



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:34 AM UTC

PDB ID : 7YOB / pdb_00007yob
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

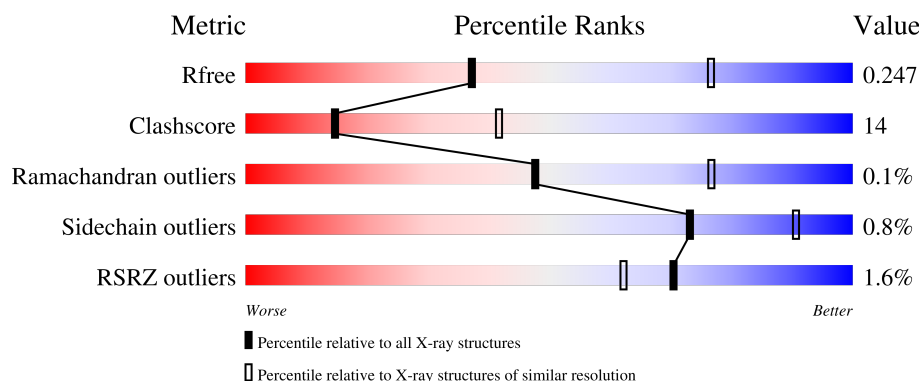
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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	2% 74% 23% .
1	B	507	% 74% 23% ..
1	C	507	2% 73% 23% ..
1	D	507	2% 74% 23% .
1	E	507	% 70% 27% .

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Mol	Chain	Length	Quality of chain
1	F	507	2% 74% 22% • •
1	G	507	2% 59% 36% • •
1	H	507	2% 68% 29% •

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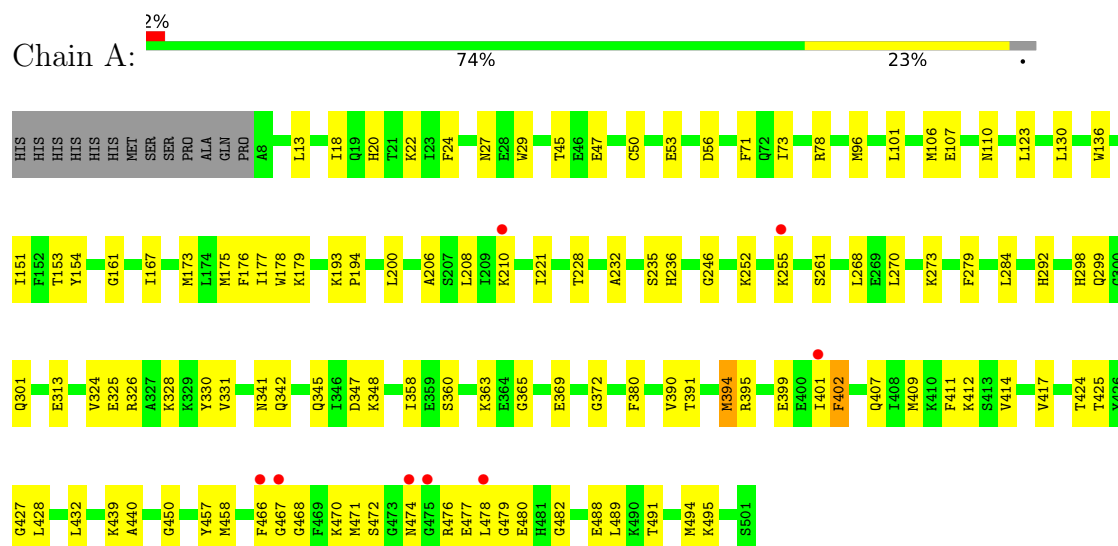
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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P24549
C	-3	HIS	-	expression tag	UNP P24549
C	-2	HIS	-	expression tag	UNP P24549
C	-1	HIS	-	expression tag	UNP P24549
C	0	HIS	-	expression tag	UNP P24549
D	-5	HIS	-	expression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

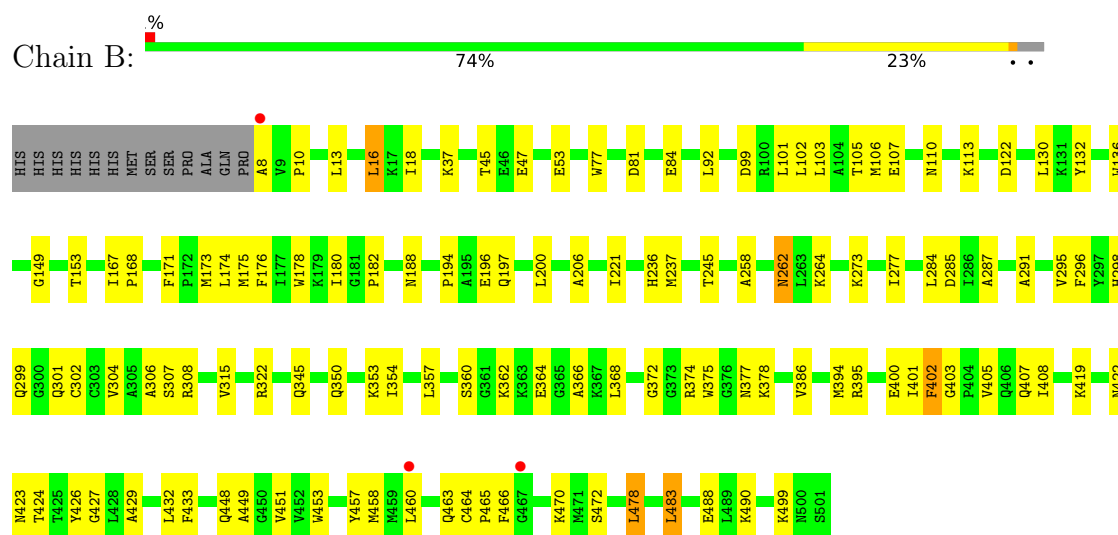
3 Residue-property plots

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.

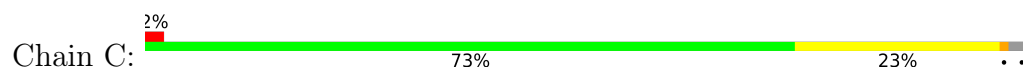
• Molecule 1: Aldehyde dehydrogenase 1A1

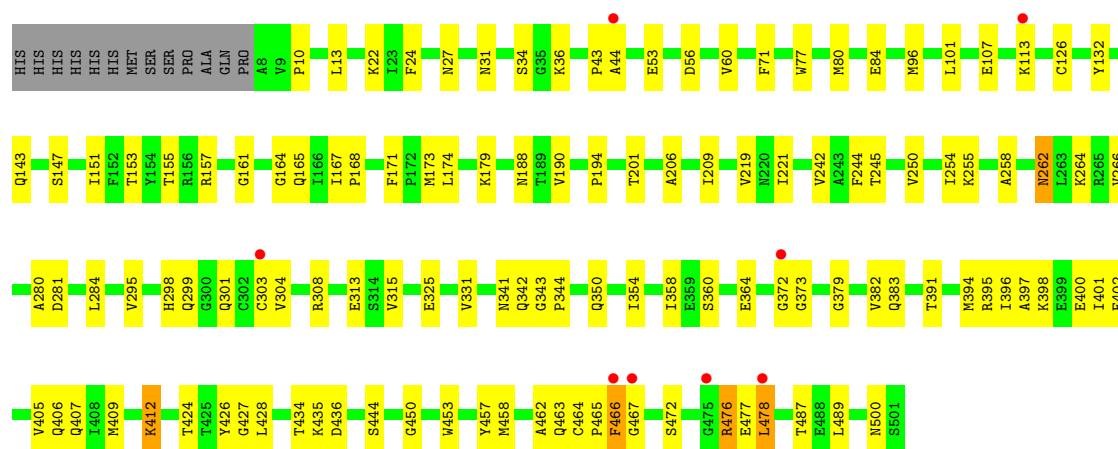


• Molecule 1: Aldehyde dehydrogenase 1A1

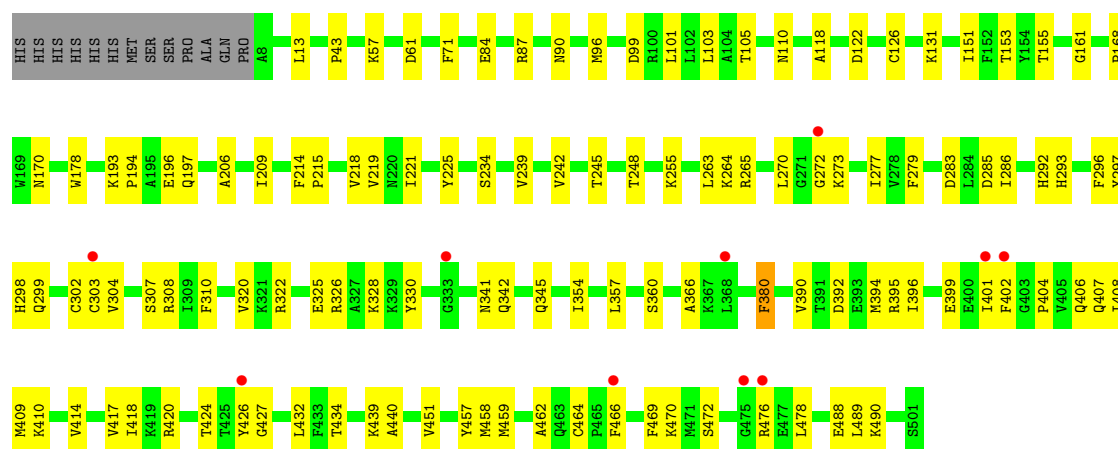
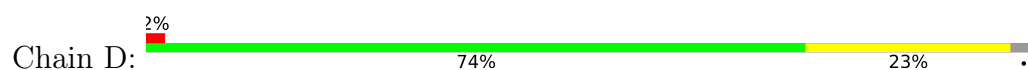


• Molecule 1: Aldehyde dehydrogenase 1A1

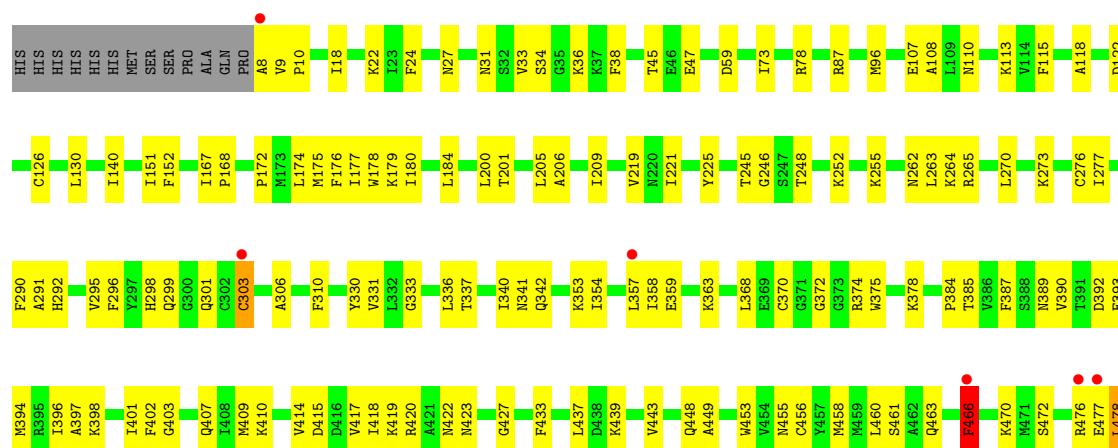




• Molecule 1: Aldehyde dehydrogenase 1A1

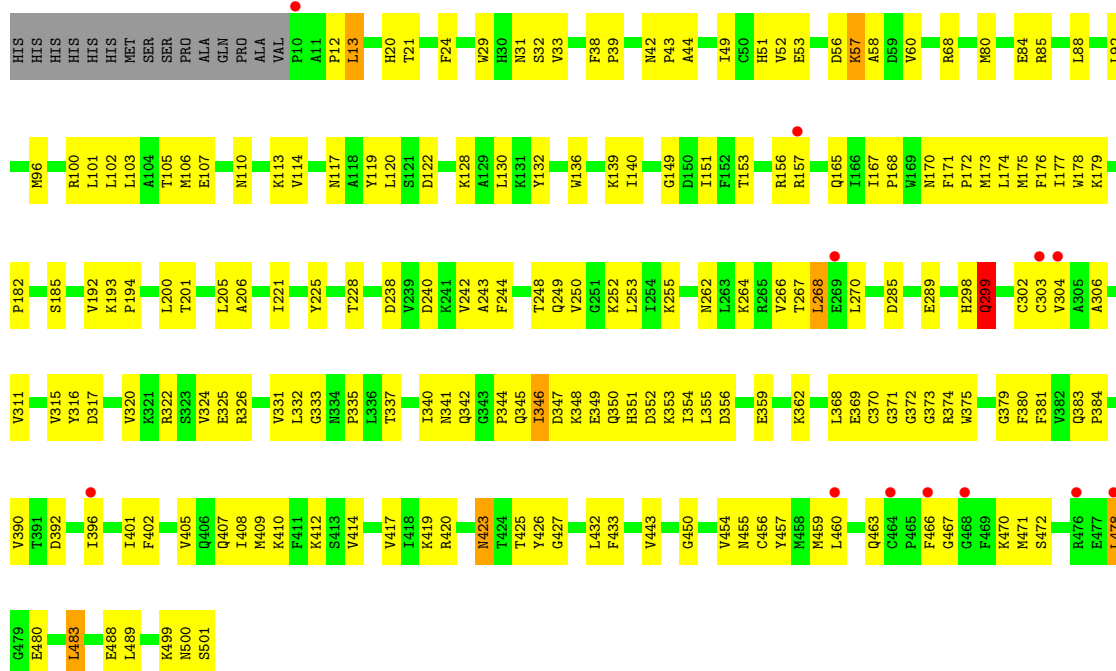


• Molecule 1: Aldehyde dehydrogenase 1A1

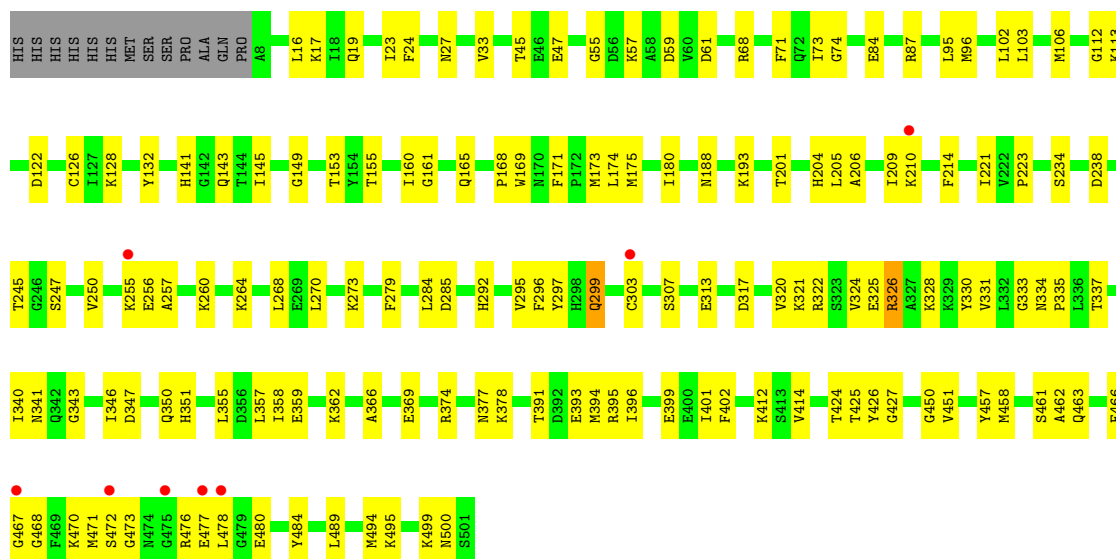




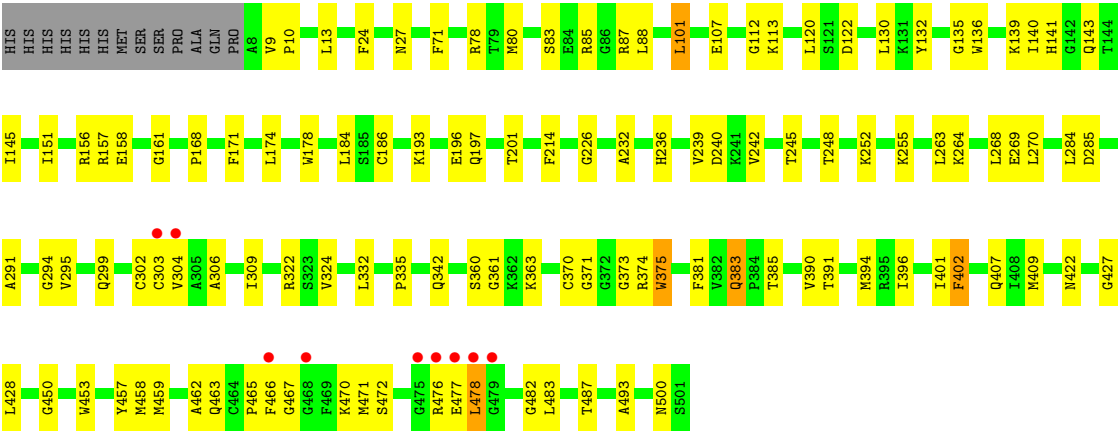
• Molecule 1: Aldehyde dehydrogenase 1A1



• Molecule 1: Aldehyde dehydrogenase 1A1



• Molecule 1: Aldehyde dehydrogenase 1A1



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 0.195 , 0.247	Depositor DCC
R_{free} test set	2000 reflections (2.19%)	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 , 61.6	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

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	0.54	0/3840	0.80	3/5195 (0.1%)
1	B	0.54	1/3825 (0.0%)	0.82	3/5179 (0.1%)
1	C	0.53	0/3831	0.80	3/5187 (0.1%)
1	D	0.47	0/3824	0.76	2/5179 (0.0%)
1	E	0.49	1/3827 (0.0%)	0.78	4/5181 (0.1%)
1	F	0.51	0/3827	0.80	5/5183 (0.1%)
1	G	0.50	0/3778	0.83	9/5125 (0.2%)
1	H	0.54	3/3845 (0.1%)	0.81	6/5201 (0.1%)
All	All	0.52	5/30597 (0.0%)	0.80	35/41430 (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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	326	ARG	CG-CD	-6.62	1.32	1.52
1	E	303	CYS	CB-SG	5.99	2.01	1.81
1	B	483	LEU	CG-CD1	-5.34	1.34	1.52
1	H	299	GLN	CD-NE2	-5.27	1.22	1.33
1	H	210	LYS	CG-CD	5.20	1.68	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	478	LEU	N-CA-C	9.99	125.09	111.90
1	F	375	TRP	CA-C-N	9.96	134.21	121.85
1	F	375	TRP	C-N-CA	9.96	134.21	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	466	PHE	CA-C-N	-9.94	113.47	121.82
1	E	466	PHE	C-N-CA	-9.94	113.47	121.82
1	E	478	LEU	CB-CA-C	-8.04	99.03	111.66
1	D	439	LYS	CD-CE-NZ	-7.79	86.97	111.90
1	A	427	GLY	N-CA-C	-7.32	95.84	113.18
1	G	478	LEU	CB-CG-CD1	-7.29	88.84	110.70
1	B	478	LEU	CB-CG-CD1	-7.01	89.68	110.70
1	F	383	GLN	CB-CG-CD	-6.40	101.72	112.60
1	B	262	ASN	N-CA-C	6.18	120.61	113.38
1	H	326	ARG	CB-CG-CD	6.12	125.37	111.30
1	G	483	LEU	CB-CG-CD1	-6.04	92.59	110.70
1	G	346	ILE	CA-C-N	6.03	133.05	121.54
1	G	346	ILE	C-N-CA	6.03	133.05	121.54
1	D	439	LYS	CA-CB-CG	-5.91	102.27	114.10
1	G	299	GLN	CA-CB-CG	5.68	125.46	114.10
1	F	269	GLU	CA-CB-CG	-5.57	102.96	114.10
1	G	423	ASN	CA-C-N	5.57	131.38	121.75
1	G	423	ASN	C-N-CA	5.57	131.38	121.75
1	H	299	GLN	CB-CA-C	-5.51	103.90	111.73
1	G	13	LEU	CB-CG-CD2	-5.40	94.51	110.70
1	A	394	MET	CG-SD-CE	-5.38	89.06	100.90
1	H	210	LYS	CA-CB-CG	5.32	124.74	114.10
1	F	478	LEU	CB-CG-CD1	-5.30	94.78	110.70
1	H	473	GLY	CA-C-N	5.30	130.16	121.58
1	H	473	GLY	C-N-CA	5.30	130.16	121.58
1	C	262	ASN	N-CA-C	-5.17	99.92	108.75
1	A	210	LYS	CD-CE-NZ	5.12	128.29	111.90
1	H	326	ARG	CG-CD-NE	5.11	123.25	112.00
1	B	378	LYS	N-CA-C	-5.10	100.02	108.75
1	G	12	PRO	N-CA-C	5.05	122.88	112.47
1	C	466	PHE	CA-C-N	-5.05	111.52	121.41
1	C	466	PHE	C-N-CA	-5.05	111.52	121.41

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	92	0
1	B	3745	0	3726	101	0
1	C	3751	0	3728	106	0
1	D	3744	0	3710	97	0
1	E	3747	0	3730	102	0
1	F	3747	0	3719	106	0
1	G	3698	0	3614	157	0
1	H	3765	0	3767	118	0
All	All	29957	0	29755	831	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 14.

All (831) 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:F:80:MET:HE2	1:F:85:ARG:HG2	1.53	0.91
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:H:173:MET:HE3	1:H:205:LEU:HD21	1.55	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:113:LYS:HZ1	1:C:171:PHE:HA	1.48	0.78
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:F:391:THR:H	1:F:394:MET:HE3	1.52	0.75
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:96:MET:HE1	1:G:177:ILE:HD11	1.71	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: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:C:308:ARG:HG2	1:C:409:MET:HE1	1.72	0.70
1:G:262:ASN:HA	1:H:471:MET:HE3	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
1:H:358:ILE:HG22	1:H:362:LYS:HE3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:17:LYS:HE2	1:H:19:GLN:CD	2.18	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:G:80:MET:HE3	1:G:84:GLU:HG3	1.75	0.68
1:G:114:VAL:HB	1:G:117:ASN:HB2	1.75	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:F:80:MET:HE1	1:F:88:LEU:HD12	1.76	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:F:483:LEU:C	1:F:483:LEU:HD23	2.20	0.66
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:B:262:ASN:HD21	1:B:264:LYS:HZ1	1.44	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:C:299:GLN:HG3	1:C:342:GLN:HG3	1.80	0.64
1:E:437:LEU:HD11	1:H:494:MET:HE1	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ILE:HD12	1:A:73:ILE:H	1.62	0.64
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:A:365:GLY:O	1:A:394:MET:HE1	1.98	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:A:391:THR:H	1:A:394:MET:HE3	1.64	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: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:A:123:LEU:HD21	1:A:173:MET:HE1	1.82	0.60
1:C:457:TYR:CD1	1:C:458:MET:HG3	2.36	0.60
1:A:391:THR:OG1	1:A:394:MET:HE3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:366:ALA:HB2	1:B:394:MET:HE1	1.83	0.60
1:C:450:GLY:HA3	1:C:467:GLY:O	2.01	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:E:151:ILE:HD11	1:F:459:MET:HE3	1.83	0.59
1:H:391:THR:H	1:H:394:MET:HE2	1.68	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:H:106:MET:HE3	1:H:201:THR:HA	1.84	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:F:294:GLY:HA2	1:F:458:MET:HE3	1.83	0.59
1:B:113:LYS:NZ	1:B:122:ASP:OD2	2.33	0.59
1:C:401:ILE:HD13	1:C:407:GLN:HE22	1.67	0.59
1:F:80:MET:HE1	1:F:88:LEU:CD1	2.32	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:H:175:MET:HE3	1:H:245:THR:HG21	1.86	0.58
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:96:MET:HE1	1:C:126:CYS:HB3	1.86	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: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:273:LYS:HB3	1:B:424:THR:HG21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:302:CYS:SG	1:B:458:MET:HE1	2.46	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:110:ASN:HD22	1:G:110:ASN:C	2.15	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:A:425:THR:HG21	1:A:471:MET:HE3	1.89	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:D:297:TYR:CD2	1:D:458:MET:HE1	2.42	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:A:107:GLU:HB2	1:A:173:MET:HE2	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:392:ASP:CG	1:E:420:ARG:HE	2.16	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:154:TYR:HE2	1:A:494:MET:HE2	1.73	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:424:THR:C	1:D:470:LYS:HZ2	2.18	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
1:B:92:LEU:HD23	1:B:130:LEU:HD11	1.93	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:366:ALA:HB2	1:D:394:MET:HE1	1.92	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:D:292:HIS:C	1:D:292:HIS:CD2	2.87	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: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:E:96:MET:HE1	1:E:126:CYS:HB3	1.93	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:407:GLN:HB3	1:A:409:MET:HE2	1.93	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:H:106:MET:HE1	1:H:204:HIS:CB	2.41	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:255:LYS:HZ1	1:H:255:LYS:NZ	2.10	0.50
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:H:96:MET:HE1	1:H:126:CYS:HB3	1.93	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:E:419:LYS:O	1:E:423:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:TYR:HE2	1:G:409:MET:C	2.21	0.49
1:F:112:GLY:HA2	1:F:335:PRO:HG2	1.94	0.49
1:A:175:MET:HE1	1:A:178:TRP:CE3	2.47	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
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:C:143:GLN:H	1:C:155:THR:HG1	1.58	0.48
1:D:96:MET:HE1	1:D:126:CYS:HB3	1.96	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:G:80:MET:HE2	1:G:85:ARG:HG2	1.95	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:E:9:VAL:HB	1:E:10:PRO:HD2	1.96	0.48
1:G:255:LYS:HZ2	1:H:255:LYS:HZ1	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:299:GLN:NE2	1:H:343:GLY:C	2.72	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: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:D:458:MET:HE2	1:D:458:MET:HB3	1.59	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: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:285:ASP:CG	1:F:322:ARG:HH21	2.22	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
1:F:391:THR:N	1:F:394:MET:HE3	2.23	0.47
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:E:262:ASN:HA	1:F:471:MET:HE2	1.97	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: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:H:193:LYS:HD3	1:H:193:LYS:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:96:MET:HE2	1:A:130:LEU:HD22	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:A:425:THR:CG2	1:A:471:MET:HE3	2.44	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:411:PHE:C	1:A:412:LYS:HD3	2.41	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
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:E:437:LEU:HD11	1:H:494:MET:CE	2.44	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: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:A:424:THR:O	1:A:470:LYS:NZ	2.42	0.45
1:B:402:PHE:HD1	1:B:402:PHE:HA	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ILE:C	1:D:151:ILE:HD12	2.42	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:G:80:MET:HE1	1:G:88:LEU:HD12	1.98	0.45
1:G:96:MET:CE	1:G:177:ILE:HD11	2.42	0.45
1:H:141:HIS:HB2	1:F:143:GLN:HG3	1.97	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: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:F:360:SER:O	1:F:361:GLY:C	2.60	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
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: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:103:LEU:HD13	1:H:173:MET:HE1	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:255:LYS:NZ	1:H:255:LYS:NZ	2.64	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:H:273:LYS:HZ1	1:H:307:SER:HB2	1.82	0.44
1:B:107:GLU:HB2	1:B:173:MET:HE3	1.99	0.44
1:B:149:GLY:O	1:B:499:LYS:HD3	2.18	0.44
1:D:273:LYS:NZ	1:D:399:GLU:O	2.37	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:G:56:ASP:O	1:G:57:LYS:C	2.61	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:F:236:HIS:O	1:F:264:LYS:NZ	2.48	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:E:458:MET:HE2	1:E:458:MET:HB3	1.77	0.43
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
1:F:268:LEU:HB3	1:F:270:LEU:HD21	1.98	0.43
1:A:106:MET:HE3	1:A:106:MET:HB2	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:106:MET:HB3	1:G:106:MET:HE2	1.57	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: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:H:297:TYR:CD2	1:H:458:MET:HE1	2.54	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:G:173:MET:HE2	1:G:173:MET:HB3	1.71	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
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:A:110:ASN:ND2	1:A:110:ASN:C	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:F:371:GLY:HA2	1:F:383:GLN:CD	2.44	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:F:453:TRP:NE1	1:F:459:MET:H	2.17	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
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:B:110:ASN:C	1:B:110:ASN:HD22	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:313:GLU:OE1	1:A:412:LYS:HD2	2.18	0.42
1:B:262:ASN:HD21	1:B:264:LYS:HZ2	1.67	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:D:292:HIS:O	1:D:293:HIS:C	2.63	0.42
1:E:87:ARG:NH2	1:H:128:LYS:HE2	2.35	0.42
1:H:96:MET:HE3	1:H:173:MET:CE	2.50	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:H:102:LEU:C	1:H:102:LEU:HD23	2.45	0.42
1:B:103:LEU:HB3	1:B:173:MET:HE1	2.00	0.41
1:G:103:LEU:HD22	1:G:205:LEU:HD11	2.02	0.41
1:C:173:MET:HE2	1:C:173:MET:HB3	1.95	0.41
1:C:395:ARG:O	1:C:396:ILE:C	2.64	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:G:96:MET:HE3	1:G:130:LEU:HD12	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:G:38:PHE:CD1	1:G:38:PHE:C	2.97	0.41
1:H:366:ALA:HB2	1:H:394:MET:HE1	2.02	0.41
1:F:239:VAL:O	1:F:264:LYS:HE3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:VAL:HB	1:F:306:ALA:O	2.21	0.41
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:419:LYS:O	1:B:423:ASN:HB2	2.21	0.41
1:B:490:LYS:NZ	1:C:444:SER:O	2.49	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:173:MET:HE3	1:G:205:LEU:HD21	2.02	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: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:102:LEU:HD23	1:B:102:LEU:C	2.45	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:A:458:MET:HE2	1:A:458:MET:HB3	1.81	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:234:SER:O	1:H:264:LYS:NZ	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:PHE:CE2	1:D:161:GLY:HA2	2.56	0.41
1:D:459:MET:HE2	1:D:459:MET:HB3	1.91	0.41
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: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:392:ASP:CG	1:G:420:ARG:HE	2.28	0.40
1:G:433:PHE:CD1	1:G:455:ASN:HA	2.55	0.40
1:H:292:HIS:CD2	1:H:292:HIS:C	2.99	0.40
1:A:167:ILE:CD1	1:A:179:LYS:HG3	2.51	0.40
1:B:106:MET:HE3	1:B:106:MET:HB2	1.76	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: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:A:232:ALA:O	1:A:236:HIS:HB2	2.22	0.40
1:B:488:GLU:CD	1:C:476:ARG:HH12	2.29	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%)	43	72
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%)	43	72
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%)	48	77

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%)	395 (100%)	1 (0%)	86	96
1	B	393/413 (95%)	392 (100%)	1 (0%)	86	96
1	C	394/413 (95%)	389 (99%)	5 (1%)	61	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	392/413 (95%)	389 (99%)	3 (1%)	73	90
1	E	394/413 (95%)	390 (99%)	4 (1%)	68	89
1	F	393/413 (95%)	390 (99%)	3 (1%)	73	90
1	G	383/413 (93%)	376 (98%)	7 (2%)	51	80
1	H	398/413 (96%)	396 (100%)	2 (0%)	81	93
All	All	3143/3304 (95%)	3117 (99%)	26 (1%)	73	90

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	PHE
1	B	402	PHE
1	C	303	CYS
1	C	402	PHE
1	C	412	LYS
1	C	476	ARG
1	C	478	LEU
1	D	303	CYS
1	D	380	PHE
1	D	402	PHE
1	E	174	LEU
1	E	303	CYS
1	E	402	PHE
1	E	466	PHE
1	G	268	LEU
1	G	299	GLN
1	G	303	CYS
1	G	347	ASP
1	G	356	ASP
1	G	402	PHE
1	G	459	MET
1	H	303	CYS
1	H	402	PHE
1	F	101	LEU
1	F	303	CYS
1	F	402	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	143	GLN
1	A	301	GLN
1	A	383	GLN
1	B	110	ASN
1	B	262	ASN
1	B	301	GLN
1	B	498	GLN
1	C	20	HIS
1	C	383	GLN
1	C	407	GLN
1	C	448	GLN
1	D	30	HIS
1	D	249	GLN
1	D	298	HIS
1	D	350	GLN
1	D	407	GLN
1	E	20	HIS
1	E	110	ASN
1	E	204	HIS
1	E	249	GLN
1	E	407	GLN
1	G	27	ASN
1	G	51	HIS
1	G	165	GLN
1	G	298	HIS
1	G	299	GLN
1	G	351	HIS
1	G	383	GLN
1	G	481	HIS
1	H	90	ASN
1	H	292	HIS
1	H	498	GLN
1	H	500	ASN
1	F	141	HIS
1	F	143	GLN
1	F	249	GLN
1	F	293	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	-0.24	8 (1%) 70 62	37, 59, 84, 100	0
1	B	494/507 (97%)	-0.21	3 (0%) 85 81	34, 61, 98, 116	0
1	C	494/507 (97%)	-0.07	8 (1%) 70 62	46, 71, 96, 114	0
1	D	494/507 (97%)	-0.03	10 (2%) 65 56	35, 69, 127, 146	0
1	E	494/507 (97%)	-0.00	6 (1%) 76 69	49, 78, 105, 127	0
1	F	494/507 (97%)	-0.00	9 (1%) 67 59	54, 77, 99, 113	0
1	G	492/507 (97%)	0.31	12 (2%) 59 50	45, 100, 157, 174	0
1	H	494/507 (97%)	-0.09	8 (1%) 70 62	42, 73, 104, 119	0
All	All	3950/4056 (97%)	-0.04	64 (1%) 70 62	34, 73, 120, 174	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	466	PHE	4.6
1	E	476	ARG	4.0
1	F	466	PHE	3.6
1	G	10	PRO	3.5
1	H	210	LYS	3.5
1	A	474	ASN	3.2
1	G	303	CYS	3.2
1	F	303	CYS	3.2
1	E	303	CYS	3.0
1	B	467	GLY	3.0
1	A	475	GLY	3.0
1	A	467	GLY	2.9
1	D	303	CYS	2.9
1	F	478	LEU	2.9
1	D	401	ILE	2.8
1	B	460	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	460	LEU	2.8
1	G	157	ARG	2.7
1	G	396	ILE	2.6
1	F	477	GLU	2.6
1	G	466	PHE	2.6
1	E	466	PHE	2.5
1	F	476	ARG	2.5
1	G	304	VAL	2.5
1	G	478	LEU	2.5
1	A	210	LYS	2.5
1	A	401	ILE	2.4
1	D	368	LEU	2.4
1	H	478	LEU	2.4
1	C	303	CYS	2.4
1	C	475	GLY	2.4
1	D	476	ARG	2.4
1	F	304	VAL	2.4
1	C	466	PHE	2.4
1	D	466	PHE	2.3
1	H	303	CYS	2.3
1	C	113	LYS	2.3
1	D	475	GLY	2.3
1	F	475	GLY	2.3
1	D	402	PHE	2.3
1	C	478	LEU	2.3
1	H	467	GLY	2.3
1	F	479	GLY	2.3
1	H	472	SER	2.3
1	D	426	TYR	2.2
1	C	372	GLY	2.2
1	H	475	GLY	2.2
1	G	476	ARG	2.2
1	A	478	LEU	2.2
1	D	333	GLY	2.2
1	G	468	GLY	2.2
1	B	8	ALA	2.2
1	E	8	ALA	2.2
1	H	477	GLU	2.2
1	A	255	LYS	2.1
1	D	272	GLY	2.1
1	E	357	LEU	2.1
1	G	464	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	468	GLY	2.1
1	C	44	ALA	2.1
1	C	467	GLY	2.1
1	G	269	GLU	2.1
1	E	477	GLU	2.0
1	H	255	LYS	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 oligosaccharides 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.