



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 24, 2022 – 10:10 AM JST

PDB ID : 7YOB
Title : Crystal structure of Aldehyde dehydrogenase 1A1 from mouse
Authors : Zhang, X.Y.; Ouyang, Z.Q.
Deposited on : 2022-08-01
Resolution : 2.89 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

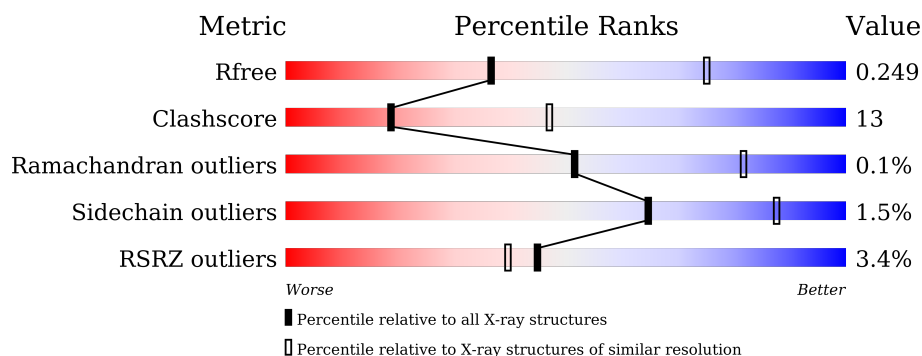
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.30
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

i

X-RAY DIFFRACTION

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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

Mol	Chain	Length	Quality of chain	
1	A	507	<div><div></div><div></div><div></div></div> 75%22% ..	
1	B	507	<div><div></div><div></div><div></div></div> 74%22% ..	
1	C	507	<div><div></div><div></div><div></div></div> 73%23% ..	
1	D	507	<div><div></div><div></div><div></div></div> 75%22% ..	
1	E	507	<div><div></div><div></div><div></div></div> 70%26% ..	
1	F	507	<div><div></div><div></div><div></div></div> 75%21% ..	

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Mol	Chain	Length	Quality of chain
1	G	507	<div><div></div><div>9%</div><div>61%</div><div>34%</div><div></div><div></div></div>
1	H	507	<div><div></div><div>2%</div><div>70%</div><div>26%</div><div></div><div></div></div>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 29957 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 1A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	494	Total	C	N	O	S	0	0	0
			3760	2395	646	696	23			
1	B	494	Total	C	N	O	S	0	0	0
			3745	2385	641	696	23			
1	C	494	Total	C	N	O	S	0	0	0
			3751	2387	642	699	23			
1	D	494	Total	C	N	O	S	0	0	0
			3744	2381	642	698	23			
1	E	494	Total	C	N	O	S	0	0	0
			3747	2387	639	698	23			
1	G	492	Total	C	N	O	S	0	0	0
			3698	2350	630	695	23			
1	H	494	Total	C	N	O	S	0	0	0
			3765	2398	644	700	23			
1	F	494	Total	C	N	O	S	0	0	0
			3747	2384	642	698	23			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP P24549
A	-4	HIS	-	expression tag	UNP P24549
A	-3	HIS	-	expression tag	UNP P24549
A	-2	HIS	-	expression tag	UNP P24549
A	-1	HIS	-	expression tag	UNP P24549
A	0	HIS	-	expression tag	UNP P24549
B	-5	HIS	-	expression tag	UNP P24549
B	-4	HIS	-	expression tag	UNP P24549
B	-3	HIS	-	expression tag	UNP P24549
B	-2	HIS	-	expression tag	UNP P24549
B	-1	HIS	-	expression tag	UNP P24549
B	0	HIS	-	expression tag	UNP P24549
C	-5	HIS	-	expression tag	UNP P24549

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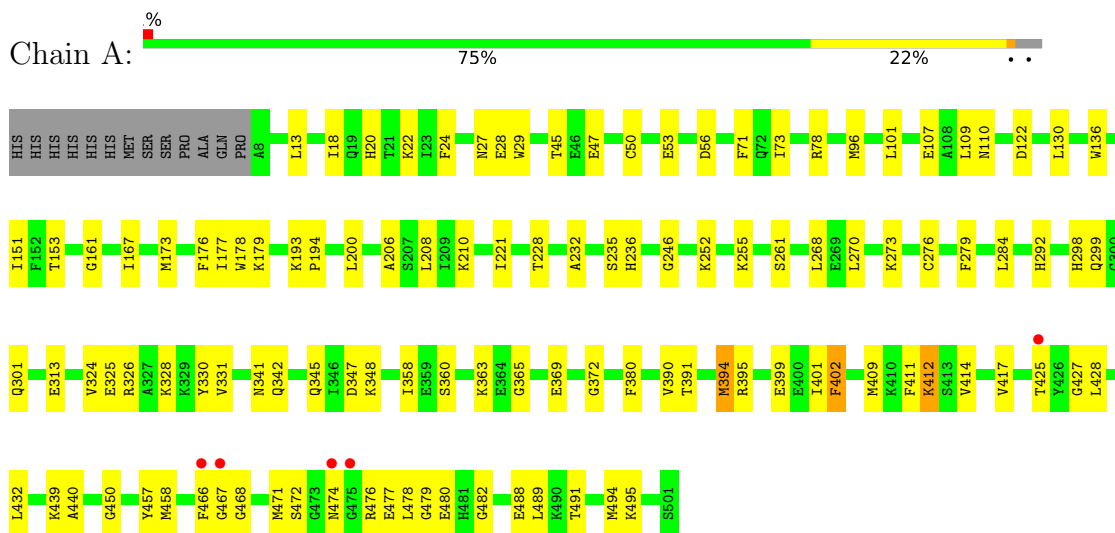
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P24549
C	-3	HIS	-	expression tag	UNP P24549
C	-2	HIS	-	expression tag	UNP P24549
C	-1	HIS	-	expression tag	UNP P24549
C	0	HIS	-	expression tag	UNP P24549
D	-5	HIS	-	expression tag	UNP P24549
D	-4	HIS	-	expression tag	UNP P24549
D	-3	HIS	-	expression tag	UNP P24549
D	-2	HIS	-	expression tag	UNP P24549
D	-1	HIS	-	expression tag	UNP P24549
D	0	HIS	-	expression tag	UNP P24549
E	-5	HIS	-	expression tag	UNP P24549
E	-4	HIS	-	expression tag	UNP P24549
E	-3	HIS	-	expression tag	UNP P24549
E	-2	HIS	-	expression tag	UNP P24549
E	-1	HIS	-	expression tag	UNP P24549
E	0	HIS	-	expression tag	UNP P24549
G	-5	HIS	-	expression tag	UNP P24549
G	-4	HIS	-	expression tag	UNP P24549
G	-3	HIS	-	expression tag	UNP P24549
G	-2	HIS	-	expression tag	UNP P24549
G	-1	HIS	-	expression tag	UNP P24549
G	0	HIS	-	expression tag	UNP P24549
H	-5	HIS	-	expression tag	UNP P24549
H	-4	HIS	-	expression tag	UNP P24549
H	-3	HIS	-	expression tag	UNP P24549
H	-2	HIS	-	expression tag	UNP P24549
H	-1	HIS	-	expression tag	UNP P24549
H	0	HIS	-	expression tag	UNP P24549
F	-5	HIS	-	expression tag	UNP P24549
F	-4	HIS	-	expression tag	UNP P24549
F	-3	HIS	-	expression tag	UNP P24549
F	-2	HIS	-	expression tag	UNP P24549
F	-1	HIS	-	expression tag	UNP P24549
F	0	HIS	-	expression tag	UNP P24549

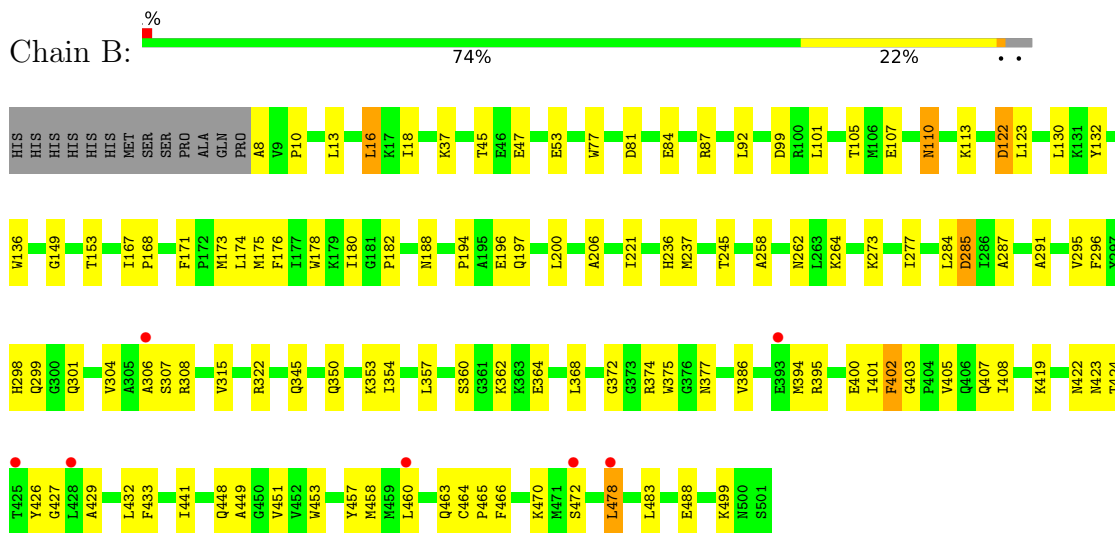
3 Residue-property plots [i](#)

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

• Molecule 1: Aldehyde dehydrogenase 1A1

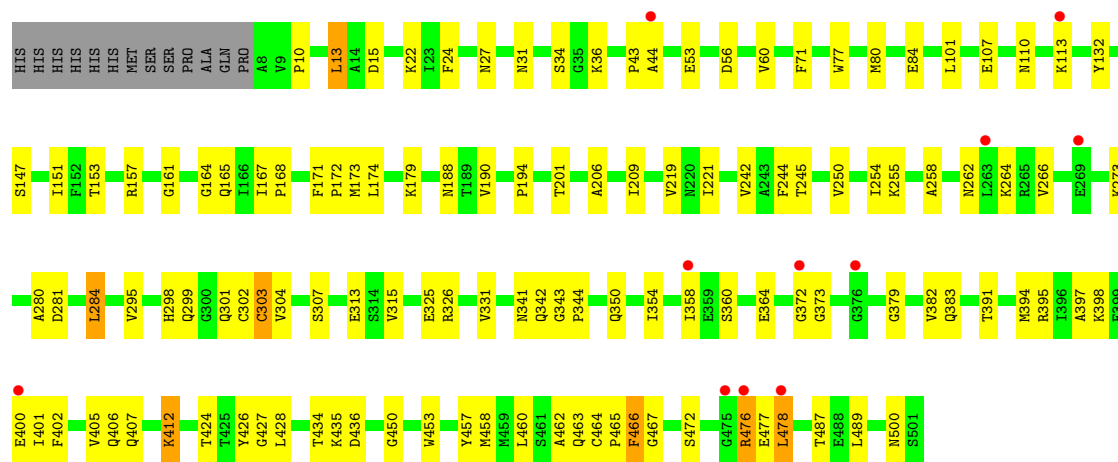


• Molecule 1: Aldehyde dehydrogenase 1A1

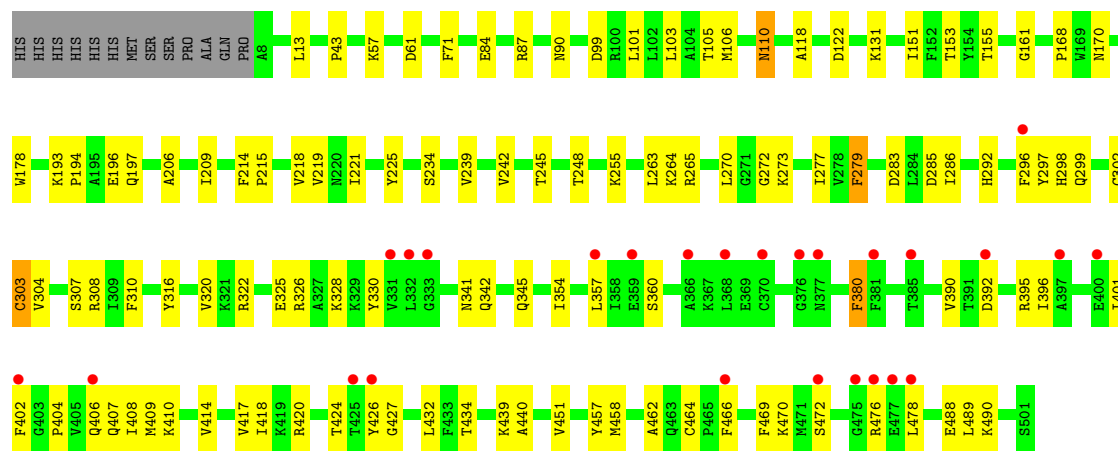
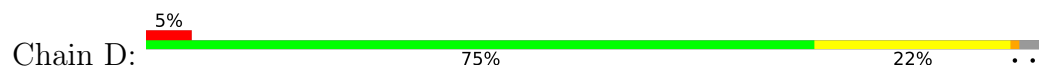


• Molecule 1: Aldehyde dehydrogenase 1A1

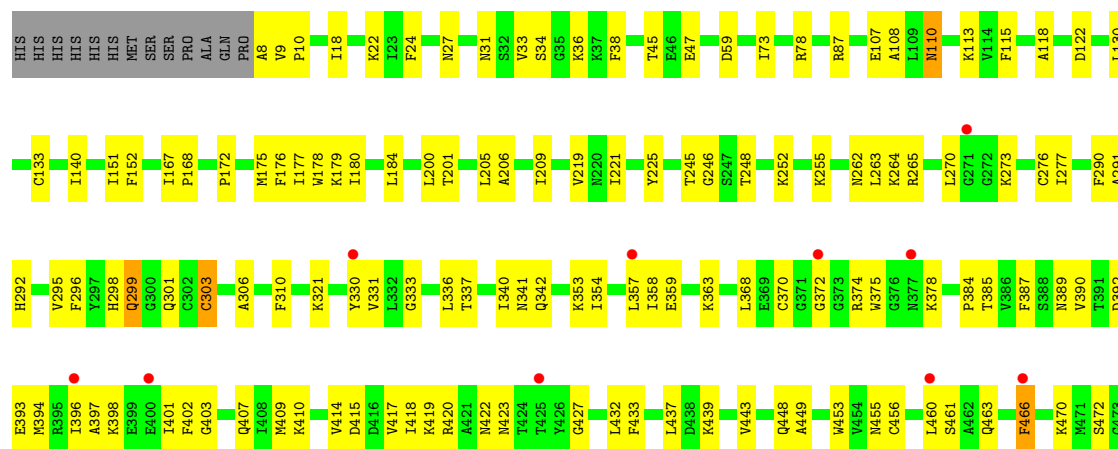




• Molecule 1: Aldehyde dehydrogenase 1A1

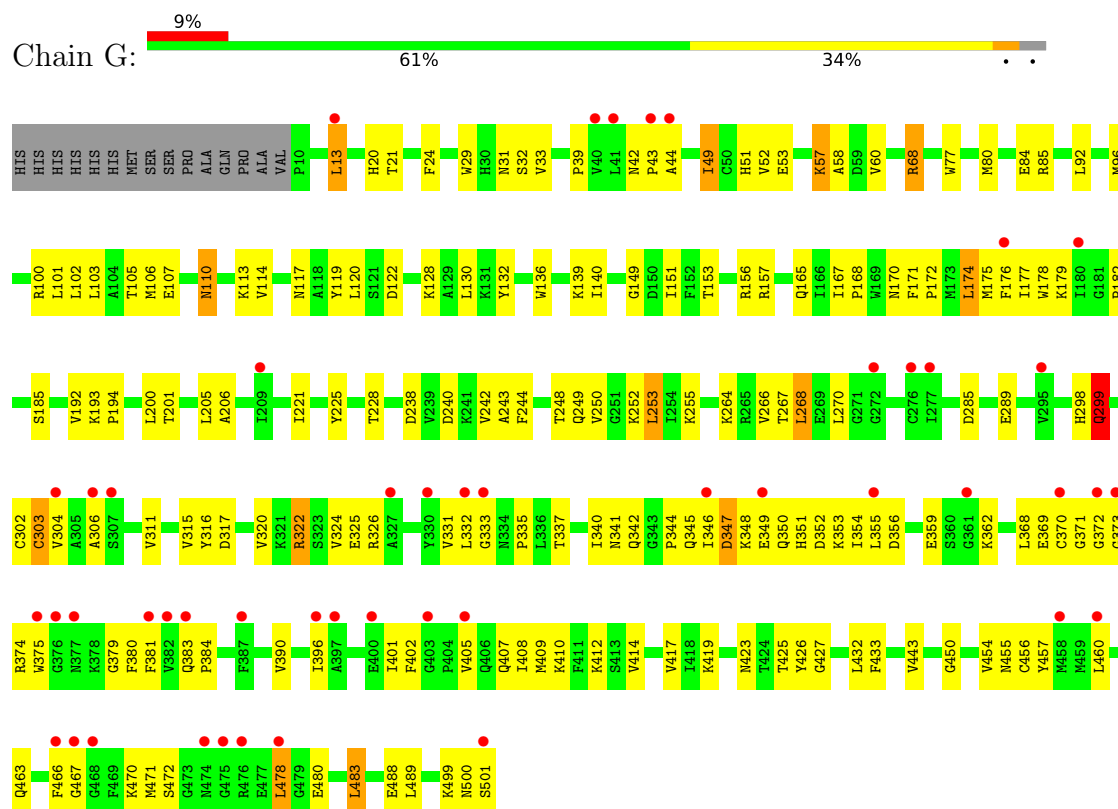


• Molecule 1: Aldehyde dehydrogenase 1A1

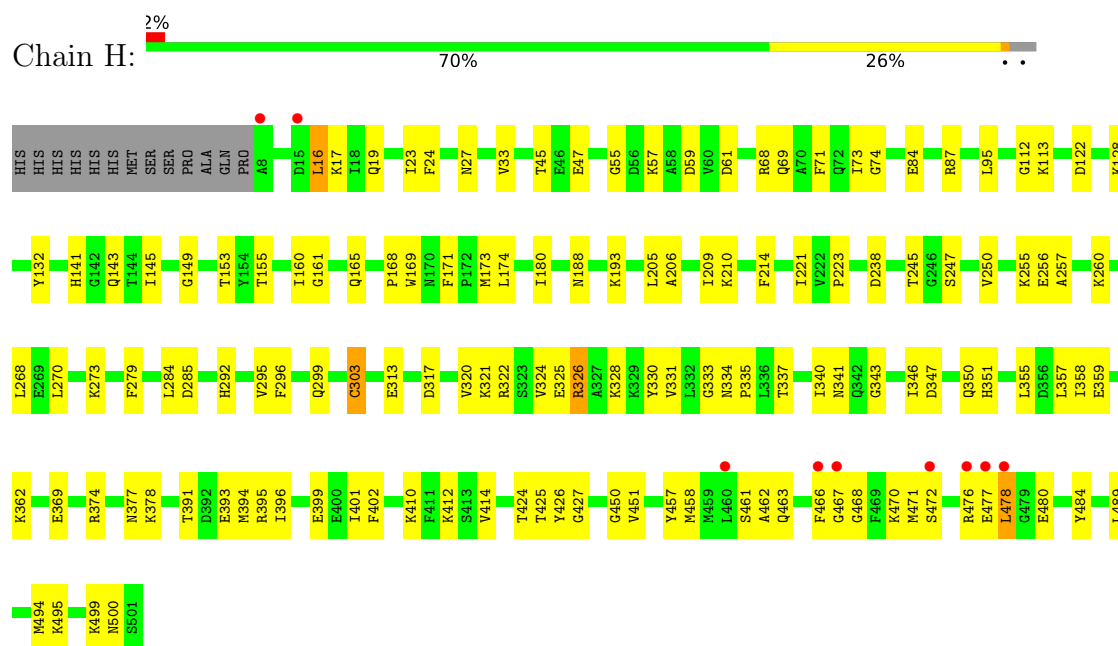




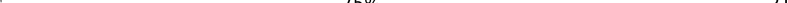
• Molecule 1: Aldehyde dehydrogenase 1A1

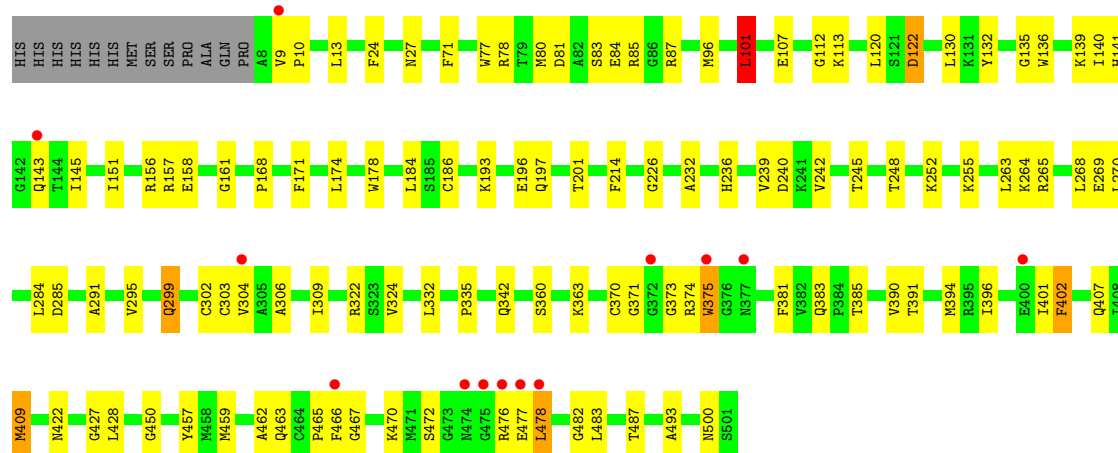


• Molecule 1: Aldehyde dehydrogenase 1A1



• Molecule 1: Aldehyde dehydrogenase 1A1

Chain F:  3% 75% 21% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.06Å 156.48Å 129.21Å 90.00° 97.97° 90.00°	Depositor
Resolution (Å)	127.96 – 2.89 127.96 – 2.89	Depositor EDS
% Data completeness (in resolution range)	93.2 (127.96-2.89) 93.3 (127.96-2.89)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.195 , 0.249 0.196 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.62$, $\langle L^2 \rangle = 0.48$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29957	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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	0.59	3/3840 (0.1%)	0.80	4/5195 (0.1%)
1	B	0.58	0/3825	0.82	2/5179 (0.0%)
1	C	0.58	2/3831 (0.1%)	0.81	5/5187 (0.1%)
1	D	0.52	1/3824 (0.0%)	0.77	3/5179 (0.1%)
1	E	0.54	1/3827 (0.0%)	0.76	6/5181 (0.1%)
1	F	0.57	1/3827 (0.0%)	0.80	5/5183 (0.1%)
1	G	0.51	1/3778 (0.0%)	0.84	10/5125 (0.2%)
1	H	0.59	2/3845 (0.1%)	0.81	6/5201 (0.1%)
All	All	0.56	11/30597 (0.0%)	0.80	41/41430 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	303	CYS	CB-SG	11.05	2.01	1.82
1	H	303	CYS	CB-SG	8.86	1.97	1.82
1	H	326	ARG	CG-CD	-7.74	1.32	1.51
1	C	303	CYS	CB-SG	7.59	1.95	1.82
1	D	303	CYS	CB-SG	7.58	1.95	1.82
1	A	210	LYS	CD-CE	6.21	1.66	1.51
1	G	303	CYS	CB-SG	5.98	1.92	1.82
1	A	276	CYS	CB-SG	-5.75	1.72	1.81
1	F	269	GLU	CG-CD	-5.60	1.43	1.51
1	C	302	CYS	CB-SG	-5.45	1.73	1.81
1	A	28	GLU	CB-CG	5.34	1.62	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	478	LEU	CB-CG-CD1	-13.03	88.84	111.00
1	B	478	LEU	CB-CG-CD1	-12.54	89.68	111.00
1	G	483	LEU	CB-CG-CD1	-10.83	92.59	111.00
1	D	439	LYS	CD-CE-NZ	-10.75	86.97	111.70
1	G	13	LEU	CB-CG-CD2	-9.70	94.51	111.00
1	F	478	LEU	CB-CG-CD1	-9.54	94.78	111.00
1	C	284	LEU	CB-CG-CD1	-8.68	96.24	111.00
1	A	210	LYS	CD-CE-NZ	7.21	128.29	111.70
1	A	109	LEU	CA-CB-CG	7.05	131.51	115.30
1	A	394	MET	CG-SD-CE	-6.96	89.06	100.20
1	E	478	LEU	CB-CG-CD1	-6.95	99.19	111.00
1	A	427	GLY	N-CA-C	-6.91	95.84	113.10
1	C	13	LEU	CB-CG-CD1	-6.62	99.74	111.00
1	E	478	LEU	CA-CB-CG	6.57	130.42	115.30
1	F	101	LEU	CA-CB-CG	6.54	130.34	115.30
1	F	122	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	B	285	ASP	CB-CG-OD1	-5.95	112.95	118.30
1	E	478	LEU	CB-CA-C	-5.88	99.03	110.20
1	E	432	LEU	CB-CG-CD1	-5.71	101.28	111.00
1	F	375	TRP	C-N-CA	5.67	134.21	122.30
1	H	16	LEU	CA-CB-CG	-5.66	102.28	115.30
1	G	13	LEU	CA-CB-CG	-5.58	102.45	115.30
1	G	347	ASP	CB-CG-OD1	5.58	123.32	118.30
1	G	253	LEU	CA-CB-CG	5.55	128.06	115.30
1	C	460	LEU	CA-CB-CG	5.53	128.02	115.30
1	H	478	LEU	CB-CG-CD2	-5.51	101.64	111.00
1	G	299	GLN	CA-CB-CG	5.48	125.46	113.40
1	G	174	LEU	CB-CG-CD1	-5.48	101.69	111.00
1	H	326	ARG	CG-CD-NE	5.45	123.25	111.80
1	G	483	LEU	CA-CB-CG	-5.39	102.89	115.30
1	G	49	ILE	CG1-CB-CG2	-5.36	99.61	111.40
1	H	326	ARG	CB-CG-CD	5.29	125.37	111.60
1	E	478	LEU	N-CA-C	5.22	125.09	111.00
1	H	210	LYS	CD-CE-NZ	5.21	123.69	111.70
1	E	133	CYS	CA-CB-SG	-5.18	104.67	114.00
1	F	96	MET	CG-SD-CE	-5.17	91.93	100.20
1	H	210	LYS	CA-CB-CG	5.16	124.74	113.40
1	C	466	PHE	C-N-CA	-5.13	111.52	122.30
1	D	279	PHE	CB-CG-CD1	-5.08	117.24	120.80
1	D	439	LYS	CA-CB-CG	-5.06	102.27	113.40
1	C	13	LEU	CB-CG-CD2	5.00	119.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	57	LYS	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3760	0	3761	82	0
1	B	3745	0	3726	96	0
1	C	3751	0	3728	101	0
1	D	3744	0	3710	91	0
1	E	3747	0	3730	99	0
1	F	3747	0	3719	100	0
1	G	3698	0	3614	150	0
1	H	3765	0	3767	106	0
All	All	29957	0	29755	781	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 13.

All (781) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:THR:O	1:B:470:LYS:NZ	1.82	1.11
1:C:434:THR:HG22	1:C:436:ASP:H	1.22	1.00
1:C:424:THR:HG22	1:C:426:TYR:H	1.26	0.98
1:H:467:GLY:HA3	1:H:476:ARG:HD3	1.51	0.92
1:B:285:ASP:OD1	1:B:322:ARG:NH1	2.03	0.91
1:G:299:GLN:HG3	1:G:342:GLN:HG3	1.54	0.89
1:H:74:GLY:H	1:F:500:ASN:HD21	1.22	0.88
1:H:427:GLY:H	1:H:472:SER:HB3	1.36	0.88
1:E:292:HIS:NE2	1:E:330:TYR:OH	2.06	0.87
1:D:401:ILE:HD13	1:D:407:GLN:HE22	1.40	0.86
1:A:325:GLU:HA	1:A:328:LYS:HE3	1.58	0.85
1:C:358:ILE:HD11	1:C:405:VAL:HG21	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:317:ASP:HA	1:G:320:VAL:HG22	1.58	0.83
1:C:31:ASN:HA	1:C:53:GLU:OE1	1.77	0.83
1:B:354:ILE:HD12	1:B:403:GLY:HA3	1.59	0.81
1:F:135:GLY:O	1:F:139:LYS:NZ	2.13	0.81
1:B:424:THR:HG23	1:B:426:TYR:H	1.45	0.80
1:E:354:ILE:HD12	1:E:403:GLY:HA3	1.65	0.79
1:E:448:GLN:HG2	1:E:470:LYS:HE3	1.62	0.79
1:E:73:ILE:HG23	1:G:500:ASN:OD1	1.84	0.78
1:D:273:LYS:HD3	1:D:307:SER:HB2	1.65	0.78
1:G:368:LEU:HD11	1:G:372:GLY:HA3	1.66	0.78
1:D:193:LYS:NZ	1:D:194:PRO:O	2.18	0.77
1:D:424:THR:HG22	1:D:426:TYR:H	1.49	0.77
1:A:299:GLN:HG3	1:A:342:GLN:HG3	1.66	0.76
1:C:342:GLN:NE2	1:C:382:VAL:O	2.19	0.76
1:B:262:ASN:HD21	1:B:264:LYS:NZ	1.85	0.75
1:B:8:ALA:HB1	1:E:8:ALA:O	1.87	0.74
1:E:273:LYS:NZ	1:E:396:ILE:O	2.20	0.74
1:D:242:VAL:HG23	1:D:264:LYS:HD3	1.69	0.74
1:G:331:VAL:H	1:G:341:ASN:HB2	1.53	0.74
1:B:153:THR:HG21	1:C:464:CYS:SG	2.27	0.74
1:G:92:LEU:HD12	1:G:130:LEU:HD11	1.67	0.74
1:A:467:GLY:HA3	1:A:476:ARG:HD3	1.70	0.73
1:D:13:LEU:HD23	1:D:101:LEU:HG	1.70	0.73
1:E:390:VAL:HG13	1:E:394:MET:HG3	1.69	0.73
1:H:256:GLU:HG2	1:H:260:LYS:HE3	1.70	0.73
1:G:390:VAL:HG23	1:G:409:MET:HG3	1.70	0.73
1:H:424:THR:HG23	1:H:426:TYR:H	1.52	0.73
1:C:466:PHE:HZ	1:C:477:GLU:OE1	1.71	0.73
1:G:33:VAL:HG11	1:G:58:ALA:HB3	1.70	0.72
1:F:80:MET:HE3	1:F:84:GLU:HG3	1.71	0.72
1:H:461:SER:OG	1:H:463:GLN:OE1	2.07	0.71
1:C:107:GLU:OE1	1:C:173:MET:HG3	1.90	0.71
1:A:466:PHE:CZ	1:A:477:GLU:HB2	2.25	0.71
1:G:396:ILE:O	1:G:407:GLN:NE2	2.24	0.71
1:E:18:ILE:HD13	1:E:200:LEU:HD13	1.72	0.71
1:B:308:ARG:HH12	1:B:424:THR:HB	1.56	0.71
1:G:348:LYS:HD2	1:G:351:HIS:HB3	1.72	0.70
1:A:489:LEU:HD23	1:D:476:ARG:HG3	1.72	0.70
1:A:178:TRP:CE3	1:A:466:PHE:CZ	2.79	0.70
1:A:178:TRP:CD1	1:A:478:LEU:HD11	2.26	0.70
1:B:237:MET:HA	1:B:262:ASN:HD22	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:358:ILE:HG22	1:H:362:LYS:HE3	1.72	0.70
1:F:391:THR:H	1:F:394:MET:HE3	1.55	0.70
1:A:193:LYS:NZ	1:A:194:PRO:O	2.25	0.70
1:C:373:GLY:N	1:C:383:GLN:HE21	1.90	0.70
1:D:13:LEU:H	1:D:105:THR:HG21	1.56	0.70
1:D:215:PRO:O	1:D:218:VAL:HG12	1.92	0.69
1:G:348:LYS:HD3	1:G:380:PHE:CE2	2.27	0.69
1:G:348:LYS:HD3	1:G:380:PHE:HE2	1.57	0.69
1:G:488:GLU:OE2	1:H:476:ARG:NH2	2.25	0.69
1:H:145:ILE:O	1:H:153:THR:OG1	2.10	0.69
1:C:206:ALA:HB2	1:C:221:ILE:HD12	1.75	0.68
1:F:140:ILE:HD11	1:F:483:LEU:HD22	1.76	0.68
1:A:391:THR:OG1	1:A:394:MET:HE2	1.94	0.68
1:G:114:VAL:HB	1:G:117:ASN:HB2	1.75	0.68
1:C:113:LYS:HZ1	1:C:171:PHE:HA	1.57	0.68
1:D:390:VAL:HG21	1:D:407:GLN:HB3	1.75	0.68
1:G:374:ARG:NH2	1:G:379:GLY:O	2.27	0.68
1:E:461:SER:OG	1:E:463:GLN:OE1	2.11	0.67
1:A:45:THR:OG1	1:A:47:GLU:HG2	1.93	0.67
1:C:281:ASP:OD1	1:C:434:THR:HG23	1.94	0.67
1:B:457:TYR:CD2	1:B:458:MET:HG3	2.29	0.67
1:G:373:GLY:N	1:G:383:GLN:HE21	1.92	0.67
1:G:390:VAL:HG21	1:G:407:GLN:HB3	1.75	0.67
1:H:374:ARG:NH2	1:H:377:ASN:O	2.27	0.67
1:B:236:HIS:O	1:B:262:ASN:ND2	2.29	0.66
1:F:477:GLU:N	1:F:477:GLU:OE1	2.28	0.66
1:B:427:GLY:N	1:B:472:SER:OG	2.27	0.66
1:G:13:LEU:HD21	1:G:102:LEU:HA	1.77	0.66
1:F:428:LEU:HD13	1:F:472:SER:OG	1.96	0.65
1:F:151:ILE:HD11	1:F:493:ALA:HB1	1.77	0.65
1:C:255:LYS:HD2	1:C:266:VAL:HG21	1.78	0.65
1:C:466:PHE:CD1	1:C:466:PHE:O	2.49	0.65
1:C:284:LEU:HD11	1:C:315:VAL:CG1	2.27	0.65
1:G:168:PRO:HG2	1:G:175:MET:HG3	1.79	0.65
1:F:299:GLN:HG3	1:F:342:GLN:HG3	1.79	0.65
1:A:428:LEU:HB2	1:A:472:SER:HB3	1.79	0.64
1:G:320:VAL:HG12	1:G:408:ILE:HG21	1.79	0.64
1:G:349:GLU:O	1:G:353:LYS:HB3	1.96	0.64
1:H:17:LYS:HE2	1:H:19:GLN:CD	2.18	0.64
1:C:299:GLN:HG3	1:C:342:GLN:HG3	1.80	0.64
1:A:73:ILE:HD12	1:A:73:ILE:H	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:ASN:HA	1:G:53:GLU:HG2	1.78	0.64
1:C:358:ILE:HD11	1:C:405:VAL:CG2	2.27	0.64
1:B:488:GLU:OE2	1:C:476:ARG:NH1	2.31	0.64
1:H:395:ARG:HD2	1:H:399:GLU:OE2	1.98	0.64
1:C:427:GLY:N	1:C:472:SER:OG	2.30	0.63
1:H:462:ALA:HA	1:H:478:LEU:HD13	1.80	0.63
1:A:206:ALA:HB2	1:A:221:ILE:HD12	1.81	0.63
1:B:464:CYS:SG	1:C:153:THR:HG21	2.39	0.63
1:F:178:TRP:CD1	1:F:478:LEU:HD11	2.33	0.63
1:C:13:LEU:CD1	1:C:101:LEU:HG	2.28	0.63
1:E:252:LYS:HA	1:F:263:LEU:HD21	1.80	0.63
1:A:13:LEU:HD23	1:A:101:LEU:HG	1.81	0.63
1:C:373:GLY:O	1:C:383:GLN:HG2	1.98	0.63
1:A:457:TYR:CD1	1:A:458:MET:HG3	2.33	0.63
1:H:68:ARG:NE	1:H:238:ASP:OD1	2.30	0.63
1:H:331:VAL:H	1:H:341:ASN:HB2	1.62	0.63
1:G:107:GLU:OE2	1:G:172:PRO:HD2	1.99	0.62
1:G:255:LYS:NZ	1:H:255:LYS:HZ1	1.97	0.62
1:E:337:THR:HB	1:E:340:ILE:HD12	1.81	0.62
1:D:151:ILE:HD13	1:D:153:THR:HG23	1.81	0.62
1:H:74:GLY:N	1:F:500:ASN:HD21	1.96	0.62
1:A:425:THR:HG22	1:A:471:MET:HB2	1.82	0.62
1:G:136:TRP:CE2	1:F:139:LYS:HD3	2.35	0.61
1:D:285:ASP:OD1	1:D:322:ARG:NH1	2.33	0.61
1:G:373:GLY:H	1:G:383:GLN:HE21	1.47	0.61
1:A:324:VAL:HG21	1:A:369:GLU:HG2	1.82	0.61
1:G:401:ILE:HG21	1:G:405:VAL:HB	1.82	0.61
1:B:45:THR:OG1	1:B:47:GLU:HG2	2.01	0.61
1:B:377:ASN:HB2	1:H:17:LYS:HE3	1.83	0.61
1:E:401:ILE:HD13	1:E:407:GLN:HE22	1.66	0.61
1:F:483:LEU:C	1:F:483:LEU:HD23	2.20	0.61
1:G:80:MET:HE1	1:G:84:GLU:HG3	1.82	0.61
1:H:285:ASP:OD1	1:H:322:ARG:NH1	2.34	0.61
1:H:467:GLY:HA3	1:H:476:ARG:CD	2.29	0.61
1:F:467:GLY:HA3	1:F:476:ARG:NH1	2.16	0.61
1:A:450:GLY:HA3	1:A:467:GLY:O	2.01	0.60
1:D:178:TRP:CD1	1:D:478:LEU:HD11	2.36	0.60
1:C:457:TYR:CD1	1:C:458:MET:HG3	2.36	0.60
1:E:107:GLU:OE2	1:E:172:PRO:HD2	2.01	0.60
1:F:466:PHE:O	1:F:477:GLU:OE1	2.20	0.60
1:C:450:GLY:HA3	1:C:467:GLY:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:MET:HE3	1:B:441:ILE:HD11	1.84	0.60
1:G:285:ASP:OD1	1:G:322:ARG:NH1	2.35	0.60
1:F:242:VAL:HG23	1:F:264:LYS:HD3	1.82	0.60
1:F:450:GLY:HA3	1:F:467:GLY:O	2.01	0.60
1:D:273:LYS:HD3	1:D:307:SER:CB	2.31	0.60
1:G:249:GLN:HA	1:G:252:LYS:HD2	1.83	0.60
1:E:389:ASN:OD1	1:E:410:LYS:NZ	2.34	0.60
1:D:206:ALA:HB2	1:D:221:ILE:HD12	1.83	0.60
1:G:130:LEU:HG	1:G:177:ILE:HD12	1.83	0.60
1:A:151:ILE:HD13	1:A:153:THR:HG23	1.83	0.59
1:A:467:GLY:CA	1:A:476:ARG:HD3	2.32	0.59
1:G:489:LEU:HD21	1:H:476:ARG:HG3	1.84	0.59
1:B:10:PRO:HG2	1:B:101:LEU:HD13	1.84	0.59
1:F:71:PHE:O	1:F:78:ARG:HD3	2.03	0.59
1:F:396:ILE:O	1:F:407:GLN:NE2	2.34	0.59
1:C:434:THR:HG22	1:C:436:ASP:N	2.07	0.59
1:C:113:LYS:HG2	1:C:298:HIS:CE1	2.37	0.59
1:C:358:ILE:HG21	1:C:372:GLY:HA2	1.83	0.59
1:C:400:GLU:O	1:C:400:GLU:HG2	2.03	0.59
1:F:467:GLY:HA3	1:F:476:ARG:CZ	2.33	0.59
1:B:364:GLU:OE1	1:B:394:MET:HB3	2.03	0.59
1:E:359:GLU:O	1:E:363:LYS:HG3	2.03	0.59
1:G:13:LEU:HD11	1:G:101:LEU:CB	2.33	0.59
1:A:292:HIS:NE2	1:A:330:TYR:OH	2.36	0.59
1:D:277:ILE:HG21	1:D:279:PHE:CZ	2.38	0.59
1:E:295:VAL:HG23	1:E:296:PHE:CD2	2.38	0.59
1:H:17:LYS:HE2	1:H:19:GLN:OE1	2.02	0.59
1:C:401:ILE:HD13	1:C:407:GLN:HE22	1.67	0.59
1:F:324:VAL:HG13	1:F:370:CYS:HB2	1.86	0.58
1:F:390:VAL:HB	1:F:409:MET:HG3	1.85	0.58
1:A:358:ILE:HG21	1:A:372:GLY:HA2	1.85	0.58
1:C:22:LYS:HA	1:C:53:GLU:HG3	1.84	0.58
1:F:107:GLU:OE1	1:F:201:THR:HG21	2.02	0.58
1:F:291:ALA:HB1	1:F:309:ILE:HD13	1.85	0.58
1:F:427:GLY:H	1:F:472:SER:HB2	1.68	0.58
1:G:255:LYS:HZ2	1:H:255:LYS:HZ1	1.50	0.58
1:A:365:GLY:O	1:A:394:MET:HE1	2.04	0.58
1:A:252:LYS:HA	1:D:263:LEU:HD21	1.84	0.58
1:C:34:SER:OG	1:C:36:LYS:HG3	2.04	0.58
1:D:196:GLU:HG2	1:D:225:TYR:CD1	2.38	0.58
1:E:427:GLY:N	1:E:472:SER:OG	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:359:GLU:HA	1:H:362:LYS:HD2	1.86	0.58
1:B:451:VAL:HG21	1:B:466:PHE:HB2	1.85	0.58
1:E:299:GLN:HG3	1:E:342:GLN:HG3	1.86	0.58
1:G:21:THR:O	1:G:52:VAL:HG13	2.04	0.58
1:A:298:HIS:O	1:A:301:GLN:HG3	2.03	0.57
1:E:418:ILE:HD11	1:E:443:VAL:HG13	1.86	0.57
1:H:74:GLY:H	1:F:500:ASN:ND2	1.99	0.57
1:B:16:LEU:HD22	1:B:105:THR:HG22	1.86	0.57
1:G:57:LYS:O	1:G:60:VAL:HG22	2.03	0.57
1:F:401:ILE:HG13	1:F:402:PHE:H	1.68	0.57
1:B:168:PRO:HG3	1:B:245:THR:HG22	1.86	0.57
1:H:206:ALA:HB2	1:H:221:ILE:HD12	1.87	0.57
1:G:119:TYR:HD1	1:G:120:LEU:HD22	1.69	0.57
1:C:13:LEU:N	1:C:13:LEU:HD12	2.20	0.57
1:E:38:PHE:HB2	1:E:225:TYR:OH	2.05	0.57
1:G:350:GLN:O	1:G:354:ILE:HG13	2.04	0.57
1:D:427:GLY:N	1:D:472:SER:OG	2.36	0.57
1:G:171:PHE:HE1	1:G:302:CYS:HA	1.70	0.57
1:G:225:TYR:HB2	1:G:228:THR:OG1	2.05	0.57
1:B:13:LEU:CD1	1:B:101:LEU:HG	2.35	0.57
1:C:373:GLY:H	1:C:383:GLN:HE21	1.50	0.57
1:F:476:ARG:HH11	1:F:476:ARG:HG2	1.70	0.57
1:E:422:ASN:O	1:E:470:LYS:NZ	2.27	0.56
1:G:324:VAL:HG21	1:G:369:GLU:HB3	1.87	0.56
1:G:373:GLY:H	1:G:383:GLN:HG2	1.69	0.56
1:H:451:VAL:HG21	1:H:466:PHE:CD1	2.40	0.56
1:B:460:LEU:O	1:B:460:LEU:HD12	2.06	0.56
1:B:113:LYS:NZ	1:B:122:ASP:OD2	2.33	0.56
1:G:128:LYS:HG2	1:F:87:ARG:HH21	1.70	0.56
1:H:24:PHE:CZ	1:H:27:ASN:HA	2.40	0.56
1:H:73:ILE:HD12	1:H:73:ILE:H	1.70	0.56
1:F:401:ILE:HG13	1:F:402:PHE:N	2.21	0.56
1:B:262:ASN:HD21	1:B:264:LYS:HZ1	1.53	0.56
1:B:273:LYS:HB3	1:B:424:THR:HG21	1.86	0.56
1:G:182:PRO:HA	1:G:483:LEU:HD21	1.88	0.56
1:D:357:LEU:HD13	1:D:401:ILE:HG22	1.86	0.56
1:E:295:VAL:HG12	1:E:306:ALA:O	2.06	0.56
1:A:110:ASN:ND2	1:A:110:ASN:O	2.37	0.56
1:E:330:TYR:HD2	1:E:384:PRO:HG3	1.71	0.56
1:A:466:PHE:HE2	1:A:478:LEU:HB2	1.70	0.56
1:E:291:ALA:O	1:E:295:VAL:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:MET:CE	1:G:84:GLU:HG3	2.35	0.56
1:C:284:LEU:HD11	1:C:315:VAL:HG11	1.87	0.55
1:F:143:GLN:HG2	1:F:145:ILE:HG13	1.88	0.55
1:C:10:PRO:HG2	1:C:101:LEU:HD13	1.88	0.55
1:B:206:ALA:HB2	1:B:221:ILE:HD13	1.88	0.55
1:F:9:VAL:HG22	1:F:120:LEU:HD11	1.86	0.55
1:E:206:ALA:HB2	1:E:221:ILE:HD13	1.88	0.55
1:E:262:ASN:OD1	1:E:264:LYS:HE3	2.06	0.55
1:C:13:LEU:HD11	1:C:101:LEU:HG	1.88	0.55
1:D:13:LEU:HB2	1:D:105:THR:HG21	1.88	0.55
1:A:24:PHE:CZ	1:A:27:ASN:HA	2.42	0.55
1:C:304:VAL:HG23	1:C:304:VAL:O	2.07	0.55
1:E:310:PHE:CD2	1:E:417:VAL:HG23	2.42	0.55
1:B:451:VAL:CG2	1:B:466:PHE:HB2	2.36	0.55
1:G:193:LYS:NZ	1:G:194:PRO:O	2.38	0.55
1:B:168:PRO:HG3	1:B:245:THR:CG2	2.37	0.55
1:G:13:LEU:CD2	1:G:102:LEU:HA	2.36	0.55
1:G:243:ALA:HA	1:G:267:THR:O	2.07	0.55
1:B:298:HIS:O	1:B:301:GLN:HG3	2.07	0.55
1:A:73:ILE:HG23	1:C:500:ASN:HD22	1.71	0.54
1:D:392:ASP:OD2	1:D:420:ARG:HD2	2.07	0.54
1:G:463:GLN:OE1	1:G:463:GLN:N	2.40	0.54
1:A:96:MET:CE	1:A:130:LEU:HD22	2.37	0.54
1:B:176:PHE:CE2	1:B:180:ILE:HD13	2.43	0.54
1:C:304:VAL:HG12	1:C:428:LEU:HD23	1.88	0.54
1:E:394:MET:HB2	1:E:397:ALA:HB3	1.89	0.54
1:G:85:ARG:NH1	1:G:185:SER:O	2.41	0.54
1:H:173:MET:HE3	1:H:205:LEU:HD21	1.89	0.54
1:H:321:LYS:O	1:H:325:GLU:HG2	2.08	0.54
1:B:308:ARG:NH1	1:B:424:THR:HB	2.22	0.54
1:E:107:GLU:OE1	1:E:201:THR:HG21	2.07	0.54
1:E:298:HIS:O	1:E:301:GLN:HG3	2.08	0.54
1:G:242:VAL:HG23	1:G:264:LYS:HD3	1.90	0.54
1:H:333:GLY:HA3	1:H:340:ILE:HD13	1.90	0.54
1:A:428:LEU:HA	1:A:468:GLY:HA2	1.90	0.54
1:G:244:PHE:O	1:G:268:LEU:HA	2.07	0.54
1:H:165:GLN:OE1	1:H:180:ILE:HG22	2.07	0.54
1:H:466:PHE:HB3	1:H:477:GLU:HG2	1.87	0.54
1:A:348:LYS:HG2	1:A:380:PHE:CE1	2.43	0.54
1:H:168:PRO:HD3	1:H:245:THR:HB	1.89	0.54
1:D:308:ARG:HH22	1:D:424:THR:HG1	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:VAL:HG23	1:D:409:MET:HG3	1.89	0.54
1:A:466:PHE:CE2	1:A:478:LEU:HB2	2.43	0.54
1:C:424:THR:HG22	1:C:426:TYR:N	2.08	0.54
1:D:84:GLU:HG2	1:D:87:ARG:NH2	2.23	0.54
1:D:168:PRO:HD3	1:D:245:THR:HB	1.89	0.54
1:G:178:TRP:CE2	1:G:478:LEU:HD11	2.43	0.54
1:C:255:LYS:CD	1:C:266:VAL:HG21	2.38	0.53
1:A:13:LEU:CD2	1:A:101:LEU:HG	2.38	0.53
1:E:265:ARG:N	1:E:265:ARG:HD2	2.23	0.53
1:H:292:HIS:NE2	1:H:296:PHE:CD2	2.76	0.53
1:B:427:GLY:O	1:B:449:ALA:HA	2.08	0.53
1:D:304:VAL:HG11	1:D:466:PHE:HZ	1.74	0.53
1:D:390:VAL:HG23	1:D:409:MET:CG	2.39	0.53
1:G:178:TRP:CD2	1:G:478:LEU:HD11	2.44	0.53
1:A:151:ILE:HG22	1:A:495:LYS:HA	1.91	0.53
1:A:73:ILE:HG23	1:C:500:ASN:ND2	2.24	0.52
1:C:43:PRO:HB2	1:C:344:PRO:CG	2.39	0.52
1:G:176:PHE:CE1	1:G:192:VAL:HG11	2.44	0.52
1:G:419:LYS:O	1:G:423:ASN:HB2	2.10	0.52
1:F:13:LEU:HD13	1:F:101:LEU:CD1	2.39	0.52
1:G:470:LYS:HG3	1:G:471:MET:H	1.74	0.52
1:H:71:PHE:CE2	1:H:161:GLY:HA2	2.44	0.52
1:A:292:HIS:CE1	1:A:326:ARG:HG3	2.44	0.52
1:C:43:PRO:O	1:C:44:ALA:HB3	2.09	0.52
1:C:250:VAL:O	1:C:254:ILE:HG13	2.09	0.52
1:F:113:LYS:HD3	1:F:122:ASP:OD2	2.09	0.52
1:H:468:GLY:HA3	1:H:472:SER:O	2.10	0.52
1:E:24:PHE:CZ	1:E:27:ASN:HA	2.45	0.52
1:C:151:ILE:HD13	1:C:153:THR:OG1	2.10	0.52
1:G:333:GLY:HA3	1:G:340:ILE:HD13	1.91	0.52
1:H:326:ARG:NH1	1:H:330:TYR:OH	2.35	0.52
1:F:466:PHE:HB3	1:F:477:GLU:OE2	2.09	0.52
1:B:123:LEU:HD21	1:B:173:MET:HE1	1.91	0.52
1:G:170:ASN:O	1:G:298:HIS:HE1	1.93	0.52
1:B:182:PRO:HB3	1:B:483:LEU:HD23	1.91	0.52
1:H:292:HIS:CD2	1:H:296:PHE:CD2	2.97	0.52
1:F:186:CYS:SG	1:F:483:LEU:HD21	2.49	0.52
1:F:304:VAL:HG11	1:F:466:PHE:CZ	2.45	0.52
1:F:465:PRO:HA	1:F:477:GLU:O	2.10	0.51
1:G:266:VAL:HG12	1:G:268:LEU:HD12	1.91	0.51
1:G:351:HIS:CD2	1:G:355:LEU:HD23	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD23	1:B:130:LEU:HD11	1.93	0.51
1:B:107:GLU:HB2	1:B:173:MET:HE3	1.92	0.51
1:B:299:GLN:HB3	1:B:345:GLN:OE1	2.10	0.51
1:D:43:PRO:HA	1:D:380:PHE:HE1	1.76	0.51
1:D:390:VAL:O	1:D:409:MET:HG2	2.09	0.51
1:E:255:LYS:NZ	1:F:255:LYS:NZ	2.59	0.51
1:F:140:ILE:CD1	1:F:483:LEU:HD22	2.39	0.51
1:F:304:VAL:HG11	1:F:466:PHE:HZ	1.75	0.51
1:B:262:ASN:HD21	1:B:264:LYS:HZ2	1.58	0.51
1:C:44:ALA:HA	1:C:379:GLY:HA3	1.93	0.51
1:G:249:GLN:O	1:G:252:LYS:HB2	2.11	0.51
1:G:250:VAL:HA	1:G:253:LEU:HD13	1.92	0.51
1:H:268:LEU:HB3	1:H:270:LEU:HD21	1.92	0.51
1:F:143:GLN:HG2	1:F:145:ILE:CG1	2.40	0.51
1:A:268:LEU:H	1:A:474:ASN:HB3	1.75	0.51
1:E:255:LYS:HZ2	1:F:255:LYS:NZ	2.08	0.51
1:D:462:ALA:O	1:D:478:LEU:O	2.29	0.51
1:G:122:ASP:O	1:G:174:LEU:HD11	2.09	0.51
1:H:369:GLU:N	1:H:369:GLU:OE1	2.44	0.51
1:E:33:VAL:HG23	1:E:59:ASP:OD1	2.11	0.51
1:G:44:ALA:CA	1:G:344:PRO:HG3	2.41	0.51
1:H:424:THR:O	1:H:470:LYS:HE3	2.11	0.51
1:F:80:MET:HE1	1:F:85:ARG:HG2	1.92	0.51
1:B:258:ALA:HB1	1:B:264:LYS:HG3	1.92	0.51
1:B:377:ASN:HB2	1:H:17:LYS:CE	2.41	0.51
1:E:437:LEU:HD11	1:H:494:MET:HE1	1.92	0.51
1:G:362:LYS:HE3	1:G:368:LEU:HD13	1.92	0.51
1:G:410:LYS:HG2	1:G:412:LYS:NZ	2.25	0.51
1:F:306:ALA:HB2	1:F:457:TYR:CZ	2.46	0.51
1:E:113:LYS:NZ	1:E:122:ASP:OD2	2.39	0.50
1:G:268:LEU:HD23	1:G:270:LEU:HD21	1.93	0.50
1:H:247:SER:OG	1:H:250:VAL:HG23	2.10	0.50
1:B:287:ALA:HA	1:B:433:PHE:CD2	2.46	0.50
1:H:326:ARG:NH1	1:H:330:TYR:CZ	2.78	0.50
1:B:18:ILE:HD13	1:B:200:LEU:HD13	1.93	0.50
1:H:320:VAL:O	1:H:324:VAL:HG23	2.11	0.50
1:F:156:ARG:NH1	1:F:158:GLU:OE2	2.43	0.50
1:G:68:ARG:HD2	1:G:238:ASP:OD2	2.12	0.50
1:F:71:PHE:CE2	1:F:161:GLY:HA2	2.46	0.50
1:E:370:CYS:O	1:E:385:THR:HA	2.11	0.50
1:G:110:ASN:HD22	1:G:110:ASN:C	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:ARG:NH2	1:C:487:THR:OG1	2.44	0.50
1:D:57:LYS:HE2	1:D:61:ASP:OD1	2.11	0.50
1:D:308:ARG:HB3	1:D:310:PHE:CE1	2.47	0.50
1:G:374:ARG:HG2	1:G:375:TRP:N	2.26	0.50
1:G:13:LEU:HD13	1:G:105:THR:OG1	2.12	0.50
1:G:299:GLN:O	1:G:345:GLN:NE2	2.41	0.50
1:G:337:THR:HB	1:G:340:ILE:HD12	1.93	0.50
1:H:462:ALA:O	1:H:478:LEU:O	2.30	0.50
1:B:178:TRP:CH2	1:B:460:LEU:HD13	2.47	0.50
1:B:350:GLN:O	1:B:354:ILE:HG22	2.12	0.50
1:C:280:ALA:HA	1:C:315:VAL:HG21	1.94	0.50
1:D:380:PHE:CD1	1:D:380:PHE:N	2.79	0.50
1:E:248:THR:HA	1:E:270:LEU:HD13	1.94	0.50
1:E:433:PHE:CD2	1:E:455:ASN:HA	2.46	0.50
1:G:167:ILE:HB	1:G:194:PRO:HA	1.93	0.50
1:H:209:ILE:HG23	1:H:214:PHE:CD2	2.47	0.50
1:F:136:TRP:HB3	1:F:483:LEU:HD13	1.93	0.50
1:B:136:TRP:CD1	1:B:483:LEU:CD1	2.95	0.49
1:E:331:VAL:H	1:E:341:ASN:HB2	1.76	0.49
1:E:394:MET:HB2	1:E:397:ALA:CB	2.42	0.49
1:H:257:ALA:HA	1:H:260:LYS:NZ	2.27	0.49
1:D:299:GLN:HG3	1:D:342:GLN:HG3	1.93	0.49
1:E:22:LYS:HE3	1:E:31:ASN:ND2	2.26	0.49
1:E:466:PHE:O	1:E:476:ARG:HA	2.12	0.49
1:A:279:PHE:CE2	1:A:439:LYS:HD3	2.47	0.49
1:D:424:THR:C	1:D:470:LYS:HZ2	2.15	0.49
1:E:419:LYS:O	1:E:423:ASN:HB2	2.12	0.49
1:F:112:GLY:HA2	1:F:335:PRO:HG2	1.94	0.49
1:C:206:ALA:HA	1:C:209:ILE:HD12	1.94	0.49
1:C:350:GLN:O	1:C:354:ILE:HG13	2.13	0.49
1:C:457:TYR:HD1	1:C:458:MET:HG3	1.78	0.49
1:G:178:TRP:CH2	1:G:460:LEU:HD13	2.47	0.49
1:H:500:ASN:O	1:F:156:ARG:NH2	2.46	0.49
1:D:410:LYS:O	1:D:420:ARG:NH2	2.45	0.49
1:G:427:GLY:N	1:G:472:SER:OG	2.45	0.49
1:A:18:ILE:HG21	1:A:50:CYS:SG	2.53	0.49
1:B:168:PRO:HD3	1:B:245:THR:HB	1.94	0.49
1:H:451:VAL:HG21	1:H:466:PHE:HD1	1.78	0.49
1:A:457:TYR:HD1	1:A:458:MET:HG3	1.78	0.49
1:C:462:ALA:O	1:C:478:LEU:O	2.30	0.49
1:B:291:ALA:O	1:B:295:VAL:HG12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:96:MET:CE	1:G:177:ILE:HD11	2.42	0.49
1:D:13:LEU:CD2	1:D:101:LEU:HG	2.42	0.49
1:D:118:ALA:HA	1:D:122:ASP:HB2	1.94	0.49
1:D:279:PHE:HD2	1:D:434:THR:HB	1.76	0.49
1:D:330:TYR:HD1	1:D:341:ASN:HB3	1.78	0.49
1:F:371:GLY:HA3	1:F:385:THR:HA	1.94	0.49
1:B:403:GLY:O	1:B:405:VAL:N	2.43	0.48
1:C:179:LYS:NZ	1:C:477:GLU:OE2	2.32	0.48
1:D:272:GLY:HA2	1:D:426:TYR:CD1	2.47	0.48
1:G:414:VAL:O	1:G:417:VAL:HG12	2.13	0.48
1:A:299:GLN:HB3	1:A:345:GLN:OE1	2.13	0.48
1:C:467:GLY:HA2	1:C:476:ARG:HB3	1.95	0.48
1:D:296:PHE:HE1	1:D:406:GLN:HE21	1.60	0.48
1:G:24:PHE:CD2	1:G:206:ALA:HB1	2.48	0.48
1:E:265:ARG:HD2	1:E:265:ARG:H	1.78	0.48
1:G:206:ALA:HB2	1:G:221:ILE:HD12	1.95	0.48
1:F:171:PHE:HE1	1:F:302:CYS:HA	1.78	0.48
1:A:107:GLU:HB2	1:A:173:MET:HE2	1.96	0.48
1:E:9:VAL:HB	1:E:10:PRO:HD2	1.96	0.48
1:B:273:LYS:HG3	1:B:308:ARG:HD3	1.95	0.48
1:E:439:LYS:O	1:E:443:VAL:HG23	2.13	0.48
1:H:425:THR:O	1:H:471:MET:HB2	2.13	0.48
1:B:178:TRP:CE2	1:B:478:LEU:HD11	2.49	0.48
1:D:265:ARG:NH2	1:D:488:GLU:OE2	2.26	0.48
1:D:308:ARG:NH2	1:D:424:THR:OG1	2.44	0.48
1:G:289:GLU:HA	1:G:326:ARG:HH11	1.78	0.48
1:G:373:GLY:O	1:G:383:GLN:HG2	2.13	0.48
1:H:292:HIS:CE1	1:H:296:PHE:CE2	3.02	0.48
1:H:295:VAL:HG13	1:H:296:PHE:CD2	2.49	0.48
1:F:467:GLY:N	1:F:476:ARG:HD3	2.28	0.48
1:B:81:ASP:O	1:B:84:GLU:HB3	2.12	0.48
1:E:392:ASP:CG	1:E:420:ARG:HE	2.16	0.48
1:D:234:SER:HA	1:D:242:VAL:HG21	1.95	0.48
1:D:326:ARG:NH1	1:D:330:TYR:OH	2.34	0.48
1:F:360:SER:O	1:F:363:LYS:N	2.47	0.48
1:C:13:LEU:HD12	1:C:101:LEU:HG	1.96	0.47
1:D:326:ARG:HH12	1:D:330:TYR:HH	1.58	0.47
1:H:351:HIS:O	1:H:355:LEU:HD23	2.14	0.47
1:H:358:ILE:O	1:H:362:LYS:HG3	2.14	0.47
1:F:422:ASN:O	1:F:470:LYS:NZ	2.47	0.47
1:G:425:THR:HG23	1:G:426:TYR:CD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:304:VAL:HG21	1:C:453:TRP:HH2	1.80	0.47
1:D:248:THR:HA	1:D:270:LEU:HD13	1.95	0.47
1:D:396:ILE:HB	1:D:407:GLN:HE21	1.79	0.47
1:F:140:ILE:HD13	1:F:140:ILE:HA	1.54	0.47
1:D:326:ARG:O	1:D:326:ARG:HD3	2.14	0.47
1:E:437:LEU:HD11	1:H:494:MET:CE	2.44	0.47
1:G:178:TRP:CZ2	1:G:460:LEU:HD13	2.50	0.47
1:G:355:LEU:O	1:G:359:GLU:HG2	2.15	0.47
1:A:208:LEU:HD23	1:A:208:LEU:HA	1.71	0.47
1:B:354:ILE:CD1	1:B:403:GLY:HA3	2.37	0.47
1:C:165:GLN:OE1	1:C:190:VAL:HG21	2.15	0.47
1:C:209:ILE:HD13	1:C:219:VAL:HG11	1.95	0.47
1:C:242:VAL:HG12	1:C:266:VAL:HG12	1.97	0.47
1:E:118:ALA:HA	1:E:122:ASP:HB2	1.96	0.47
1:G:332:LEU:HD23	1:G:381:PHE:HD2	1.80	0.47
1:B:362:LYS:HD3	1:B:368:LEU:HD13	1.96	0.47
1:D:178:TRP:NE1	1:D:478:LEU:HD11	2.30	0.47
1:D:360:SER:OG	1:D:395:ARG:HB2	2.13	0.47
1:G:324:VAL:HG13	1:G:370:CYS:SG	2.55	0.47
1:H:23:ILE:HG13	1:H:223:PRO:HD2	1.96	0.47
1:F:80:MET:CE	1:F:85:ARG:HG2	2.44	0.47
1:A:273:LYS:HE2	1:A:399:GLU:O	2.15	0.47
1:A:331:VAL:H	1:A:341:ASN:HB2	1.80	0.47
1:B:374:ARG:HG2	1:B:375:TRP:N	2.30	0.47
1:D:13:LEU:N	1:D:105:THR:HG21	2.26	0.47
1:D:155:THR:HB	1:D:489:LEU:HD11	1.97	0.47
1:E:310:PHE:HA	1:E:409:MET:HG3	1.96	0.47
1:G:322:ARG:O	1:G:325:GLU:HB3	2.15	0.47
1:F:476:ARG:O	1:F:482:GLY:HA2	2.15	0.47
1:A:360:SER:OG	1:A:395:ARG:HD3	2.15	0.47
1:E:414:VAL:HG13	1:E:415:ASP:OD1	2.14	0.47
1:F:13:LEU:HD13	1:F:101:LEU:HD12	1.97	0.47
1:C:391:THR:OG1	1:C:394:MET:HG3	2.14	0.47
1:G:100:ARG:HH21	1:G:120:LEU:HA	1.79	0.47
1:G:128:LYS:HG2	1:F:87:ARG:NH2	2.30	0.47
1:F:143:GLN:NE2	1:F:145:ILE:HG12	2.29	0.47
1:H:149:GLY:O	1:H:499:LYS:HD3	2.15	0.47
1:G:32:SER:H	1:G:53:GLU:HG3	1.81	0.46
1:H:33:VAL:HG23	1:H:59:ASP:OD1	2.15	0.46
1:H:113:LYS:HD3	1:H:122:ASP:OD2	2.14	0.46
1:D:292:HIS:C	1:D:292:HIS:CD2	2.87	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:ILE:CD1	1:E:403:GLY:HA3	2.41	0.46
1:G:176:PHE:HE1	1:G:192:VAL:HG11	1.80	0.46
1:H:95:LEU:HD23	1:H:95:LEU:HA	1.59	0.46
1:B:237:MET:HA	1:B:262:ASN:ND2	2.28	0.46
1:C:24:PHE:CZ	1:C:27:ASN:HA	2.50	0.46
1:G:42:ASN:HB2	1:G:49:ILE:HD11	1.97	0.46
1:G:96:MET:HE1	1:G:177:ILE:HD11	1.98	0.46
1:G:132:TYR:CE1	1:G:463:GLN:HG3	2.49	0.46
1:A:136:TRP:CZ2	1:A:480:GLU:HB2	2.50	0.46
1:B:132:TYR:CE1	1:B:463:GLN:HG3	2.50	0.46
1:B:360:SER:OG	1:B:395:ARG:HD3	2.16	0.46
1:E:368:LEU:HB2	1:E:387:PHE:CE1	2.51	0.46
1:G:170:ASN:O	1:G:298:HIS:CE1	2.68	0.46
1:F:391:THR:N	1:F:394:MET:HE3	2.28	0.46
1:B:295:VAL:HG13	1:B:296:PHE:CD2	2.50	0.46
1:D:457:TYR:CD2	1:D:458:MET:HG3	2.50	0.46
1:H:393:GLU:O	1:H:393:GLU:HG2	2.15	0.46
1:F:161:GLY:HA3	1:F:240:ASP:OD2	2.16	0.46
1:F:428:LEU:HA	1:F:428:LEU:HD12	1.54	0.46
1:A:22:LYS:HA	1:A:53:GLU:HG3	1.98	0.46
1:A:432:LEU:HD21	1:A:440:ALA:HA	1.97	0.46
1:B:77:TRP:NE1	1:B:188:ASN:O	2.41	0.46
1:E:205:LEU:HA	1:E:205:LEU:HD23	1.66	0.46
1:E:333:GLY:HA3	1:E:340:ILE:HD13	1.97	0.46
1:H:457:TYR:HD1	1:H:458:MET:HG3	1.81	0.46
1:F:132:TYR:CE1	1:F:463:GLN:HG3	2.50	0.46
1:A:22:LYS:HA	1:A:53:GLU:CG	2.46	0.46
1:C:284:LEU:HD13	1:C:284:LEU:HA	1.39	0.46
1:E:78:ARG:NE	1:G:501:SER:OG	2.44	0.46
1:E:176:PHE:HD2	1:E:177:ILE:HD12	1.80	0.46
1:E:418:ILE:CD1	1:E:443:VAL:HG13	2.45	0.46
1:H:391:THR:H	1:H:394:MET:HE2	1.80	0.46
1:C:331:VAL:H	1:C:341:ASN:HB2	1.80	0.46
1:E:401:ILE:HG21	1:E:407:GLN:HE22	1.81	0.46
1:A:491:THR:HB	1:D:451:VAL:HG12	1.97	0.46
1:B:368:LEU:HD11	1:B:372:GLY:HA3	1.97	0.46
1:B:457:TYR:HD2	1:B:458:MET:HG3	1.78	0.46
1:D:432:LEU:HD21	1:D:440:ALA:HA	1.98	0.46
1:E:168:PRO:HG2	1:E:175:MET:HG3	1.98	0.46
1:E:392:ASP:O	1:E:398:LYS:NZ	2.49	0.46
1:G:140:ILE:HD13	1:G:140:ILE:HA	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:149:GLY:O	1:G:499:LYS:HD3	2.16	0.46
1:F:465:PRO:HB2	1:F:476:ARG:HB3	1.98	0.46
1:B:171:PHE:HB3	1:B:174:LEU:HB2	1.98	0.45
1:H:45:THR:OG1	1:H:47:GLU:HG2	2.16	0.45
1:H:457:TYR:CD1	1:H:458:MET:HG3	2.51	0.45
1:B:307:SER:O	1:B:407:GLN:HB2	2.15	0.45
1:G:374:ARG:HG3	1:G:381:PHE:O	2.16	0.45
1:F:168:PRO:HD3	1:F:245:THR:HB	1.98	0.45
1:E:427:GLY:O	1:E:449:ALA:HA	2.16	0.45
1:D:296:PHE:CD2	1:D:404:PRO:HB3	2.51	0.45
1:G:255:LYS:NZ	1:H:255:LYS:NZ	2.64	0.45
1:G:390:VAL:HG22	1:G:408:ILE:O	2.15	0.45
1:G:456:CYS:HB3	1:H:495:LYS:HB2	1.97	0.45
1:B:353:LYS:NZ	1:B:401:ILE:O	2.49	0.45
1:B:457:TYR:CE2	1:B:458:MET:HG3	2.52	0.45
1:G:374:ARG:HG2	1:G:375:TRP:H	1.81	0.45
1:F:483:LEU:HD23	1:F:483:LEU:O	2.16	0.45
1:A:347:ASP:HA	1:A:380:PHE:CE2	2.51	0.45
1:A:478:LEU:HA	1:A:478:LEU:HD23	1.66	0.45
1:C:295:VAL:HG11	1:C:406:GLN:OE1	2.16	0.45
1:B:402:PHE:HD1	1:B:402:PHE:HA	1.54	0.45
1:E:140:ILE:HD13	1:E:140:ILE:HA	1.79	0.45
1:E:393:GLU:HA	1:E:398:LYS:NZ	2.32	0.45
1:G:432:LEU:HD22	1:G:454:VAL:HG22	1.99	0.45
1:H:55:GLY:HA2	1:H:59:ASP:OD2	2.17	0.45
1:H:155:THR:HB	1:H:489:LEU:HD11	1.98	0.45
1:H:324:VAL:HG12	1:H:328:LYS:HE3	1.99	0.45
1:H:141:HIS:HB2	1:F:143:GLN:HG3	1.97	0.45
1:H:173:MET:CE	1:H:205:LEU:HD21	2.47	0.45
1:F:232:ALA:O	1:F:236:HIS:HB2	2.17	0.45
1:B:178:TRP:CZ2	1:B:460:LEU:HD13	2.52	0.45
1:C:325:GLU:HA	1:C:325:GLU:OE1	2.17	0.45
1:D:283:ASP:HB3	1:D:286:ILE:CG1	2.47	0.45
1:G:43:PRO:HB3	1:G:346:ILE:HA	1.99	0.45
1:G:316:TYR:HE2	1:G:409:MET:C	2.21	0.45
1:C:295:VAL:HG21	1:C:406:GLN:HB2	1.98	0.45
1:C:478:LEU:HD22	1:C:478:LEU:HA	1.85	0.45
1:A:71:PHE:CE2	1:A:161:GLY:HA2	2.52	0.44
1:A:401:ILE:HG13	1:A:402:PHE:N	2.32	0.44
1:B:130:LEU:HD23	1:B:130:LEU:HA	1.79	0.44
1:C:395:ARG:O	1:C:397:ALA:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ASP:HB3	1:D:286:ILE:HG12	1.99	0.44
1:D:292:HIS:CD2	1:D:296:PHE:HB2	2.51	0.44
1:D:292:HIS:NE2	1:D:296:PHE:HB2	2.32	0.44
1:E:290:PHE:CD2	1:E:456:CYS:HA	2.52	0.44
1:G:77:TRP:CZ3	1:G:80:MET:HE2	2.52	0.44
1:G:151:ILE:HG23	1:G:153:THR:HG23	1.99	0.44
1:A:279:PHE:HE2	1:A:414:VAL:HG22	1.82	0.44
1:B:16:LEU:HD12	1:B:16:LEU:HA	1.62	0.44
1:D:277:ILE:HG21	1:D:279:PHE:CE1	2.53	0.44
1:E:263:LEU:HD21	1:F:252:LYS:HA	1.98	0.44
1:H:84:GLU:OE2	1:H:87:ARG:NH2	2.51	0.44
1:H:169:TRP:CE2	1:H:346:ILE:HG21	2.53	0.44
1:H:337:THR:HB	1:H:340:ILE:HD12	2.00	0.44
1:C:56:ASP:O	1:C:60:VAL:HG23	2.17	0.44
1:C:147:SER:OG	1:C:151:ILE:HD11	2.17	0.44
1:H:71:PHE:CZ	1:H:161:GLY:HA2	2.52	0.44
1:A:363:LYS:HD3	1:A:363:LYS:O	2.18	0.44
1:D:414:VAL:O	1:D:418:ILE:HG13	2.18	0.44
1:F:248:THR:HA	1:F:270:LEU:HD13	1.99	0.44
1:A:390:VAL:O	1:A:409:MET:HG2	2.17	0.44
1:A:428:LEU:HB2	1:A:472:SER:CB	2.46	0.44
1:C:43:PRO:HB2	1:C:344:PRO:HG2	2.00	0.44
1:B:284:LEU:HD22	1:B:315:VAL:HG13	1.98	0.44
1:B:304:VAL:HG11	1:B:453:TRP:CZ3	2.52	0.44
1:D:90:ASN:OD1	1:D:131:LYS:NZ	2.50	0.44
1:G:113:LYS:O	1:G:335:PRO:HB3	2.18	0.44
1:H:16:LEU:HA	1:H:16:LEU:HD12	1.65	0.44
1:B:149:GLY:O	1:B:499:LYS:HD3	2.18	0.44
1:D:401:ILE:O	1:D:401:ILE:HG13	2.17	0.44
1:E:167:ILE:CD1	1:E:179:LYS:HG3	2.48	0.44
1:E:177:ILE:HD12	1:E:177:ILE:N	2.33	0.44
1:E:178:TRP:NE1	1:E:478:LEU:HD11	2.33	0.44
1:A:365:GLY:O	1:A:394:MET:CE	2.66	0.44
1:C:13:LEU:HD12	1:C:13:LEU:H	1.80	0.44
1:H:334:ASN:O	1:H:340:ILE:HD12	2.18	0.44
1:B:357:LEU:HD13	1:B:357:LEU:HA	1.71	0.44
1:E:34:SER:OG	1:E:36:LYS:HG3	2.18	0.44
1:E:368:LEU:HB2	1:E:387:PHE:HE1	1.82	0.44
1:F:374:ARG:HG2	1:F:375:TRP:N	2.32	0.44
1:G:157:ARG:HD3	1:G:489:LEU:HB3	2.00	0.43
1:G:171:PHE:HZ	1:G:302:CYS:SG	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:268:LEU:HB3	1:F:270:LEU:HD21	1.98	0.43
1:C:77:TRP:NE1	1:C:188:ASN:O	2.47	0.43
1:D:304:VAL:O	1:D:304:VAL:HG23	2.17	0.43
1:G:432:LEU:HD23	1:G:454:VAL:HG13	1.99	0.43
1:F:291:ALA:HB1	1:F:309:ILE:CD1	2.48	0.43
1:B:277:ILE:HB	1:B:432:LEU:HD12	1.99	0.43
1:D:414:VAL:O	1:D:417:VAL:HG12	2.18	0.43
1:E:179:LYS:NZ	1:E:477:GLU:OE1	2.51	0.43
1:H:143:GLN:HG2	1:F:141:HIS:CD2	2.53	0.43
1:A:479:GLY:H	1:A:482:GLY:HA3	1.84	0.43
1:B:304:VAL:HG13	1:B:429:ALA:HB3	1.99	0.43
1:B:405:VAL:HG12	1:B:407:GLN:OE1	2.18	0.43
1:D:239:VAL:O	1:D:264:LYS:HE3	2.17	0.43
1:E:110:ASN:O	1:E:110:ASN:ND2	2.49	0.43
1:G:32:SER:H	1:G:53:GLU:CG	2.30	0.43
1:G:139:LYS:HD3	1:F:136:TRP:CE2	2.53	0.43
1:H:171:PHE:HB3	1:H:174:LEU:HB2	2.01	0.43
1:F:332:LEU:HD23	1:F:381:PHE:HB3	2.00	0.43
1:A:56:ASP:OD1	1:A:228:THR:HB	2.19	0.43
1:A:284:LEU:HD12	1:A:284:LEU:HA	1.76	0.43
1:E:374:ARG:HG2	1:E:375:TRP:N	2.32	0.43
1:G:136:TRP:NE1	1:F:139:LYS:HD3	2.34	0.43
1:G:368:LEU:HD21	1:G:371:GLY:O	2.18	0.43
1:H:299:GLN:NE2	1:H:343:GLY:C	2.72	0.43
1:A:246:GLY:O	1:A:270:LEU:HA	2.18	0.43
1:A:491:THR:HG21	1:D:464:CYS:HB3	2.00	0.43
1:C:450:GLY:CA	1:C:467:GLY:O	2.65	0.43
1:C:467:GLY:CA	1:C:476:ARG:HB3	2.49	0.43
1:D:296:PHE:HE1	1:D:406:GLN:NE2	2.17	0.43
1:G:201:THR:O	1:G:205:LEU:HD13	2.18	0.43
1:G:466:PHE:CE1	1:G:478:LEU:HD12	2.53	0.43
1:H:174:LEU:HD23	1:H:174:LEU:HA	1.94	0.43
1:A:20:HIS:HB3	1:A:29:TRP:CH2	2.53	0.43
1:A:255:LYS:HE3	1:D:255:LYS:HG3	2.01	0.43
1:B:196:GLU:HG2	1:B:197:GLN:N	2.33	0.43
1:C:31:ASN:CA	1:C:53:GLU:OE1	2.60	0.43
1:H:279:PHE:HE2	1:H:414:VAL:HG22	1.83	0.43
1:F:193:LYS:HE3	1:F:226:GLY:HA2	1.99	0.43
1:A:411:PHE:CD2	1:A:417:VAL:HB	2.54	0.43
1:C:262:ASN:O	1:C:264:LYS:N	2.50	0.43
1:C:299:GLN:HG2	1:C:343:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:273:LYS:HD2	1:H:273:LYS:HA	1.82	0.43
1:C:80:MET:SD	1:C:84:GLU:HG3	2.59	0.43
1:D:110:ASN:O	1:D:110:ASN:ND2	2.49	0.43
1:E:394:MET:O	1:E:398:LYS:N	2.52	0.43
1:G:136:TRP:CZ2	1:G:480:GLU:HB2	2.54	0.43
1:G:348:LYS:HE2	1:G:351:HIS:HD2	1.83	0.43
1:H:160:ILE:N	1:H:188:ASN:OD1	2.51	0.43
1:F:373:GLY:H	1:F:383:GLN:HG2	1.84	0.43
1:B:37:LYS:HE2	1:B:53:GLU:OE2	2.18	0.43
1:B:360:SER:O	1:B:364:GLU:HG3	2.18	0.43
1:C:168:PRO:HD3	1:C:245:THR:HB	1.99	0.43
1:C:395:ARG:O	1:C:398:LYS:N	2.30	0.43
1:C:466:PHE:CZ	1:C:477:GLU:OE1	2.62	0.43
1:D:209:ILE:HD13	1:D:219:VAL:HG11	2.01	0.43
1:D:325:GLU:O	1:D:328:LYS:HG2	2.19	0.43
1:E:168:PRO:HD3	1:E:245:THR:HB	2.01	0.43
1:E:276:CYS:O	1:E:277:ILE:HD13	2.18	0.43
1:G:289:GLU:HA	1:G:326:ARG:NH1	2.33	0.43
1:E:453:TRP:HZ2	1:E:460:LEU:CD2	2.32	0.42
1:G:106:MET:CE	1:G:200:LEU:HB3	2.49	0.42
1:G:165:GLN:NE2	1:G:179:LYS:HB3	2.34	0.42
1:F:285:ASP:CG	1:F:322:ARG:HH21	2.22	0.42
1:C:43:PRO:HB2	1:C:344:PRO:HG3	2.01	0.42
1:D:99:ASP:O	1:D:103:LEU:HD12	2.19	0.42
1:G:20:HIS:HB3	1:G:29:TRP:CH2	2.54	0.42
1:G:450:GLY:HA3	1:G:467:GLY:O	2.19	0.42
1:H:193:LYS:HD3	1:H:193:LYS:C	2.39	0.42
1:H:347:ASP:OD1	1:H:350:GLN:HG2	2.19	0.42
1:F:24:PHE:CZ	1:F:27:ASN:HA	2.54	0.42
1:F:174:LEU:HD12	1:F:174:LEU:HA	1.84	0.42
1:F:284:LEU:HD23	1:F:284:LEU:HA	1.72	0.42
1:B:386:VAL:HG13	1:B:408:ILE:CD1	2.49	0.42
1:C:313:GLU:OE1	1:C:412:LYS:HD2	2.18	0.42
1:E:130:LEU:HD23	1:E:130:LEU:HA	1.61	0.42
1:G:268:LEU:HD13	1:G:268:LEU:H	1.83	0.42
1:H:313:GLU:HB2	1:H:412:LYS:HD2	2.01	0.42
1:H:357:LEU:HD13	1:H:357:LEU:HA	1.66	0.42
1:C:167:ILE:HB	1:C:194:PRO:HA	2.00	0.42
1:D:170:ASN:O	1:D:298:HIS:HE1	2.02	0.42
1:G:44:ALA:HA	1:G:344:PRO:HG3	2.01	0.42
1:F:113:LYS:CD	1:F:122:ASP:OD2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:LEU:HD13	1:F:214:PHE:CE2	2.55	0.42
1:F:196:GLU:HG2	1:F:197:GLN:N	2.35	0.42
1:F:466:PHE:HD2	1:F:477:GLU:OE2	2.03	0.42
1:B:295:VAL:HB	1:B:306:ALA:O	2.20	0.42
1:D:304:VAL:CG1	1:D:466:PHE:HZ	2.33	0.42
1:E:353:LYS:O	1:E:357:LEU:HD23	2.19	0.42
1:G:432:LEU:O	1:G:454:VAL:HA	2.18	0.42
1:C:360:SER:O	1:C:364:GLU:HG3	2.19	0.42
1:D:197:GLN:OE1	1:D:197:GLN:N	2.45	0.42
1:G:39:PRO:HB3	1:G:51:HIS:CE1	2.54	0.42
1:G:248:THR:HG22	1:G:252:LYS:HE3	2.00	0.42
1:G:306:ALA:HB2	1:G:457:TYR:CZ	2.54	0.42
1:F:157:ARG:NH1	1:F:487:THR:OG1	2.42	0.42
1:C:132:TYR:CE1	1:C:463:GLN:HG3	2.55	0.42
1:C:298:HIS:O	1:C:301:GLN:HG3	2.19	0.42
1:E:151:ILE:HG22	1:E:152:PHE:N	2.35	0.42
1:E:246:GLY:O	1:E:270:LEU:HA	2.19	0.42
1:E:295:VAL:CG2	1:E:296:PHE:CD2	3.02	0.42
1:A:71:PHE:CD1	1:A:78:ARG:HD3	2.54	0.42
1:A:96:MET:HE1	1:A:130:LEU:HD22	2.02	0.42
1:A:313:GLU:OE1	1:A:412:LYS:HD2	2.18	0.42
1:E:453:TRP:HZ2	1:E:460:LEU:HD23	1.85	0.42
1:G:304:VAL:HG23	1:G:304:VAL:O	2.20	0.42
1:C:464:CYS:HA	1:C:465:PRO:HD3	1.94	0.42
1:D:84:GLU:OE2	1:D:87:ARG:NE	2.50	0.42
1:E:87:ARG:NH2	1:H:128:LYS:HE2	2.35	0.42
1:F:13:LEU:HA	1:F:13:LEU:HD12	1.64	0.42
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.73	0.42
1:C:107:GLU:OE1	1:C:201:THR:HG21	2.20	0.42
1:E:292:HIS:CE1	1:E:330:TYR:HH	2.38	0.41
1:G:103:LEU:HD22	1:G:205:LEU:HD11	2.02	0.41
1:D:214:PHE:HB3	1:D:218:VAL:HG11	2.03	0.41
1:E:180:ILE:HB	1:E:184:LEU:HD13	2.02	0.41
1:H:193:LYS:HD3	1:H:193:LYS:O	2.20	0.41
1:H:284:LEU:HD23	1:H:322:ARG:HH21	1.85	0.41
1:F:396:ILE:HD12	1:F:407:GLN:HG2	2.00	0.41
1:A:235:SER:HA	1:A:261:SER:OG	2.20	0.41
1:A:412:LYS:HD3	1:A:412:LYS:N	2.36	0.41
1:E:115:PHE:HB2	1:E:336:LEU:HD23	2.02	0.41
1:F:239:VAL:O	1:F:264:LYS:HE3	2.20	0.41
1:F:295:VAL:HB	1:F:306:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ASP:N	1:B:99:ASP:OD1	2.53	0.41
1:C:434:THR:HG22	1:C:435:LYS:N	2.35	0.41
1:E:330:TYR:N	1:E:330:TYR:CD1	2.88	0.41
1:G:130:LEU:HD23	1:G:130:LEU:HA	1.79	0.41
1:H:377:ASN:OD1	1:H:378:LYS:N	2.53	0.41
1:A:466:PHE:CE2	1:A:477:GLU:HB2	2.55	0.41
1:B:262:ASN:ND2	1:B:264:LYS:HZ2	2.18	0.41
1:B:419:LYS:O	1:B:423:ASN:HB2	2.21	0.41
1:C:258:ALA:HB1	1:C:264:LYS:HG3	2.02	0.41
1:E:45:THR:HA	1:E:378:LYS:NZ	2.35	0.41
1:E:466:PHE:HD1	1:E:466:PHE:HA	1.73	0.41
1:G:106:MET:HE3	1:G:106:MET:HB3	1.75	0.41
1:G:348:LYS:O	1:G:352:ASP:N	2.45	0.41
1:G:355:LEU:HD13	1:G:355:LEU:HA	1.81	0.41
1:H:355:LEU:HA	1:H:355:LEU:HD13	1.79	0.41
1:H:450:GLY:HA3	1:H:467:GLY:O	2.21	0.41
1:D:155:THR:HA	1:D:490:LYS:O	2.21	0.41
1:E:45:THR:OG1	1:E:47:GLU:HG2	2.20	0.41
1:E:151:ILE:HD11	1:F:459:MET:HG3	2.01	0.41
1:H:396:ILE:HB	1:H:401:ILE:HD11	2.02	0.41
1:F:83:SER:O	1:F:87:ARG:HG3	2.21	0.41
1:A:176:PHE:HD2	1:A:177:ILE:HD12	1.86	0.41
1:A:411:PHE:C	1:A:412:LYS:HD3	2.41	0.41
1:B:136:TRP:CD1	1:B:483:LEU:HD12	2.56	0.41
1:B:178:TRP:CD1	1:B:478:LEU:HD11	2.55	0.41
1:B:374:ARG:HG2	1:B:375:TRP:H	1.85	0.41
1:B:422:ASN:OD1	1:B:448:GLN:HB3	2.21	0.41
1:C:71:PHE:CZ	1:C:161:GLY:HA2	2.55	0.41
1:G:156:ARG:O	1:G:489:LEU:HA	2.21	0.41
1:H:112:GLY:HA2	1:H:335:PRO:HG2	2.02	0.41
1:B:400:GLU:OE1	1:B:401:ILE:N	2.54	0.41
1:E:209:ILE:HD13	1:E:219:VAL:HG11	2.01	0.41
1:C:113:LYS:HZ1	1:C:172:PRO:HD2	1.86	0.41
1:D:320:VAL:HG22	1:D:408:ILE:HG21	2.02	0.41
1:G:171:PHE:CE1	1:G:302:CYS:HA	2.52	0.41
1:G:371:GLY:HA3	1:G:384:PRO:O	2.21	0.41
1:H:317:ASP:O	1:H:320:VAL:HG12	2.21	0.41
1:F:462:ALA:O	1:F:478:LEU:O	2.39	0.41
1:B:13:LEU:HD12	1:B:13:LEU:N	2.36	0.41
1:C:273:LYS:HZ3	1:C:307:SER:HB2	1.86	0.41
1:D:71:PHE:CE2	1:D:161:GLY:HA2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:LYS:HB2	1:D:470:LYS:HE3	1.87	0.41
1:G:68:ARG:NH2	1:G:240:ASP:OD2	2.41	0.41
1:G:106:MET:HE1	1:G:200:LEU:HB3	2.03	0.41
1:G:255:LYS:HZ1	1:H:255:LYS:NZ	2.19	0.41
1:F:130:LEU:HA	1:F:130:LEU:HD23	1.71	0.41
1:B:167:ILE:HB	1:B:194:PRO:HA	2.02	0.40
1:B:465:PRO:HG2	1:C:489:LEU:HD21	2.04	0.40
1:C:244:PHE:CG	1:C:254:ILE:HD12	2.56	0.40
1:D:345:GLN:HG3	1:D:354:ILE:HD12	2.02	0.40
1:E:393:GLU:HA	1:E:398:LYS:HZ3	1.84	0.40
1:G:248:THR:HA	1:G:270:LEU:HD13	2.03	0.40
1:G:433:PHE:CD1	1:G:455:ASN:HA	2.55	0.40
1:A:167:ILE:CD1	1:A:179:LYS:HG3	2.51	0.40
1:C:164:GLY:O	1:C:242:VAL:HA	2.21	0.40
1:G:311:VAL:CG1	1:G:315:VAL:HG23	2.49	0.40
1:A:488:GLU:HG3	1:D:469:PHE:CE1	2.56	0.40
1:B:110:ASN:O	1:B:110:ASN:ND2	2.52	0.40
1:E:108:ALA:HB3	1:E:336:LEU:HD21	2.03	0.40
1:G:432:LEU:HD11	1:G:443:VAL:HB	2.03	0.40
1:H:132:TYR:CE1	1:H:463:GLN:HG3	2.56	0.40
1:H:480:GLU:O	1:H:484:TYR:HD2	2.04	0.40
1:B:168:PRO:HG2	1:B:175:MET:HG3	2.03	0.40
1:C:174:LEU:HA	1:C:174:LEU:HD23	1.85	0.40
1:D:151:ILE:HD12	1:D:151:ILE:C	2.42	0.40
1:E:358:ILE:HG21	1:E:372:GLY:HA2	2.02	0.40
1:H:57:LYS:HD3	1:H:61:ASP:OD2	2.21	0.40
1:F:77:TRP:CZ3	1:F:80:MET:HE1	2.57	0.40
1:A:232:ALA:O	1:A:236:HIS:HB2	2.22	0.40
1:C:428:LEU:HA	1:C:428:LEU:HD12	1.80	0.40
1:D:297:TYR:HD2	1:D:302:CYS:SG	2.45	0.40
1:G:425:THR:O	1:G:471:MET:HB2	2.22	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	492/507 (97%)	484 (98%)	8 (2%)	0	100	100
1	B	492/507 (97%)	480 (98%)	11 (2%)	1 (0%)	47	78
1	C	492/507 (97%)	480 (98%)	12 (2%)	0	100	100
1	D	492/507 (97%)	486 (99%)	6 (1%)	0	100	100
1	E	492/507 (97%)	486 (99%)	6 (1%)	0	100	100
1	F	492/507 (97%)	484 (98%)	7 (1%)	1 (0%)	47	78
1	G	490/507 (97%)	479 (98%)	11 (2%)	0	100	100
1	H	492/507 (97%)	481 (98%)	11 (2%)	0	100	100
All	All	3934/4056 (97%)	3860 (98%)	72 (2%)	2 (0%)	51	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	16	LEU
1	F	10	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/413 (96%)	393 (99%)	3 (1%)	81	94
1	B	393/413 (95%)	389 (99%)	4 (1%)	76	92
1	C	394/413 (95%)	386 (98%)	8 (2%)	55	82
1	D	392/413 (95%)	386 (98%)	6 (2%)	65	87
1	E	394/413 (95%)	388 (98%)	6 (2%)	65	87
1	F	393/413 (95%)	386 (98%)	7 (2%)	59	85
1	G	383/413 (93%)	374 (98%)	9 (2%)	50	80
1	H	398/413 (96%)	394 (99%)	4 (1%)	76	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3143/3304 (95%)	3096 (98%)	47 (2%)	65 87

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	402	PHE
1	A	412	LYS
1	B	87	ARG
1	B	110	ASN
1	B	122	ASP
1	B	402	PHE
1	C	15	ASP
1	C	110	ASN
1	C	303	CYS
1	C	326	ARG
1	C	402	PHE
1	C	412	LYS
1	C	476	ARG
1	C	478	LEU
1	D	106	MET
1	D	110	ASN
1	D	303	CYS
1	D	316	TYR
1	D	380	PHE
1	D	402	PHE
1	E	110	ASN
1	E	299	GLN
1	E	303	CYS
1	E	321	LYS
1	E	402	PHE
1	E	466	PHE
1	G	68	ARG
1	G	110	ASN
1	G	268	LEU
1	G	299	GLN
1	G	303	CYS
1	G	322	ARG
1	G	347	ASP
1	G	356	ASP
1	G	402	PHE
1	H	69	GLN

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Mol	Chain	Res	Type
1	H	303	CYS
1	H	402	PHE
1	H	410	LYS
1	F	81	ASP
1	F	101	LEU
1	F	265	ARG
1	F	299	GLN
1	F	303	CYS
1	F	402	PHE
1	F	409	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	262	ASN
1	C	383	GLN
1	D	298	HIS
1	D	301	GLN
1	D	407	GLN
1	G	298	HIS
1	G	351	HIS
1	G	383	GLN
1	H	292	HIS
1	F	141	HIS
1	F	500	ASN

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 monosaccharides 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	494/507 (97%)	0.08	5 (1%) 82 82	37, 59, 84, 100	0
1	B	494/507 (97%)	0.14	7 (1%) 75 75	34, 61, 98, 116	0
1	C	494/507 (97%)	0.15	11 (2%) 62 59	46, 71, 96, 114	0
1	D	494/507 (97%)	0.31	26 (5%) 26 22	35, 69, 127, 146	0
1	E	494/507 (97%)	0.28	15 (3%) 50 45	49, 78, 105, 127	0
1	F	494/507 (97%)	0.23	13 (2%) 56 52	54, 77, 99, 113	0
1	G	492/507 (97%)	0.61	48 (9%) 7 5	45, 100, 157, 174	0
1	H	494/507 (97%)	0.20	9 (1%) 68 67	42, 73, 104, 119	0
All	All	3950/4056 (97%)	0.25	134 (3%) 45 40	34, 73, 120, 174	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	466	PHE	6.9
1	E	476	ARG	6.4
1	D	333	GLY	5.5
1	G	377	ASN	5.2
1	G	476	ARG	5.2
1	C	372	GLY	5.0
1	A	466	PHE	4.9
1	F	466	PHE	4.5
1	G	387	PHE	4.4
1	G	467	GLY	4.4
1	G	41	LEU	4.3
1	G	304	VAL	4.2
1	G	400	GLU	4.2
1	G	370	CYS	4.0
1	G	478	LEU	4.0
1	G	306	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	425	THR	3.9
1	D	466	PHE	3.9
1	G	375	TRP	3.9
1	G	468	GLY	3.8
1	F	478	LEU	3.8
1	E	357	LEU	3.7
1	E	474	ASN	3.7
1	G	474	ASN	3.7
1	G	44	ALA	3.7
1	G	396	ILE	3.6
1	G	403	GLY	3.6
1	E	478	LEU	3.6
1	G	333	GLY	3.6
1	C	475	GLY	3.5
1	G	382	VAL	3.5
1	G	43	PRO	3.5
1	F	377	ASN	3.4
1	E	475	GLY	3.4
1	G	295	VAL	3.4
1	A	474	ASN	3.4
1	F	476	ARG	3.3
1	E	477	GLU	3.3
1	C	476	ARG	3.2
1	E	396	ILE	3.2
1	B	478	LEU	3.2
1	D	476	ARG	3.1
1	E	466	PHE	3.1
1	D	357	LEU	3.1
1	B	472	SER	3.1
1	G	332	LEU	3.0
1	F	477	GLU	3.0
1	D	376	GLY	3.0
1	D	397	ALA	3.0
1	G	307	SER	2.9
1	D	381	PHE	2.9
1	G	405	VAL	2.9
1	G	272	GLY	2.9
1	G	460	LEU	2.9
1	H	472	SER	2.9
1	E	372	GLY	2.9
1	H	477	GLU	2.8
1	A	475	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	406	GLN	2.8
1	H	478	LEU	2.8
1	B	393	GLU	2.8
1	C	478	LEU	2.7
1	G	349	GLU	2.7
1	D	368	LEU	2.7
1	D	400	GLU	2.7
1	E	330	TYR	2.7
1	H	460	LEU	2.7
1	G	372	GLY	2.6
1	D	385	THR	2.6
1	E	425	THR	2.6
1	H	476	ARG	2.6
1	G	373	GLY	2.6
1	F	304	VAL	2.6
1	D	477	GLU	2.6
1	D	332	LEU	2.5
1	F	400	GLU	2.5
1	A	467	GLY	2.5
1	E	400	GLU	2.5
1	G	475	GLY	2.5
1	C	44	ALA	2.4
1	D	359	GLU	2.4
1	B	428	LEU	2.4
1	B	306	ALA	2.4
1	D	370	CYS	2.4
1	G	458	MET	2.4
1	H	15	ASP	2.3
1	G	327	ALA	2.3
1	D	392	ASP	2.3
1	G	397	ALA	2.3
1	D	478	LEU	2.3
1	A	425	THR	2.3
1	E	460	LEU	2.3
1	G	180	ILE	2.3
1	H	466	PHE	2.3
1	F	372	GLY	2.3
1	D	475	GLY	2.3
1	G	277	ILE	2.3
1	G	355	LEU	2.2
1	D	426	TYR	2.2
1	H	467	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	296	PHE	2.2
1	D	402	PHE	2.2
1	E	377	ASN	2.2
1	G	383	GLN	2.2
1	C	113	LYS	2.2
1	E	271	GLY	2.2
1	F	375	TRP	2.2
1	D	331	VAL	2.2
1	F	9	VAL	2.2
1	H	8	ALA	2.1
1	F	143	GLN	2.1
1	C	376	GLY	2.1
1	C	358	ILE	2.1
1	C	400	GLU	2.1
1	G	381	PHE	2.1
1	D	472	SER	2.1
1	B	460	LEU	2.1
1	G	346	ILE	2.1
1	D	377	ASN	2.1
1	F	475	GLY	2.1
1	G	376	GLY	2.1
1	C	263	LEU	2.1
1	D	425	THR	2.1
1	G	361	GLY	2.1
1	G	209	ILE	2.0
1	G	501	SER	2.0
1	D	366	ALA	2.0
1	G	330	TYR	2.0
1	C	269	GLU	2.0
1	G	276	CYS	2.0
1	G	40	VAL	2.0
1	G	176	PHE	2.0
1	G	13	LEU	2.0
1	F	474	ASN	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 [i](#)

There are no monosaccharides 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.