR:O	1:D:470:MET:HB2	2.07	0.54
1:H:271:GLY:HA2	1:H:425:TYR:CG	2.43	0.54
1:A:100:THR:HG23	1:A:114:TYR:OH	2.08	0.54
1:A:162:CYS:HB3	2:A:9063:HOH:O	2.07	0.54
1:D:63:VAL:HG11	1:D:235:HIS:CE1	2.43	0.54
1:F:404:VAL:HG12	1:F:406:GLN:OE1	2.07	0.54
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.43	0.54
1:D:276:ILE:CG2	1:D:416:VAL:HG21	2.38	0.54
1:B:329:ARG:NE	1:B:341:GLN:HB2	2.22	0.54
1:C:36:THR:CB	1:C:50:GLN:HG3	2.38	0.54
1:D:106:GLU:O	1:D:110:ASN:HB3	2.07	0.54
1:D:41:ASN:HD22	1:D:43:SER:H	1.55	0.54
1:F:23:PHE:CD2	1:F:205:ALA:HB1	2.43	0.54
1:H:99:ARG:HG3	1:H:122:LEU:HD22	1.90	0.54
1:A:303:CYS:SG	1:A:459:PHE:HZ	2.31	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:442:LEU:O	1:A:446:LEU:HG	2.08	0.54
1:A:464:PRO:HG2	1:B:490:THR:OG1	2.08	0.54
1:B:302:CYS:HB2	1:B:427:LEU:CD2	2.37	0.54
1:B:269:LEU:HD12	1:B:470:MET:O	2.08	0.54
1:B:56:LYS:HE2	1:B:60:ASP:OD1	2.07	0.54
1:C:493:VAL:HG13	1:D:453:VAL:HB	1.90	0.54
1:D:393:MET:O	1:D:397:LYS:HG3	2.07	0.54
1:E:135:TRP:CG	1:E:482:LEU:HD11	2.43	0.54
1:E:240:LYS:HG3	1:E:264:ARG:HB3	1.90	0.54
1:G:107:THR:HG23	1:G:112:LYS:O	2.07	0.54
1:H:33:SER:O	1:H:34:ARG:HB2	2.08	0.54
1:A:366:LYS:HB2	2:A:9086:HOH:O	2.08	0.53
1:B:435:ASP:HB3	1:B:438:LYS:HB2	1.90	0.53
1:D:247:THR:HA	1:D:269:LEU:HD22	1.91	0.53
1:E:154:THR:HA	1:E:489:LYS:O	2.09	0.53
1:F:294:LEU:HD13	1:F:405:MET:HA	1.90	0.53
1:G:238:VAL:O	1:G:263:LYS:HE3	2.08	0.53
1:H:11:PRO:HB3	1:H:114:TYR:CE2	2.43	0.53
1:H:271:GLY:O	1:H:399:GLU:HB2	2.08	0.53
1:C:33:SER:O	1:C:34:ARG:HB2	2.08	0.53
1:E:21:GLN:HB3	1:E:29:HIS:O	2.08	0.53
1:G:170:PHE:HB3	1:G:173:LEU:HB3	1.89	0.53
1:A:148:GLY:O	1:A:498:LYS:HD3	2.08	0.53
1:B:33:SER:O	1:B:34:ARG:HB2	2.09	0.53
1:D:294:LEU:HD11	1:D:404:VAL:O	2.07	0.53
1:F:276:ILE:HG12	1:F:416:VAL:HG21	1.89	0.53
1:H:102:LEU:HD21	1:H:203:TYR:HD2	1.73	0.53
1:B:109:ASP:OD2	1:B:199:LEU:HG	2.09	0.53
1:C:254:GLN:OE1	1:D:262:LEU:HD22	2.08	0.53
1:D:464:PRO:HA	1:D:476:GLU:O	2.09	0.53
1:F:247:THR:CG2	1:F:269:LEU:HD13	2.38	0.53
1:H:449:GLY:HA2	1:H:468:TYR:CE1	2.44	0.53
1:A:33:SER:O	1:A:34:ARG:HB2	2.08	0.53
1:B:202:LEU:O	1:B:205:ALA:HB3	2.08	0.53
1:C:251:ARG:HA	1:D:262:LEU:HD21	1.90	0.53
1:F:240:LYS:HG2	1:F:241:VAL:N	2.23	0.53
1:H:274:PRO:HA	1:H:307:ARG:O	2.08	0.53
1:D:473:SER:HA	2:D:9478:HOH:O	2.07	0.53
1:A:107:THR:HG23	1:A:112:LYS:O	2.09	0.53
1:F:36:THR:OG1	1:F:50:GLN:HG3	2.07	0.53
1:E:146:ILE:CG1	1:F:460:GLY:HA3	2.39	0.53
1:H:120:VAL:HG12	1:H:124:MET:CE	2.39	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:39:THR:HG23	1:H:48:ILE:HB	1.91	0.53
1:A:8:VAL:HG21	1:A:115:VAL:CG2	2.38	0.53
1:A:460:GLY:HA3	1:B:146:ILE:HG13	1.90	0.53
1:C:99:ARG:HG2	1:C:118:TYR:CE1	2.43	0.53
1:F:63:VAL:HG21	1:F:235:HIS:CD2	2.44	0.53
1:H:317:GLU:CG	1:H:321:ARG:HE	2.21	0.53
1:A:187:ASN:HD21	1:A:485:TYR:HB3	1.74	0.53
1:C:257:ALA:HA	1:C:260:SER:OG	2.09	0.53
1:D:139:TYR:CD1	1:D:482:LEU:HD12	2.43	0.53
1:F:424:THR:O	1:F:470:MET:HB2	2.09	0.53
1:H:243:PHE:CG	1:H:253:ILE:HG13	2.44	0.53
1:A:135:TRP:CG	1:A:482:LEU:HD11	2.44	0.52
1:B:460:GLY:HA3	1:B:462:GLN:HE21	1.72	0.52
1:B:138:LYS:HD3	1:D:135:TRP:CE2	2.44	0.52
1:E:247:THR:CB	1:E:269:LEU:HB3	2.39	0.52
1:F:294:LEU:HD22	1:F:405:MET:HB2	1.90	0.52
1:G:271:GLY:HA2	1:G:425:TYR:CG	2.44	0.52
1:H:336:ASP:HB3	1:H:339:THR:OG1	2.08	0.52
1:B:26:ASN:O	1:B:209:LYS:HE3	2.10	0.52
1:D:90:ARG:NH1	1:D:94:LEU:HD21	2.24	0.52
1:E:22:ILE:HG22	1:E:24:ILE:HG13	1.89	0.52
1:F:247:THR:HA	1:F:269:LEU:CD2	2.37	0.52
1:F:497:GLN:HG2	1:F:499:ASN:HD21	1.74	0.52
1:C:240:LYS:HG2	1:C:241:VAL:N	2.23	0.52
1:C:247:THR:HG23	1:C:269:LEU:HB3	1.90	0.52
1:D:33:SER:O	1:D:34:ARG:HB2	2.08	0.52
1:A:185:THR:CG2	1:A:482:LEU:HD22	2.39	0.52
1:A:13:GLN:HE22	1:A:333:ASN:HD21	1.57	0.52
1:C:271:GLY:HA2	1:C:425:TYR:CG	2.44	0.52
1:F:26:ASN:ND2	1:F:215:PRO:HA	2.25	0.52
1:H:94:LEU:HB3	1:H:207:LEU:HD22	1.91	0.52
1:D:11:PRO:HB3	1:D:114:TYR:CD1	2.45	0.52
1:G:470:MET:HG2	1:H:261:ASN:O	2.10	0.52
1:C:398:GLU:HA	2:C:8720:HOH:O	2.09	0.52
1:D:327:LYS:HE2	1:D:369:CYS:CB	2.40	0.52
1:E:247:THR:HA	1:E:269:LEU:CD2	2.36	0.52
1:F:131:TYR:CE1	1:F:462:GLN:HB3	2.45	0.52
1:F:21:GLN:HB3	1:F:29:HIS:O	2.09	0.52
1:B:311:GLN:NE2	1:B:312:GLU:HG2	2.25	0.52
1:D:22:ILE:HG22	1:D:24:ILE:HG13	1.91	0.52
1:G:120:VAL:HG12	1:G:124:MET:CE	2.40	0.52
1:A:40:VAL:HG22	1:A:47:VAL:HA	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:358:ASN:O	1:C:362:GLN:HG2	2.09	0.52
1:A:235:HIS:HB3	1:A:238:VAL:CG2	2.37	0.52
1:B:244:THR:HG23	1:B:268:GLU:CB	2.40	0.52
1:B:410:PHE:CD1	1:B:416:VAL:HB	2.45	0.52
1:D:323:VAL:CG1	1:D:327:LYS:HE3	2.40	0.52
1:D:271:GLY:HA2	1:D:425:TYR:CD2	2.45	0.52
1:E:424:THR:HG23	1:E:470:MET:HE2	1.91	0.52
1:F:26:ASN:HD22	1:F:26:ASN:N	2.07	0.52
1:H:257:ALA:HA	1:H:260:SER:OG	2.09	0.52
1:H:244:THR:HG23	1:H:268:GLU:CB	2.37	0.52
1:A:89:ASN:ND2	1:A:133:ALA:HB1	2.25	0.52
1:B:116:ILE:O	1:B:120:VAL:HB	2.10	0.52
1:C:53:GLU:HG3	2:C:8714:HOH:O	2.09	0.52
1:G:453:VAL:HB	1:H:493:VAL:HG13	1.92	0.52
1:C:315:TYR:CE1	1:C:409:LYS:HE2	2.45	0.51
1:E:247:THR:OG1	1:E:269:LEU:HB3	2.10	0.51
1:F:175:GLN:NE2	1:F:204:VAL:HG21	2.25	0.51
1:G:463:SER:O	1:G:477:LEU:HB2	2.10	0.51
1:E:240:LYS:HG2	1:E:241:VAL:N	2.23	0.51
1:E:244:THR:HG23	1:E:268:GLU:CB	2.40	0.51
1:E:247:THR:CG2	1:E:269:LEU:HD13	2.34	0.51
1:F:40:VAL:HG13	1:F:46:GLU:O	2.10	0.51
1:H:458:VAL:HA	2:H:8806:HOH:O	2.10	0.51
1:A:254:GLN:HG2	1:B:258:GLY:HA3	1.91	0.51
1:E:18:PHE:HA	2:E:9287:HOH:O	2.10	0.51
1:F:258:GLY:HA2	1:F:262:LEU:HD23	1.91	0.51
1:A:461:ALA:HA	1:A:477:LEU:CD2	2.34	0.51
1:A:487:GLU:HG3	1:B:468:TYR:CE1	2.46	0.51
1:B:291:HIS:HE1	1:B:326:ALA:HA	1.75	0.51
1:F:121:ASP:O	1:F:125:VAL:HG23	2.10	0.51
1:G:254:GLN:OE1	1:H:262:LEU:HD22	2.10	0.51
1:H:431:VAL:HG21	1:H:442:LEU:HB3	1.93	0.51
1:C:498:LYS:HD3	2:C:8984:HOH:O	2.11	0.51
1:D:100:THR:HG23	1:D:114:TYR:OH	2.11	0.51
1:D:167:PRO:HD3	1:D:244:THR:HB	1.92	0.51
1:E:268:GLU:OE2	1:E:476:GLU:OE1	2.28	0.51
1:F:291:HIS:NE2	1:F:329:ARG:HD2	2.25	0.51
1:F:39:THR:HG23	1:F:48:ILE:HB	1.93	0.51
1:D:327:LYS:HE2	1:D:369:CYS:HB3	1.91	0.51
1:G:244:THR:OG1	1:G:268:GLU:OE1	2.29	0.51
1:G:63:VAL:HG11	1:G:235:HIS:CE1	2.46	0.51
1:H:266:THR:O	1:H:267:LEU:HD23	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:99:ARG:HD3	1:D:118:TYR:CZ	2.46	0.51
1:E:11:PRO:HB3	1:E:114:TYR:CE1	2.45	0.51
1:E:250:GLY:HA2	1:E:253:ILE:HG12	1.92	0.51
1:H:36:THR:OG1	1:H:50:GLN:HG3	2.10	0.51
1:B:431:VAL:CG1	1:B:442:LEU:HD12	2.41	0.51
1:A:39:THR:OG1	1:A:109:ASP:OD1	2.29	0.51
1:C:294:LEU:HD22	1:C:405:MET:HB2	1.92	0.51
1:D:235:HIS:HB3	1:D:238:VAL:CG2	2.41	0.51
1:E:312:GLU:OE1	1:E:411:LYS:HG3	2.10	0.51
1:F:315:TYR:CD1	1:F:409:LYS:HE2	2.46	0.51
1:H:409:LYS:HG2	2:H:8802:HOH:O	2.10	0.51
1:C:355:GLY:HA2	1:E:50:GLN:NE2	2.25	0.51
1:E:262:LEU:HD13	1:F:269:LEU:HD11	1.92	0.51
1:C:358:ASN:OD1	1:E:50:GLN:HG3	2.11	0.51
1:B:468:TYR:O	1:B:471:SER:HB2	2.10	0.50
1:C:15:PRO:HG2	1:C:108:LEU:HD22	1.93	0.50
1:A:496:PRO:HG2	1:C:441:TYR:HB2	1.93	0.50
1:H:178:LYS:HD3	1:H:476:GLU:OE2	2.11	0.50
1:C:313:ASP:HB3	2:C:9454:HOH:O	2.11	0.50
1:C:487:GLU:HG3	1:D:468:TYR:CZ	2.46	0.50
1:F:199:LEU:HB2	2:F:8749:HOH:O	2.10	0.50
1:G:246:SER:HG	1:G:249:ILE:H	1.59	0.50
1:A:366:LYS:HE2	1:A:368:LEU:CD2	2.40	0.50
1:E:142:LYS:HG3	1:F:480:TYR:OH	2.12	0.50
1:E:350:PHE:CE2	1:E:354:LEU:HD11	2.46	0.50
1:F:294:LEU:CD1	1:F:405:MET:HA	2.42	0.50
1:H:413:ILE:O	1:H:417:VAL:HG23	2.11	0.50
1:B:8:VAL:HG13	1:B:118:TYR:CD2	2.46	0.50
1:B:311:GLN:OE1	1:B:313:ASP:HB2	2.12	0.50
1:F:271:GLY:HA2	1:F:425:TYR:CG	2.46	0.50
1:G:298:GLN:HG3	1:G:341:GLN:HG3	1.92	0.50
1:H:247:THR:OG1	1:H:269:LEU:HB3	2.11	0.50
1:H:356:TYR:CB	1:H:400:ILE:HG12	2.42	0.50
1:A:464:PRO:HG3	1:A:480:TYR:CE1	2.46	0.50
1:D:13:GLN:HA	1:D:335:PHE:CE1	2.46	0.50
1:D:190:VAL:HG22	1:D:219:ASN:HB2	1.94	0.50
1:B:444:GLN:NE2	1:D:499:ASN:HB2	2.26	0.50
1:G:195:GLU:HG2	1:G:196:GLN:NE2	2.26	0.50
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.47	0.50
1:H:344:GLN:HG3	1:H:353:ILE:HD12	1.94	0.50
1:H:44:THR:O	1:H:377:ARG:NH1	2.44	0.50
1:A:363:GLU:HG3	2:A:9084:HOH:O	2.10	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:465:PHE:HB2	1:A:477:LEU:HD12	1.94	0.50
1:B:268:GLU:OE1	1:B:476:GLU:OE1	2.30	0.50
1:C:185:THR:HG23	1:C:482:LEU:HD22	1.94	0.50
1:F:130:ARG:HD3	1:H:86:ARG:CZ	2.42	0.50
1:C:120:VAL:HG12	1:C:124:MET:CE	2.40	0.50
1:C:476:GLU:O	1:C:477:LEU:HB2	2.12	0.50
2:A:8696:HOH:O	1:D:498:LYS:HE3	2.12	0.50
1:E:487:GLU:HG3	1:F:468:TYR:CE1	2.46	0.50
1:F:94:LEU:HD22	1:F:97:ARG:NH2	2.27	0.50
1:H:132:TYR:CE2	1:H:181:PRO:HB3	2.46	0.50
1:H:373:ILE:HG22	1:H:375:ALA:H	1.77	0.50
1:H:68:ALA:HA	1:H:71:GLN:HG2	1.93	0.50
1:A:126:LEU:O	1:A:130:ARG:HG3	2.11	0.50
1:A:294:LEU:HD12	1:A:306:SER:HA	1.93	0.50
1:A:140:HIS:ND1	1:D:142:LYS:HD3	2.27	0.50
1:E:131:TYR:CZ	1:E:462:GLN:HA	2.47	0.50
1:F:247:THR:CA	1:F:269:LEU:HB3	2.41	0.50
1:H:425:TYR:O	1:H:469:LYS:HD2	2.11	0.50
1:A:251:ARG:CG	1:B:262:LEU:HD21	2.42	0.50
1:C:347:GLU:OE1	1:E:347:GLU:OE1	2.30	0.50
1:E:257:ALA:HA	1:E:260:SER:OG	2.12	0.50
1:F:315:TYR:CD2	1:F:409:LYS:HG3	2.46	0.50
1:F:350:PHE:HZ	1:F:373:ILE:HG12	1.77	0.50
1:G:467:GLY:O	1:G:472:GLY:O	2.30	0.50
1:G:490:THR:OG1	1:H:464:PRO:HG2	2.11	0.50
1:A:25:ASN:HA	1:A:216:GLY:N	2.27	0.49
1:E:251:ARG:O	1:E:255:VAL:HG23	2.11	0.49
1:E:424:THR:HG21	1:E:470:MET:CE	2.39	0.49
1:G:79:MET:SD	1:G:83:HIS:HD2	2.35	0.49
1:E:79:MET:SD	1:E:83:HIS:HD2	2.35	0.49
1:F:175:GLN:HE22	1:F:204:VAL:HG21	1.76	0.49
1:A:11:PRO:HD3	2:A:8905:HOH:O	2.12	0.49
1:A:280:ASP:O	1:A:434:LYS:HG3	2.11	0.49
1:A:36:THR:HB	1:A:51:VAL:O	2.13	0.49
1:A:236:GLU:OE2	1:A:260:SER:HB2	2.13	0.49
1:A:374:ALA:HB2	1:A:382:GLN:CG	2.43	0.49
1:A:413:ILE:HD11	1:A:442:LEU:HG	1.94	0.49
1:D:106:GLU:OE2	1:D:171:PRO:HB2	2.12	0.49
1:D:323:VAL:HG13	1:D:327:LYS:HE3	1.95	0.49
1:E:264:ARG:HH22	1:F:474:GLY:N	2.11	0.49
1:G:275:ASN:HD22	1:G:430:ALA:HB3	1.75	0.49
1:G:487:GLU:HG3	1:H:468:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:431:VAL:HG21	1:A:442:LEU:HB3	1.94	0.49
1:B:370:GLY:HA2	1:B:382:GLN:OE1	2.13	0.49
1:D:425:TYR:O	1:D:469:LYS:HD2	2.11	0.49
1:F:361:LYS:HD2	1:F:367:LEU:HD22	1.94	0.49
1:A:300:GLN:HE22	1:A:345:VAL:H	1.61	0.49
1:F:294:LEU:HD12	1:F:306:SER:HA	1.93	0.49
1:G:344:GLN:HG3	1:G:353:ILE:HD12	1.94	0.49
1:H:124:MET:HE3	1:H:173:LEU:HD22	1.94	0.49
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.94	0.49
1:G:483:GLN:NE2	2:G:8808:HOH:O	2.45	0.49
1:H:21:GLN:HB3	1:H:29:HIS:O	2.12	0.49
1:H:27:GLU:O	1:H:29:HIS:HD2	1.96	0.49
1:A:173:LEU:HD11	1:A:177:TRP:NE1	2.27	0.49
1:B:465:PHE:O	1:B:476:GLU:N	2.44	0.49
1:C:424:THR:CG2	1:C:470:MET:HB2	2.34	0.49
1:D:249:ILE:O	1:D:252:VAL:HB	2.13	0.49
1:E:162:CYS:HG	1:E:485:TYR:HD2	1.60	0.49
1:B:41:ASN:HD22	1:B:42:PRO:HD2	1.77	0.49
1:B:413:ILE:HG12	1:B:441:TYR:CE2	2.47	0.49
1:B:462:GLN:HB2	2:D:9062:HOH:O	2.13	0.49
1:E:410:PHE:CD1	1:E:416:VAL:HB	2.48	0.49
1:E:489:LYS:HB2	1:F:468:TYR:OH	2.13	0.49
1:A:21:GLN:O	1:A:28:TRP:HZ3	1.95	0.48
1:B:235:HIS:HB3	1:B:238:VAL:HG23	1.95	0.48
1:F:350:PHE:CZ	1:F:373:ILE:HG12	2.48	0.48
1:G:300:GLN:HE22	1:G:345:VAL:H	1.61	0.48
1:A:374:ALA:HB2	1:A:382:GLN:HG2	1.94	0.48
1:A:79:MET:SD	1:A:83:HIS:HD2	2.36	0.48
1:D:99:ARG:HG2	1:D:118:TYR:CE1	2.48	0.48
1:F:276:ILE:HG12	1:F:416:VAL:CG2	2.43	0.48
1:H:168:TRP:O	1:H:171:PRO:HD3	2.13	0.48
1:A:468:TYR:O	1:A:471:SER:HB2	2.14	0.48
1:C:154:THR:HA	1:C:489:LYS:O	2.13	0.48
1:D:155:ARG:HD2	2:D:8727:HOH:O	2.13	0.48
1:D:460:GLY:O	1:D:477:LEU:HD13	2.13	0.48
1:D:240:LYS:HE3	1:D:484:ALA:O	2.11	0.48
1:E:330:VAL:HG21	2:E:9316:HOH:O	2.13	0.48
1:A:241:VAL:CG1	1:A:265:VAL:HG22	2.43	0.48
1:B:302:CYS:HB2	1:B:427:LEU:HD21	1.95	0.48
1:C:25:ASN:HA	1:C:216:GLY:N	2.29	0.48
1:C:37:PHE:HD2	1:C:53:GLU:HB2	1.78	0.48
1:D:22:ILE:HG12	1:D:222:PRO:HD2	1.94	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:302:CYS:HB2	1:E:427:LEU:CD2	2.44	0.48
1:F:107:THR:CG2	1:F:334:PRO:HB2	2.44	0.48
1:A:255:VAL:HG22	1:B:255:VAL:HG13	1.95	0.48
1:B:394:THR:HG23	1:B:398:GLU:OE1	2.14	0.48
1:C:366:LYS:HE2	1:C:368:LEU:HD21	1.95	0.48
1:D:249:ILE:H	1:D:249:ILE:HD12	1.78	0.48
1:E:241:VAL:CG1	1:E:265:VAL:HG13	2.43	0.48
1:A:322:SER:HB3	1:A:405:MET:CE	2.43	0.48
1:G:33:SER:O	1:G:34:ARG:HB2	2.12	0.48
1:G:392:GLY:O	1:G:397:LYS:HE2	2.14	0.48
1:G:269:LEU:CD1	1:H:262:LEU:HD13	2.44	0.48
1:H:276:ILE:CD1	1:H:446:LEU:HD11	2.37	0.48
1:B:11:PRO:HB3	1:B:114:TYR:CE2	2.49	0.48
1:B:413:ILE:HG12	1:B:441:TYR:HE2	1.78	0.48
1:B:449:GLY:HA2	1:B:468:TYR:CE1	2.49	0.48
1:C:344:GLN:HG3	1:C:353:ILE:HD12	1.95	0.48
1:C:356:TYR:CG	1:C:400:ILE:HG12	2.48	0.48
1:D:294:LEU:CD1	1:D:405:MET:HA	2.43	0.48
1:E:33:SER:O	1:E:34:ARG:HB2	2.13	0.48
1:G:366:LYS:HE2	1:G:368:LEU:CD2	2.39	0.48
1:A:315:TYR:CE1	1:A:319:VAL:HG21	2.49	0.48
1:B:79:MET:HG3	1:B:83:HIS:HB3	1.95	0.48
1:C:131:TYR:CZ	1:C:462:GLN:HA	2.49	0.48
1:D:240:LYS:HG2	1:D:241:VAL:N	2.28	0.48
1:E:123:ASP:O	1:E:127:LYS:HG3	2.14	0.48
1:E:145:PRO:HG3	2:H:9581:HOH:O	2.14	0.48
1:F:39:THR:HG22	1:F:49:CYS:O	2.13	0.48
1:F:464:PRO:HA	1:F:476:GLU:O	2.13	0.48
1:G:23:PHE:CE1	1:G:26:ASN:HA	2.49	0.48
1:A:353:ILE:O	1:A:357:ILE:HG13	2.13	0.48
1:B:441:TYR:CD2	1:B:442:LEU:HD23	2.48	0.48
1:D:123:ASP:OD2	1:D:127:LYS:HE3	2.14	0.48
1:D:315:TYR:CE1	1:D:409:LYS:HE2	2.49	0.48
1:G:235:HIS:HB3	1:G:238:VAL:HG23	1.95	0.48
1:H:356:TYR:CD1	1:H:400:ILE:HG12	2.49	0.48
1:A:298:GLN:HG3	1:A:341:GLN:HG3	1.96	0.48
1:C:280:ASP:HB3	2:C:9447:HOH:O	2.14	0.48
1:G:244:THR:HA	1:G:268:GLU:O	2.14	0.48
1:H:310:VAL:HG21	1:H:318:PHE:CD2	2.49	0.48
1:A:138:LYS:HD3	1:C:135:TRP:CE2	2.48	0.47
1:B:353:ILE:O	1:B:357:ILE:HG13	2.13	0.47
1:D:163:GLY:O	1:D:241:VAL:HA	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:80:ASP:OD1	1:H:498:LYS:NZ	2.47	0.47
1:A:172:LEU:CD2	1:A:200:THR:HB	2.39	0.47
1:A:281:ALA:HB2	1:A:432:PHE:O	2.14	0.47
1:D:291:HIS:CE1	1:D:326:ALA:HA	2.48	0.47
1:E:263:LYS:O	1:E:265:VAL:HG23	2.14	0.47
1:F:44:THR:HA	1:F:377:ARG:CD	2.42	0.47
1:G:345:VAL:HG12	1:G:349:GLN:HG3	1.97	0.47
1:A:405:MET:HE3	1:A:407:ILE:HD11	1.95	0.47
1:B:257:ALA:HB1	1:B:263:LYS:CG	2.43	0.47
1:C:100:THR:HG22	2:C:8954:HOH:O	2.14	0.47
1:C:347:GLU:OE1	1:E:379:TYR:OH	2.30	0.47
1:C:32:VAL:HA	1:C:34:ARG:NH1	2.28	0.47
1:D:11:PRO:HB3	1:D:114:TYR:CZ	2.50	0.47
1:F:107:THR:HG23	1:F:334:PRO:HB2	1.95	0.47
1:F:395:ILE:HD12	1:F:406:GLN:HG3	1.96	0.47
1:G:44:THR:HA	1:G:377:ARG:HD3	1.95	0.47
1:H:71:GLN:NE2	1:H:71:GLN:HA	2.30	0.47
1:A:17:VAL:HG13	2:A:9055:HOH:O	2.15	0.47
1:B:94:LEU:HB3	1:B:207:LEU:HD22	1.96	0.47
1:E:15:PRO:HD2	1:E:108:LEU:HD13	1.96	0.47
1:A:241:VAL:HG13	1:A:241:VAL:O	2.15	0.47
1:A:367:LEU:HD11	1:A:369:CYS:O	2.13	0.47
1:B:452:TRP:HB3	1:B:455:CYS:O	2.14	0.47
1:C:100:THR:HG23	1:C:114:TYR:OH	2.15	0.47
1:C:11:PRO:HB3	1:C:114:TYR:CE2	2.49	0.47
1:F:435:ASP:HB3	1:F:438:LYS:HB2	1.94	0.47
1:G:195:GLU:OE1	1:G:224:PHE:HD2	1.97	0.47
1:G:249:ILE:HA	1:G:252:VAL:CG2	2.44	0.47
1:E:257:ALA:HB1	1:E:263:LYS:HG3	1.97	0.47
1:F:28:TRP:CZ3	1:F:202:LEU:HD22	2.50	0.47
1:F:327:LYS:HE3	1:F:369:CYS:HB3	1.96	0.47
1:G:255:VAL:HG13	1:H:255:VAL:CG2	2.44	0.47
1:A:215:PRO:HG3	2:A:8907:HOH:O	2.15	0.47
1:D:498:LYS:HE2	1:D:498:LYS:HB3	1.70	0.47
1:E:436:LEU:N	2:E:8837:HOH:O	2.48	0.47
1:F:247:THR:HG23	1:F:269:LEU:CB	2.45	0.47
1:F:60:ASP:O	1:F:64:LYS:HG3	2.14	0.47
1:C:414:GLU:HG3	1:C:441:TYR:OH	2.14	0.47
1:A:116:ILE:O	1:A:120:VAL:HB	2.15	0.47
1:A:196:GLN:NE2	1:A:196:GLN:H	1.93	0.47
1:A:272:LYS:HE3	1:A:306:SER:CB	2.32	0.47
1:B:132:TYR:OH	1:B:477:LEU:HA	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:73:GLY:HA2	1:D:78:ARG:HD2	1.97	0.47
1:E:271:GLY:HA2	1:E:425:TYR:HB3	1.97	0.47
1:G:347:GLU:O	1:G:351:LYS:HE2	2.15	0.47
1:D:161:VAL:N	1:D:239:ASP:OD2	2.44	0.47
1:D:246:SER:OG	1:D:249:ILE:CD1	2.59	0.47
1:D:449:GLY:HA2	1:D:468:TYR:CE1	2.50	0.47
1:E:70:PHE:CZ	1:E:160:GLY:HA2	2.50	0.47
1:G:40:VAL:HG13	1:G:46:GLU:O	2.14	0.47
1:E:440:ASN:HD22	1:G:495:VAL:HG12	1.79	0.47
1:H:75:PRO:HG2	2:H:9364:HOH:O	2.15	0.47
1:A:48:ILE:HG21	1:A:199:LEU:HD11	1.96	0.47
1:A:240:LYS:HG3	1:A:241:VAL:N	2.28	0.47
1:B:106:GLU:O	1:B:110:ASN:HB3	2.15	0.47
1:E:283:MET:N	2:E:8830:HOH:O	2.48	0.47
1:G:240:LYS:HG3	1:G:241:VAL:N	2.30	0.47
1:G:96:GLU:O	1:G:99:ARG:HB2	2.14	0.47
2:E:8837:HOH:O	1:H:436:LEU:N	2.47	0.47
1:B:241:VAL:HG13	1:B:265:VAL:HG13	1.96	0.46
1:C:487:GLU:HG3	1:D:468:TYR:CE1	2.51	0.46
1:D:126:LEU:HD12	2:D:9168:HOH:O	2.14	0.46
1:D:302:CYS:HB2	1:D:427:LEU:CD2	2.45	0.46
1:G:315:TYR:CD2	1:G:409:LYS:HG3	2.49	0.46
1:H:40:VAL:HG13	1:H:46:GLU:O	2.15	0.46
1:A:187:ASN:ND2	1:A:485:TYR:HB3	2.29	0.46
1:A:312:GLU:HB3	2:A:9097:HOH:O	2.15	0.46
1:B:359:THR:O	1:B:363:GLU:HG3	2.15	0.46
1:B:431:VAL:HG21	1:B:442:LEU:HB3	1.97	0.46
1:D:356:TYR:CG	1:D:400:ILE:HG12	2.51	0.46
1:E:264:ARG:HH22	1:F:474:GLY:H	1.63	0.46
1:E:271:GLY:HA2	1:E:425:TYR:CG	2.51	0.46
1:G:370:GLY:HA2	2:G:8782:HOH:O	2.15	0.46
1:A:260:SER:O	1:B:251:ARG:NH2	2.49	0.46
1:C:198:PRO:O	1:C:202:LEU:HG	2.16	0.46
1:C:41:ASN:HD22	1:C:43:SER:H	1.62	0.46
1:D:251:ARG:O	1:D:255:VAL:HG23	2.15	0.46
1:A:106:GLU:O	1:A:110:ASN:HB3	2.16	0.46
1:D:76:TRP:HA	1:D:79:MET:HE3	1.97	0.46
1:F:208:ILE:CD1	1:F:218:VAL:HG11	2.46	0.46
1:F:87:LEU:HB3	1:F:213:PHE:CZ	2.50	0.46
1:H:344:GLN:HG3	1:H:353:ILE:CD1	2.46	0.46
1:B:107:THR:CG2	1:B:334:PRO:HB2	2.46	0.46
1:E:307:ARG:NH1	2:E:9314:HOH:O	2.48	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:24:ILE:O	1:F:27:GLU:HB2	2.16	0.46
1:G:74:SER:OG	1:G:77:ARG:HG2	2.15	0.46
1:H:435:ASP:HB3	1:H:438:LYS:HB2	1.98	0.46
1:A:476:GLU:O	1:A:477:LEU:HB2	2.16	0.46
1:A:56:LYS:HE2	1:A:60:ASP:OD2	2.15	0.46
1:B:167:PRO:HD3	1:B:244:THR:HB	1.97	0.46
1:B:255:VAL:O	1:B:259:SER:OG	2.23	0.46
1:E:356:TYR:CG	1:E:400:ILE:HG12	2.50	0.46
1:G:424:THR:HG22	1:G:424:THR:O	2.15	0.46
1:A:18:PHE:HD1	1:A:101:TYR:HH	1.63	0.46
1:A:350:PHE:HE1	1:A:380:PHE:O	1.98	0.46
1:B:312:GLU:HG3	1:B:313:ASP:N	2.31	0.46
1:B:369:CYS:SG	1:B:385:VAL:HG23	2.56	0.46
1:C:241:VAL:HG13	1:C:265:VAL:HG13	1.98	0.46
1:C:424:THR:O	1:C:424:THR:HG22	2.15	0.46
1:E:120:VAL:HG12	1:E:124:MET:CE	2.43	0.46
1:F:120:VAL:HG12	1:F:124:MET:CE	2.46	0.46
1:H:33:SER:HB2	1:H:35:LYS:HD3	1.97	0.46
1:D:347:GLU:O	1:D:350:PHE:HB3	2.15	0.46
1:D:132:TYR:OH	1:D:477:LEU:HA	2.16	0.46
1:E:306:SER:O	1:E:406:GLN:HB2	2.15	0.46
1:E:428:ALA:HB1	1:E:452:TRP:CZ3	2.51	0.46
1:E:76:TRP:CH2	1:E:84:ARG:HD2	2.51	0.46
1:F:348:THR:HA	1:F:351:LYS:HE3	1.97	0.46
1:G:294:LEU:HD11	1:G:405:MET:HA	1.98	0.46
1:B:413:ILE:CG1	1:B:442:LEU:HD21	2.46	0.46
1:D:374:ALA:HB3	1:D:380:PHE:HB3	1.97	0.46
1:C:144:ILE:CG2	1:D:462:GLN:HB2	2.45	0.46
1:F:323:VAL:HG21	1:F:368:LEU:HB3	1.98	0.46
1:H:132:TYR:OH	1:H:477:LEU:HA	2.16	0.46
1:A:170:PHE:HB3	1:A:173:LEU:HB3	1.98	0.46
1:A:376:ASP:N	1:A:376:ASP:OD1	2.49	0.46
1:B:109:ASP:OD2	1:B:199:LEU:HB2	2.16	0.46
1:D:123:ASP:CG	1:D:127:LYS:HE3	2.37	0.46
1:F:246:SER:HB3	2:F:8646:HOH:O	2.15	0.46
1:H:131:TYR:CZ	1:H:462:GLN:HA	2.51	0.46
1:A:363:GLU:CB	2:A:9084:HOH:O	2.60	0.45
1:C:32:VAL:HA	1:C:34:ARG:HH11	1.80	0.45
1:F:23:PHE:CG	1:F:205:ALA:HB1	2.51	0.45
1:F:464:PRO:HG3	1:F:480:TYR:CE1	2.51	0.45
1:G:466:GLY:HA3	2:G:8784:HOH:O	2.16	0.45
1:A:405:MET:HE2	1:A:407:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:350:PHE:CD1	1:C:379:TYR:HB3	2.52	0.45
1:D:167:PRO:HB2	2:D:9259:HOH:O	2.17	0.45
1:D:302:CYS:HB2	1:D:427:LEU:HD21	1.98	0.45
2:C:9206:HOH:O	1:E:352:LYS:HE2	2.16	0.45
1:A:388:ASP:O	1:A:390:GLN:NE2	2.50	0.45
1:A:413:ILE:O	1:A:416:VAL:HG12	2.16	0.45
1:B:413:ILE:HG12	1:B:442:LEU:HD21	1.97	0.45
1:B:463:SER:O	1:B:477:LEU:HB2	2.17	0.45
1:D:308:THR:HB	1:D:407:ILE:HA	1.98	0.45
1:E:43:SER:HA	1:E:343:PRO:HG3	1.99	0.45
1:E:131:TYR:CE1	1:E:462:GLN:HB3	2.51	0.45
1:H:317:GLU:HG2	1:H:321:ARG:HE	1.80	0.45
1:H:43:SER:OG	1:H:334:PRO:HG3	2.16	0.45
1:A:173:LEU:HD11	1:A:177:TRP:HE1	1.82	0.45
1:D:185:THR:OG1	1:D:187:ASN:ND2	2.50	0.45
1:E:155:ARG:NE	1:E:157:GLU:OE2	2.44	0.45
1:E:344:GLN:HG3	1:E:353:ILE:CD1	2.46	0.45
1:E:381:ILE:HG22	1:E:403:PRO:HG2	1.97	0.45
1:G:275:ASN:ND2	1:G:430:ALA:HB3	2.32	0.45
1:H:159:VAL:N	1:H:187:ASN:OD1	2.49	0.45
1:H:460:GLY:HA3	1:H:462:GLN:HE21	1.81	0.45
1:A:317:GLU:OE1	1:A:321:ARG:NH2	2.47	0.45
1:A:323:VAL:HG12	1:A:327:LYS:HD2	1.98	0.45
1:A:356:TYR:HE2	1:A:398:GLU:OE2	2.00	0.45
1:A:424:THR:HG22	1:A:424:THR:O	2.16	0.45
1:B:315:TYR:CD1	1:B:409:LYS:HE2	2.51	0.45
1:B:465:PHE:N	1:B:476:GLU:O	2.50	0.45
1:A:483:GLN:NE2	1:B:483:GLN:OE1	2.50	0.45
1:D:192:LYS:NZ	2:D:9260:HOH:O	2.50	0.45
1:D:476:GLU:O	1:D:477:LEU:HB2	2.17	0.45
1:D:8:VAL:HG13	1:D:118:TYR:CD2	2.52	0.45
1:E:100:THR:HG22	2:E:9298:HOH:O	2.15	0.45
1:E:281:ALA:HB2	1:E:432:PHE:O	2.16	0.45
1:F:170:PHE:HZ	1:F:301:CYS:HG	1.65	0.45
1:A:424:THR:CG2	1:A:470:MET:HE2	2.44	0.45
1:C:465:PHE:N	1:C:476:GLU:O	2.50	0.45
1:D:421:ASN:ND2	1:D:445:ALA:O	2.50	0.45
1:E:217:VAL:HG12	1:E:218:VAL:HG23	1.99	0.45
1:E:440:ASN:ND2	2:E:9358:HOH:O	2.50	0.45
1:F:23:PHE:HA	1:F:27:GLU:O	2.16	0.45
1:G:103:ALA:HB2	1:G:122:LEU:HD13	1.98	0.45
1:G:408:LEU:HD23	1:G:419:ARG:HH11	1.80	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:303:CYS:SG	1:H:459:PHE:HZ	2.40	0.45
1:A:59:VAL:HG21	1:A:231:ALA:HB3	1.98	0.45
1:A:32:VAL:HG23	1:A:61:LYS:HZ3	1.82	0.45
1:B:107:THR:HG23	1:B:112:LYS:O	2.16	0.45
1:B:185:THR:OG1	1:B:187:ASN:ND2	2.50	0.45
1:B:32:VAL:HG11	1:B:57:GLU:OE1	2.17	0.45
1:D:300:GLN:HB3	1:D:401:PHE:CE2	2.52	0.45
1:D:351:LYS:HD3	1:F:347:GLU:CD	2.37	0.45
1:F:476:GLU:O	1:F:477:LEU:HB2	2.16	0.45
1:F:498:LYS:HG2	1:F:499:ASN:N	2.32	0.45
1:G:240:LYS:HG2	2:G:9550:HOH:O	2.16	0.45
1:H:241:VAL:HG13	1:H:241:VAL:O	2.17	0.45
1:H:244:THR:HG23	1:H:268:GLU:HG3	1.99	0.45
1:A:290:ALA:N	2:A:9077:HOH:O	2.50	0.45
1:A:90:ARG:HH21	1:A:94:LEU:CD2	2.25	0.45
1:B:431:VAL:HG11	1:B:442:LEU:HD12	1.99	0.45
1:D:170:PHE:HZ	1:D:301:CYS:HG	1.63	0.45
1:E:358:ASN:HD22	1:E:361:LYS:NZ	2.15	0.45
1:G:260:SER:O	1:H:251:ARG:NH2	2.50	0.45
1:G:294:LEU:O	1:G:299:GLY:HA2	2.17	0.45
1:H:257:ALA:HB1	1:H:263:LYS:CG	2.46	0.45
1:A:159:VAL:HG12	1:A:187:ASN:OD1	2.16	0.45
1:A:22:ILE:HD11	1:A:54:GLY:CA	2.47	0.45
1:A:260:SER:OG	1:A:263:LYS:NZ	2.50	0.45
1:B:117:SER:HA	1:B:121:ASP:HB2	1.98	0.45
1:C:294:LEU:HD11	1:C:404:VAL:O	2.16	0.45
1:D:144:ILE:HD11	1:D:154:THR:HG23	1.99	0.45
1:D:159:VAL:N	1:D:187:ASN:OD1	2.50	0.45
1:F:315:TYR:CG	1:F:409:LYS:HE2	2.51	0.45
1:G:254:GLN:OE1	1:H:262:LEU:CD2	2.64	0.45
1:G:315:TYR:CE1	1:G:319:VAL:HG21	2.52	0.45
1:G:76:TRP:CH2	1:G:84:ARG:HD2	2.52	0.45
1:H:41:ASN:ND2	2:H:8792:HOH:O	2.49	0.45
1:C:449:GLY:HA2	1:C:468:TYR:CE1	2.51	0.45
1:E:363:GLU:CD	1:E:394:THR:H	2.20	0.45
1:E:70:PHE:CZ	1:E:158:PRO:HB2	2.52	0.45
1:G:11:PRO:HB3	1:G:114:TYR:CZ	2.52	0.45
1:H:444:GLN:NE2	2:H:8804:HOH:O	2.50	0.45
1:D:71:GLN:O	1:D:74:SER:HB3	2.17	0.44
1:F:124:MET:HE3	1:F:173:LEU:CD2	2.38	0.44
1:F:247:THR:HG23	1:F:269:LEU:CD1	2.43	0.44
1:A:267:LEU:O	1:A:473:SER:N	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:99:ARG:HD3	1:B:118:TYR:CZ	2.52	0.44
1:C:260:SER:OG	1:C:263:LYS:NZ	2.49	0.44
1:D:260:SER:OG	1:D:263:LYS:NZ	2.50	0.44
1:D:417:VAL:HG11	1:D:445:ALA:HB1	1.99	0.44
1:E:273:SER:HB2	1:E:304:ALA:O	2.17	0.44
1:E:79:MET:HB3	2:E:8814:HOH:O	2.17	0.44
1:F:465:PHE:N	1:F:476:GLU:O	2.50	0.44
1:A:48:ILE:HD11	1:A:109:ASP:HA	1.98	0.44
1:A:344:GLN:HG3	1:A:353:ILE:HD12	2.00	0.44
1:E:159:VAL:N	1:E:187:ASN:OD1	2.50	0.44
1:E:208:ILE:HG23	1:E:213:PHE:CD1	2.52	0.44
1:E:294:LEU:HD13	1:E:405:MET:HA	2.00	0.44
1:F:208:ILE:HD13	1:F:218:VAL:HG11	2.00	0.44
1:H:465:PHE:N	1:H:476:GLU:O	2.49	0.44
1:A:272:LYS:HA	1:A:306:SER:OG	2.17	0.44
1:A:332:GLY:HA3	2:A:9079:HOH:O	2.17	0.44
1:A:373:ILE:HG22	1:A:375:ALA:H	1.82	0.44
1:B:253:ILE:HD13	1:B:253:ILE:N	2.32	0.44
1:D:39:THR:OG1	1:D:109:ASP:OD1	2.35	0.44
1:D:363:GLU:CD	1:D:394:THR:H	2.20	0.44
1:E:498:LYS:HB3	1:E:498:LYS:HE2	1.81	0.44
1:F:8:VAL:HG13	1:F:118:TYR:CG	2.51	0.44
1:E:251:ARG:CA	1:F:262:LEU:HD21	2.46	0.44
1:F:26:ASN:N	2:F:8842:HOH:O	2.50	0.44
1:G:272:LYS:HE2	1:G:396:ALA:C	2.38	0.44
1:F:498:LYS:NZ	1:G:80:ASP:OD1	2.46	0.44
1:F:135:TRP:CE2	1:H:138:LYS:HD3	2.52	0.44
1:A:291:HIS:O	1:A:295:PHE:HB2	2.17	0.44
1:B:257:ALA:HA	1:B:260:SER:OG	2.17	0.44
1:C:118:TYR:HD2	1:C:119:LEU:HD23	1.83	0.44
1:C:99:ARG:HA	1:C:122:LEU:HD22	2.00	0.44
1:C:262:LEU:HD21	1:D:251:ARG:HG2	1.99	0.44
1:G:172:LEU:CG	1:G:200:THR:HB	2.48	0.44
1:A:112:LYS:HE2	1:A:112:LYS:HB3	1.69	0.44
1:B:11:PRO:HB3	1:B:114:TYR:CZ	2.52	0.44
1:C:142:LYS:NZ	2:C:8658:HOH:O	2.50	0.44
1:C:21:GLN:HB3	1:C:29:HIS:O	2.17	0.44
1:E:138:LYS:HD3	1:G:135:TRP:CE2	2.53	0.44
1:E:363:GLU:OE2	1:E:394:THR:N	2.50	0.44
1:F:159:VAL:N	1:F:187:ASN:OD1	2.50	0.44
1:F:60:ASP:OD1	1:F:235:HIS:NE2	2.50	0.44
1:G:476:GLU:O	1:G:477:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:13:GLN:HB3	2:A:8906:HOH:O	2.17	0.44
1:A:273:SER:N	2:A:9073:HOH:O	2.50	0.44
1:B:308:THR:HB	1:B:407:ILE:HA	1.99	0.44
1:A:468:TYR:CE1	1:B:487:GLU:HG3	2.52	0.44
1:C:297:ASN:ND2	1:C:300:GLN:O	2.50	0.44
1:F:102:LEU:HD21	1:F:203:TYR:HD2	1.81	0.44
1:G:357:ILE:HG22	1:G:361:LYS:HE2	1.99	0.44
1:A:460:GLY:HA3	1:A:463:SER:HB2	1.98	0.44
1:D:198:PRO:O	1:D:202:LEU:HG	2.18	0.44
1:D:160:GLY:HA3	1:D:239:ASP:OD2	2.17	0.44
1:D:246:SER:HG	1:D:249:ILE:HD12	1.82	0.44
1:D:417:VAL:HG22	1:D:442:LEU:HD23	1.99	0.44
1:E:170:PHE:O	1:E:174:MET:HG2	2.18	0.44
1:E:260:SER:OG	1:E:263:LYS:NZ	2.50	0.44
1:E:291:HIS:ND1	1:E:325:ARG:HG3	2.32	0.44
1:E:247:THR:HG21	1:E:425:TYR:HE2	1.82	0.44
1:A:142:LYS:O	1:A:153:TYR:HA	2.18	0.44
1:C:106:GLU:OE2	1:C:171:PRO:HB2	2.17	0.44
1:E:233:ALA:O	1:E:263:LYS:NZ	2.50	0.44
1:H:77:ARG:HG3	1:H:77:ARG:HH11	1.83	0.44
1:A:453:VAL:HB	1:B:493:VAL:HG13	2.00	0.43
1:D:22:ILE:HD13	1:D:58:ASP:HB3	2.00	0.43
1:E:348:THR:O	1:E:352:LYS:HB2	2.18	0.43
1:E:452:TRP:HB3	1:E:455:CYS:O	2.18	0.43
1:F:33:SER:O	1:F:34:ARG:HB2	2.17	0.43
1:G:159:VAL:HG12	1:G:187:ASN:OD1	2.17	0.43
1:G:294:LEU:HD21	1:G:404:VAL:C	2.38	0.43
1:B:122:LEU:O	1:B:126:LEU:HG	2.18	0.43
1:C:196:GLN:H	1:C:196:GLN:NE2	2.14	0.43
1:E:253:ILE:N	1:E:253:ILE:HD13	2.33	0.43
1:A:55:ASP:N	1:A:58:ASP:OD2	2.49	0.43
1:B:193:VAL:HG22	1:B:222:PRO:HA	1.99	0.43
1:D:103:ALA:HB2	1:D:122:LEU:HD13	1.99	0.43
1:D:404:VAL:HG12	1:D:406:GLN:OE1	2.17	0.43
1:D:94:LEU:O	1:D:97:ARG:HB3	2.18	0.43
1:E:275:ASN:HD22	1:E:430:ALA:HB3	1.82	0.43
1:F:95:ILE:HG23	1:F:102:LEU:HD13	2.00	0.43
1:E:444:GLN:HG3	1:F:155:ARG:CZ	2.48	0.43
1:H:135:TRP:CG	1:H:482:LEU:HD11	2.53	0.43
1:B:346:ASP:OD1	1:B:349:GLN:HB2	2.18	0.43
1:E:432:PHE:HA	1:E:454:ASN:OD1	2.18	0.43
1:E:490:THR:HG1	1:F:464:PRO:HG2	1.83	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:67:ARG:O	1:E:71:GLN:NE2	2.50	0.43
1:F:302:CYS:O	1:F:427:LEU:HD23	2.18	0.43
1:G:249:ILE:O	1:G:252:VAL:HB	2.18	0.43
1:G:294:LEU:CD1	1:G:306:SER:HA	2.43	0.43
1:H:28:TRP:HH2	1:H:202:LEU:O	2.01	0.43
1:B:330:VAL:HG12	1:B:339:THR:HA	2.00	0.43
1:E:264:ARG:NH2	1:F:474:GLY:H	2.16	0.43
1:H:461:ALA:CA	1:H:477:LEU:HD22	2.47	0.43
1:A:245:GLY:HA3	2:A:9070:HOH:O	2.18	0.43
1:A:399:GLU:HG3	2:A:9095:HOH:O	2.17	0.43
1:C:465:PHE:C	1:C:475:GLN:HB3	2.39	0.43
1:D:112:LYS:HE2	1:D:112:LYS:HB3	1.77	0.43
1:D:168:TRP:CZ2	1:D:345:VAL:HG11	2.54	0.43
1:E:241:VAL:HG12	1:E:265:VAL:HG22	1.99	0.43
1:A:27:GLU:O	1:A:29:HIS:HD2	2.01	0.43
1:E:418:GLY:O	1:E:422:ASN:HB2	2.18	0.43
1:E:424:THR:O	1:E:470:MET:HB2	2.18	0.43
1:F:315:TYR:CE1	1:F:319:VAL:HG21	2.53	0.43
1:G:460:GLY:HA3	1:H:146:ILE:HG13	2.00	0.43
1:H:102:LEU:HD21	1:H:203:TYR:CD2	2.53	0.43
1:H:42:PRO:HD2	2:H:8792:HOH:O	2.18	0.43
1:B:294:LEU:O	1:B:299:GLY:HA2	2.19	0.43
1:D:208:ILE:HD13	1:D:218:VAL:HG11	2.00	0.43
1:C:490:THR:OG1	1:D:464:PRO:HG2	2.19	0.43
1:G:161:VAL:HA	1:G:188:VAL:CG2	2.49	0.43
1:G:31:ALA:O	1:G:34:ARG:NH1	2.52	0.43
1:H:71:GLN:O	1:H:74:SER:HB3	2.19	0.43
1:B:71:GLN:O	1:B:74:SER:HB3	2.18	0.43
1:D:361:LYS:HD2	1:D:367:LEU:HD22	2.01	0.43
1:G:269:LEU:HD13	1:H:262:LEU:HD13	2.01	0.43
1:H:235:HIS:HB3	1:H:238:VAL:HG23	2.00	0.43
1:A:175:GLN:HE22	1:A:201:ALA:HA	1.84	0.43
1:A:198:PRO:O	1:A:202:LEU:HG	2.19	0.43
1:A:258:GLY:HA3	1:B:254:GLN:HG2	2.00	0.43
1:B:459:PHE:HE2	1:B:465:PHE:CD1	2.37	0.43
1:D:123:ASP:OD1	1:D:127:LYS:HE3	2.19	0.43
1:D:81:ALA:O	1:D:136:ALA:HB1	2.19	0.43
1:E:23:PHE:CG	1:E:205:ALA:HB1	2.54	0.43
1:H:334:PRO:HG2	2:H:8787:HOH:O	2.19	0.43
1:A:350:PHE:CE1	1:A:381:ILE:HG13	2.54	0.42
1:B:82:SER:N	2:B:9159:HOH:O	2.50	0.42
1:E:102:LEU:HD21	1:E:203:TYR:CD2	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:389:VAL:HG11	1:G:396:ALA:HB2	2.00	0.42
1:E:437:ASP:HB3	1:G:496:PRO:HG3	2.01	0.42
1:H:247:THR:HA	1:H:269:LEU:CD2	2.32	0.42
1:H:317:GLU:OE1	1:H:321:ARG:NH2	2.50	0.42
1:A:13:GLN:HE21	1:A:335:PHE:HD1	1.60	0.42
1:B:171:PRO:HG3	1:B:197:THR:HG21	2.01	0.42
1:B:443:SER:HA	1:B:451:VAL:HG11	2.01	0.42
1:B:8:VAL:HA	1:B:9:PRO:HD3	1.92	0.42
1:C:346:ASP:O	1:C:350:PHE:HB2	2.19	0.42
1:C:366:LYS:HE2	1:C:368:LEU:CD2	2.49	0.42
1:E:106:GLU:O	1:E:110:ASN:HB3	2.19	0.42
1:E:28:TRP:CH2	1:E:202:LEU:HB3	2.54	0.42
1:F:298:GLN:NE2	2:F:8848:HOH:O	2.52	0.42
1:H:315:TYR:O	1:H:319:VAL:HG23	2.19	0.42
1:B:131:TYR:O	1:D:138:LYS:NZ	2.52	0.42
1:B:331:VAL:HA	1:B:341:GLN:O	2.19	0.42
1:C:164:GLN:CD	1:C:178:LYS:HB3	2.39	0.42
1:C:287:VAL:HG22	1:C:318:PHE:CD1	2.54	0.42
1:D:431:VAL:HG21	1:D:442:LEU:HB3	2.01	0.42
1:D:421:ASN:O	1:D:469:LYS:NZ	2.52	0.42
1:G:70:PHE:CE2	1:G:160:GLY:HA2	2.54	0.42
1:H:95:ILE:HG22	1:H:126:LEU:HD21	2.01	0.42
1:H:408:LEU:N	1:H:408:LEU:HD12	2.34	0.42
1:A:42:PRO:HG3	1:A:110:ASN:O	2.19	0.42
1:B:330:VAL:O	1:B:340:GLU:N	2.46	0.42
1:B:389:VAL:HB	1:B:408:LEU:HG	2.01	0.42
1:D:353:ILE:O	1:D:357:ILE:HG13	2.20	0.42
1:F:41:ASN:ND2	1:F:43:SER:H	2.16	0.42
1:G:23:PHE:HB2	1:G:28:TRP:CZ3	2.54	0.42
1:A:275:ASN:ND2	2:A:9074:HOH:O	2.51	0.42
1:B:246:SER:OG	1:B:249:ILE:HG12	2.19	0.42
1:C:107:THR:CG2	1:C:334:PRO:HB2	2.49	0.42
1:C:241:VAL:O	1:C:241:VAL:HG13	2.19	0.42
1:C:435:ASP:HB3	1:C:438:LYS:HD2	2.01	0.42
1:D:71:GLN:HA	1:D:71:GLN:NE2	2.35	0.42
1:E:240:LYS:HZ3	1:E:242:ALA:HB2	1.83	0.42
1:F:498:LYS:HE2	1:F:498:LYS:HB3	1.67	0.42
1:G:371:GLY:N	1:G:384:THR:OG1	2.53	0.42
1:H:250:GLY:O	1:H:253:ILE:HB	2.20	0.42
1:H:256:ALA:O	1:H:260:SER:HB3	2.19	0.42
1:B:167:PRO:HG2	1:B:174:MET:HG3	2.01	0.42
1:E:494:LYS:NZ	2:E:8642:HOH:O	2.48	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:475:GLN:OE1	1:F:480:TYR:HB3	2.20	0.42
1:G:248:GLU:CG	1:G:249:ILE:HD13	2.40	0.42
1:G:49:CYS:N	2:G:8768:HOH:O	2.49	0.42
1:H:216:GLY:HA2	1:H:219:ASN:OD1	2.19	0.42
1:A:465:PHE:N	1:A:476:GLU:O	2.49	0.42
1:B:26:ASN:N	2:B:8933:HOH:O	2.50	0.42
1:C:240:LYS:HG3	1:C:264:ARG:HB3	2.02	0.42
1:E:350:PHE:HZ	1:E:373:ILE:HG23	1.84	0.42
1:F:332:GLY:O	1:F:380:PHE:HE2	2.03	0.42
1:H:347:GLU:O	1:H:350:PHE:HB3	2.19	0.42
1:H:347:GLU:O	1:H:351:LYS:HG3	2.20	0.42
1:A:496:PRO:HD2	2:A:9139:HOH:O	2.19	0.42
1:B:185:THR:HG23	1:B:482:LEU:HD22	2.01	0.42
1:D:246:SER:OG	1:D:248:GLU:HB3	2.19	0.42
1:D:415:GLU:OE2	1:D:419:ARG:NH2	2.50	0.42
1:F:132:TYR:OH	1:F:477:LEU:HA	2.20	0.42
1:A:22:ILE:HD11	1:A:54:GLY:HA3	2.02	0.42
1:A:464:PRO:HB3	1:A:480:TYR:HD1	1.85	0.42
1:D:362:GLN:NE2	2:D:8631:HOH:O	2.53	0.42
1:H:243:PHE:CB	1:H:253:ILE:HG13	2.50	0.42
1:A:446:LEU:O	1:B:489:LYS:NZ	2.48	0.42
1:B:170:PHE:HB3	1:B:173:LEU:HB3	2.01	0.42
1:B:346:ASP:O	1:B:350:PHE:HB2	2.20	0.42
1:C:273:SER:HA	1:C:274:PRO:HD3	1.95	0.42
1:D:124:MET:HE3	1:D:173:LEU:CD2	2.41	0.42
1:E:468:TYR:O	1:E:471:SER:HB2	2.19	0.42
1:E:465:PHE:N	1:E:476:GLU:O	2.50	0.42
1:G:112:LYS:HB3	1:G:112:LYS:HE2	1.70	0.42
1:G:238:VAL:HB	1:G:263:LYS:HE2	2.02	0.42
1:A:142:LYS:HD2	1:B:480:TYR:CZ	2.54	0.41
1:A:473:SER:HA	2:A:8661:HOH:O	2.19	0.41
1:B:363:GLU:CD	1:B:394:THR:H	2.22	0.41
1:C:272:LYS:NZ	1:C:395:ILE:O	2.50	0.41
1:C:50:GLN:NE2	1:E:355:GLY:HA2	2.34	0.41
1:A:347:GLU:O	1:A:351:LYS:HG3	2.20	0.41
1:B:112:LYS:HE2	1:B:112:LYS:HB3	1.79	0.41
1:B:465:PHE:O	1:B:475:GLN:HA	2.20	0.41
1:C:125:VAL:HG22	1:C:173:LEU:HA	2.01	0.41
1:E:244:THR:HA	1:E:268:GLU:HB2	2.02	0.41
1:G:185:THR:OG1	1:G:187:ASN:ND2	2.53	0.41
1:G:294:LEU:HD13	2:G:8881:HOH:O	2.19	0.41
1:H:113:PRO:O	1:H:116:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:199:LEU:HB2	2:A:8636:HOH:O	2.19	0.41
1:B:96:GLU:OE2	1:B:130:ARG:NH1	2.50	0.41
1:H:175:GLN:O	1:H:179:LEU:HG	2.20	0.41
1:A:274:PRO:HA	1:A:307:ARG:O	2.21	0.41
1:A:307:ARG:HD3	1:A:396:ALA:O	2.20	0.41
1:A:35:LYS:HE2	2:A:8909:HOH:O	2.20	0.41
1:A:131:TYR:CE1	1:A:462:GLN:HB3	2.55	0.41
1:B:134:GLY:HA3	2:D:9467:HOH:O	2.21	0.41
1:C:21:GLN:O	1:C:28:TRP:HZ3	2.03	0.41
1:D:226:PRO:O	1:D:230:ALA:HB3	2.20	0.41
1:D:44:THR:CB	1:D:46:GLU:HG2	2.50	0.41
1:D:20:ASN:O	1:D:51:VAL:HA	2.21	0.41
1:E:350:PHE:CE1	1:E:381:ILE:HG13	2.55	0.41
1:E:393:MET:O	1:E:397:LYS:HG3	2.20	0.41
1:F:28:TRP:HZ3	1:F:202:LEU:HD22	1.85	0.41
1:F:44:THR:HA	1:F:377:ARG:NE	2.36	0.41
1:F:473:SER:HA	2:F:8764:HOH:O	2.20	0.41
1:G:82:SER:O	1:G:86:ARG:HG2	2.20	0.41
1:H:346:ASP:HA	1:H:379:TYR:CE1	2.55	0.41
1:H:435:ASP:OD1	1:H:438:LYS:HG3	2.20	0.41
1:A:464:PRO:HB3	1:A:480:TYR:CD1	2.56	0.41
1:B:435:ASP:HB3	1:B:438:LYS:HD2	2.02	0.41
1:B:460:GLY:CA	1:B:462:GLN:HE21	2.34	0.41
1:D:25:ASN:C	1:D:215:PRO:HB3	2.41	0.41
1:D:131:TYR:CZ	1:D:462:GLN:HA	2.56	0.41
1:F:146:ILE:HG21	1:F:150:PHE:HB2	2.01	0.41
1:F:166:ILE:HG22	1:F:178:LYS:HE2	2.01	0.41
1:F:48:ILE:HD13	1:F:108:LEU:HD23	2.02	0.41
1:H:375:ALA:HB3	1:H:380:PHE:HB2	2.01	0.41
1:H:24:ILE:HD13	1:H:61:LYS:HB3	2.02	0.41
1:A:13:GLN:NE2	1:A:335:PHE:HB2	2.36	0.41
1:B:294:LEU:CD1	1:B:306:SER:HA	2.46	0.41
1:B:465:PHE:HB3	1:B:476:GLU:HB2	2.03	0.41
1:C:142:LYS:HD2	1:D:480:TYR:OH	2.21	0.41
1:E:243:PHE:HD2	1:E:267:LEU:HD22	1.85	0.41
1:F:243:PHE:HB3	1:F:267:LEU:HD22	2.01	0.41
1:G:249:ILE:N	1:G:249:ILE:HD13	2.35	0.41
1:G:449:GLY:HA2	1:G:468:TYR:CE1	2.54	0.41
1:G:8:VAL:HA	1:G:9:PRO:HD3	1.95	0.41
1:H:87:LEU:HB3	1:H:213:PHE:CE1	2.56	0.41
1:A:370:GLY:HA3	1:A:383:PRO:O	2.21	0.41
1:A:498:LYS:HB3	1:A:498:LYS:HE2	1.90	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:249:ILE:HD13	1:B:249:ILE:N	2.35	0.41
1:E:56:LYS:O	1:E:60:ASP:OD1	2.39	0.41
1:F:106:GLU:O	1:F:110:ASN:HB3	2.20	0.41
1:F:249:ILE:N	1:F:249:ILE:HD13	2.36	0.41
1:G:333:ASN:HA	1:G:334:PRO:HD2	1.91	0.41
1:H:249:ILE:HD13	1:H:249:ILE:N	2.36	0.41
1:H:131:TYR:CE1	1:H:462:GLN:HB3	2.56	0.41
1:A:253:ILE:HG22	1:A:265:VAL:HG11	2.02	0.41
1:A:350:PHE:HZ	1:A:373:ILE:HD13	1.80	0.41
1:B:323:VAL:CG1	1:B:327:LYS:HE3	2.50	0.41
1:D:275:ASN:HD21	1:D:432:PHE:HE1	1.66	0.41
1:E:166:ILE:CG2	1:E:178:LYS:HG3	2.51	0.41
1:F:415:GLU:O	1:F:419:ARG:HG3	2.21	0.41
1:G:89:ASN:OD1	1:G:130:ARG:HG2	2.21	0.41
1:G:87:LEU:HB3	1:G:213:PHE:CZ	2.56	0.41
1:A:87:LEU:HB3	1:A:213:PHE:CZ	2.56	0.41
1:B:67:ARG:NH2	1:B:161:VAL:HG23	2.36	0.41
1:B:24:ILE:CD1	1:B:61:LYS:HB3	2.50	0.41
1:B:498:LYS:HD2	2:B:8938:HOH:O	2.21	0.41
1:C:175:GLN:HE22	1:C:201:ALA:HA	1.86	0.41
1:C:261:ASN:OD1	1:C:263:LYS:HG2	2.21	0.41
1:C:79:MET:HG2	1:C:84:ARG:HG2	2.02	0.41
1:F:164:GLN:CD	1:F:178:LYS:HB3	2.41	0.41
1:G:11:PRO:HB3	1:G:114:TYR:CG	2.56	0.41
1:G:444:GLN:HG3	1:H:155:ARG:CZ	2.51	0.41
1:G:466:GLY:N	2:G:8892:HOH:O	2.45	0.41
1:H:113:PRO:HA	1:H:334:PRO:O	2.21	0.41
1:B:498:LYS:HE2	1:B:498:LYS:HB3	1.93	0.41
1:C:34:ARG:NH2	2:C:9202:HOH:O	2.51	0.41
1:C:148:GLY:O	1:C:498:LYS:HE2	2.21	0.41
1:E:431:VAL:HG21	1:E:442:LEU:HB3	2.03	0.41
1:E:78:ARG:HD2	1:H:497:GLN:NE2	2.36	0.41
1:F:141:GLY:HA3	1:G:143:THR:OG1	2.20	0.41
1:F:175:GLN:HE22	1:F:204:VAL:CG2	2.34	0.41
1:B:331:VAL:HG22	1:B:341:GLN:HB3	2.03	0.41
1:C:23:PHE:CG	1:C:205:ALA:HB1	2.56	0.41
1:C:27:GLU:HB3	1:C:29:HIS:NE2	2.36	0.41
1:C:344:GLN:CG	1:C:381:ILE:HD12	2.51	0.41
1:D:365:ALA:HB2	1:D:393:MET:SD	2.61	0.41
1:D:331:VAL:HG21	1:D:383:PRO:HD3	2.02	0.41
1:E:245:GLY:O	1:E:269:LEU:HA	2.21	0.41
1:F:169:ASN:OD1	1:F:169:ASN:N	2.53	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:315:TYR:O	1:G:319:VAL:HG23	2.21	0.41
1:G:450:THR:HG1	1:G:465:PHE:HD1	1.69	0.41
1:H:329:ARG:HE	1:H:341:GLN:HB2	1.85	0.41
1:A:21:GLN:HB2	1:A:28:TRP:HE3	1.87	0.40
1:A:289:GLN:HB2	2:A:9077:HOH:O	2.21	0.40
1:C:214:PRO:O	1:C:217:VAL:HG23	2.21	0.40
1:C:221:VAL:HA	1:C:222:PRO:HD2	1.93	0.40
1:D:17:VAL:CG1	1:D:199:LEU:HD22	2.51	0.40
1:D:427:LEU:HD11	1:D:465:PHE:CZ	2.56	0.40
1:G:389:VAL:CG1	1:G:396:ALA:HB2	2.50	0.40
1:H:18:PHE:HD1	1:H:101:TYR:HH	1.64	0.40
1:H:333:ASN:O	1:H:339:THR:OG1	2.30	0.40
1:C:376:ASP:N	1:C:376:ASP:OD1	2.50	0.40
1:C:462:GLN:CD	1:C:462:GLN:H	2.24	0.40
1:C:70:PHE:CZ	1:C:160:GLY:HA2	2.56	0.40
1:D:169:ASN:HD22	1:D:401:PHE:HZ	1.69	0.40
1:D:107:THR:HG23	1:D:334:PRO:HB2	2.04	0.40
1:F:246:SER:OG	1:F:249:ILE:HG12	2.22	0.40
1:H:67:ARG:HD2	2:H:8896:HOH:O	2.21	0.40
1:C:247:THR:HG23	1:C:269:LEU:HB2	2.01	0.40
1:D:430:ALA:HA	1:D:452:TRP:O	2.21	0.40
1:E:444:GLN:HG3	1:F:155:ARG:NH2	2.36	0.40
1:G:113:PRO:HB2	1:G:116:ILE:HG12	2.03	0.40
1:G:200:THR:O	1:G:204:VAL:HG23	2.21	0.40
1:G:99:ARG:HD2	2:G:8772:HOH:O	2.20	0.40
1:B:476:GLU:O	1:B:477:LEU:HB2	2.21	0.40
1:D:241:VAL:O	1:D:241:VAL:HG13	2.21	0.40
1:D:70:PHE:CZ	1:D:160:GLY:HA2	2.56	0.40
1:E:37:PHE:O	1:E:51:VAL:N	2.50	0.40
1:F:241:VAL:O	1:F:241:VAL:HG13	2.21	0.40
1:G:101:TYR:N	2:G:9547:HOH:O	2.50	0.40
2:F:9536:HOH:O	1:G:72:LEU:HD23	2.21	0.40
1:H:443:SER:HA	1:H:451:VAL:HG11	2.03	0.40
1:D:120:VAL:HG12	1:D:124:MET:HE1	2.04	0.40
1:D:208:ILE:CD1	1:D:218:VAL:HG11	2.52	0.40
1:E:247:THR:HG23	1:E:269:LEU:CB	2.51	0.40
1:F:27:GLU:HB3	1:F:29:HIS:NE2	2.36	0.40
1:G:70:PHE:CE1	1:G:158:PRO:HB2	2.57	0.40
1:G:35:LYS:HE2	1:G:35:LYS:HB3	1.98	0.40
1:G:424:THR:CG2	1:G:470:MET:HB2	2.44	0.40
1:H:116:ILE:O	1:H:120:VAL:HB	2.21	0.40
1:H:149:ASP:HA	1:H:498:LYS:HB2	2.04	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:333:ASN:HA	1:H:334:PRO:HD2	1.91	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	492/500 (98%)	475 (96%)	16 (3%)	1 (0%)	56	55
1	B	492/500 (98%)	476 (97%)	16 (3%)	0	100	100
1	C	492/500 (98%)	471 (96%)	21 (4%)	0	100	100
1	D	492/500 (98%)	473 (96%)	18 (4%)	1 (0%)	56	55
1	E	492/500 (98%)	472 (96%)	19 (4%)	1 (0%)	56	55
1	F	492/500 (98%)	476 (97%)	16 (3%)	0	100	100
1	G	492/500 (98%)	472 (96%)	20 (4%)	0	100	100
1	H	492/500 (98%)	477 (97%)	14 (3%)	1 (0%)	56	55
All	All	3936/4000 (98%)	3792 (96%)	140 (4%)	4 (0%)	59	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	270	GLY
1	H	426	GLY
1	A	426	GLY
1	D	426	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/402 (99%)	371 (93%)	28 (7%)	21	16
1	B	399/402 (99%)	373 (94%)	26 (6%)	24	18
1	C	399/402 (99%)	378 (95%)	21 (5%)	32	28
1	D	399/402 (99%)	381 (96%)	18 (4%)	38	35
1	E	399/402 (99%)	377 (94%)	22 (6%)	30	26
1	F	399/402 (99%)	376 (94%)	23 (6%)	28	23
1	G	399/402 (99%)	378 (95%)	21 (5%)	32	28
1	H	399/402 (99%)	377 (94%)	22 (6%)	30	26
All	All	3192/3216 (99%)	3011 (94%)	181 (6%)	29	25

All (181) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	22	ILE
1	A	41	ASN
1	A	50	GLN
1	A	55	ASP
1	A	79	MET
1	A	115	VAL
1	A	122	LEU
1	A	192	LYS
1	A	196	GLN
1	A	240	LYS
1	A	246	SER
1	A	249	ILE
1	A	264	ARG
1	A	294	LEU
1	A	298	GLN
1	A	302	CYS
1	A	320	GLU
1	A	338	LYS
1	A	361	LYS
1	A	373	ILE
1	A	376	ASP
1	A	377	ARG
1	A	390	GLN

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Mol	Chain	Res	Type
1	A	401	PHE
1	A	463	SER
1	A	473	SER
1	A	483	GLN
1	B	13	GLN
1	B	34	ARG
1	B	41	ASN
1	B	50	GLN
1	B	56	LYS
1	B	79	MET
1	B	121	ASP
1	B	122	LEU
1	B	142	LYS
1	B	192	LYS
1	B	196	GLN
1	B	246	SER
1	B	249	ILE
1	B	264	ARG
1	B	269	LEU
1	B	273	SER
1	B	294	LEU
1	B	302	CYS
1	B	320	GLU
1	B	361	LYS
1	B	376	ASP
1	B	377	ARG
1	B	399	GLU
1	B	401	PHE
1	B	463	SER
1	B	473	SER
1	C	14	GLN
1	C	34	ARG
1	C	41	ASN
1	C	79	MET
1	C	87	LEU
1	C	122	LEU
1	C	142	LYS
1	C	146	ILE
1	C	192	LYS
1	C	196	GLN
1	C	246	SER
1	C	249	ILE

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Mol	Chain	Res	Type
1	C	264	ARG
1	C	294	LEU
1	C	302	CYS
1	C	351	LYS
1	C	377	ARG
1	C	401	PHE
1	C	463	SER
1	C	470	MET
1	C	473	SER
1	D	34	ARG
1	D	41	ASN
1	D	122	LEU
1	D	192	LYS
1	D	196	GLN
1	D	246	SER
1	D	264	ARG
1	D	275	ASN
1	D	302	CYS
1	D	338	LYS
1	D	351	LYS
1	D	358	ASN
1	D	376	ASP
1	D	377	ARG
1	D	401	PHE
1	D	463	SER
1	D	473	SER
1	D	475	GLN
1	E	22	ILE
1	E	41	ASN
1	E	50	GLN
1	E	122	LEU
1	E	135	TRP
1	E	142	LYS
1	E	192	LYS
1	E	196	GLN
1	E	246	SER
1	E	249	ILE
1	E	264	ARG
1	E	268	GLU
1	E	294	LEU
1	E	302	CYS
1	E	320	GLU

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Mol	Chain	Res	Type
1	E	338	LYS
1	E	376	ASP
1	E	377	ARG
1	E	399	GLU
1	E	401	PHE
1	E	463	SER
1	E	473	SER
1	F	26	ASN
1	F	34	ARG
1	F	41	ASN
1	F	55	ASP
1	F	121	ASP
1	F	122	LEU
1	F	192	LYS
1	F	196	GLN
1	F	246	SER
1	F	249	ILE
1	F	264	ARG
1	F	288	GLU
1	F	302	CYS
1	F	320	GLU
1	F	338	LYS
1	F	347	GLU
1	F	377	ARG
1	F	399	GLU
1	F	401	PHE
1	F	462	GLN
1	F	463	SER
1	F	473	SER
1	F	498	LYS
1	G	14	GLN
1	G	41	ASN
1	G	55	ASP
1	G	122	LEU
1	G	192	LYS
1	G	195	GLU
1	G	196	GLN
1	G	240	LYS
1	G	246	SER
1	G	248	GLU
1	G	249	ILE
1	G	251	ARG

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Mol	Chain	Res	Type
1	G	259	SER
1	G	264	ARG
1	G	351	LYS
1	G	376	ASP
1	G	377	ARG
1	G	401	PHE
1	G	463	SER
1	G	470	MET
1	G	473	SER
1	H	34	ARG
1	H	41	ASN
1	H	79	MET
1	H	122	LEU
1	H	192	LYS
1	H	196	GLN
1	H	220	ILE
1	H	240	LYS
1	H	246	SER
1	H	249	ILE
1	H	264	ARG
1	H	268	GLU
1	H	275	ASN
1	H	302	CYS
1	H	338	LYS
1	H	376	ASP
1	H	377	ARG
1	H	401	PHE
1	H	463	SER
1	H	470	MET
1	H	473	SER
1	H	486	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	26	ASN
1	A	29	HIS
1	A	41	ASN
1	A	83	HIS
1	A	89	ASN
1	A	175	GLN

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Mol	Chain	Res	Type
1	A	196	GLN
1	A	275	ASN
1	A	300	GLN
1	A	462	GLN
1	B	26	ASN
1	B	41	ASN
1	B	50	GLN
1	B	175	GLN
1	B	196	GLN
1	B	275	ASN
1	B	300	GLN
1	B	462	GLN
1	C	26	ASN
1	C	41	ASN
1	C	50	GLN
1	C	71	GLN
1	C	175	GLN
1	C	196	GLN
1	C	275	ASN
1	C	300	GLN
1	C	349	GLN
1	C	462	GLN
1	D	26	ASN
1	D	41	ASN
1	D	50	GLN
1	D	71	GLN
1	D	89	ASN
1	D	164	GLN
1	D	175	GLN
1	D	196	GLN
1	D	289	GLN
1	D	291	HIS
1	D	300	GLN
1	D	349	GLN
1	D	362	GLN
1	E	26	ASN
1	E	41	ASN
1	E	50	GLN
1	E	89	ASN
1	E	175	GLN
1	E	196	GLN
1	E	275	ASN

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Mol	Chain	Res	Type
1	E	300	GLN
1	E	358	ASN
1	E	440	ASN
1	E	462	GLN
1	F	26	ASN
1	F	41	ASN
1	F	175	GLN
1	F	196	GLN
1	F	300	GLN
1	F	362	GLN
1	G	26	ASN
1	G	41	ASN
1	G	50	GLN
1	G	175	GLN
1	G	196	GLN
1	G	275	ASN
1	G	300	GLN
1	G	462	GLN
1	G	483	GLN
1	H	26	ASN
1	H	29	HIS
1	H	41	ASN
1	H	83	HIS
1	H	175	GLN
1	H	196	GLN
1	H	300	GLN
1	H	462	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no ligands in this entry.

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	494/500 (98%)	-0.12	14 (2%) 50 55	8, 20, 44, 68	0
1	B	494/500 (98%)	-0.18	8 (1%) 68 75	8, 20, 44, 68	0
1	C	494/500 (98%)	-0.17	7 (1%) 72 77	9, 19, 44, 68	0
1	D	494/500 (98%)	-0.16	9 (1%) 65 71	9, 20, 43, 68	0
1	E	494/500 (98%)	-0.18	8 (1%) 68 75	8, 19, 43, 68	0
1	F	494/500 (98%)	-0.18	6 (1%) 75 80	8, 19, 43, 68	0
1	G	494/500 (98%)	-0.13	19 (3%) 38 42	8, 20, 44, 68	0
1	H	494/500 (98%)	-0.13	6 (1%) 75 80	8, 20, 44, 68	0
All	All	3952/4000 (98%)	-0.15	77 (1%) 64 69	8, 20, 44, 68	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	474	GLY	6.0
1	G	474	GLY	5.1
1	F	247	THR	4.8
1	A	474	GLY	4.7
1	G	472	GLY	4.2
1	G	255	VAL	4.1
1	C	475	GLN	4.0
1	B	475	GLN	4.0
1	F	250	GLY	3.9
1	D	247	THR	3.9
1	A	253	ILE	3.9
1	B	474	GLY	3.9
1	D	475	GLN	3.7
1	C	476	GLU	3.6
1	E	247	THR	3.6
1	H	253	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	474	GLY	3.4
1	A	247	THR	3.3
1	H	476	GLU	3.3
1	G	246	SER	3.3
1	B	476	GLU	3.2
1	F	472	GLY	3.1
1	F	474	GLY	3.1
1	B	257	ALA	3.1
1	E	474	GLY	3.0
1	A	250	GLY	3.0
1	G	258	GLY	3.0
1	A	254	GLN	3.0
1	G	473	SER	3.0
1	C	253	ILE	3.0
1	G	254	GLN	2.9
1	A	473	SER	2.9
1	A	463	SER	2.9
1	A	255	VAL	2.9
1	G	256	ALA	2.8
1	B	258	GLY	2.8
1	C	254	GLN	2.8
1	A	267	LEU	2.7
1	G	253	ILE	2.7
1	A	251	ARG	2.7
1	G	250	GLY	2.6
1	B	253	ILE	2.6
1	C	224	PHE	2.6
1	F	475	GLN	2.5
1	G	476	GLU	2.5
1	H	465	PHE	2.5
1	B	7	ALA	2.5
1	E	477	LEU	2.5
1	E	248	GLU	2.5
1	G	245	GLY	2.4
1	H	247	THR	2.4
1	D	253	ILE	2.4
1	G	477	LEU	2.4
1	E	224	PHE	2.4
1	H	258	GLY	2.4
1	E	424	THR	2.4
1	E	257	ALA	2.3
1	A	249	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	257	ALA	2.3
1	G	247	THR	2.3
1	E	473	SER	2.3
1	D	225	GLY	2.3
1	A	465	PHE	2.2
1	H	478	GLY	2.2
1	D	267	LEU	2.2
1	F	253	ILE	2.1
1	D	7	ALA	2.1
1	B	424	THR	2.1
1	G	257	ALA	2.1
1	C	250	GLY	2.1
1	G	424	THR	2.1
1	G	470	MET	2.1
1	A	476	GLU	2.1
1	D	248	GLU	2.1
1	D	470	MET	2.1
1	G	251	ARG	2.1
1	G	478	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.