Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:56 AM GMT

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 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:

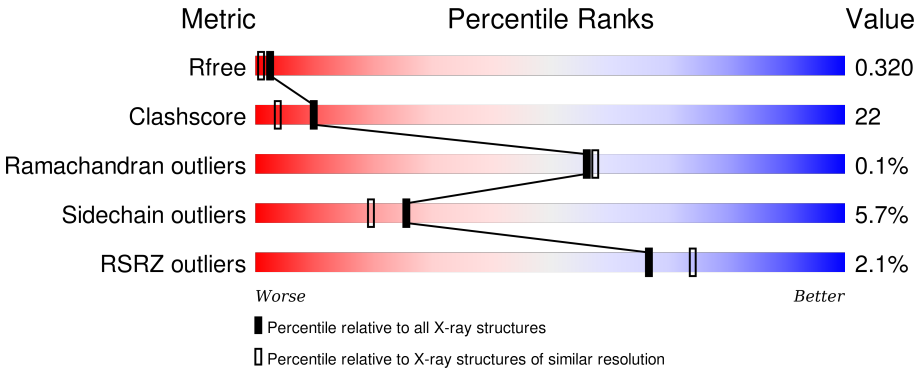
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.15 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}	91344	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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

Mol	Chain	Length	Quality of chain
1	A	500	3% 51% 43%
1	B	500	2% 57% 39%
1	C	500	% 65% 32%
1	D	500	2% 55% 41%
1	E	500	2% 57% 39%

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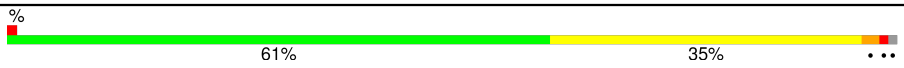
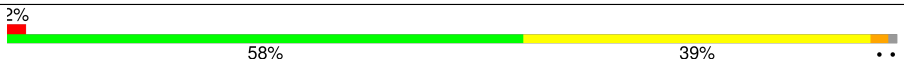
Mol	Chain	Length	Quality of chain
1	F	500	
1	G	500	
1	H	500	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 31388 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 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.

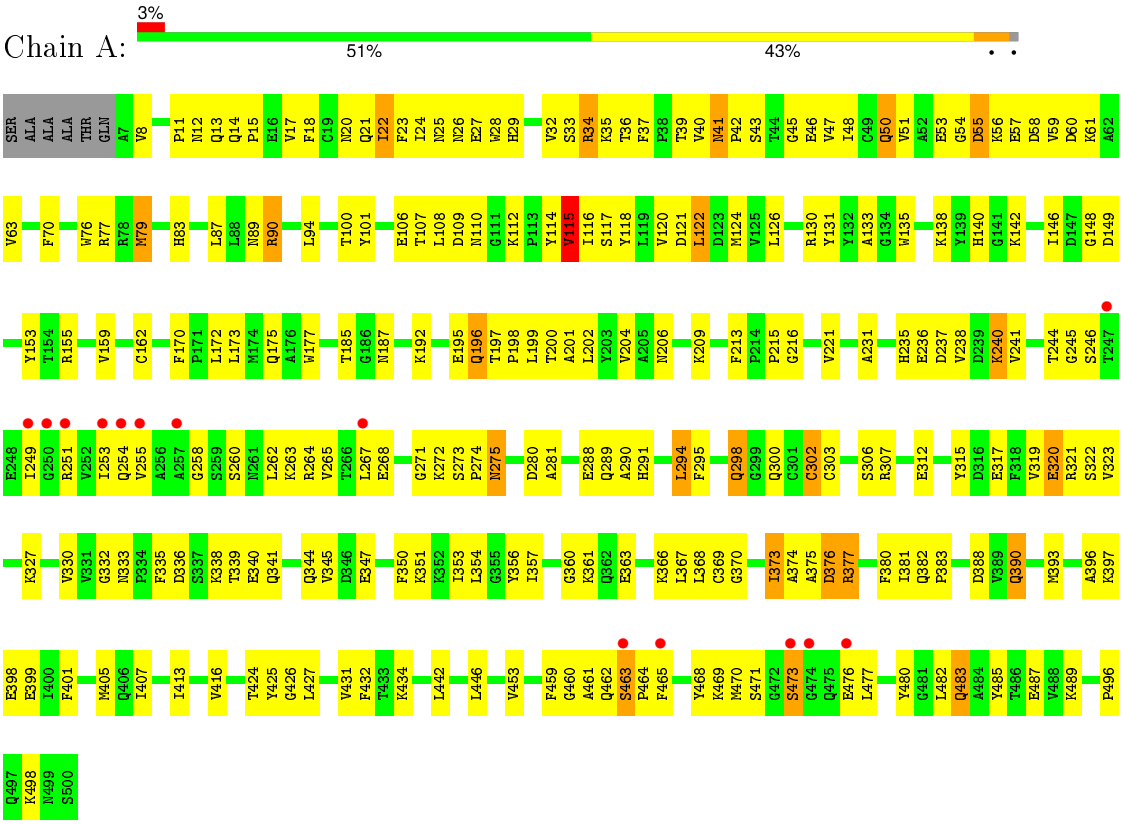
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	134	Total O 134 134	0	0
2	B	131	Total O 131 131	0	0
2	C	145	Total O 145 145	0	0
2	D	133	Total O 133 133	0	0
2	E	140	Total O 140 140	0	0
2	F	114	Total O 114 114	0	0
2	G	118	Total O 118 118	0	0
2	H	105	Total O 105 105	0	0

3 Residue-property plots (i)

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

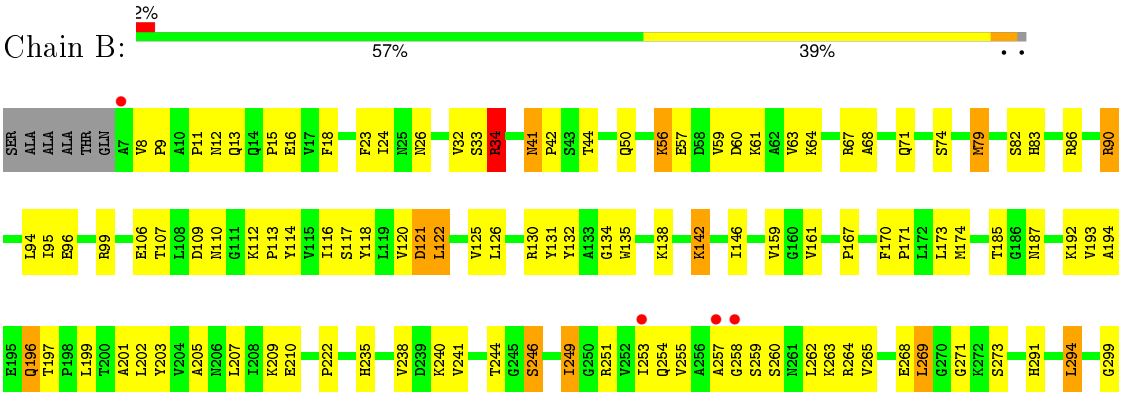
- Molecule 1: Aldehyde dehydrogenase

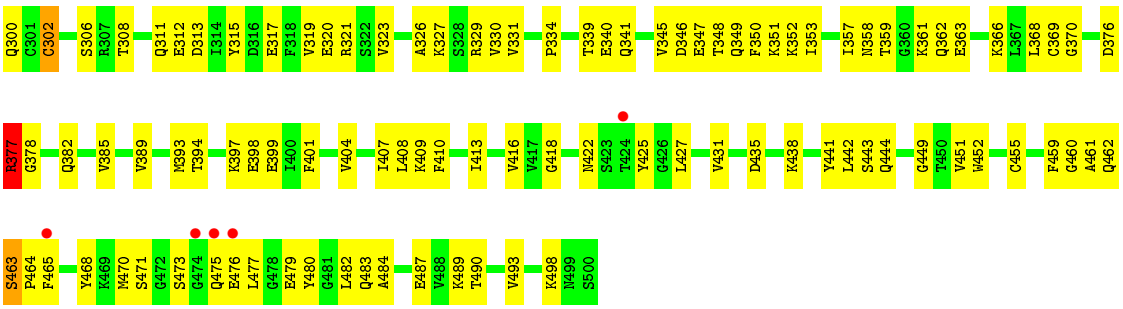
Chain A:



- Molecule 1: Aldehyde dehydrogenase

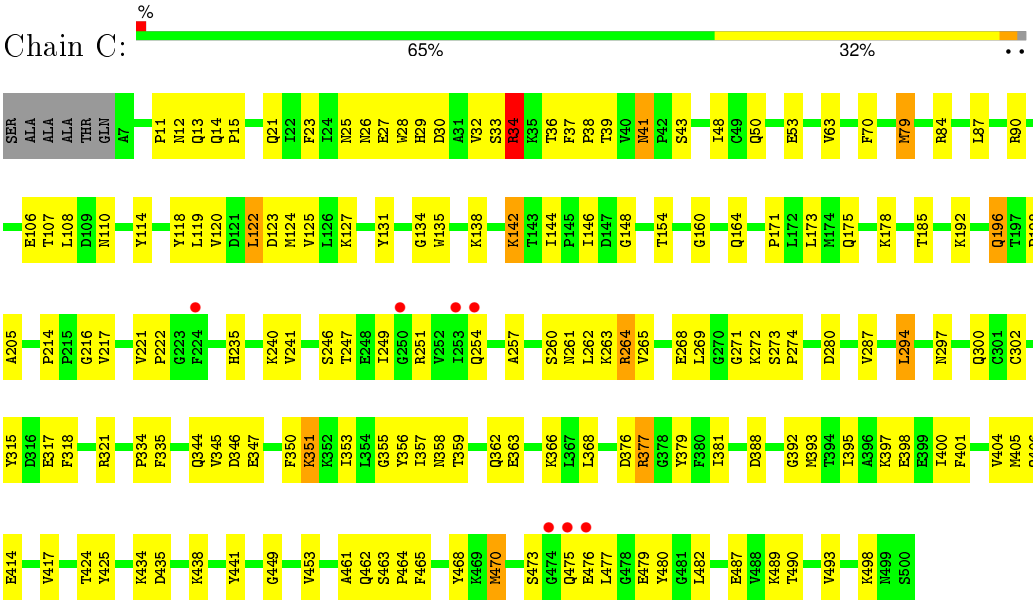
Chain B:





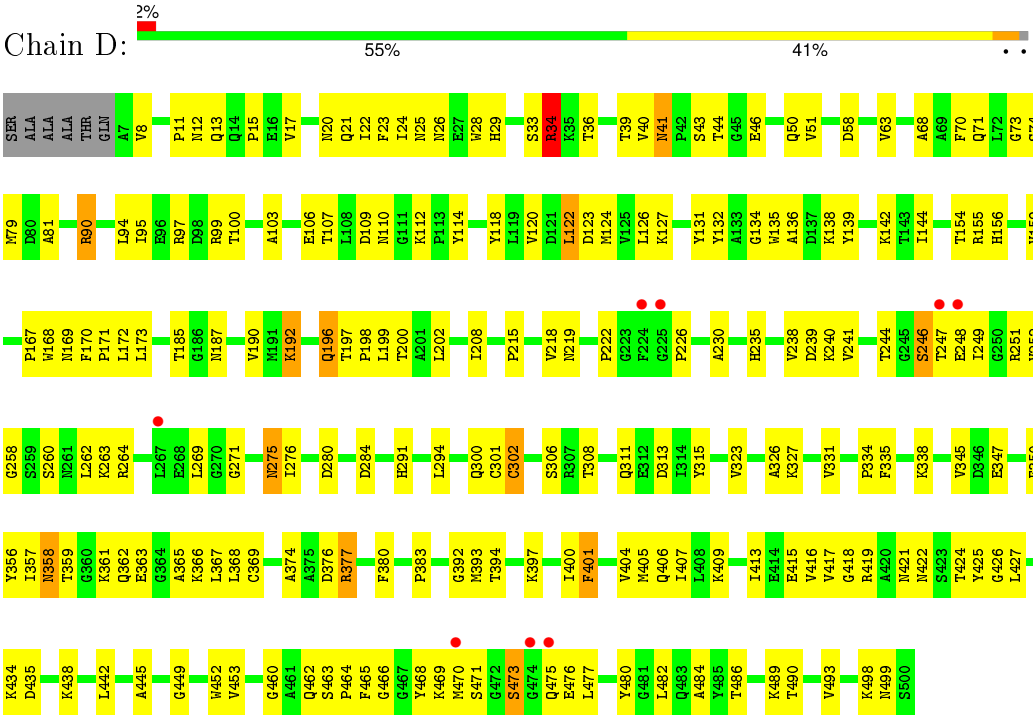
• Molecule 1: Aldehyde dehydrogenase

Chain C:



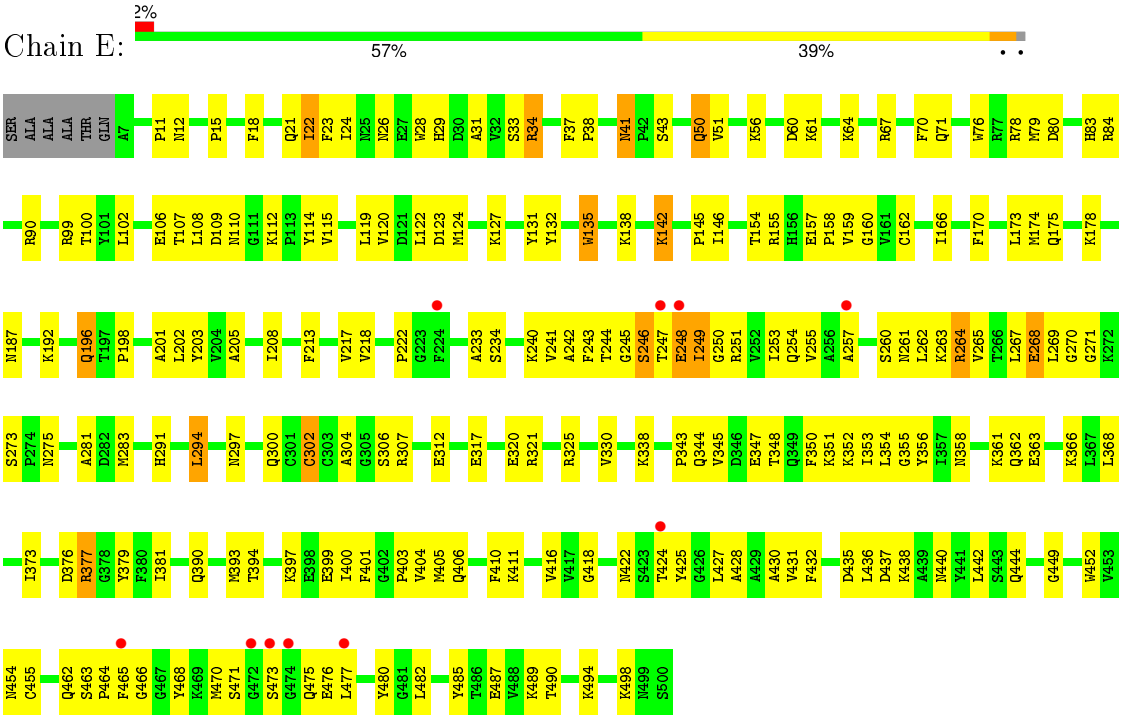
• Molecule 1: Aldehyde dehydrogenase

Chain D:



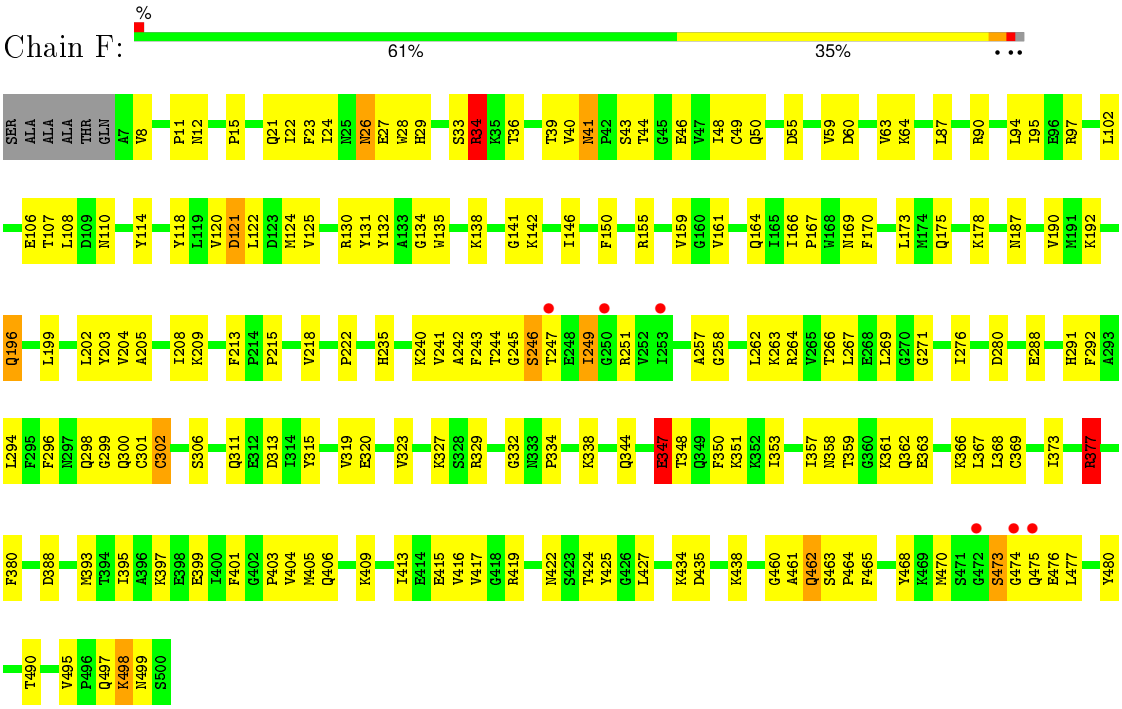
- Molecule 1: Aldehyde dehydrogenase

Chain E:



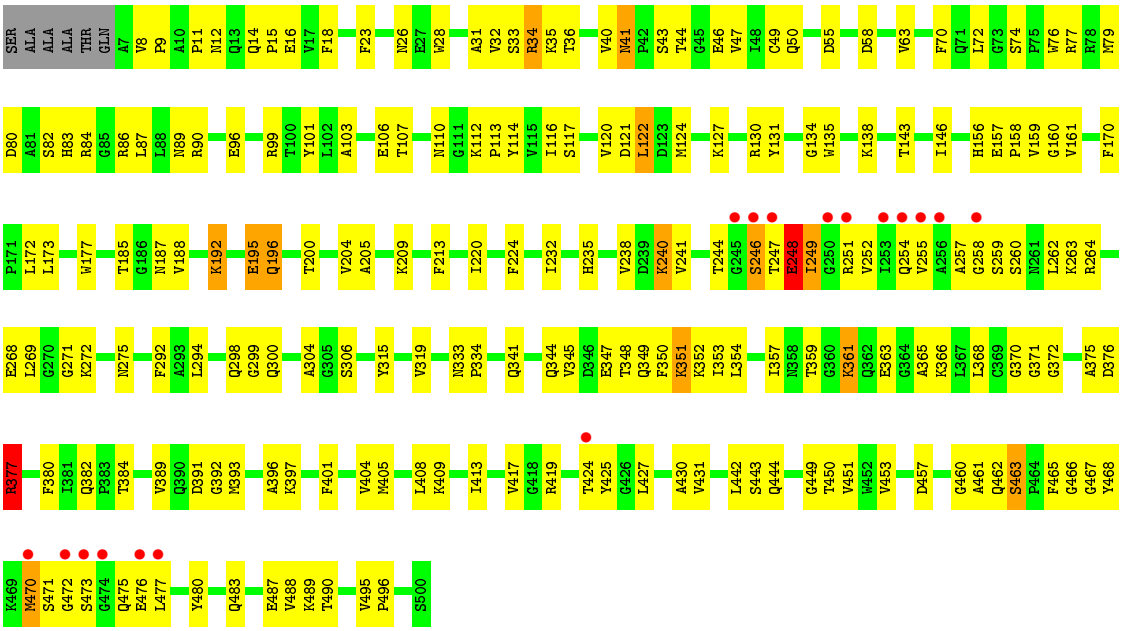
- Molecule 1: Aldehyde dehydrogenase

Chain F:



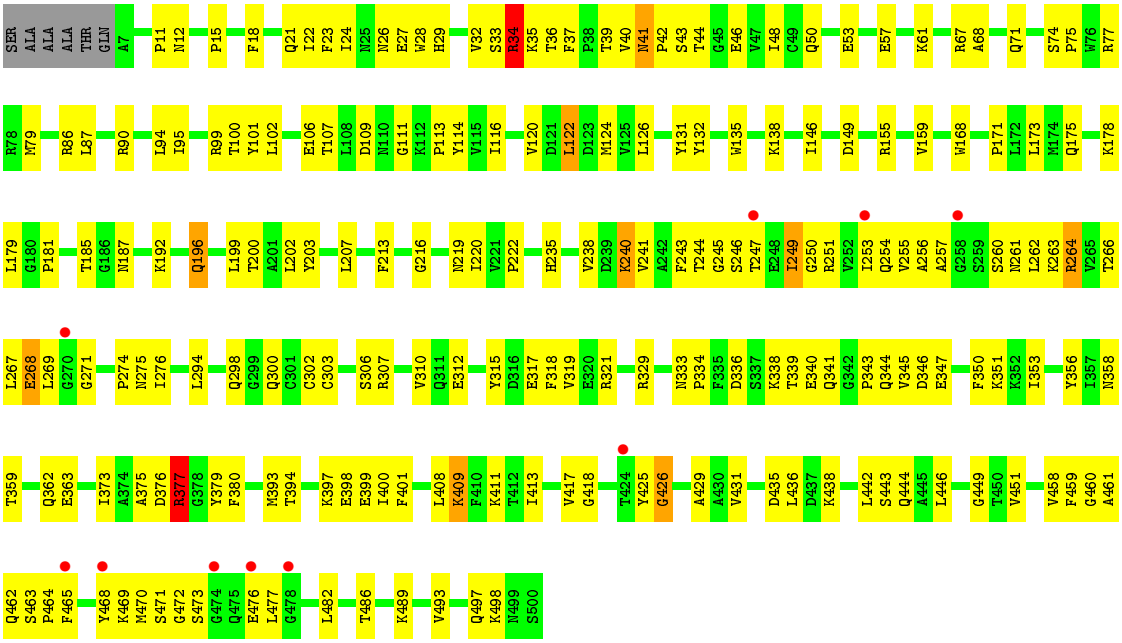
- Molecule 1: Aldehyde dehydrogenase

Chain G:



• Molecule 1: Aldehyde dehydrogenase

Chain H:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	4.22 (at 2.15Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.251 , 0.314 0.264 , 0.320	Depositor DCC
R_{free} test set	9468 reflections (5.44%)	DCC
Wilson B-factor (Å^2)	18.8	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.467 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
2	A	134	0	0	27	0
2	B	131	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 22.

All (1330) 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: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:H:247:THR:HG23	1:H:269:LEU:HD13	1.47	0.95
1:F:26:ASN:HB3	1:F:209:LYS:HD2	1.49	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	Interatomic distance (Å)	Clash overlap (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:H:294:LEU:HD12	1:H:306:SER:HA	1.63	0.79
1:G:294:LEU:HD12	1:G:306:SER:HA	1.64	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:E:247:THR:HA	1:E:269:LEU:HB3	1.66	0.77
1:D:21:GLN:HB3	1:D:29:HIS:O	1.84	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:F:266:THR:O	1:F:267:LEU:HD23	1.85	0.77
1:A:41:ASN:HD22	1:A:43:SER:H	1.33	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:H:238:VAL:O	1:H:263:LYS:HE3	1.85	0.76
1:G:77:ARG:HD2	2:G:8877:HOH:O	1.85	0.76
1:C:351:LYS:HB3	1:E:38:PRO:HG2	1.67	0.76
1:D:172:LEU:HD21	1:D:200:THR:HB	1.65	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:F:240:LYS:NZ	1:F:242:ALA:HB2	2.01	0.76
1:D:12:ASN:O	1:D:15:PRO:HD3	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:22:ILE:HG12	1:H:222:PRO:HD2	1.69	0.75
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:F:247:THR:HA	1:F:269:LEU:HB3	1.71	0.73
1:E:317:GLU:O	1:E:321:ARG:HG3	1.89	0.73
1:E:244:THR:HG23	1:E:268:GLU:HB3	1.69	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:H:120:VAL:HG12	1:H:124:MET:HE2	1.71	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:A:32:VAL:HG11	1:A:57:GLU:OE2	1.89	0.72
1:H:100:THR:HG22	2:H:9608:HOH:O	1.88	0.72
1:B:194:ALA:HB3	1:B:197:THR:OG1	1.90	0.72
1:D:40:VAL:HG13	1:D:46:GLU:O	1.90	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:12:ASN:O	1:E:15:PRO:HD3	1.88	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:41:ASN:ND2	1:G:43:SER:H	1.88	0.71
1:G:366:LYS:HE2	1:G:368:LEU:HD21	1.71	0.71
1:C:353:ILE:O	1:C:357:ILE:HG13	1.91	0.71
1:D:156:HIS:HB3	1:D:486:THR:HG21	1.73	0.71
1:D:300:GLN:HE22	1:D:345:VAL:H	1.37	0.71
1:B:313:ASP:HB3	2:B:9435:HOH:O	1.91	0.71
1:F:247:THR:HG23	1:F:269:LEU:HD13	1.72	0.71
1:B:257:ALA:HB1	1:B:263:LYS:HG3	1.71	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:142:LYS:HD2	1:B:480:TYR:OH	1.91	0.70
1:B:294:LEU:HD12	1:B:306:SER:HA	1.74	0.70
1:B:44:THR:HB	1:B:377:ARG:NH2	2.07	0.70
1:G:41:ASN:HD21	1:G:43:SER:HB2	1.57	0.70
1:D:359:THR:O	1:D:363:GLU:HG3	1.92	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:H:257:ALA:HB1	1:H:263:LYS:HG3	1.75	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: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:G:196:GLN:HE21	1:G:196:GLN:N	1.89	0.69
1:B:121:ASP:O	1:B:125:VAL:HG23	1.93	0.69
1:A:425:TYR:O	1:A:469:LYS:HD2	1.93	0.68
1:E:424:THR:CG2	1:E:470:MET:CG	2.71	0.68
1:B:378:GLY:HA2	2:B:8708:HOH:O	1.93	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: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:A:109:ASP:OD2	1:A:197:THR:HA	1.92	0.68
1:E:196:GLN:HE21	1:E:196:GLN:H	1.41	0.68
1:F:298:GLN:HE21	1:F:300:GLN:HE21	1.40	0.68
1:D:235:HIS:HB3	1:D:238:VAL:HG23	1.75	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: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:26:ASN:HB3	1:G:209:LYS:HD2	1.76	0.68
1:G:124:MET:HE3	1:G:173:LEU:HD22	1.76	0.67
1:C:294:LEU:HD12	1:C:306:SER:HA	1.74	0.67
1:C:241:VAL:HG12	1:C:265:VAL:HG22	1.77	0.67
1:H:46:GLU:HB2	2:H:8788:HOH:O	1.93	0.67
1:B:196:GLN:H	1:B:196:GLN:NE2	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:426:GLY:O	1:H:468:TYR:HB2	1.94	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: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:E:366:LYS:HD3	1:E:368:LEU:HD21	1.77	0.67
1:C:280:ASP:O	1:C:434:LYS:HD2	1.94	0.67
1:H:358:ASN:O	1:H:362:GLN:HG2	1.94	0.67
1:G:120:VAL:HG12	1:G:124:MET:HE2	1.77	0.67
1:A:303:CYS:HG	1:A:459:PHE:HZ	1.40	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:C:300:GLN:HE22	1:C:345:VAL:H	1.43	0.66
1:A:251:ARG:HG2	1:B:262:LEU:HD21	1.77	0.66
1:G:77:ARG:HA	2:G:8877:HOH:O	1.95	0.66
1:H:245:GLY:O	1:H:269:LEU:HA	1.95	0.66
1:G:463:SER:HB3	2:G:9569:HOH:O	1.95	0.66
1:E:261:ASN:HA	1:F:251:ARG:HH22	1.59	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:G:244:THR:OG1	1:G:268:GLU:HB2	1.95	0.65
1:C:462:GLN:O	1:D:144:ILE:HG21	1.96	0.65
1:G:361:LYS:HA	2:G:9353:HOH:O	1.95	0.65
1:C:103:ALA:HB2	1:C:122:LEU:HD13	1.79	0.65
1:A:15:PRO:HD2	1:A:108:LEU:HD13	1.77	0.65
1:A:36:THR:OG1	1:A:50:GLN:HG3	1.96	0.65
1:G:195:GLU:HA	2:G:8776:HOH:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:GLY:O	1:C:138:LYS:HD2	1.96	0.65
1:A:146:ILE:HG22	2:A:8700:HOH:O	1.97	0.65
1:E:251:ARG:HA	1:F:262:LEU:HD21	1.79	0.65
1:D:306:SER:O	1:D:406:GLN:HB2	1.96	0.65
1:B:68:ALA:HA	1:B:71:GLN:HG2	1.79	0.65
1:G:247:THR:HA	1:G:269:LEU:HD22	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:431:VAL:HG21	1:G:442:LEU:HB3	1.79	0.64
1:D:155:ARG:HD3	1:D:489:LYS:HD2	1.78	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:NE2	1:H:196:GLN:H	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:D:134:GLY:O	1:D:138:LYS:HD2	1.97	0.64
1:B:271:GLY:HA2	1:B:425:TYR:CG	2.33	0.64
1:H:37:PHE:HD2	1:H:53:GLU:HB2	1.63	0.64
1:A:393:MET:O	1:A:397:LYS:HG3	1.97	0.64
1:E:247:THR:CA	1:E:269:LEU:HB3	2.27	0.64
1:C:23:PHE:CZ	1:C:26:ASN:HA	2.33	0.64
1:H:408:LEU:HB3	2:H:8635:HOH:O	1.97	0.63
1:H:356:TYR:CG	1:H:400:ILE:HG12	2.33	0.63
1:D:155:ARG:HB2	1:D:489:LYS:HB3	1.80	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:G:315:TYR:CG	1:G:409:LYS:HE2	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:G:32:VAL:HG23	1:G:58:ASP:OD1	1.98	0.63
1:E:344:GLN:HG3	1:E:353:ILE:HD12	1.79	0.63
1:E:424:THR:CG2	1:E:470:MET:CB	2.73	0.63
1:A:480:TYR:OH	1:B:142:LYS:HG3	1.98	0.63
1:D:23:PHE:CZ	1:D:26:ASN:HA	2.33	0.63
1:B:23:PHE:CZ	1:B:26:ASN:HA	2.33	0.63
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:24:ILE:HG22	1:A:25:ASN:OD1	1.99	0.62
1:A:350:PHE:CZ	1:A:373:ILE:HD13	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:353:ILE:O	1:F:357:ILE:HG13	2.00	0.62
1:B:59:VAL:O	1:B:63:VAL:HG23	1.98	0.62
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:G:461:ALA:HA	1:G:477:LEU:HD22	1.82	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: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:G:248:GLU:O	1:G:252:VAL:HG23	2.00	0.62
1:F:359:THR:O	1:F:363:GLU:HG3	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:F:460:GLY:O	1:F:477:LEU:HD13	2.00	0.61
1:E:41:ASN:ND2	1:E:43:SER:HB2	2.16	0.61
1:D:23:PHE:HB2	1:D:28:TRP:CZ3	2.36	0.61
1:D:95:ILE:HG22	1:D:126:LEU:HD21	1.82	0.61
1:B:347:GLU:O	1:B:351:LYS:HG3	1.99	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:H:41:ASN:HD22	1:H:43:SER:H	1.47	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:E:31:ALA:HA	2:E:8812:HOH:O	2.01	0.61
1:B:203:TYR:HB2	2:B:8930:HOH:O	2.00	0.61
1:C:30:ASP:HB2	1:C:34:ARG:NH2	2.16	0.61
1:G:375:ALA:HB3	1:G:380:PHE:HB2	1.82	0.60
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:A:70:PHE:CD1	1:A:77:ARG:HD3	2.36	0.60
1:A:23:PHE:CZ	1:A:26:ASN:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:393:MET:O	1:H:397:LYS:HG3	2.02	0.60
1:H:429:ALA:HB1	1:H:446:LEU:HD13	1.84	0.60
1:E:246:SER:HG	1:E:249:ILE:H	1.49	0.60
1:F:298:GLN:HE21	1:F:300:GLN:NE2	1.99	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: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:D:294:LEU:HD13	1:D:405:MET:HA	1.83	0.60
1:H:107:THR:HG23	1:H:334:PRO:HB2	1.83	0.60
1:F:11:PRO:HB3	1:F:114:TYR:CE1	2.36	0.60
1:B:12:ASN:O	1:B:15:PRO:HD3	2.01	0.60
1:G:468:TYR:O	1:G:471:SER:HB2	2.02	0.60
1:F:294:LEU:O	1:F:299:GLY:HA2	2.02	0.60
1:B:94:LEU:HD13	1:B:210:GLU:OE2	2.01	0.60
1:F:298:GLN:HB2	1:F:300:GLN:NE2	2.15	0.59
1:E:294:LEU:HD22	1:E:405:MET:HB2	1.83	0.59
1:A:424:THR:HG22	1:A:470:MET:HB2	1.84	0.59
1:H:23:PHE:CZ	1:H:26:ASN:HA	2.37	0.59
1:E:435:ASP:OD1	1:E:438:LYS:HG3	2.01	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:E:146:ILE:HG13	1:F:460:GLY:HA3	1.84	0.59
1:F:347:GLU:O	1:F:351:LYS:HG3	2.01	0.59
1:C:388:ASP:HA	2:C:8979:HOH:O	2.02	0.59
1:D:468:TYR:O	1:D:471:SER:HB2	2.02	0.59
1:C:135:TRP:CZ2	1:C:479:GLU:HB2	2.38	0.59
1:E:11:PRO:HB3	1:E:114:TYR:CZ	2.37	0.59
1:C:247:THR:HA	1:C:269:LEU:HB3	1.84	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:F:209:LYS:HD3	2:F:8843:HOH:O	2.02	0.59
1:A:109:ASP:OD2	1:A:198:PRO:HD2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:247:THR:HG23	1:C:269:LEU:CB	2.33	0.58
1:C:261:ASN:HD21	1:C:263:LYS:HE3	1.68	0.58
1:A:11:PRO:HB3	1:A:114:TYR:CZ	2.38	0.58
1:E:240:LYS:NZ	1:E:242:ALA:HB2	2.18	0.58
1:D:196:GLN:HE21	1:D:196:GLN:N	1.95	0.58
1:A:39:THR:HG23	1:A:48:ILE:HB	1.85	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:76:TRP:O	1:A:79:MET:HB3	2.04	0.58
1:A:366:LYS:HE2	1:A:368:LEU:HD21	1.84	0.58
1:F:497:GLN:HG2	1:F:499:ASN:ND2	2.19	0.58
1:H:269:LEU:HD12	1:H:472:GLY:N	2.19	0.58
1:F:11:PRO:HB3	1:F:114:TYR:CZ	2.39	0.58
1:E:115:VAL:HG13	1:E:119:LEU:HD12	1.86	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:D:280:ASP:O	1:D:434:LYS:HG3	2.03	0.57
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:H:300:GLN:HE22	1:H:345:VAL:N	2.01	0.57
1:F:294:LEU:HD11	1:F:404:VAL:O	2.04	0.57
1:A:241:VAL:HG12	1:A:265:VAL:HG22	1.86	0.57
1:A:363:GLU:HB2	2:A:9084:HOH:O	2.03	0.57
1:E:294:LEU:HD11	1:E:404:VAL:O	2.04	0.57
1:D:291:HIS:HE1	1:D:326:ALA:HA	1.69	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: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:G:11:PRO:HB3	1:G:114:TYR:CE1	2.39	0.57
1:G:41:ASN:ND2	1:G:43:SER:HB2	2.18	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:146:ILE:HG13	1:H:460:GLY:HA3	1.85	0.57
1:C:106:GLU:O	1:C:110:ASN:HB3	2.03	0.57
1:B:366:LYS:HG2	1:B:368:LEU:HD21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLU:CG	2:A:9084:HOH:O	2.51	0.57
1:A:20:ASN:HA	1:A:202:LEU:HD12	1.87	0.57
1:H:477:LEU:HD21	2:H:8838:HOH:O	2.05	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:A:8:VAL:HG21	1:A:115:VAL:HG22	1.85	0.57
1:D:44:THR:HB	1:D:46:GLU:HG2	1.87	0.57
1:C:12:ASN:O	1:C:15:PRO:HD3	2.04	0.57
1:G:86:ARG:HG3	2:G:9545:HOH:O	2.04	0.57
1:G:468:TYR:OH	1:H:489:LYS:HB2	2.04	0.57
1:A:366:LYS:HG2	1:A:368:LEU:CD2	2.35	0.57
2:E:8837:HOH:O	1:H:436:LEU:HB2	2.04	0.57
1:D:262:LEU:HB3	2:D:9469:HOH:O	2.05	0.57
1:F:41:ASN:HD22	1:F:43:SER:H	1.51	0.57
1:C:39:THR:HG23	1:C:48:ILE:HB	1.87	0.57
1:E:275:ASN:ND2	1:E:430:ALA:HB3	2.20	0.57
1:A:12:ASN:O	1:A:15:PRO:HD3	2.04	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:37:PHE:HD2	1:A:53:GLU:HB2	1.70	0.56
1:H:329:ARG:HA	1:H:340:GLU:OE2	2.05	0.56
1:F:245:GLY:O	1:F:269:LEU:HA	2.04	0.56
1:A:424:THR:CG2	1:A:470:MET:CE	2.83	0.56
1:A:117:SER:O	1:A:122:LEU:HD12	2.05	0.56
1:D:246:SER:HG	1:D:248:GLU:HB3	1.69	0.56
1:F:240:LYS:HZ3	1:F:242:ALA:HB2	1.70	0.56
1:F:167:PRO:HD3	1:F:244:THR:HB	1.85	0.56
1:D:392:GLY:O	1:D:397:LYS:HE2	2.05	0.56
1:H:394:THR:HG23	1:H:398:GLU:HG3	1.88	0.56
1:G:131:TYR:CZ	1:G:462:GLN:HA	2.40	0.56
1:B:201:ALA:HB2	2:B:8940:HOH:O	2.04	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: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:358:ASN:O	1:E:362:GLN:HG2	2.05	0.56
1:A:63:VAL:HG11	1:A:235:HIS:CE1	2.41	0.56
1:A:22:ILE:CD1	1:A:221:VAL:HG13	2.36	0.56
1:E:102:LEU:HD21	1:E:203:TYR:HD2	1.70	0.56
1:G:156:HIS:HD2	1:G:488:VAL:HG22	1.69	0.56
1:G:315:TYR:CD1	1:G:409:LYS:HE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:LYS:HE2	2:H:9549:HOH:O	2.05	0.56
1:B:16:GLU:HB3	1:B:18:PHE:CZ	2.41	0.56
1:A:131:TYR:CZ	1:A:462:GLN:HA	2.41	0.56
1:D:418:GLY:O	1:D:422:ASN:HB2	2.06	0.56
1:F:196:GLN:HE21	1:F:196:GLN:N	2.00	0.56
1:A:302:CYS:HB2	1:A:427:LEU:CD2	2.35	0.56
1:G:70:PHE:CZ	1:G:160:GLY:HA2	2.40	0.56
1:H:294:LEU:CD1	1:H:306:SER:HA	2.34	0.56
1:G:294:LEU:CD1	1:G:405:MET:HA	2.36	0.56
1:A:13:GLN:HG2	1:A:335:PHE:CG	2.41	0.56
1:E:61:LYS:HD2	2:E:9482:HOH:O	2.05	0.56
1:E:132:TYR:OH	1:E:477:LEU:HA	2.06	0.56
1:D:276:ILE:HG23	1:D:416:VAL:HG21	1.86	0.56
1:A:405:MET:CE	1:A:407:ILE:HD11	2.36	0.55
1:E:22:ILE:CD1	1:E:222:PRO:HD2	2.35	0.55
1:A:271:GLY:HA2	1:A:425:TYR:CG	2.41	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:D:36:THR:OG1	1:D:50:GLN:HG3	2.05	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:A:11:PRO:HB3	1:A:114:TYR:CE1	2.41	0.55
1:H:240:LYS:HD2	1:H:264:ARG:HB3	1.88	0.55
1:C:36:THR:OG1	1:C:50:GLN:HG3	2.06	0.55
1:C:123:ASP:O	1:C:127:LYS:HG3	2.05	0.55
1:A:124:MET:HE3	1:A:173:LEU:HD22	1.88	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:A:424:THR:HG21	1:A:470:MET:CE	2.36	0.55
1:G:11:PRO:HB3	1:G:114:TYR:CD1	2.40	0.55
1:B:366:LYS:HG2	1:B:368:LEU:CD2	2.35	0.55
1:F:344:GLN:OE1	1:F:403:PRO:HD3	2.06	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:F:240:LYS:HZ1	1:F:242:ALA:HB2	1.70	0.55
1:B:131:TYR:CZ	1:B:462:GLN:HA	2.41	0.55
1:G:427:LEU:HD11	1:G:465:PHE:CZ	2.42	0.55
1:G:292:PHE:CE1	1:G:457:ASP:HB2	2.41	0.55
1:A:489:LYS:HB2	1:B:468:TYR:OH	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:PHE:O	1:E:354:LEU:HG	2.07	0.55
1:D:271:GLY:HA2	1:D:425:TYR:CG	2.42	0.55
1:C:241:VAL:CG1	1:C:265:VAL:HG22	2.37	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:G:255:VAL:CG2	1:H:255:VAL:HG13	2.36	0.55
1:B:294:LEU:HD11	1:B:404:VAL:O	2.07	0.55
1:A:271:GLY:HA2	1:A:425:TYR:CD2	2.41	0.55
1:G:106:GLU:O	1:G:110:ASN:HB3	2.07	0.55
1:B:113:PRO:HB2	1:B:116:ILE:HG12	1.88	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:B:90:ARG:CZ	1:B:94:LEU:HD21	2.37	0.55
1:G:192:LYS:HB2	1:G:232:ILE:CD1	2.37	0.55
1:B:32:VAL:HG21	1:B:57:GLU:HB3	1.89	0.55
1:E:300:GLN:HE22	1:E:345:VAL:N	2.05	0.55
1:B:461:ALA:HA	1:B:477:LEU:HD22	1.89	0.55
1:E:254:GLN:OE1	1:F:262:LEU:HD22	2.07	0.55
1:C:63:VAL:HG11	1:C:235:HIS:CE1	2.42	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:G:255:VAL:HG13	1:H:255:VAL:HG22	1.89	0.54
1:D:258:GLY:HA2	1:D:262:LEU:HD23	1.88	0.54
1:A:8:VAL:HG13	1:A:118:TYR:CD2	2.43	0.54
1:G:292:PHE:HE1	1:G:457:ASP:HB2	1.73	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:311:GLN:OE1	1:D:313:ASP:HB2	2.06	0.54
1:G:372:GLY:O	1:G:382:GLN:HG3	2.07	0.54
1:A:146:ILE:CG1	1:B:460:GLY:HA3	2.38	0.54
1:A:22:ILE:HD13	1:A:221:VAL:HG13	1.89	0.54
1:B:82:SER:HB3	2:B:9159:HOH:O	2.08	0.54
1:H:271:GLY:HA2	1:H:425:TYR:CG	2.43	0.54
1:D:424:THR:O	1:D:470:MET:HB2	2.07	0.54
1:D:63:VAL:HG11	1:D:235:HIS:CE1	2.43	0.54
1:G:23:PHE:CZ	1:G:26:ASN:HA	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:404:VAL:HG12	1:F:406:GLN:OE1	2.07	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:276:ILE:CG2	1:D:416:VAL:HG21	2.38	0.54
1:F:23:PHE:CD2	1:F:205:ALA:HB1	2.43	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:H:99:ARG:HG3	1:H:122:LEU:HD22	1.90	0.54
1:D:41:ASN:HD22	1:D:43:SER:H	1.55	0.54
1:A:303:CYS:SG	1:A:459:PHE:HZ	2.31	0.54
1:B:56:LYS:HE2	1:B:60:ASP:OD1	2.07	0.54
1:A:464:PRO:HG2	1:B:490:THR:OG1	2.08	0.54
1:E:240:LYS:HG3	1:E:264:ARG:HB3	1.90	0.54
1:D:393:MET:O	1:D:397:LYS:HG3	2.07	0.54
1:C:493:VAL:HG13	1:D:453:VAL:HB	1.90	0.54
1:B:302:CYS:HB2	1:B:427:LEU:CD2	2.37	0.54
1:A:442:LEU:O	1:A:446:LEU:HG	2.08	0.54
1:H:33:SER:O	1:H:34:ARG:HB2	2.08	0.54
1:E:135:TRP:CG	1:E:482:LEU:HD11	2.43	0.54
1:G:107:THR:HG23	1:G:112:LYS:O	2.07	0.54
1:B:269:LEU:HD12	1:B:470:MET:O	2.08	0.54
1:D:247:THR:HA	1:D:269:LEU:HD22	1.91	0.53
1:G:238:VAL:O	1:G:263:LYS:HE3	2.08	0.53
1:F:294:LEU:HD13	1:F:405:MET:HA	1.90	0.53
1:A:366:LYS:HB2	2:A:9086:HOH:O	2.08	0.53
1:H:271:GLY:O	1:H:399:GLU:HB2	2.08	0.53
1:B:435:ASP:HB3	1:B:438:LYS:HB2	1.90	0.53
1:E:154:THR:HA	1:E:489:LYS:O	2.09	0.53
1:H:11:PRO:HB3	1:H:114:TYR:CE2	2.43	0.53
1:G:170:PHE:HB3	1:G:173:LEU:HB3	1.89	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:D:294:LEU:HD11	1:D:404:VAL:O	2.07	0.53
1:A:148:GLY:O	1:A:498:LYS:HD3	2.08	0.53
1:F:276:ILE:HG12	1:F:416:VAL:HG21	1.89	0.53
1:B:33:SER:O	1:B:34:ARG:HB2	2.09	0.53
1:H:102:LEU:HD21	1:H:203:TYR:HD2	1.73	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:C:254:GLN:OE1	1:D:262:LEU:HD22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:464:PRO:HA	1:D:476:GLU:O	2.09	0.53
1:B:109:ASP:OD2	1:B:199:LEU:HG	2.09	0.53
1:F:240:LYS:HG2	1:F:241:VAL:N	2.23	0.53
1:C:251:ARG:HA	1:D:262:LEU:HD21	1.90	0.53
1:H:274:PRO:HA	1:H:307:ARG:O	2.08	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:D:473:SER:HA	2:D:9478:HOH:O	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
1:F:36:THR:OG1	1:F:50:GLN:HG3	2.07	0.53
1:A:107:THR:HG23	1:A:112:LYS:O	2.09	0.53
1:H:39:THR:HG23	1:H:48:ILE:HB	1.91	0.53
1:F:63:VAL:HG21	1:F:235:HIS:CD2	2.44	0.53
1:C:99:ARG:HG2	1:C:118:TYR:CE1	2.43	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:H:317:GLU:CG	1:H:321:ARG:HE	2.21	0.53
1:C:257:ALA:HA	1:C:260:SER:OG	2.09	0.53
1:A:187:ASN:HD21	1:A:485:TYR:HB3	1.74	0.53
1:D:139:TYR:CD1	1:D:482:LEU:HD12	2.43	0.53
1:H:243:PHE:CG	1:H:253:ILE:HG13	2.44	0.53
1:F:424:THR:O	1:F:470:MET:HB2	2.09	0.53
1:E:247:THR:CB	1:E:269:LEU:HB3	2.39	0.52
1:H:336:ASP:HB3	1:H:339:THR:OG1	2.08	0.52
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: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:B:138:LYS:HD3	1:D:135:TRP:CE2	2.44	0.52
1:F:247:THR:HA	1:F:269:LEU:CD2	2.37	0.52
1:E:22:ILE:HG22	1:E:24:ILE:HG13	1.89	0.52
1:B:26:ASN:O	1:B:209:LYS:HE3	2.10	0.52
1:F:497:GLN:HG2	1:F:499:ASN:HD21	1.74	0.52
1:D:90:ARG:NH1	1:D:94:LEU:HD21	2.24	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:F:26:ASN:ND2	1:F:215:PRO:HA	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:GLY:HA2	1:C:425:TYR:CG	2.44	0.52
1:H:94:LEU:HB3	1:H:207:LEU:HD22	1.91	0.52
1:G:470:MET:HG2	1:H:261:ASN:O	2.10	0.52
1:D:11:PRO:HB3	1:D:114:TYR:CD1	2.45	0.52
1:F:21:GLN:HB3	1:F:29:HIS:O	2.09	0.52
1:E:247:THR:HA	1:E:269:LEU:CD2	2.36	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:F:131:TYR:CE1	1:F:462:GLN:HB3	2.45	0.52
1:B:311:GLN:NE2	1:B:312:GLU:HG2	2.25	0.52
1:G:120:VAL:HG12	1:G:124:MET:CE	2.40	0.52
1:D:22:ILE:HG22	1:D:24:ILE:HG13	1.91	0.52
1:A:40:VAL:HG22	1:A:47:VAL:HA	1.92	0.52
1:C:358:ASN:O	1:C:362:GLN:HG2	2.09	0.52
1:E:424:THR:HG23	1:E:470:MET:HE2	1.91	0.52
1:A:235:HIS:HB3	1:A:238:VAL:CG2	2.37	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:B:244:THR:HG23	1:B:268:GLU:CB	2.40	0.52
1:D:271:GLY:HA2	1:D:425:TYR:CD2	2.45	0.52
1:D:323:VAL:CG1	1:D:327:LYS:HE3	2.40	0.52
1:B:410:PHE:CD1	1:B:416:VAL:HB	2.45	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:A:89:ASN:ND2	1:A:133:ALA:HB1	2.25	0.52
1:G:453:VAL:HB	1:H:493:VAL:HG13	1.92	0.52
1:E:247:THR:OG1	1:E:269:LEU:HB3	2.10	0.51
1:G:463:SER:O	1:G:477:LEU:HB2	2.10	0.51
1:C:315:TYR:CE1	1:C:409:LYS:HE2	2.45	0.51
1:F:175:GLN:NE2	1:F:204:VAL:HG21	2.25	0.51
1:E:247:THR:CG2	1:E:269:LEU:HD13	2.34	0.51
1:E:244:THR:HG23	1:E:268:GLU:CB	2.40	0.51
1:E:240:LYS:HG2	1:E:241:VAL:N	2.23	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:F:258:GLY:HA2	1:F:262:LEU:HD23	1.91	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:A:461:ALA:HA	1:A:477:LEU:CD2	2.34	0.51
1:G:254:GLN:OE1	1:H:262:LEU:HD22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:431:VAL:HG21	1:H:442:LEU:HB3	1.93	0.51
1:F:121:ASP:O	1:F:125:VAL:HG23	2.10	0.51
1:E:268:GLU:OE2	1:E:476:GLU:OE1	2.28	0.51
1:D:100:THR:HG23	1:D:114:TYR:OH	2.11	0.51
1:C:498:LYS:HD3	2:C:8984:HOH:O	2.11	0.51
1:F:39:THR:HG23	1:F:48:ILE:HB	1.93	0.51
1:F:291:HIS:NE2	1:F:329:ARG:HD2	2.25	0.51
1:D:167:PRO:HD3	1:D:244:THR:HB	1.92	0.51
1:G:63:VAL:HG11	1:G:235:HIS:CE1	2.46	0.51
1:G:244:THR:OG1	1:G:268:GLU:OE1	2.29	0.51
1:D:327:LYS:HE2	1:D:369:CYS:HB3	1.91	0.51
1:H:266:THR:O	1:H:267:LEU:HD23	2.11	0.51
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:H:36:THR:OG1	1:H:50:GLN:HG3	2.10	0.51
1:E:250:GLY:HA2	1:E:253:ILE:HG12	1.92	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:D:235:HIS:HB3	1:D:238:VAL:CG2	2.41	0.51
1:C:294:LEU:HD22	1:C:405:MET:HB2	1.92	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:E:312:GLU:OE1	1:E:411:LYS:HG3	2.10	0.51
1:E:262:LEU:HD13	1:F:269:LEU:HD11	1.92	0.51
1:C:355:GLY:HA2	1:E:50:GLN:NE2	2.25	0.51
1:C:358:ASN:OD1	1:E:50:GLN:HG3	2.11	0.51
1:H:178:LYS:HD3	1:H:476:GLU:OE2	2.11	0.50
1:C:15:PRO:HG2	1:C:108:LEU:HD22	1.93	0.50
1:B:468:TYR:O	1:B:471:SER:HB2	2.10	0.50
1:A:496:PRO:HG2	1:C:441:TYR:HB2	1.93	0.50
1:G:246:SER:HG	1:G:249:ILE:H	1.59	0.50
1:C:487:GLU:HG3	1:D:468:TYR:CZ	2.46	0.50
1:C:313:ASP:HB3	2:C:9454:HOH:O	2.11	0.50
1:F:199:LEU:HB2	2:F:8749:HOH:O	2.10	0.50
1:E:142:LYS:HG3	1:F:480:TYR:OH	2.12	0.50
1:F:294:LEU:CD1	1:F:405:MET:HA	2.42	0.50
1:A:366:LYS:HE2	1:A:368:LEU:CD2	2.40	0.50
1:E:350:PHE:CE2	1:E:354:LEU:HD11	2.46	0.50
1:H:413:ILE:O	1:H:417:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:247:THR:OG1	1:H:269:LEU:HB3	2.11	0.50
1:B:311:GLN:OE1	1:B:313:ASP:HB2	2.12	0.50
1:H:356:TYR:CB	1:H:400:ILE:HG12	2.42	0.50
1:F:271:GLY:HA2	1:F:425:TYR:CG	2.46	0.50
1:B:8:VAL:HG13	1:B:118:TYR:CD2	2.46	0.50
1:G:298:GLN:HG3	1:G:341:GLN:HG3	1.92	0.50
1:G:195:GLU:HG2	1:G:196:GLN:NE2	2.26	0.50
1:A:464:PRO:HG3	1:A:480:TYR:CE1	2.46	0.50
1:B:444:GLN:NE2	1:D:499:ASN:HB2	2.26	0.50
1:H:11:PRO:HB3	1:H:114:TYR:CZ	2.47	0.50
1:D:190:VAL:HG22	1:D:219:ASN:HB2	1.94	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:D:13:GLN:HA	1:D:335:PHE:CE1	2.46	0.50
1:A:465:PHE:HB2	1:A:477:LEU:HD12	1.94	0.50
1:A:363:GLU:HG3	2:A:9084:HOH:O	2.10	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:476:GLU:O	1:C:477:LEU:HB2	2.12	0.50
1:C:120:VAL:HG12	1:C:124:MET:CE	2.40	0.50
1:H:132:TYR:CE2	1:H:181:PRO:HB3	2.46	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
2:A:8696:HOH:O	1:D:498:LYS:HE3	2.12	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:294:LEU:HD12	1:A:306:SER:HA	1.93	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:126:LEU:O	1:A:130:ARG:HG3	2.11	0.50
1:E:131:TYR:CZ	1:E:462:GLN:HA	2.47	0.50
1:A:140:HIS:ND1	1:D:142:LYS:HD3	2.27	0.50
1:C:347:GLU:OE1	1:E:347:GLU:OE1	2.30	0.50
1:A:251:ARG:CG	1:B:262:LEU:HD21	2.42	0.50
1:F:315:TYR:CD2	1:F:409:LYS:HG3	2.46	0.50
1:E:257:ALA:HA	1:E:260:SER:OG	2.12	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:E:424:THR:HG21	1:E:470:MET:CE	2.39	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:251:ARG:O	1:E:255:VAL:HG23	2.11	0.49
1:A:25:ASN:HA	1:A:216:GLY:N	2.27	0.49
1:G:79:MET:SD	1:G:83:HIS:HD2	2.35	0.49
1:F:175:GLN:HE22	1:F:204:VAL:HG21	1.76	0.49
1:E:79:MET:SD	1:E:83:HIS:HD2	2.35	0.49
1:A:36:THR:HB	1:A:51:VAL:O	2.13	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:236:GLU:OE2	1:A:260:SER:HB2	2.13	0.49
1:G:487:GLU:HG3	1:H:468:TYR:CE1	2.47	0.49
1:E:264:ARG:HH22	1:F:474:GLY:N	2.11	0.49
1:D:106:GLU:OE2	1:D:171:PRO:HB2	2.12	0.49
1:A:413:ILE:HD11	1:A:442:LEU:HG	1.94	0.49
1:D:323:VAL:HG13	1:D:327:LYS:HE3	1.95	0.49
1:G:275:ASN:HD22	1:G:430:ALA:HB3	1.75	0.49
1:A:374:ALA:HB2	1:A:382:GLN:CG	2.43	0.49
1:D:425:TYR:O	1:D:469:LYS:HD2	2.11	0.49
1:A:431:VAL:HG21	1:A:442:LEU:HB3	1.94	0.49
1:F:361:LYS:HD2	1:F:367:LEU:HD22	1.94	0.49
1:B:370:GLY:HA2	1:B:382:GLN:OE1	2.13	0.49
1:H:124:MET:HE3	1:H:173:LEU:HD22	1.94	0.49
1:F:294:LEU:HD12	1:F:306:SER:HA	1.93	0.49
1:A:300:GLN:HE22	1:A:345:VAL:H	1.61	0.49
1:G:344:GLN:HG3	1:G:353:ILE:HD12	1.94	0.49
1:G:161:VAL:HA	1:G:188:VAL:HG23	1.94	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:G:483:GLN:NE2	2:G:8808:HOH:O	2.45	0.49
1:D:249:ILE:O	1:D:252:VAL:HB	2.13	0.49
1:C:424:THR:CG2	1:C:470:MET:HB2	2.34	0.49
1:B:465:PHE:O	1:B:476:GLU:N	2.44	0.49
1:A:173:LEU:HD11	1:A:177:TRP:NE1	2.27	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:462:GLN:HB2	2:D:9062:HOH:O	2.13	0.49
1:E:489:LYS:HB2	1:F:468:TYR:OH	2.13	0.49
1:B:413:ILE:HG12	1:B:441:TYR:CE2	2.47	0.49
1:E:410:PHE:CD1	1:E:416:VAL:HB	2.48	0.49
1:A:21:GLN:O	1:A:28:TRP:HZ3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:HIS:HB3	1:B:238:VAL:HG23	1.95	0.48
1:D:99:ARG:HG2	1:D:118:TYR:CE1	2.48	0.48
1:A:79:MET:SD	1:A:83:HIS:HD2	2.36	0.48
1:F:276:ILE:HG12	1:F:416:VAL:CG2	2.43	0.48
1:A:374:ALA:HB2	1:A:382:GLN:HG2	1.94	0.48
1:H:168:TRP:O	1:H:171:PRO:HD3	2.13	0.48
1:D:155:ARG:HD2	2:D:8727:HOH:O	2.13	0.48
1:C:154:THR:HA	1:C:489:LYS:O	2.13	0.48
1:D:460:GLY:O	1:D:477:LEU:HD13	2.13	0.48
1:A:468:TYR:O	1:A:471:SER:HB2	2.14	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:D:22:ILE:HG12	1:D:222:PRO:HD2	1.94	0.48
1:C:37:PHE:HD2	1:C:53:GLU:HB2	1.78	0.48
1:C:25:ASN:HA	1:C:216:GLY:N	2.29	0.48
1:F:107:THR:CG2	1:F:334:PRO:HB2	2.44	0.48
1:E:302:CYS:HB2	1:E:427:LEU:CD2	2.44	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: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:A:322:SER:HB3	1:A:405:MET:CE	2.43	0.48
1:H:276:ILE:CD1	1:H:446:LEU:HD11	2.37	0.48
1:G:269:LEU:CD1	1:H:262:LEU:HD13	2.44	0.48
1:G:392:GLY:O	1:G:397:LYS:HE2	2.14	0.48
1:G:33:SER:O	1:G:34:ARG:HB2	2.12	0.48
1:D:294:LEU:CD1	1:D:405:MET:HA	2.43	0.48
1:G:366:LYS:HE2	1:G:368:LEU:CD2	2.39	0.48
1:C:344:GLN:HG3	1:C:353:ILE:HD12	1.95	0.48
1:B:449:GLY:HA2	1:B:468:TYR:CE1	2.49	0.48
1:B:413:ILE:HG12	1:B:441:TYR:HE2	1.78	0.48
1:E:33:SER:O	1:E:34:ARG:HB2	2.13	0.48
1:C:356:TYR:CG	1:C:400:ILE:HG12	2.48	0.48
1:B:11:PRO:HB3	1:B:114:TYR:CE2	2.49	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:C:131:TYR:CZ	1:C:462:GLN:HA	2.49	0.48
1:F:39:THR:HG22	1:F:49:CYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:240:LYS:HG2	1:D:241:VAL:N	2.28	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: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: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:B:441:TYR:CD2	1:B:442:LEU:HD23	2.48	0.48
1:A:353:ILE:O	1:A:357:ILE:HG13	2.13	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: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:298:GLN:HG3	1:A:341:GLN:HG3	1.96	0.48
1:A:138:LYS:HD3	1:C:135:TRP:CE2	2.48	0.47
1:D:163:GLY:O	1:D:241:VAL:HA	2.13	0.47
1:E:80:ASP:OD1	1:H:498:LYS:NZ	2.47	0.47
1:B:353:ILE:O	1:B:357:ILE:HG13	2.13	0.47
1:A:172:LEU:CD2	1:A:200:THR:HB	2.39	0.47
1:F:44:THR:HA	1:F:377:ARG:CD	2.42	0.47
1:E:263:LYS:O	1:E:265:VAL:HG23	2.14	0.47
1:D:291:HIS:CE1	1:D:326:ALA:HA	2.48	0.47
1:G:345:VAL:HG12	1:G:349:GLN:HG3	1.97	0.47
1:A:281:ALA:HB2	1:A:432:PHE:O	2.14	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: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:395:ILE:HD12	1:F:406:GLN:HG3	1.96	0.47
1:C:100:THR:HG22	2:C:8954:HOH:O	2.14	0.47
1:H:71:GLN:NE2	1:H:71:GLN:HA	2.30	0.47
1:F:107:THR:HG23	1:F:334:PRO:HB2	1.95	0.47
1:G:44:THR:HA	1:G:377:ARG:HD3	1.95	0.47
1:E:15:PRO:HD2	1:E:108:LEU:HD13	1.96	0.47
1:B:94:LEU:HB3	1:B:207:LEU:HD22	1.96	0.47
1:A:17:VAL:HG13	2:A:9055:HOH:O	2.15	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:C:100:THR:HG23	1:C:114:TYR:OH	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:PRO:HB3	1:C:114:TYR:CE2	2.49	0.47
1:A:241:VAL:HG13	1:A:241:VAL:O	2.15	0.47
1:F:435:ASP:HB3	1:F:438:LYS:HB2	1.94	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:G:255:VAL:HG13	1:H:255:VAL:CG2	2.44	0.47
1:E:257:ALA:HB1	1:E:263:LYS:HG3	1.97	0.47
1:F:327:LYS:HE3	1:F:369:CYS:HB3	1.96	0.47
1:F:28:TRP:CZ3	1:F:202:LEU:HD22	2.50	0.47
1:F:247:THR:HG23	1:F:269:LEU:CB	2.45	0.47
1:E:436:LEU:N	2:E:8837:HOH:O	2.48	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:D:498:LYS:HE2	1:D:498:LYS:HB3	1.70	0.47
1:A:215:PRO:HG3	2:A:8907:HOH:O	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:E:271:GLY:HA2	1:E:425:TYR:HB3	1.97	0.47
1:B:132:TYR:OH	1:B:477:LEU:HA	2.15	0.47
1:A:116:ILE:O	1:A:120:VAL:HB	2.15	0.47
1:G:347:GLU:O	1:G:351:LYS:HE2	2.15	0.47
1:D:73:GLY:HA2	1:D:78:ARG:HD2	1.97	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:H:75:PRO:HG2	2:H:9364:HOH:O	2.15	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:D:161:VAL:N	1:D:239:ASP:OD2	2.44	0.47
1:E:440:ASN:HD22	1:G:495:VAL:HG12	1.79	0.47
2:E:8837:HOH:O	1:H:436:LEU:N	2.47	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:G:96:GLU:O	1:G:99:ARG:HB2	2.14	0.47
1:G:240:LYS:HG3	1:G:241:VAL:N	2.30	0.47
1:E:283:MET:N	2:E:8830:HOH:O	2.48	0.47
1:B:106:GLU:O	1:B:110:ASN:HB3	2.15	0.47
1:H:40:VAL:HG13	1:H:46:GLU:O	2.15	0.46
1:G:315:TYR:CD2	1:G:409:LYS:HG3	2.49	0.46
1:D:126:LEU:HD12	2:D:9168:HOH:O	2.14	0.46
1:C:487:GLU:HG3	1:D:468:TYR:CE1	2.51	0.46
1:B:241:VAL:HG13	1:B:265:VAL:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:CYS:HB2	1:D:427:LEU:CD2	2.45	0.46
1:E:271:GLY:HA2	1:E:425:TYR:CG	2.51	0.46
1:E:264:ARG:HH22	1:F:474:GLY:H	1.63	0.46
1:A:187:ASN:ND2	1:A:485:TYR:HB3	2.29	0.46
1:B:431:VAL:HG21	1:B:442:LEU:HB3	1.97	0.46
1:B:359:THR:O	1:B:363:GLU:HG3	2.15	0.46
1:A:312:GLU:HB3	2:A:9097:HOH:O	2.15	0.46
1:D:356:TYR:CG	1:D:400:ILE:HG12	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:H:344:GLN:HG3	1:H:353:ILE:CD1	2.46	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:A:106:GLU:O	1:A:110:ASN:HB3	2.16	0.46
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:B:107:THR:CG2	1:B:334:PRO:HB2	2.46	0.46
1:H:435:ASP:HB3	1:H:438:LYS:HB2	1.98	0.46
1:E:307:ARG:NH1	2:E:9314:HOH:O	2.48	0.46
1:A:476:GLU:O	1:A:477:LEU:HB2	2.16	0.46
1:G:424:THR:HG22	1:G:424:THR:O	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:A:56:LYS:HE2	1:A:60:ASP:OD2	2.15	0.46
1:C:424:THR:O	1:C:424:THR:HG22	2.15	0.46
1:F:120:VAL:HG12	1:F:124:MET:CE	2.46	0.46
1:E:120:VAL:HG12	1:E:124:MET:CE	2.43	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:C:241:VAL:HG13	1:C:265:VAL:HG13	1.98	0.46
1:H:33:SER:HB2	1:H:35:LYS:HD3	1.97	0.46
1:A:18:PHE:HD1	1:A:101:TYR:HH	1.63	0.46
1:B:369:CYS:SG	1:B:385:VAL:HG23	2.56	0.46
1:G:294:LEU:HD11	1:G:405:MET:HA	1.98	0.46
1:E:306:SER:O	1:E:406:GLN:HB2	2.15	0.46
1:F:348:THR:HA	1:F:351:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:TYR:OH	1:D:477:LEU:HA	2.16	0.46
1:E:76:TRP:CH2	1:E:84:ARG:HD2	2.51	0.46
1:E:428:ALA:HB1	1:E:452:TRP:CZ3	2.51	0.46
1:D:347:GLU:O	1:D:350:PHE:HB3	2.15	0.46
1:H:132:TYR:OH	1:H:477:LEU:HA	2.16	0.46
1:B:413:ILE:CG1	1:B:442:LEU:HD21	2.46	0.46
1:C:144:ILE:CG2	1:D:462:GLN:HB2	2.45	0.46
1:D:374:ALA:HB3	1:D:380:PHE:HB3	1.97	0.46
1:F:323:VAL:HG21	1:F:368:LEU:HB3	1.98	0.46
1:H:131:TYR:CZ	1:H:462:GLN:HA	2.51	0.46
1:A:170:PHE:HB3	1:A:173:LEU:HB3	1.98	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:A:376:ASP:N	1:A:376:ASP:OD1	2.49	0.46
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: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: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
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:C:350:PHE:CD1	1:C:379:TYR:HB3	2.52	0.45
1:E:43:SER:HA	1:E:343:PRO:HG3	1.99	0.45
1:H:43:SER:OG	1:H:334:PRO:HG3	2.16	0.45
1:B:463:SER:O	1:B:477:LEU:HB2	2.17	0.45
1:A:413:ILE:O	1:A:416:VAL:HG12	2.16	0.45
1:H:317:GLU:HG2	1:H:321:ARG:HE	1.80	0.45
1:B:413:ILE:HG12	1:B:442:LEU:HD21	1.97	0.45
1:E:131:TYR:CE1	1:E:462:GLN:HB3	2.51	0.45
1:D:308:THR:HB	1:D:407:ILE:HA	1.98	0.45
1:A:388:ASP:O	1:A:390:GLN:NE2	2.50	0.45
1:E:344:GLN:HG3	1:E:353:ILE:CD1	2.46	0.45
1:H:460:GLY:HA3	1:H:462:GLN:HE21	1.81	0.45
1:A:173:LEU:HD11	1:A:177:TRP:HE1	1.82	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:E:155:ARG:NE	1:E:157:GLU:OE2	2.44	0.45
1:H:159:VAL:N	1:H:187:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:THR:OG1	1:D:187:ASN:ND2	2.50	0.45
1:A:317:GLU:OE1	1:A:321:ARG:NH2	2.47	0.45
1:B:465:PHE:N	1:B:476:GLU:O	2.50	0.45
1:B:315:TYR:CD1	1:B:409:LYS:HE2	2.51	0.45
1:A:424:THR:O	1:A:424:THR:HG22	2.16	0.45
1:D:8:VAL:HG13	1:D:118:TYR:CD2	2.52	0.45
1:D:476:GLU:O	1:D:477:LEU:HB2	2.17	0.45
1:D:192:LYS:NZ	2:D:9260:HOH:O	2.50	0.45
1:A:323:VAL:HG12	1:A:327:LYS:HD2	1.98	0.45
1:E:100:THR:HG22	2:E:9298:HOH:O	2.15	0.45
1:A:356:TYR:HE2	1:A:398:GLU:OE2	2.00	0.45
1:A:483:GLN:NE2	1:B:483:GLN:OE1	2.50	0.45
1:F:170:PHE:HZ	1:F:301:CYS:HG	1.65	0.45
1:E:281:ALA:HB2	1:E:432:PHE:O	2.16	0.45
1:C:465:PHE:N	1:C:476:GLU:O	2.50	0.45
1:F:23:PHE:HA	1:F:27:GLU:O	2.16	0.45
1:D:421:ASN:ND2	1:D:445:ALA:O	2.50	0.45
1:G:408:LEU:HD23	1:G:419:ARG:HH11	1.80	0.45
1:A:424:THR:CG2	1:A:470:MET:HE2	2.44	0.45
1:E:440:ASN:ND2	2:E:9358:HOH:O	2.50	0.45
1:H:303:CYS:SG	1:H:459:PHE:HZ	2.40	0.45
1:E:217:VAL:HG12	1:E:218:VAL:HG23	1.99	0.45
1:G:103:ALA:HB2	1:G:122:LEU:HD13	1.98	0.45
1:F:476:GLU:O	1:F:477:LEU:HB2	2.16	0.45
1:H:244:THR:HG23	1:H:268:GLU:HG3	1.99	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: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:498:LYS:HG2	1:F:499:ASN:N	2.32	0.45
1:B:32:VAL:HG11	1:B:57:GLU:OE1	2.17	0.45
1:G:240:LYS:HG2	2:G:9550:HOH:O	2.16	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:H:241:VAL:HG13	1:H:241:VAL:O	2.17	0.45
1:A:90:ARG:HH21	1:A:94:LEU:CD2	2.25	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:E:358:ASN:HD22	1:E:361:LYS:NZ	2.15	0.45
1:B:431:VAL:HG11	1:B:442:LEU:HD12	1.99	0.45
1:G:260:SER:O	1:H:251:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:PHE:HZ	1:D:301:CYS:HG	1.63	0.45
1:A:290:ALA:N	2:A:9077:HOH:O	2.50	0.45
1:A:260:SER:OG	1:A:263:LYS:NZ	2.50	0.45
1:G:254:GLN:OE1	1:H:262:LEU:CD2	2.64	0.45
1:H:41:ASN:ND2	2:H:8792:HOH:O	2.49	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:F:315:TYR:CG	1:F:409:LYS:HE2	2.51	0.45
1:G:315:TYR:CE1	1:G:319:VAL:HG21	2.52	0.45
1:A:22:ILE:HD11	1:A:54:GLY:CA	2.47	0.45
1:A:159:VAL:HG12	1:A:187:ASN:OD1	2.16	0.45
1:D:159:VAL:N	1:D:187:ASN:OD1	2.50	0.45
1:G:76:TRP:CH2	1:G:84:ARG:HD2	2.52	0.45
1:G:11:PRO:HB3	1:G:114:TYR:CZ	2.52	0.45
1:E:70:PHE:CZ	1:E:158:PRO:HB2	2.52	0.45
1:E:363:GLU:CD	1:E:394:THR:H	2.20	0.45
1:H:444:GLN:NE2	2:H:8804:HOH:O	2.50	0.45
1:C:449:GLY:HA2	1:C:468:TYR:CE1	2.51	0.45
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:D:71:GLN:O	1:D:74:SER:HB3	2.17	0.44
1:F:465:PHE:N	1:F:476:GLU:O	2.50	0.44
1:D:417:VAL:HG11	1:D:445:ALA:HB1	1.99	0.44
1:C:260:SER:OG	1:C:263:LYS:NZ	2.49	0.44
1:B:99:ARG:HD3	1:B:118:TYR:CZ	2.52	0.44
1:E:79:MET:HB3	2:E:8814:HOH:O	2.17	0.44
1:E:273:SER:HB2	1:E:304:ALA:O	2.17	0.44
1:A:267:LEU:O	1:A:473:SER:N	2.50	0.44
1:D:260:SER:OG	1:D:263:LYS:NZ	2.50	0.44
1:A:48:ILE:HD11	1:A:109:ASP:HA	1.98	0.44
1:H:465:PHE:N	1:H:476:GLU:O	2.49	0.44
1:E:294:LEU:HD13	1:E:405:MET:HA	2.00	0.44
1:A:344:GLN:HG3	1:A:353:ILE:HD12	2.00	0.44
1:F:208:ILE:HD13	1:F:218:VAL:HG11	2.00	0.44
1:E:208:ILE:HG23	1:E:213:PHE:CD1	2.52	0.44
1:E:159:VAL:N	1:E:187:ASN:OD1	2.50	0.44
1:A:272:LYS:HA	1:A:306:SER:OG	2.17	0.44
1:F:26:ASN:N	2:F:8842:HOH:O	2.50	0.44
1:A:373:ILE:HG22	1:A:375:ALA:H	1.82	0.44
1:D:363:GLU:CD	1:D:394:THR:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:THR:OG1	1:D:109:ASP:OD1	2.35	0.44
1:E:251:ARG:CA	1:F:262:LEU:HD21	2.46	0.44
1:F:8:VAL:HG13	1:F:118:TYR:CG	2.51	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:332:GLY:HA3	2:A:9079:HOH:O	2.17	0.44
1:G:272:LYS:HE2	1:G:396:ALA:C	2.38	0.44
1:B:253:ILE:HD13	1:B:253:ILE:N	2.32	0.44
1:E:498:LYS:HB3	1:E:498:LYS:HE2	1.81	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:G:172:LEU:CG	1:G:200:THR:HB	2.48	0.44
1:C:262:LEU:HD21	1:D:251:ARG:HG2	1.99	0.44
1:A:291:HIS:O	1:A:295:PHE:HB2	2.17	0.44
1:G:476:GLU:O	1:G:477:LEU:HB2	2.18	0.44
1:F:60:ASP:OD1	1:F:235:HIS:NE2	2.50	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: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:C:142:LYS:NZ	2:C:8658:HOH:O	2.50	0.44
1:E:138:LYS:HD3	1:G:135:TRP:CE2	2.53	0.44
1:C:21:GLN:HB3	1:C:29:HIS:O	2.17	0.44
1:C:297:ASN:ND2	1:C:300:GLN:O	2.50	0.44
1:G:357:ILE:HG22	1:G:361:LYS:HE2	1.99	0.44
1:A:13:GLN:HB3	2:A:8906:HOH:O	2.17	0.44
1:A:468:TYR:CE1	1:B:487:GLU:HG3	2.52	0.44
1:B:308:THR:HB	1:B:407:ILE:HA	1.99	0.44
1:A:273:SER:N	2:A:9073:HOH:O	2.50	0.44
1:F:102:LEU:HD21	1:F:203:TYR:HD2	1.81	0.44
1:D:246:SER:HG	1:D:249:ILE:HD12	1.82	0.44
1:E:247:THR:HG21	1:E:425:TYR:HE2	1.82	0.44
1:D:417:VAL:HG22	1:D:442:LEU:HD23	1.99	0.44
1:E:260:SER:OG	1:E:263:LYS:NZ	2.50	0.44
1:A:460:GLY:HA3	1:A:463:SER:HB2	1.98	0.44
1:D:160:GLY:HA3	1:D:239:ASP:OD2	2.17	0.44
1:E:170:PHE:O	1:E:174:MET:HG2	2.18	0.44
1:D:198:PRO:O	1:D:202:LEU:HG	2.18	0.44
1:E:291:HIS:ND1	1:E:325:ARG:HG3	2.32	0.44
1:A:142:LYS:O	1:A:153:TYR:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:ALA:O	1:E:263:LYS:NZ	2.50	0.44
1:C:106:GLU:OE2	1:C:171:PRO:HB2	2.17	0.44
1:H:77:ARG:HG3	1:H:77:ARG:HH11	1.83	0.44
1:G:294:LEU:HD21	1:G:404:VAL:C	2.38	0.43
1:D:22:ILE:HD13	1:D:58:ASP:HB3	2.00	0.43
1:E:452:TRP:HB3	1:E:455:CYS:O	2.18	0.43
1:E:348:THR:O	1:E:352:LYS:HB2	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:A:453:VAL:HB	1:B:493:VAL:HG13	2.00	0.43
1:C:196:GLN:H	1:C:196:GLN:NE2	2.14	0.43
1:B:122:LEU:O	1:B:126:LEU:HG	2.18	0.43
1:E:253:ILE:N	1:E:253:ILE:HD13	2.33	0.43
1:D:404:VAL:HG12	1:D:406:GLN:OE1	2.17	0.43
1:A:55:ASP:N	1:A:58:ASP:OD2	2.49	0.43
1:H:135:TRP:CG	1:H:482:LEU:HD11	2.53	0.43
1:D:103:ALA:HB2	1:D:122:LEU:HD13	1.99	0.43
1:E:275:ASN:HD22	1:E:430:ALA:HB3	1.82	0.43
1:D:94:LEU:O	1:D:97:ARG:HB3	2.18	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:B:193:VAL:HG22	1:B:222:PRO:HA	1.99	0.43
1:E:490:THR:HG1	1:F:464:PRO:HG2	1.83	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: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:67:ARG:O	1:E:71:GLN:NE2	2.50	0.43
1:H:28:TRP:HH2	1:H:202:LEU:O	2.01	0.43
1:F:302:CYS:O	1:F:427:LEU:HD23	2.18	0.43
1:H:461:ALA:CA	1:H:477:LEU:HD22	2.47	0.43
1:E:264:ARG:NH2	1:F:474:GLY:H	2.16	0.43
1:B:330:VAL:HG12	1:B:339:THR:HA	2.00	0.43
1:C:465:PHE:C	1:C:475:GLN:HB3	2.39	0.43
1:D:168:TRP:CZ2	1:D:345:VAL:HG11	2.54	0.43
1:A:399:GLU:HG3	2:A:9095:HOH:O	2.17	0.43
1:E:241:VAL:HG12	1:E:265:VAL:HG22	1.99	0.43
1:A:245:GLY:HA3	2:A:9070:HOH:O	2.18	0.43
1:D:112:LYS:HE2	1:D:112:LYS:HB3	1.77	0.43
1:E:424:THR:O	1:E:470:MET:HB2	2.18	0.43
1:H:42:PRO:HD2	2:H:8792:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:TYR:CE1	1:F:319:VAL:HG21	2.53	0.43
1:H:102:LEU:HD21	1:H:203:TYR:CD2	2.53	0.43
1:A:27:GLU:O	1:A:29:HIS:HD2	2.01	0.43
1:G:460:GLY:HA3	1:H:146:ILE:HG13	2.00	0.43
1:E:418:GLY:O	1:E:422:ASN:HB2	2.18	0.43
1:B:294:LEU:O	1:B:299:GLY:HA2	2.19	0.43
1:G:31:ALA:O	1:G:34:ARG:NH1	2.52	0.43
1:C:490:THR:OG1	1:D:464:PRO:HG2	2.19	0.43
1:H:71:GLN:O	1:H:74:SER:HB3	2.19	0.43
1:G:161:VAL:HA	1:G:188:VAL:CG2	2.49	0.43
1:D:208:ILE:HD13	1:D:218:VAL:HG11	2.00	0.43
1:H:235:HIS:HB3	1:H:238:VAL:HG23	2.00	0.43
1:G:269:LEU:HD13	1:H:262:LEU:HD13	2.01	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:H:334:PRO:HG2	2:H:8787:HOH:O	2.19	0.43
1:B:459:PHE:HE2	1:B:465:PHE:CD1	2.37	0.43
1:A:198:PRO:O	1:A:202:LEU:HG	2.19	0.43
1:E:23:PHE:CG	1:E:205:ALA:HB1	2.54	0.43
1:D:123:ASP:OD1	1:D:127:LYS:HE3	2.19	0.43
1:A:258:GLY:HA3	1:B:254:GLN:HG2	2.00	0.43
1:A:175:GLN:HE22	1:A:201:ALA:HA	1.84	0.43
1:D:81:ALA:O	1:D:136:ALA:HB1	2.19	0.43
1:H:247:THR:HA	1:H:269:LEU:CD2	2.32	0.42
1:A:350:PHE:CE1	1:A:381:ILE:HG13	2.54	0.42
1:E:102:LEU:HD21	1:E:203:TYR:CD2	2.52	0.42
1:B:82:SER:N	2:B:9159:HOH:O	2.50	0.42
1:H:317:GLU:OE1	1:H:321:ARG:NH2	2.50	0.42
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:F:298:GLN:NE2	2:F:8848:HOH:O	2.52	0.42
1:B:171:PRO:HG3	1:B:197:THR:HG21	2.01	0.42
1:A:13:GLN:HE21	1:A:335:PHE:HD1	1.60	0.42
1:B:8:VAL:HA	1:B:9:PRO:HD3	1.92	0.42
1:C:366:LYS:HE2	1:C:368:LEU:CD2	2.49	0.42
1:C:346:ASP:O	1:C:350:PHE:HB2	2.19	0.42
1:H:315:TYR:O	1:H:319:VAL:HG23	2.19	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:B:443:SER:HA	1:B:451:VAL:HG11	2.01	0.42
1:B:331:VAL:HA	1:B:341:GLN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:131:TYR:O	1:D:138:LYS:NZ	2.52	0.42
1:H:408:LEU:N	1:H:408:LEU:HD12	2.34	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:C:287:VAL:HG22	1:C:318:PHE:CD1	2.54	0.42
1:C:164:GLN:CD	1:C:178:LYS:HB3	2.39	0.42
1:G:23:PHE:HB2	1:G:28:TRP:CZ3	2.54	0.42
1:F:41:ASN:ND2	1:F:43:SER:H	2.16	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:H:256:ALA:O	1:H:260:SER:HB3	2.19	0.42
1:C:241:VAL:O	1:C:241:VAL:HG13	2.19	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:D:71:GLN:HA	1:D:71:GLN:NE2	2.35	0.42
1:H:250:GLY:O	1:H:253:ILE:HB	2.20	0.42
1:C:107:THR:CG2	1:C:334:PRO:HB2	2.49	0.42
1:B:246:SER:OG	1:B:249:ILE:HG12	2.19	0.42
1:A:275:ASN:ND2	2:A:9074:HOH:O	2.51	0.42
1:G:371:GLY:N	1:G:384:THR:OG1	2.53	0.42
1:C:435:ASP:HB3	1:C:438:LYS:HD2	2.01	0.42
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:B:167:PRO:HG2	1:B:174:MET:HG3	2.01	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:E:494:LYS:NZ	2:E:8642:HOH:O	2.48	0.42
1:A:465:PHE:N	1:A:476:GLU:O	2.49	0.42
1:C:240:LYS:HG3	1:C:264:ARG:HB3	2.02	0.42
1:B:26:ASN:N	2:B:8933:HOH:O	2.50	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:D:246:SER:OG	1:D:248:GLU:HB3	2.19	0.42
1:F:132:TYR:OH	1:F:477:LEU:HA	2.20	0.42
1:A:496:PRO:HD2	2:A:9139:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:THR:HG23	1:B:482:LEU:HD22	2.01	0.42
1:D:415:GLU:OE2	1:D:419:ARG:NH2	2.50	0.42
1:D:362:GLN:NE2	2:D:8631:HOH:O	2.53	0.42
1:A:464:PRO:HB3	1:A:480:TYR:HD1	1.85	0.42
1:A:22:ILE:HD11	1:A:54:GLY:HA3	2.02	0.42
1:H:243:PHE:CB	1:H:253:ILE:HG13	2.50	0.42
1:D:124:MET:HE3	1:D:173:LEU:CD2	2.41	0.42
1:G:238:VAL:HB	1:G:263:LYS:HE2	2.02	0.42
1:E:465:PHE:N	1:E:476:GLU:O	2.50	0.42
1:B:346:ASP:O	1:B:350:PHE:HB2	2.20	0.42
1:A:446:LEU:O	1:B:489:LYS:NZ	2.48	0.42
1:G:112:LYS:HB3	1:G:112:LYS:HE2	1.70	0.42
1:E:468:TYR:O	1:E:471:SER:HB2	2.19	0.42
1:B:170:PHE:HB3	1:B:173:LEU:HB3	2.01	0.42
1:C:273:SER:HA	1:C:274:PRO:HD3	1.95	0.42
1:A:142:LYS:HD2	1:B:480:TYR:CZ	2.54	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:B:363:GLU:CD	1:B:394:THR:H	2.22	0.41
1:A:473:SER:HA	2:A:8661:HOH:O	2.19	0.41
1:C:125:VAL:HG22	1:C:173:LEU:HA	2.01	0.41
1:G:294:LEU:HD13	2:G:8881:HOH:O	2.19	0.41
1:E:244:THR:HA	1:E:268:GLU:HB2	2.02	0.41
1:H:113:PRO:O	1:H:116:ILE:HB	2.20	0.41
1:B:465:PHE:O	1:B:475:GLN:HA	2.20	0.41
1:B:112:LYS:HE2	1:B:112:LYS:HB3	1.79	0.41
1:G:185:THR:OG1	1:G:187:ASN:ND2	2.53	0.41
1:A:347:GLU:O	1:A:351:LYS:HG3	2.20	0.41
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:D:44:THR:CB	1:D:46:GLU:HG2	2.50	0.41
1:F:44:THR:HA	1:F:377:ARG:NE	2.36	0.41
1:G:82:SER:O	1:G:86:ARG:HG2	2.20	0.41
1:A:131:TYR:CE1	1:A:462:GLN:HB3	2.55	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:H:435:ASP:OD1	1:H:438:LYS:HG3	2.20	0.41
1:C:21:GLN:O	1:C:28:TRP:HZ3	2.03	0.41
1:D:20:ASN:O	1:D:51:VAL:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:GLY:HA3	2:D:9467:HOH:O	2.21	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:F:473:SER:HA	2:F:8764:HOH:O	2.20	0.41
1:A:35:LYS:HE2	2:A:8909:HOH:O	2.20	0.41
1:D:226:PRO:O	1:D:230:ALA:HB3	2.20	0.41
1:H:346:ASP:HA	1:H:379:TYR:CE1	2.55	0.41
1:B:460:GLY:CA	1:B:462:GLN:HE21	2.34	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: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:D:131:TYR:CZ	1:D:462:GLN:HA	2.56	0.41
1:F:166:ILE:HG22	1:F:178:LYS:HE2	2.01	0.41
1:D:25:ASN:C	1:D:215:PRO:HB3	2.41	0.41
1:H:24:ILE:HD13	1:H:61:LYS:HB3	2.02	0.41
1:F:146:ILE:HG21	1:F:150:PHE:HB2	2.01	0.41
1:G:249:ILE:HD13	1:G:249:ILE:N	2.35	0.41
1:F:243:PHE:HB3	1:F:267:LEU:HD22	2.01	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:H:87:LEU:HB3	1:H:213:PHE:CE1	2.56	0.41
1:G:449:GLY:HA2	1:G:468:TYR:CE1	2.54	0.41
1:A:13:GLN:NE2	1:A:335:PHE:HB2	2.36	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:G:8:VAL:HA	1:G:9:PRO:HD3	1.95	0.41
1:E:56:LYS:O	1:E:60:ASP:OD1	2.39	0.41
1:A:498:LYS:HB3	1:A:498:LYS:HE2	1.90	0.41
1:H:131:TYR:CE1	1:H:462:GLN:HB3	2.56	0.41
1:F:249:ILE:N	1:F:249:ILE:HD13	2.36	0.41
1:B:249:ILE:HD13	1:B:249:ILE:N	2.35	0.41
1:G:333:ASN:HA	1:G:334:PRO:HD2	1.91	0.41
1:F:106:GLU:O	1:F:110:ASN:HB3	2.20	0.41
1:A:370:GLY:HA3	1:A:383:PRO:O	2.21	0.41
1:H:249:ILE:HD13	1:H:249:ILE:N	2.36	0.41
1:A:350:PHE:HZ	1:A:373:ILE:HD13	1.80	0.41
1:A:253:ILE:HG22	1:A:265:VAL:HG11	2.02	0.41
1:B:323:VAL:CG1	1:B:327:LYS:HE3	2.50	0.41
1:F:415:GLU:O	1:F:419:ARG:HG3	2.21	0.41
1:E:166:ILE:CG2	1:E:178:LYS:HG3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:LEU:HB3	1:G:213:PHE:CZ	2.56	0.41
1:D:275:ASN:HD21	1:D:432:PHE:HE1	1.66	0.41
1:G:89:ASN:OD1	1:G:130:ARG:HG2	2.21	0.41
1:H:113:PRO:HA	1:H:334:PRO:O	2.21	0.41
1:C:34:ARG:NH2	2:C:9202:HOH:O	2.51	0.41
1:C:261:ASN:OD1	1:C:263:LYS:HG2	2.21	0.41
1:G:11:PRO:HB3	1:G:114:TYR:CG	2.56	0.41
1:F:175:GLN:HE22	1:F:204:VAL:CG2	2.34	0.41
1:C:148:GLY:O	1:C:498:LYS:HE2	2.21	0.41
1:G:466:GLY:N	2:G:8892:HOH:O	2.45	0.41
1:F:164:GLN:CD	1:F:178:LYS:HB3	2.41	0.41
1:B:498:LYS:HD2	2:B:8938:HOH:O	2.21	0.41
1:C:79:MET:HG2	1:C:84:ARG:HG2	2.02	0.41
1:G:444:GLN:HG3	1:H:155:ARG:CZ	2.51	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:C:175:GLN:HE22	1:C:201:ALA:HA	1.86	0.41
1:A:87:LEU:HB3	1:A:213:PHE:CZ	2.56	0.41
1:B:498:LYS:HE2	1:B:498:LYS:HB3	1.93	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:E:431:VAL:HG21	1:E:442:LEU:HB3	2.03	0.41
1:H:329:ARG:HE	1:H:341:GLN:HB2	1.85	0.41
1:E:245:GLY:O	1:E:269:LEU:HA	2.21	0.41
1:B:331:VAL:HG22	1:B:341:GLN:HB3	2.03	0.41
1:C:344:GLN:CG	1:C:381:ILE:HD12	2.51	0.41
1:C:23:PHE:CG	1:C:205:ALA:HB1	2.56	0.41
1:G:315:TYR:O	1:G:319:VAL:HG23	2.21	0.41
1:D:365:ALA:HB2	1:D:393:MET:SD	2.61	0.41
1:G:450:THR:HG1	1:G:465:PHE:HD1	1.69	0.41
1:C:27:GLU:HB3	1:C:29:HIS:NE2	2.36	0.41
1:D:331:VAL:HG21	1:D:383:PRO:HD3	2.02	0.41
1:F:169:ASN:OD1	1:F:169:ASN:N	2.53	0.41
1:H:333:ASN:O	1:H:339:THR:OG1	2.30	0.40
1:A:21:GLN:HB2	1:A:28:TRP:HE3	1.87	0.40
1:D:427:LEU:HD11	1:D:465:PHE:CZ	2.56	0.40
1:A:289:GLN:HB2	2:A:9077:HOH:O	2.21	0.40
1:G:389:VAL:CG1	1:G:396:ALA:HB2	2.50	0.40
1:D:17:VAL:CG1	1:D:199:LEU:HD22	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:18:PHE:HD1	1:H:101:TYR:HH	1.64	0.40
1:D:169:ASN:HD22	1:D:401:PHE:HZ	1.69	0.40
1:C:462:GLN:CD	1:C:462:GLN:H	2.24	0.40
1:F:246:SER:OG	1:F:249:ILE:HG12	2.22	0.40
1:C:70:PHE:CZ	1:C:160:GLY:HA2	2.56	0.40
1:D:107:THR:HG23	1:D:334:PRO:HB2	2.04	0.40
1:H:67:ARG:HD2	2:H:8896:HOH:O	2.21	0.40
1:C:376:ASP:N	1:C:376:ASP:OD1	2.50	0.40
1:C:247:THR:HG23	1:C:269:LEU:HB2	2.01	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:E:444:GLN:HG3	1:F:155:ARG:NH2	2.36	0.40
1:D:430:ALA:HA	1:D:452:TRP:O	2.21	0.40
1:G:113:PRO:HB2	1:G:116:ILE:HG12	2.03	0.40
1:F:241:VAL:O	1:F:241:VAL:HG13	2.21	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:H:443:SER:HA	1:H:451:VAL:HG11	2.03	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:F:27:GLU:HB3	1:F:29:HIS:NE2	2.36	0.40
1:E:247:THR:HG23	1:E:269:LEU:CB	2.51	0.40
1:D:120:VAL:HG12	1:D:124:MET:HE1	2.04	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:333:ASN:HA	1:H:334:PRO:HD2	1.91	0.40
1:G:70:PHE:CE1	1:G:158:PRO:HB2	2.57	0.40
1:H:149:ASP:HA	1:H:498:LYS:HB2	2.04	0.40
1:D:208:ILE:CD1	1:D:218:VAL:HG11	2.52	0.40
1:G:35:LYS:HE2	1:G:35:LYS:HB3	1.98	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	492/500 (98%)	475 (96%)	16 (3%)	1 (0%)	52	51
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%)	52	51
1	E	492/500 (98%)	472 (96%)	19 (4%)	1 (0%)	52	51
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%)	52	51
All	All	3936/4000 (98%)	3792 (96%)	140 (4%)	4 (0%)	56	57

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	399/402 (99%)	371 (93%)	28 (7%)	19	12
1	B	399/402 (99%)	373 (94%)	26 (6%)	21	15
1	C	399/402 (99%)	378 (95%)	21 (5%)	28	23
1	D	399/402 (99%)	381 (96%)	18 (4%)	34	30
1	E	399/402 (99%)	377 (94%)	22 (6%)	27	21
1	F	399/402 (99%)	376 (94%)	23 (6%)	25	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	399/402 (99%)	378 (95%)	21 (5%)	28 23
1	H	399/402 (99%)	377 (94%)	22 (6%)	27 21
All	All	3192/3216 (99%)	3011 (94%)	181 (6%)	25 19

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	494/500 (98%)	-0.19	14 (2%)	56	66	8, 20, 44, 68	0
1	B	494/500 (98%)	-0.25	9 (1%)	71	79	8, 20, 44, 68	0
1	C	494/500 (98%)	-0.25	7 (1%)	78	83	9, 19, 44, 68	0
1	D	494/500 (98%)	-0.24	9 (1%)	71	79	9, 20, 43, 68	0
1	E	494/500 (98%)	-0.26	10 (2%)	68	75	8, 19, 43, 68	0
1	F	494/500 (98%)	-0.25	6 (1%)	81	85	8, 19, 43, 68	0
1	G	494/500 (98%)	-0.20	17 (3%)	49	59	8, 20, 44, 68	0
1	H	494/500 (98%)	-0.21	10 (2%)	68	75	8, 20, 44, 68	0
All	All	3952/4000 (98%)	-0.23	82 (2%)	67	74	8, 20, 44, 68	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	474	GLY	5.6
1	F	247	THR	5.5
1	G	474	GLY	5.3
1	A	474	GLY	5.1
1	C	475	GLN	4.3
1	G	255	VAL	4.0
1	D	475	GLN	4.0
1	B	474	GLY	3.9
1	H	253	ILE	3.9
1	A	247	THR	3.9
1	B	475	GLN	3.9
1	G	472	GLY	3.8
1	D	247	THR	3.8
1	A	253	ILE	3.7
1	F	250	GLY	3.6
1	E	247	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	476	GLU	3.5
1	G	246	SER	3.4
1	C	253	ILE	3.2
1	B	476	GLU	3.2
1	C	474	GLY	3.2
1	A	254	GLN	3.2
1	A	251	ARG	3.1
1	H	476	GLU	3.1
1	C	254	GLN	3.1
1	G	254	GLN	3.0
1	A	250	GLY	3.0
1	F	474	GLY	3.0
1	A	463	SER	3.0
1	B	258	GLY	3.0
1	E	477	LEU	2.9
1	B	253	ILE	2.8
1	G	473	SER	2.8
1	F	472	GLY	2.8
1	B	257	ALA	2.8
1	G	247	THR	2.8
1	A	267	LEU	2.8
1	G	253	ILE	2.8
1	E	474	GLY	2.7
1	C	224	PHE	2.7
1	H	465	PHE	2.7
1	G	250	GLY	2.7
1	G	256	ALA	2.7
1	F	253	ILE	2.7
1	A	473	SER	2.6
1	E	248	GLU	2.6
1	G	477	LEU	2.6
1	B	424	THR	2.6
1	D	253	ILE	2.6
1	B	7	ALA	2.6
1	B	465	PHE	2.6
1	G	258	GLY	2.5
1	G	476	GLU	2.5
1	E	224	PHE	2.5
1	E	424	THR	2.5
1	H	247	THR	2.4
1	E	473	SER	2.4
1	A	465	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	255	VAL	2.4
1	A	249	ILE	2.4
1	D	267	LEU	2.4
1	H	424	THR	2.3
1	G	470	MET	2.3
1	G	251	ARG	2.3
1	E	472	GLY	2.3
1	F	475	GLN	2.3
1	H	258	GLY	2.2
1	D	224	PHE	2.2
1	G	245	GLY	2.2
1	H	474	GLY	2.2
1	E	465	PHE	2.2
1	G	424	THR	2.2
1	H	468	TYR	2.2
1	D	225	GLY	2.1
1	A	257	ALA	2.1
1	D	248	GLU	2.1
1	C	250	GLY	2.1
1	E	257	ALA	2.1
1	H	270	GLY	2.1
1	A	476	GLU	2.0
1	H	478	GLY	2.0
1	D	470	MET	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.