



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 01:47 am BST

PDB ID : 3MFM
Title : Crystal Structures and Mutational Analyses of Acyl-CoA Carboxylase Subunit of *Streptomyces coelicolor*
Authors : Diacovich, L.; Arabolaza, A.; Shillito, E.M.; Lin, T.-W.; Mitchell, D.L.; Melgar, M.M.
Deposited on : 2010-04-02
Resolution : 2.38 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 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	:	2.11
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)	:	2.11

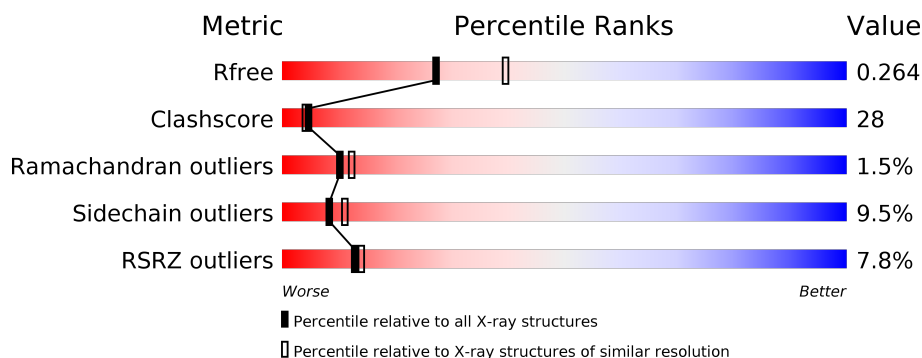
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	530	<div> <div>9%</div> <div> <div>51%</div> <div>40%</div> <div>8%</div> </div> </div>
1	B	530	<div> <div>10%</div> <div> <div>50%</div> <div>41%</div> <div>7%</div> </div> </div>
1	C	530	<div> <div>6%</div> <div> <div>61%</div> <div>32%</div> <div>5%</div> </div> </div>
1	D	530	<div> <div>8%</div> <div> <div>55%</div> <div>38%</div> <div>5%</div> </div> </div>
1	E	530	<div> <div>5%</div> <div> <div>59%</div> <div>33%</div> <div>6%</div> </div> </div>
1	F	530	<div> <div>8%</div> <div> <div>58%</div> <div>35%</div> <div>5%</div> </div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 23718 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 Propionyl-CoA carboxylase complex B subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	F	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	A	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	B	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	D	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			
1	E	521	Total	C	N	O	S	0	0	0
			3953	2481	699	760	13			

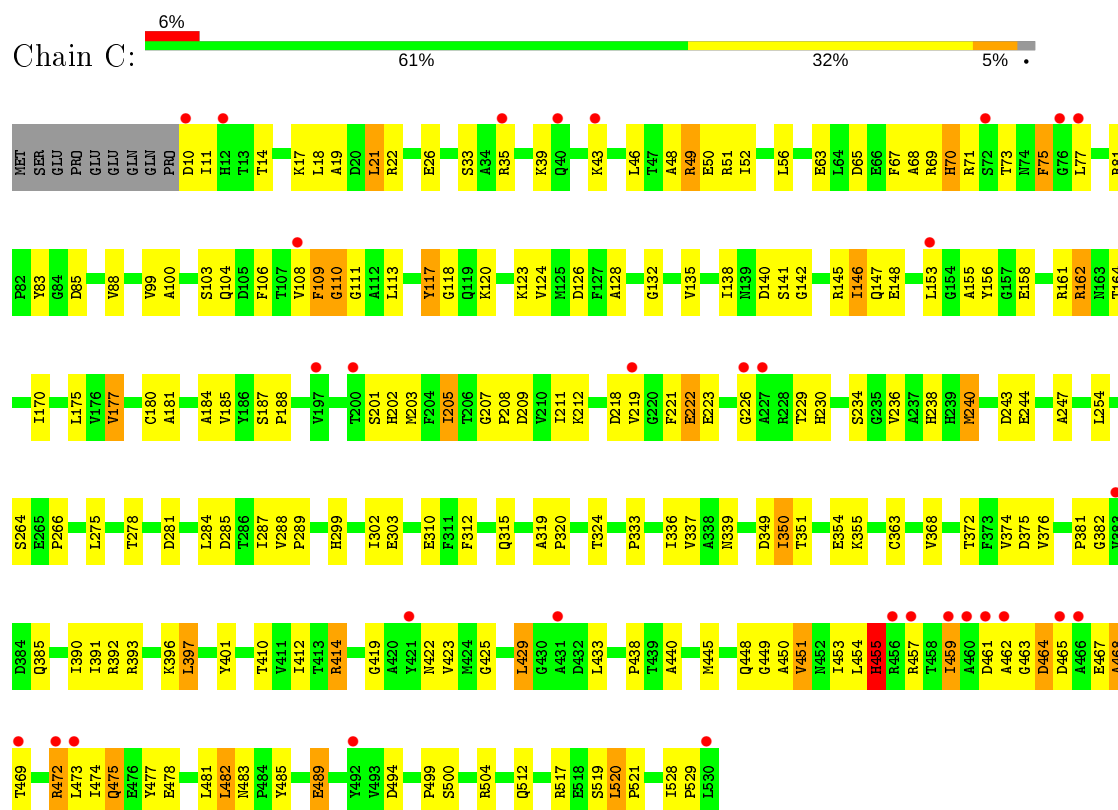
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
F	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
A	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
B	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
D	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7
E	422	ASN	ASP	ENGINEERED MUTATION	UNP Q9X4K7

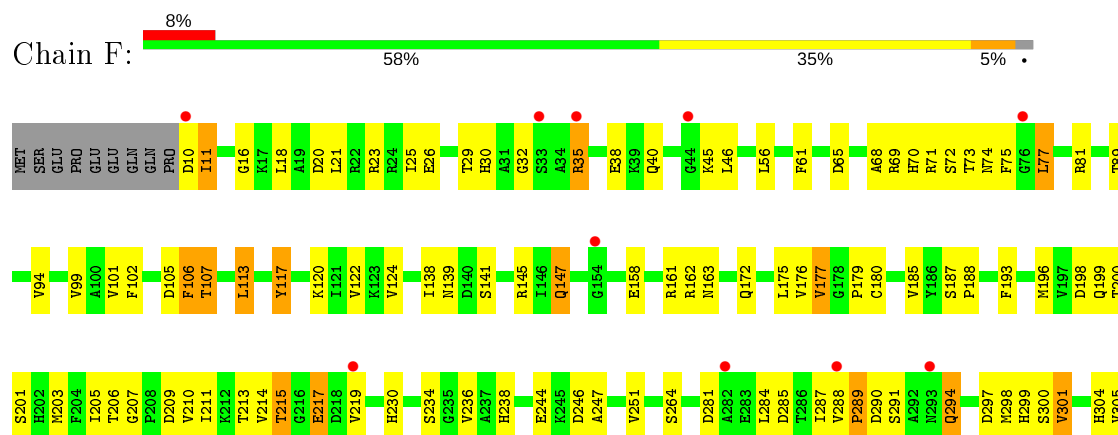
3 Residue-property plots

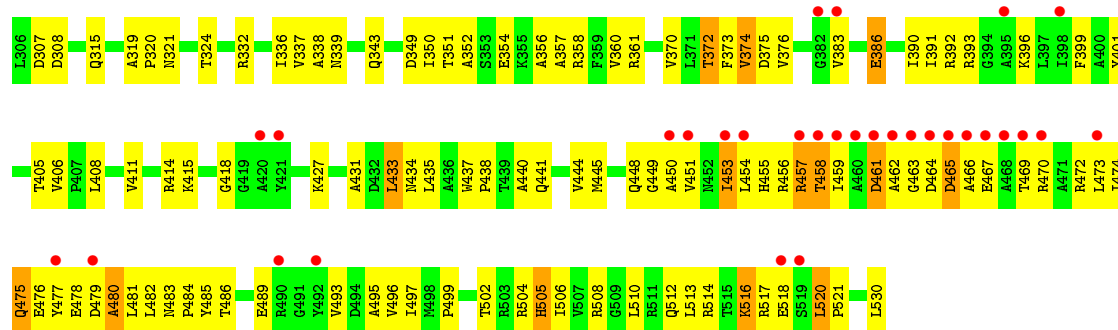
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

- Molecule 1: Propionyl-CoA carboxylase complex B subunit

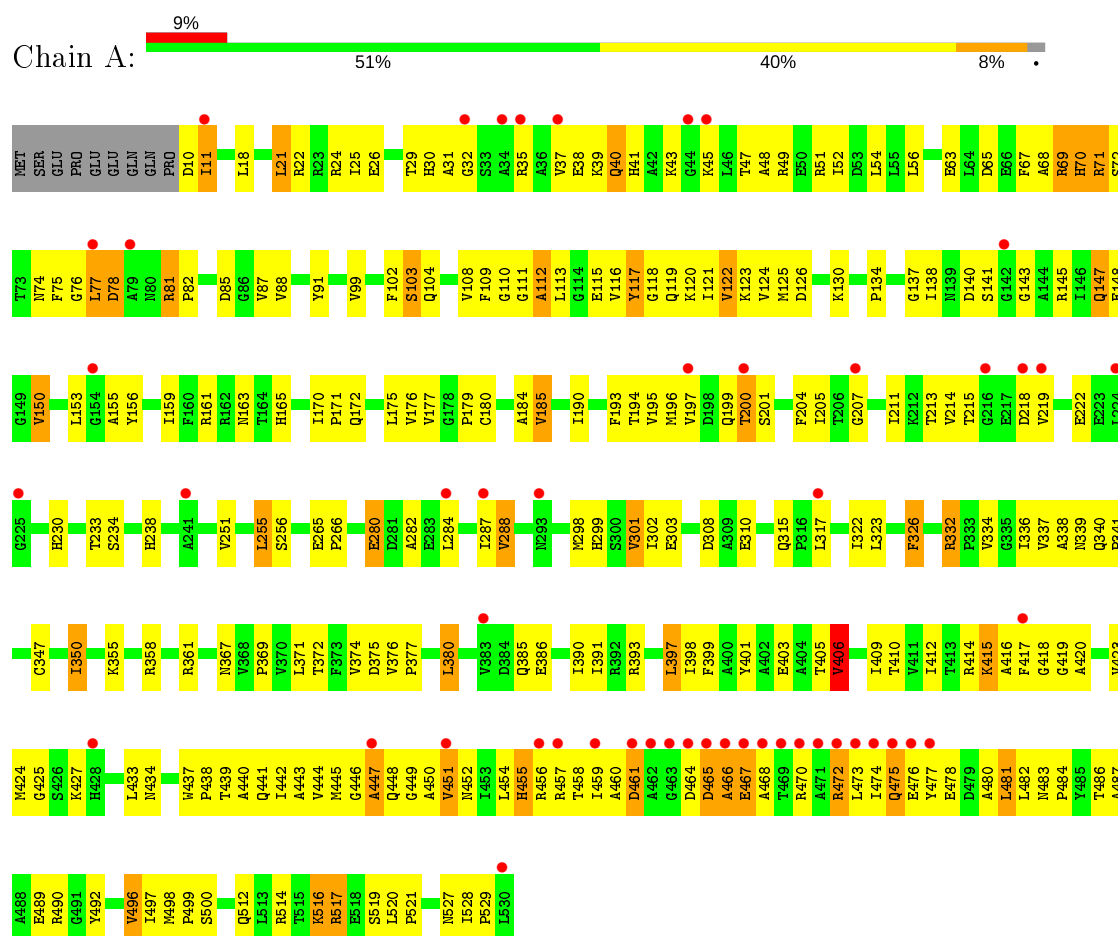


- Molecule 1: Propionyl-CoA carboxylase complex B subunit

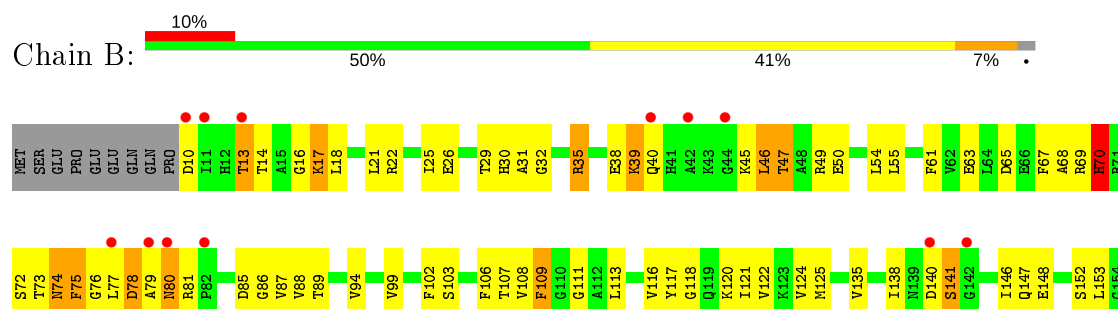


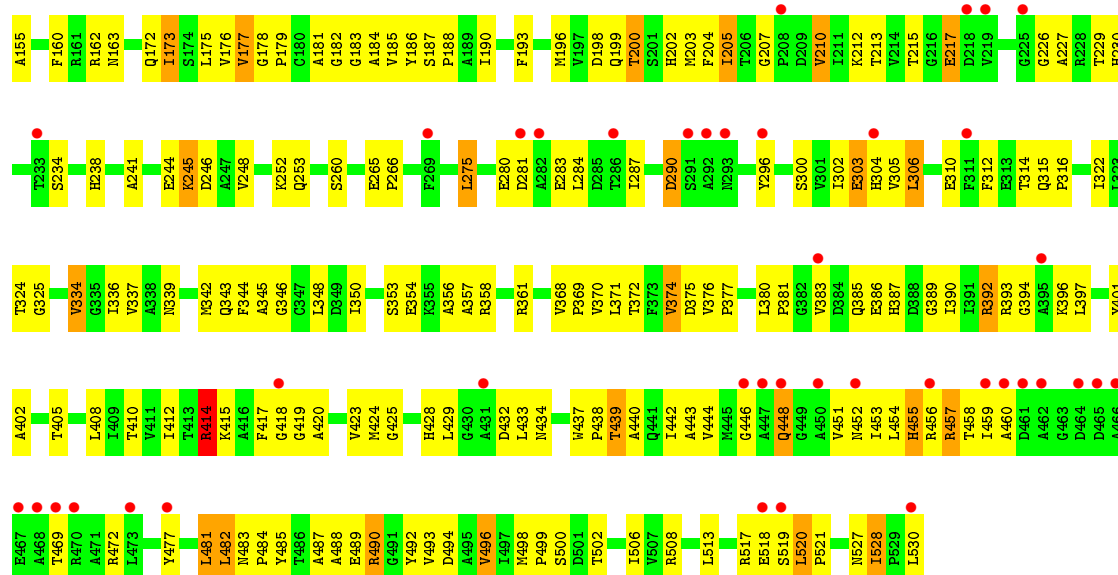


● Molecule 1: Propionyl-CoA carboxylase complex B subunit

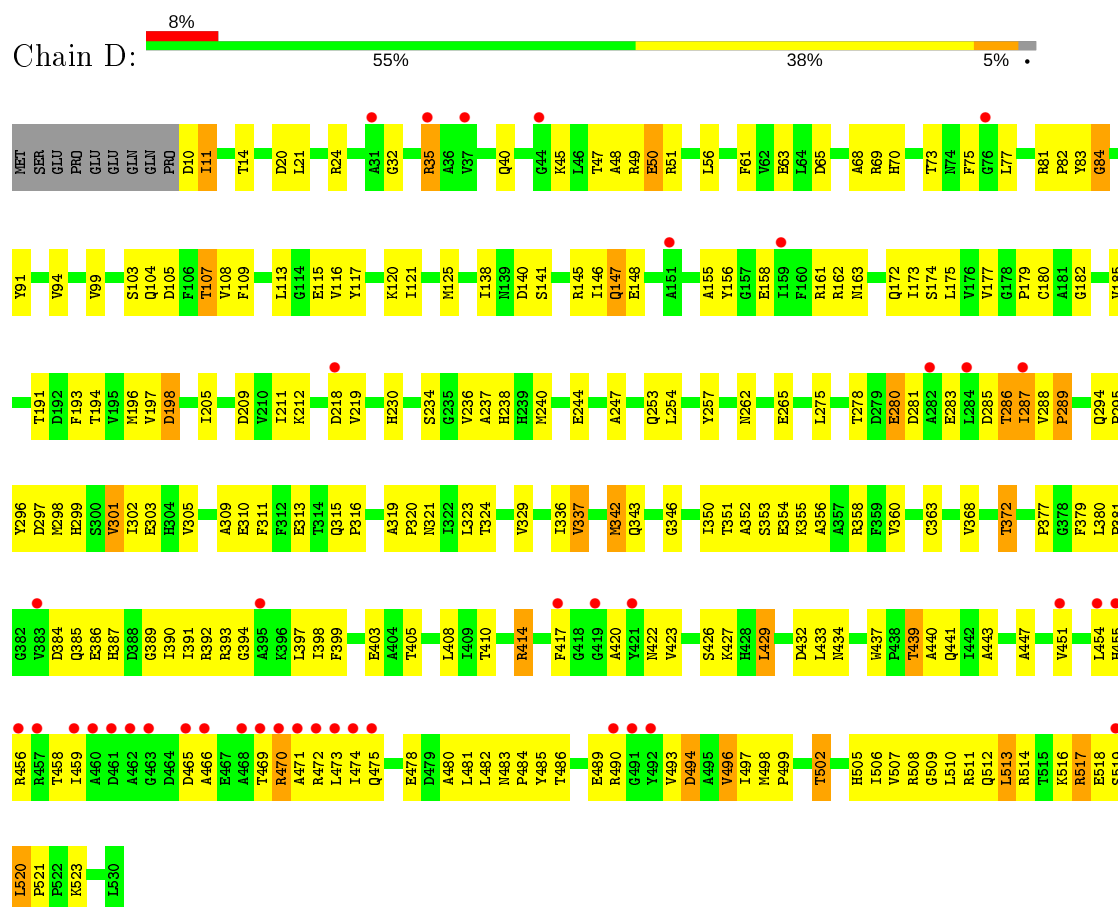


● Molecule 1: Propionyl-CoA carboxylase complex B subunit



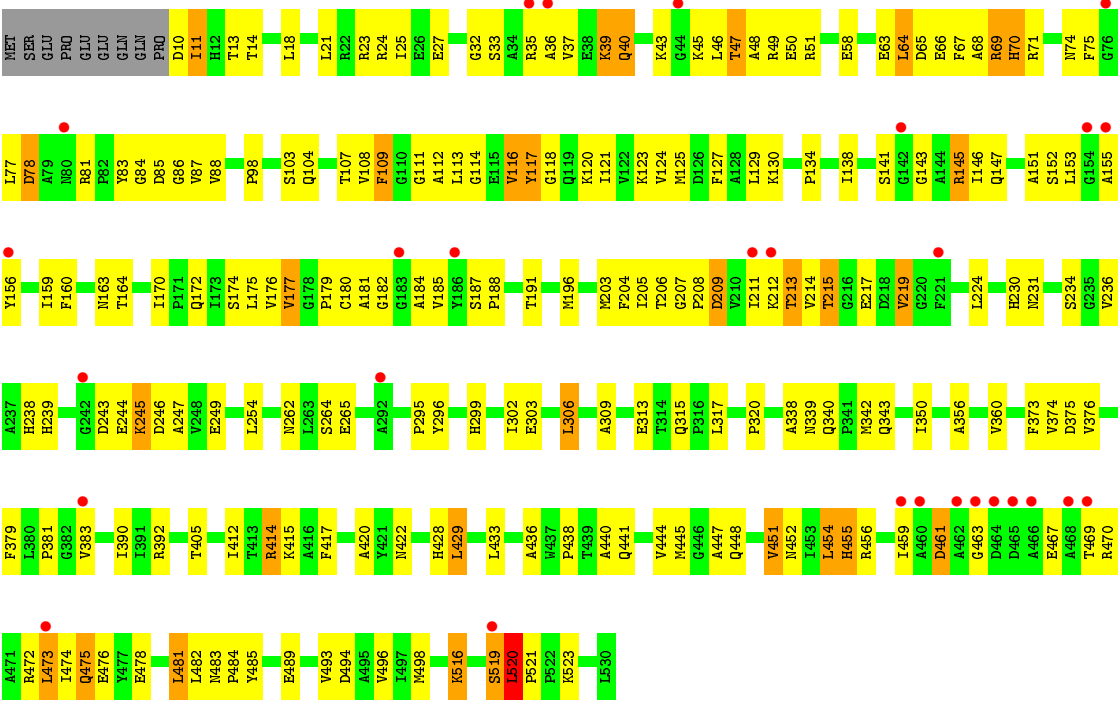


• Molecule 1: Propionyl-CoA carboxylase complex B subunit



• Molecule 1: Propionyl-CoA carboxylase complex B subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.67Å 220.96Å 136.74Å 90.00° 103.08° 90.00°	Depositor
Resolution (Å)	38.82 – 2.38 45.00 – 2.38	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.82-2.38) 99.1 (45.00-2.38)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.6.1_357, CNS, REFMAC 5.2.0019	Depositor
R, R_{free}	0.224 , 0.268 0.219 , 0.264	Depositor DCC
R_{free} test set	9136 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.3	Xtriage
Anisotropy	1.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23718	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.90 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2372e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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	0.42	0/4033	0.61	0/5478
1	B	0.44	0/4033	0.62	0/5478
1	C	0.41	0/4033	0.61	1/5478 (0.0%)
1	D	0.44	0/4033	0.62	1/5478 (0.0%)
1	E	0.41	0/4033	0.60	0/5478
1	F	0.41	0/4033	0.60	0/5478
All	All	0.42	0/24198	0.61	2/32868 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	84	GLY	N-CA-C	-5.39	99.61	113.10
1	C	109	PHE	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3953	0	3882	310	0
1	B	3953	0	3882	299	0
1	C	3953	0	3882	192	0
1	D	3953	0	3882	218	0
1	E	3953	0	3882	227	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3953	0	3882	213	0
All	All	23718	0	23292	1319	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 28.

All (1319) 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:337:VAL:HG21	1:B:401:TYR:OH	1.46	1.15
1:E:69:ARG:HH11	1:E:69:ARG:HG3	1.01	1.13
1:B:35:ARG:HH11	1:B:35:ARG:HG2	1.06	1.13
1:C:520:LEU:HD12	1:C:521:PRO:HD2	1.16	1.12
1:A:163:ASN:HB3	1:A:190:ILE:HD11	1.23	1.11
1:E:376:VAL:HG11	1:E:420:ALA:HB1	1.34	1.08
1:A:415:LYS:HE3	1:A:416:ALA:H	1.13	1.07
1:A:415:LYS:HE3	1:A:416:ALA:N	1.69	1.07
1:A:81:ARG:HG2	1:A:81:ARG:HH11	0.95	1.06
1:E:51:ARG:HG2	1:E:51:ARG:HH11	1.17	1.06
1:D:286:THR:O	1:D:288:VAL:HG12	1.55	1.04
1:A:111:GLY:HA3	1:A:141:SER:HA	1.39	1.03
1:A:451:VAL:HG21	1:A:474:ILE:HD13	1.41	1.02
1:D:397:LEU:HD23	1:D:423:VAL:HG12	1.42	1.01
1:A:69:ARG:HH11	1:A:69:ARG:HG2	1.27	1.00
1:A:350:ILE:HD11	1:A:393:ARG:HH11	1.24	0.99
1:B:35:ARG:HG2	1:B:35:ARG:NH1	1.69	0.98
1:E:35:ARG:HG2	1:E:39:LYS:HE3	1.46	0.96
1:A:81:ARG:HG2	1:A:81:ARG:NH1	1.72	0.96
1:D:320:PRO:HB2	1:D:343:GLN:HE21	1.31	0.95
1:E:519:SER:O	1:E:520:LEU:HB2	1.66	0.95
1:E:208:PRO:HA	1:E:211:ILE:HG12	1.48	0.94
1:B:138:ILE:HG23	1:B:175:LEU:HD23	1.50	0.92
1:A:380:LEU:HD11	1:A:385:GLN:HG3	1.50	0.92
1:B:374:VAL:HG13	1:B:412:ILE:HD13	1.51	0.92
1:E:69:ARG:NH1	1:E:69:ARG:HG3	1.80	0.92
1:A:456:ARG:HD3	1:A:459:ILE:HG12	1.52	0.92
1:D:32:GLY:HA3	1:D:107:THR:HG23	1.52	0.92
1:E:113:LEU:HD23	1:E:156:TYR:CE1	2.05	0.91
1:E:295:PRO:HB2	1:E:342:MET:CE	2.01	0.91
1:D:32:GLY:HA3	1:D:107:THR:CG2	2.01	0.90
1:B:35:ARG:CG	1:B:35:ARG:HH11	1.83	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:288:VAL:O	1:D:14:THR:HG21	1.73	0.89
1:D:194:THR:H	1:D:238:HIS:HD2	1.20	0.89
1:A:163:ASN:HB3	1:A:190:ILE:CD1	2.03	0.88
1:B:72:SER:OG	1:B:77:LEU:HD13	1.73	0.88
1:B:72:SER:OG	1:B:77:LEU:CD1	2.21	0.88
1:A:452:ASN:HB2	1:A:456:ARG:HH21	1.38	0.88
1:E:215:THR:HB	1:E:217:GLU:HG2	1.54	0.88
1:A:350:ILE:HD11	1:A:393:ARG:NH1	1.89	0.87
1:A:391:ILE:HD12	1:A:391:ILE:H	1.37	0.87
1:C:14:THR:HG21	1:A:288:VAL:O	1.75	0.87
1:F:56:LEU:HD21	1:F:101:VAL:HG21	1.56	0.87
1:F:475:GLN:HA	1:F:478:GLU:HG2	1.56	0.86
1:F:288:VAL:O	1:B:14:THR:HG21	1.75	0.86
1:A:150:VAL:HG11	1:B:442:ILE:HG22	1.57	0.86
1:D:337:VAL:HG13	1:D:372:THR:HB	1.55	0.85
1:B:305:VAL:O	1:B:306:LEU:HG	1.76	0.85
1:D:472:ARG:HE	1:D:475:GLN:HB3	1.39	0.85
1:F:451:VAL:HA	1:F:454:LEU:HG	1.58	0.85
1:B:10:ASP:O	1:B:16:GLY:HA3	1.77	0.85
1:F:497:ILE:HG21	1:F:505:HIS:CE1	2.12	0.84
1:A:465:ASP:OD2	1:A:467:GLU:HG2	1.77	0.84
1:F:32:GLY:HA3	1:F:107:THR:HG23	1.60	0.84
1:A:451:VAL:HG21	1:A:474:ILE:CD1	2.08	0.83
1:C:49:ARG:O	1:C:50:GLU:HB3	1.76	0.83
1:D:77:LEU:HD11	1:D:147:GLN:HG3	1.58	0.83
1:A:138:ILE:HG22	1:A:175:LEU:HB3	1.59	0.83
1:A:163:ASN:CB	1:A:190:ILE:HD11	2.08	0.83
1:A:380:LEU:HD11	1:A:385:GLN:CG	2.08	0.82
1:B:520:LEU:HG	1:B:521:PRO:HD2	1.59	0.82
1:E:113:LEU:HD13	1:E:117:TYR:CD2	2.14	0.82
1:A:81:ARG:CG	1:A:81:ARG:HH11	1.86	0.82
1:C:187:SER:HB3	1:C:188:PRO:HD3	1.60	0.82
1:E:520:LEU:HD22	1:E:521:PRO:HD2	1.60	0.82
1:A:498:MET:HE2	1:A:500:SER:HB3	1.62	0.82
1:F:458:THR:HG21	1:F:469:THR:HG21	1.62	0.82
1:E:405:THR:O	1:E:516:LYS:HE3	1.79	0.81
1:B:415:LYS:HD2	1:B:417:PHE:CE1	2.15	0.81
1:E:36:ALA:HA	1:E:39:LYS:HD3	1.62	0.81
1:D:286:THR:O	1:D:287:ILE:HG22	1.80	0.81
1:A:478:GLU:HA	1:A:482:LEU:HD23	1.62	0.81
1:D:466:ALA:O	1:D:470:ARG:HB3	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:451:VAL:HB	1:F:470:ARG:CZ	2.10	0.81
1:A:442:ILE:HG12	1:A:484:PRO:HA	1.63	0.81
1:C:489:GLU:HA	1:D:68:ALA:HA	1.60	0.81
1:A:112:ALA:HA	1:A:143:GLY:O	1.81	0.80
1:E:47:THR:HG22	1:E:50:GLU:HG2	1.62	0.80
1:A:288:VAL:HG21	1:A:439:THR:HG21	1.64	0.80
1:D:138:ILE:HD12	1:D:175:LEU:HD23	1.63	0.80
1:D:49:ARG:O	1:D:50:GLU:HB2	1.79	0.80
1:B:300:SER:HA	1:B:303:GLU:HG2	1.63	0.80
1:C:75:PHE:HE1	1:F:454:LEU:HD13	1.46	0.80
1:F:139:ASN:HB2	1:F:176:VAL:HG12	1.64	0.79
1:A:380:LEU:CD1	1:A:385:GLN:HG3	2.12	0.79
1:E:40:GLN:HG3	1:E:45:LYS:HB2	1.65	0.79
1:D:397:LEU:HD23	1:D:423:VAL:CG1	2.13	0.79
1:D:363:CYS:HB3	1:D:368:VAL:HG22	1.62	0.79
1:D:469:THR:HG22	1:D:473:LEU:HD22	1.64	0.79
1:B:21:LEU:O	1:B:25:ILE:HD12	1.82	0.79
1:B:69:ARG:HD3	1:B:81:ARG:HB2	1.65	0.79
1:D:520:LEU:HB2	1:D:521:PRO:HD2	1.65	0.79
1:D:105:ASP:OD1	1:D:107:THR:HB	1.82	0.78
1:D:386:GLU:OE2	1:D:391:ILE:HD11	1.83	0.78
1:E:243:ASP:HB3	1:E:246:ASP:OD1	1.84	0.78
1:E:339:ASN:OD1	1:E:376:VAL:HG23	1.84	0.78
1:E:51:ARG:HG2	1:E:51:ARG:NH1	1.96	0.78
1:E:69:ARG:HH11	1:E:69:ARG:CG	1.91	0.78
1:A:323:LEU:HD21	1:A:340:GLN:HB2	1.63	0.78
1:A:456:ARG:HD3	1:A:459:ILE:CG1	2.13	0.78
1:E:182:GLY:O	1:E:185:VAL:HG12	1.83	0.78
1:B:437:TRP:HE1	1:B:502:THR:HG21	1.49	0.78
1:F:18:LEU:HG	1:E:498:MET:CE	2.14	0.77
1:A:103:SER:OG	1:A:138:ILE:HD11	1.84	0.77
1:A:369:PRO:HA	1:A:406:VAL:HG13	1.66	0.77
1:C:158:GLU:HG3	1:C:162:ARG:HH21	1.49	0.77
1:C:474:ILE:O	1:C:475:GLN:HB3	1.84	0.77
1:D:194:THR:H	1:D:238:HIS:CD2	2.03	0.77
1:A:111:GLY:HA3	1:A:141:SER:CA	2.14	0.77
1:D:354:GLU:OE2	1:D:393:ARG:HD3	1.85	0.77
1:C:39:LYS:O	1:C:43:LYS:HG3	1.83	0.76
1:A:361:ARG:HD2	1:A:403:GLU:OE2	1.84	0.76
1:F:32:GLY:HA3	1:F:107:THR:CG2	2.15	0.76
1:A:323:LEU:CD2	1:A:340:GLN:HB2	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:PHE:C	1:C:111:GLY:H	1.88	0.76
1:A:211:ILE:HG21	1:B:383:VAL:HG23	1.67	0.75
1:A:498:MET:CE	1:A:500:SER:HB3	2.15	0.75
1:F:448:GLN:HG2	1:F:449:GLY:H	1.51	0.75
1:B:393:ARG:O	1:B:396:LYS:HG3	1.87	0.75
1:E:203:MET:HB2	1:E:230:HIS:CE1	2.20	0.75
1:A:415:LYS:HD2	1:A:441:GLN:HB2	1.68	0.75
1:E:39:LYS:N	1:E:39:LYS:HD2	2.02	0.74
1:F:290:ASP:OD1	1:B:14:THR:HG23	1.86	0.74
1:A:380:LEU:HD12	1:A:380:LEU:O	1.86	0.74
1:B:202:HIS:ND1	1:B:226:GLY:HA2	2.02	0.74
1:C:350:ILE:HB	1:C:393:ARG:HG2	1.67	0.74
1:A:69:ARG:NH1	1:A:69:ARG:HG2	1.94	0.74
1:A:517:ARG:CG	1:A:517:ARG:HH11	2.01	0.73
1:A:529:PRO:HA	1:B:358:ARG:NH1	2.03	0.73
1:D:286:THR:C	1:D:288:VAL:H	1.92	0.73
1:F:94:VAL:HG23	1:F:99:VAL:HG11	1.71	0.73
1:C:75:PHE:CE1	1:F:454:LEU:HD13	2.24	0.73
1:E:113:LEU:HD12	1:E:114:GLY:N	2.03	0.73
1:E:207:GLY:O	1:E:211:ILE:HG23	1.88	0.73
1:F:18:LEU:HG	1:E:498:MET:HE1	1.68	0.73
1:F:350:ILE:HG13	1:F:393:ARG:HD2	1.71	0.73
1:E:376:VAL:HG11	1:E:420:ALA:CB	2.15	0.73
1:C:185:VAL:HG22	1:F:391:ILE:HG23	1.69	0.72
1:A:145:ARG:HD2	1:A:148:GLU:OE2	1.89	0.72
1:B:305:VAL:HG11	1:B:506:ILE:HD12	1.71	0.72
1:C:109:PHE:O	1:C:111:GLY:N	2.21	0.72
1:D:145:ARG:HD2	1:D:148:GLU:OE2	1.89	0.72
1:D:391:ILE:CG2	1:E:185:VAL:HG22	2.19	0.72
1:B:337:VAL:CG2	1:B:401:TYR:OH	2.32	0.72
1:B:437:TRP:HE1	1:B:502:THR:CG2	2.01	0.72
1:C:73:THR:HG21	1:B:73:THR:HG21	1.70	0.72
1:F:451:VAL:HB	1:F:470:ARG:NH2	2.05	0.72
1:D:456:ARG:O	1:D:459:ILE:HG12	1.90	0.72
1:D:405:THR:O	1:D:516:LYS:HE2	1.90	0.72
1:D:350:ILE:HG23	1:D:393:ARG:HD2	1.72	0.72
1:F:73:THR:HG21	1:D:73:THR:HG21	1.72	0.71
1:F:324:THR:HA	1:F:336:ILE:O	1.89	0.71
1:B:389:GLY:O	1:B:393:ARG:HG2	1.91	0.71
1:A:40:GLN:NE2	1:A:41:HIS:H	1.89	0.71
1:E:520:LEU:HD22	1:E:521:PRO:CD	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:HIS:HE2	1:A:148:GLU:CD	1.94	0.71
1:C:65:ASP:OD2	1:C:123:LYS:HD3	1.91	0.71
1:A:452:ASN:HB2	1:A:456:ARG:NH2	2.06	0.71
1:A:468:ALA:O	1:A:472:ARG:HB3	1.91	0.71
1:C:208:PRO:CG	1:C:221:PHE:HE2	2.03	0.70
1:E:33:SER:O	1:E:37:VAL:HG13	1.91	0.70
1:C:397:LEU:HG	1:C:423:VAL:CG1	2.21	0.70
1:D:381:PRO:HB2	1:E:214:VAL:HG21	1.73	0.70
1:E:47:THR:HG22	1:E:50:GLU:CG	2.22	0.70
1:D:437:TRP:HZ2	1:D:502:THR:HG21	1.56	0.70
1:B:348:LEU:HD21	1:B:424:MET:HE1	1.73	0.70
1:C:419:GLY:O	1:C:423:VAL:HG23	1.91	0.70
1:D:484:PRO:HD2	1:D:485:TYR:CD2	2.26	0.70
1:A:122:VAL:HG23	1:A:159:ILE:HG13	1.73	0.70
1:B:440:ALA:HB3	1:B:484:PRO:HB3	1.73	0.70
1:C:284:LEU:O	1:C:287:ILE:HG22	1.91	0.70
1:F:205:ILE:HG23	1:F:206:THR:HG23	1.73	0.70
1:C:208:PRO:CD	1:C:221:PHE:HE2	2.03	0.70
1:B:230:HIS:HD2	1:B:234:SER:OG	1.74	0.70
1:E:211:ILE:HG13	1:E:212:LYS:N	2.07	0.69
1:E:474:ILE:HG22	1:E:475:GLN:H	1.55	0.69
1:D:230:HIS:HA	1:D:234:SER:OG	1.92	0.69
1:A:104:GLN:HE21	1:A:140:ASP:H	1.40	0.69
1:E:113:LEU:HD23	1:E:156:TYR:CD1	2.28	0.69
1:E:295:PRO:HB2	1:E:342:MET:HE2	1.71	0.69
1:B:85:ASP:OD2	1:B:116:VAL:HG22	1.93	0.69
1:D:51:ARG:NH1	1:D:177:VAL:HG21	2.08	0.69
1:A:18:LEU:HD13	1:D:498:MET:CE	2.23	0.69
1:C:374:VAL:CG2	1:C:412:ILE:HG12	2.23	0.69
1:B:196:MET:CE	1:B:230:HIS:HB2	2.23	0.69
1:F:497:ILE:HG21	1:F:505:HIS:HE1	1.57	0.69
1:C:454:LEU:HD21	1:F:75:PHE:CZ	2.28	0.69
1:F:374:VAL:HG23	1:F:376:VAL:HG12	1.74	0.68
1:C:354:GLU:CD	1:C:393:ARG:HD2	2.13	0.68
1:F:451:VAL:HG13	1:F:455:HIS:HB2	1.74	0.68
1:B:26:GLU:O	1:B:30:HIS:HD2	1.76	0.68
1:A:65:ASP:HB2	1:A:120:LYS:HE3	1.75	0.68
1:E:295:PRO:HB2	1:E:342:MET:HE1	1.74	0.67
1:D:520:LEU:HB2	1:D:521:PRO:CD	2.23	0.67
1:D:437:TRP:CZ2	1:D:502:THR:HG21	2.29	0.67
1:A:25:ILE:O	1:A:29:THR:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:187:SER:HB3	1:F:188:PRO:HD3	1.75	0.67
1:A:299:HIS:CE1	1:A:323:LEU:HD11	2.30	0.67
1:F:287:ILE:O	1:F:289:PRO:HD3	1.93	0.67
1:A:415:LYS:NZ	1:A:441:GLN:O	2.28	0.67
1:B:343:GLN:OE1	1:B:344:PHE:HE2	1.78	0.67
1:A:91:TYR:CD1	1:D:512:GLN:HG3	2.30	0.67
1:A:68:ALA:HA	1:D:489:GLU:HA	1.77	0.66
1:B:374:VAL:CG1	1:B:412:ILE:HD13	2.22	0.66
1:B:451:VAL:HG13	1:B:455:HIS:CD2	2.29	0.66
1:C:69:ARG:HH11	1:C:81:ARG:HB2	1.60	0.66
1:F:65:ASP:HB2	1:F:120:LYS:HE3	1.77	0.66
1:A:37:VAL:O	1:A:40:GLN:NE2	2.27	0.66
1:F:290:ASP:CG	1:B:13:THR:HG22	2.16	0.66
1:D:320:PRO:CB	1:D:343:GLN:HE21	2.07	0.66
1:F:147:GLN:H	1:F:147:GLN:CD	1.98	0.66
1:D:209:ASP:HA	1:D:212:LYS:HE3	1.78	0.66
1:E:23:ARG:O	1:E:27:GLU:HG3	1.96	0.65
1:A:405:THR:O	1:A:516:LYS:HD2	1.97	0.65
1:F:451:VAL:HG22	1:F:454:LEU:HD11	1.77	0.65
1:C:397:LEU:HG	1:C:423:VAL:HG13	1.78	0.65
1:A:103:SER:HA	1:A:138:ILE:HG13	1.77	0.65
1:B:74:ASN:HB2	1:B:77:LEU:CD1	2.27	0.65
1:E:77:LEU:HD21	1:E:147:GLN:OE1	1.96	0.65
1:A:350:ILE:HG22	1:A:385:GLN:HE22	1.60	0.65
1:B:348:LEU:HD21	1:B:424:MET:CE	2.27	0.65
1:A:230:HIS:HA	1:A:234:SER:OG	1.96	0.65
1:B:519:SER:O	1:B:520:LEU:HB2	1.97	0.65
1:C:339:ASN:HD22	1:C:374:VAL:HA	1.60	0.65
1:E:47:THR:O	1:E:51:ARG:HG3	1.97	0.65
1:F:470:ARG:HH12	1:F:474:ILE:N	1.95	0.65
1:B:446:GLY:HA3	1:B:448:GLN:HE21	1.61	0.65
1:E:209:ASP:O	1:E:212:LYS:HG2	1.97	0.65
1:B:22:ARG:O	1:B:26:GLU:HG2	1.96	0.65
1:C:21:LEU:O	1:C:21:LEU:HD12	1.97	0.65
1:E:467:GLU:C	1:E:469:THR:H	2.01	0.65
1:F:437:TRP:HE1	1:F:502:THR:CG2	2.09	0.65
1:F:520:LEU:HD12	1:F:521:PRO:HD2	1.79	0.65
1:C:75:PHE:N	1:C:75:PHE:HD2	1.95	0.65
1:D:280:GLU:O	1:D:283:GLU:HG2	1.96	0.64
1:D:324:THR:HA	1:D:336:ILE:O	1.97	0.64
1:F:105:ASP:OD1	1:F:107:THR:HB	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:479:ASP:O	1:F:480:ALA:HB2	1.98	0.64
1:E:113:LEU:HD12	1:E:114:GLY:H	1.62	0.64
1:C:185:VAL:HG21	1:F:391:ILE:HG12	1.79	0.64
1:D:478:GLU:HG2	1:D:482:LEU:HD12	1.80	0.64
1:A:442:ILE:HD13	1:A:487:ALA:HB2	1.79	0.64
1:E:51:ARG:CG	1:E:51:ARG:HH11	2.01	0.64
1:A:165:HIS:HB3	1:B:520:LEU:HD11	1.80	0.64
1:D:478:GLU:CG	1:D:482:LEU:HD12	2.28	0.64
1:E:205:ILE:HG23	1:E:206:THR:HG23	1.78	0.64
1:A:265:GLU:HB2	1:A:266:PRO:HD2	1.80	0.63
1:C:467:GLU:HA	1:C:467:GLU:OE1	1.98	0.63
1:A:339:ASN:O	1:A:341:PRO:HD3	1.97	0.63
1:A:69:ARG:HB2	1:D:489:GLU:HB2	1.81	0.63
1:B:376:VAL:HG21	1:B:420:ALA:HB1	1.80	0.63
1:D:288:VAL:HG21	1:D:439:THR:HG21	1.79	0.63
1:E:238:HIS:HA	1:E:315:GLN:HG2	1.79	0.63
1:F:453:ILE:HG13	1:F:454:LEU:N	2.13	0.63
1:A:399:PHE:O	1:A:403:GLU:HG2	1.98	0.63
1:C:207:GLY:O	1:C:211:ILE:HG13	1.99	0.63
1:F:386:GLU:HA	1:F:390:ILE:HG22	1.81	0.63
1:B:26:GLU:O	1:B:30:HIS:CD2	2.51	0.63
1:B:25:ILE:O	1:B:29:THR:HG23	1.98	0.63
1:E:234:SER:HB2	1:E:236:VAL:HG23	1.80	0.63
1:F:504:ARG:O	1:F:508:ARG:HG3	1.97	0.63
1:A:450:ALA:O	1:A:454:LEU:HG	1.99	0.63
1:A:194:THR:H	1:A:238:HIS:CD2	2.17	0.63
1:B:457:ARG:O	1:B:457:ARG:HG3	1.97	0.63
1:B:29:THR:HG22	1:B:49:ARG:HH12	1.64	0.63
1:B:118:GLY:HA3	1:B:155:ALA:HB1	1.81	0.63
1:B:437:TRP:HB2	1:B:439:THR:HG23	1.81	0.63
1:A:43:LYS:HE3	1:A:45:LYS:HE2	1.80	0.62
1:B:499:PRO:O	1:B:502:THR:HG23	1.99	0.62
1:D:389:GLY:O	1:D:393:ARG:HG3	1.99	0.62
1:B:414:ARG:O	1:B:440:ALA:HA	1.99	0.62
1:C:120:LYS:O	1:C:123:LYS:HB3	1.99	0.62
1:F:470:ARG:HH12	1:F:474:ILE:CA	2.12	0.62
1:D:69:ARG:HD3	1:D:81:ARG:O	1.99	0.62
1:F:207:GLY:O	1:F:211:ILE:HG12	1.99	0.62
1:A:24:ARG:HD2	1:D:485:TYR:CE1	2.34	0.62
1:D:391:ILE:HG21	1:E:185:VAL:CG2	2.30	0.62
1:A:197:VAL:HB	1:A:200:THR:HG22	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:LEU:O	1:B:252:LYS:NZ	2.32	0.62
1:B:69:ARG:HD3	1:B:81:ARG:CB	2.29	0.62
1:B:300:SER:HA	1:B:303:GLU:CG	2.28	0.62
1:F:489:GLU:HG2	1:B:69:ARG:HB2	1.80	0.62
1:C:106:PHE:HD1	1:C:140:ASP:OD1	1.83	0.62
1:C:519:SER:O	1:C:520:LEU:CB	2.48	0.62
1:B:87:VAL:HG13	1:B:120:LYS:HD2	1.81	0.62
1:B:94:VAL:HG23	1:B:99:VAL:HG11	1.80	0.62
1:D:234:SER:O	1:E:392:ARG:NH1	2.33	0.62
1:F:113:LEU:HD22	1:F:117:TYR:CE2	2.35	0.62
1:B:138:ILE:CG2	1:B:175:LEU:HD23	2.27	0.62
1:C:49:ARG:O	1:C:50:GLU:CB	2.43	0.62
1:D:158:GLU:O	1:D:162:ARG:HG2	1.99	0.62
1:A:18:LEU:HD13	1:D:498:MET:HE1	1.81	0.61
1:F:230:HIS:HA	1:F:234:SER:OG	2.00	0.61
1:C:397:LEU:HD12	1:C:397:LEU:C	2.21	0.61
1:C:14:THR:HA	1:C:17:LYS:HE2	1.82	0.61
1:D:363:CYS:CB	1:D:368:VAL:HG22	2.29	0.61
1:F:45:LYS:HD3	1:F:200:THR:CB	2.30	0.61
1:A:299:HIS:O	1:A:303:GLU:HG3	2.00	0.61
1:B:173:ILE:HG23	1:B:193:PHE:HB2	1.80	0.61
1:B:207:GLY:O	1:B:210:VAL:HG23	2.00	0.61
1:D:94:VAL:HG23	1:D:99:VAL:HG11	1.81	0.61
1:F:448:GLN:HG2	1:F:449:GLY:N	2.16	0.61
1:C:397:LEU:HD12	1:C:397:LEU:O	2.01	0.61
1:F:56:LEU:HD12	1:F:61:PHE:HB2	1.82	0.61
1:A:414:ARG:O	1:A:440:ALA:HA	2.00	0.61
1:B:350:ILE:HD13	1:B:390:ILE:HD13	1.81	0.61
1:E:47:THR:HG22	1:E:50:GLU:H	1.64	0.61
1:C:354:GLU:OE2	1:C:393:ARG:HD2	2.01	0.61
1:D:472:ARG:NE	1:D:475:GLN:HB3	2.14	0.61
1:D:391:ILE:CG2	1:E:185:VAL:CG2	2.78	0.61
1:B:121:ILE:O	1:B:125:MET:HG3	2.01	0.61
1:C:374:VAL:HG23	1:C:412:ILE:HG23	1.83	0.61
1:D:451:VAL:HG13	1:D:455:HIS:HB2	1.83	0.61
1:E:203:MET:HB2	1:E:230:HIS:HE1	1.62	0.61
1:E:219:VAL:HG11	1:E:224:LEU:HD13	1.83	0.61
1:B:339:ASN:HD21	1:B:424:MET:CE	2.14	0.61
1:B:393:ARG:HA	1:B:396:LYS:HE3	1.83	0.60
1:B:437:TRP:NE1	1:B:502:THR:HG21	2.15	0.60
1:A:459:ILE:HG13	1:A:460:ALA:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ARG:NH1	1:A:81:ARG:HB3	2.15	0.60
1:F:337:VAL:O	1:F:372:THR:HA	2.01	0.60
1:A:26:GLU:OE1	1:A:26:GLU:N	2.34	0.60
1:A:520:LEU:HG	1:A:521:PRO:HD2	1.82	0.60
1:E:474:ILE:HG22	1:E:475:GLN:N	2.15	0.60
1:C:483:ASN:ND2	1:C:485:TYR:HB2	2.17	0.60
1:D:75:PHE:HD2	1:D:147:GLN:HB3	1.66	0.60
1:D:483:ASN:ND2	1:D:485:TYR:HB2	2.15	0.60
1:E:215:THR:HB	1:E:217:GLU:CG	2.29	0.60
1:E:230:HIS:HA	1:E:234:SER:OG	2.01	0.60
1:E:46:LEU:HB3	1:E:50:GLU:HG3	1.82	0.60
1:D:470:ARG:HG2	1:D:471:ALA:N	2.17	0.60
1:A:442:ILE:HD13	1:A:487:ALA:CB	2.32	0.60
1:D:518:GLU:O	1:D:519:SER:HB2	2.02	0.60
1:C:374:VAL:HG22	1:C:412:ILE:HA	1.83	0.60
1:A:391:ILE:CD1	1:A:391:ILE:H	2.13	0.60
1:B:405:THR:HG22	1:B:518:GLU:OE1	2.02	0.60
1:B:40:GLN:OE1	1:B:45:LYS:HB2	2.01	0.60
1:C:187:SER:HB3	1:C:188:PRO:CD	2.31	0.60
1:E:203:MET:O	1:E:230:HIS:CE1	2.55	0.60
1:C:158:GLU:HG3	1:C:162:ARG:NH2	2.15	0.59
1:D:466:ALA:HB1	1:D:470:ARG:HD2	1.84	0.59
1:F:485:TYR:HE2	1:B:17:LYS:HZ1	1.50	0.59
1:A:445:MET:HG3	1:A:450:ALA:HB2	1.84	0.59
1:E:451:VAL:HB	1:E:455:HIS:HE1	1.66	0.59
1:E:441:GLN:HG2	1:E:482:LEU:O	2.02	0.59
1:E:63:GLU:HG2	1:E:66:GLU:HB2	1.83	0.59
1:D:405:THR:O	1:D:516:LYS:CE	2.50	0.59
1:F:45:LYS:HD2	1:F:244:GLU:OE2	2.03	0.59
1:F:479:ASP:O	1:F:480:ALA:CB	2.51	0.59
1:A:35:ARG:NH1	1:A:38:GLU:OE1	2.34	0.59
1:B:496:VAL:HG13	1:E:67:PHE:CE2	2.38	0.59
1:B:29:THR:HG22	1:B:49:ARG:NH1	2.17	0.59
1:C:350:ILE:HG13	1:C:351:THR:N	2.16	0.59
1:A:214:VAL:HG21	1:B:381:PRO:HG2	1.83	0.59
1:C:451:VAL:O	1:C:454:LEU:O	2.20	0.59
1:E:163:ASN:HA	1:E:172:GLN:HE22	1.67	0.59
1:F:457:ARG:HH11	1:F:457:ARG:HG3	1.67	0.59
1:C:77:LEU:HD11	1:C:147:GLN:HG2	1.85	0.59
1:E:74:ASN:HB3	1:E:75:PHE:HD1	1.67	0.59
1:F:497:ILE:HD12	1:F:497:ILE:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:288:VAL:CG2	1:D:439:THR:HG21	2.32	0.59
1:E:459:ILE:HD11	1:E:470:ARG:HD2	1.85	0.59
1:A:472:ARG:O	1:A:476:GLU:OE1	2.21	0.59
1:B:177:VAL:O	1:B:200:THR:O	2.20	0.59
1:D:286:THR:OG1	1:D:287:ILE:N	2.36	0.59
1:F:158:GLU:OE1	1:F:161:ARG:NH2	2.36	0.59
1:E:51:ARG:CZ	1:E:177:VAL:HG21	2.33	0.58
1:A:205:ILE:HD11	1:B:390:ILE:HG21	1.85	0.58
1:A:380:LEU:HD12	1:A:380:LEU:C	2.24	0.58
1:B:334:VAL:HG21	1:B:371:LEU:HD11	1.84	0.58
1:B:402:ALA:HA	1:B:429:LEU:O	2.03	0.58
1:A:350:ILE:HG22	1:A:385:GLN:NE2	2.17	0.58
1:D:454:LEU:HD21	1:E:75:PHE:CE2	2.39	0.58
1:F:456:ARG:O	1:F:459:ILE:HG13	2.03	0.58
1:B:245:LYS:HG2	1:B:246:ASP:N	2.17	0.58
1:C:464:ASP:CG	1:C:465:ASP:H	2.07	0.58
1:D:315:GLN:OE1	1:D:355:LYS:HG3	2.04	0.58
1:B:140:ASP:O	1:B:141:SER:C	2.41	0.58
1:C:75:PHE:CD2	1:C:75:PHE:N	2.68	0.58
1:A:52:ILE:HD11	1:A:103:SER:HB2	1.86	0.58
1:A:51:ARG:HH11	1:A:138:ILE:CD1	2.16	0.58
1:B:74:ASN:HB2	1:B:77:LEU:HD11	1.84	0.58
1:F:437:TRP:HE1	1:F:502:THR:HG22	1.68	0.58
1:D:422:ASN:HA	1:D:426:SER:HB3	1.85	0.58
1:F:339:ASN:HD22	1:F:374:VAL:HA	1.67	0.58
1:F:499:PRO:O	1:F:502:THR:HG23	2.03	0.58
1:A:10:ASP:CG	1:A:11:ILE:H	2.07	0.58
1:B:77:LEU:HD21	1:B:147:GLN:HG2	1.86	0.58
1:F:470:ARG:NH1	1:F:474:ILE:N	2.51	0.58
1:E:243:ASP:OD1	1:E:244:GLU:N	2.37	0.57
1:F:69:ARG:HG2	1:E:489:GLU:HG2	1.85	0.57
1:F:350:ILE:O	1:F:354:GLU:HG3	2.04	0.57
1:F:414:ARG:O	1:F:440:ALA:HA	2.04	0.57
1:A:104:GLN:HE21	1:A:140:ASP:N	2.02	0.57
1:A:288:VAL:CG2	1:A:439:THR:HG21	2.32	0.57
1:A:77:LEU:HD11	1:A:147:GLN:HG3	1.87	0.57
1:B:176:VAL:HB	1:B:196:MET:HG2	1.85	0.57
1:D:196:MET:CE	1:D:230:HIS:HB2	2.34	0.57
1:E:340:GLN:CD	1:E:342:MET:HB2	2.25	0.57
1:E:483:ASN:HB2	1:E:484:PRO:HD2	1.86	0.57
1:F:176:VAL:CG2	1:F:196:MET:HG2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:470:ARG:HH12	1:F:474:ILE:HA	1.69	0.57
1:A:372:THR:HG21	1:A:401:TYR:CE1	2.39	0.57
1:F:45:LYS:HD3	1:F:200:THR:HB	1.85	0.57
1:A:372:THR:HG21	1:A:401:TYR:OH	2.04	0.57
1:A:372:THR:OG1	1:A:410:THR:HG22	2.04	0.57
1:B:182:GLY:O	1:B:184:ALA:N	2.37	0.57
1:B:196:MET:HE1	1:B:230:HIS:HB2	1.85	0.57
1:B:203:MET:O	1:B:230:HIS:HE1	1.88	0.57
1:D:379:PHE:HZ	1:D:423:VAL:HG21	1.68	0.57
1:B:489:GLU:HB3	1:E:69:ARG:HB2	1.87	0.57
1:B:40:GLN:HE22	1:B:45:LYS:HE2	1.68	0.57
1:E:176:VAL:HB	1:E:196:MET:HG2	1.84	0.57
1:C:302:ILE:HD13	1:C:336:ILE:HG21	1.85	0.57
1:D:138:ILE:HD13	1:D:175:LEU:HB3	1.86	0.57
1:A:130:LYS:O	1:D:517:ARG:HD2	2.04	0.57
1:A:194:THR:H	1:A:238:HIS:HD2	1.52	0.57
1:B:54:LEU:HG	1:B:248:VAL:HG11	1.87	0.57
1:C:103:SER:HB2	1:C:138:ILE:HD12	1.85	0.57
1:C:477:TYR:CE2	1:C:481:LEU:HD12	2.38	0.57
1:E:63:GLU:OE1	1:E:88:VAL:HG13	2.04	0.57
1:A:185:VAL:HG11	1:A:205:ILE:HG23	1.85	0.57
1:A:391:ILE:HD12	1:A:391:ILE:N	2.15	0.57
1:B:72:SER:HB2	1:B:148:GLU:OE1	2.05	0.57
1:B:196:MET:CE	1:B:227:ALA:HA	2.35	0.57
1:F:451:VAL:HG13	1:F:455:HIS:CD2	2.40	0.57
1:B:203:MET:HB2	1:B:230:HIS:CE1	2.40	0.57
1:C:46:LEU:HD12	1:C:50:GLU:OE2	2.05	0.57
1:C:528:ILE:HG13	1:C:529:PRO:HD2	1.86	0.57
1:F:20:ASP:OD1	1:F:23:ARG:NH2	2.38	0.57
1:F:40:GLN:HG3	1:F:45:LYS:HB2	1.86	0.57
1:A:150:VAL:HG12	1:A:153:LEU:HD12	1.85	0.57
1:A:454:LEU:HD21	1:B:146:ILE:CG2	2.35	0.57
1:E:451:VAL:HB	1:E:455:HIS:CE1	2.40	0.57
1:C:71:ARG:HH21	1:A:490:ARG:HG2	1.70	0.56
1:A:517:ARG:HG3	1:A:517:ARG:HH11	1.70	0.56
1:B:482:LEU:N	1:B:482:LEU:HD23	2.20	0.56
1:C:19:ALA:HA	1:C:22:ARG:NH1	2.20	0.56
1:B:517:ARG:HH11	1:B:517:ARG:HG3	1.70	0.56
1:C:410:THR:HG21	1:C:425:GLY:O	2.05	0.56
1:C:208:PRO:CG	1:C:221:PHE:CE2	2.87	0.56
1:C:472:ARG:HD3	1:C:475:GLN:HE21	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:PRO:HB3	1:A:171:PRO:HB2	1.86	0.56
1:D:509:GLY:O	1:D:513:LEU:HB2	2.04	0.56
1:E:113:LEU:O	1:E:145:ARG:HB2	2.05	0.56
1:E:155:ALA:O	1:E:159:ILE:HG12	2.05	0.56
1:E:177:VAL:O	1:E:177:VAL:HG23	2.06	0.56
1:E:181:ALA:HA	1:E:204:PHE:O	2.05	0.56
1:E:245:LYS:CG	1:E:246:ASP:N	2.68	0.56
1:F:18:LEU:HG	1:E:498:MET:HE3	1.86	0.56
1:E:47:THR:CG2	1:E:50:GLU:H	2.17	0.56
1:F:475:GLN:HA	1:F:478:GLU:CG	2.33	0.56
1:B:520:LEU:HG	1:B:521:PRO:CD	2.34	0.56
1:C:118:GLY:HA3	1:C:155:ALA:HB1	1.87	0.56
1:D:313:GLU:OE2	1:D:316:PRO:HA	2.04	0.56
1:D:440:ALA:HB3	1:D:484:PRO:HB3	1.86	0.56
1:A:520:LEU:HD12	1:A:521:PRO:HD2	1.88	0.56
1:B:314:THR:HG23	1:B:325:GLY:HA2	1.86	0.56
1:C:397:LEU:HD11	1:C:401:TYR:CE2	2.41	0.56
1:C:475:GLN:HA	1:C:478:GLU:HB2	1.88	0.56
1:A:102:PHE:CZ	1:A:137:GLY:HA3	2.40	0.56
1:C:464:ASP:OD2	1:C:468:ALA:HB2	2.06	0.56
1:C:376:VAL:HG13	1:C:376:VAL:O	2.05	0.56
1:A:69:ARG:CG	1:A:69:ARG:HH11	2.07	0.56
1:B:410:THR:OG1	1:B:434:ASN:ND2	2.39	0.56
1:C:70:HIS:C	1:C:70:HIS:HD1	2.09	0.56
1:A:71:ARG:NH2	1:D:490:ARG:HE	2.04	0.56
1:A:520:LEU:CG	1:A:521:PRO:HD2	2.35	0.56
1:B:182:GLY:HA2	1:B:205:ILE:O	2.06	0.56
1:C:10:ASP:O	1:C:11:ILE:HD13	2.06	0.56
1:D:356:ALA:O	1:D:360:VAL:HG23	2.05	0.56
1:A:88:VAL:O	1:A:103:SER:N	2.39	0.56
1:A:113:LEU:HD13	1:A:156:TYR:CE1	2.41	0.56
1:C:109:PHE:C	1:C:111:GLY:N	2.55	0.56
1:D:69:ARG:CD	1:D:81:ARG:O	2.54	0.56
1:F:462:ALA:HB1	1:F:465:ASP:OD2	2.05	0.56
1:E:23:ARG:HG3	1:E:24:ARG:N	2.21	0.55
1:A:451:VAL:O	1:A:454:LEU:HB2	2.06	0.55
1:D:434:ASN:O	1:D:494:ASP:OD1	2.25	0.55
1:D:354:GLU:OE1	1:E:392:ARG:NH2	2.39	0.55
1:D:196:MET:HE1	1:D:230:HIS:HB2	1.89	0.55
1:A:284:LEU:O	1:A:287:ILE:HG22	2.06	0.55
1:D:297:ASP:OD1	1:D:299:HIS:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:LEU:O	1:D:337:VAL:HA	2.06	0.55
1:D:77:LEU:HD11	1:D:147:GLN:CG	2.35	0.55
1:F:438:PRO:HG3	1:B:21:LEU:HD22	1.88	0.55
1:A:464:ASP:O	1:A:465:ASP:HB3	2.06	0.55
1:B:106:PHE:HB2	1:B:140:ASP:OD2	2.06	0.55
1:B:140:ASP:O	1:B:179:PRO:O	2.24	0.55
1:B:485:TYR:O	1:B:489:GLU:HG3	2.07	0.55
1:D:56:LEU:HD12	1:D:61:PHE:HB2	1.88	0.55
1:B:74:ASN:N	1:B:77:LEU:HD12	2.21	0.55
1:B:88:VAL:HG13	1:B:103:SER:HB3	1.89	0.55
1:C:520:LEU:CD1	1:C:521:PRO:HD2	2.11	0.55
1:B:456:ARG:HG2	1:B:459:ILE:HG12	1.87	0.55
1:D:82:PRO:O	1:D:84:GLY:O	2.24	0.55
1:A:298:MET:HE3	1:A:301:VAL:HG11	1.89	0.55
1:B:456:ARG:C	1:B:458:THR:H	2.10	0.55
1:B:459:ILE:HG13	1:B:460:ALA:N	2.22	0.55
1:C:208:PRO:HA	1:C:211:ILE:HB	1.87	0.55
1:C:22:ARG:O	1:C:26:GLU:HG2	2.07	0.55
1:C:381:PRO:HB3	1:F:211:ILE:HD13	1.88	0.55
1:E:379:PHE:O	1:E:381:PRO:HD3	2.07	0.55
1:A:457:ARG:NH1	1:A:461:ASP:HB2	2.23	0.54
1:E:415:LYS:HE2	1:E:417:PHE:HE2	1.72	0.54
1:F:373:PHE:CD1	1:F:411:VAL:CG2	2.90	0.54
1:E:376:VAL:O	1:E:376:VAL:HG12	2.06	0.54
1:F:434:ASN:O	1:F:493:VAL:HG13	2.07	0.54
1:A:415:LYS:CD	1:A:441:GLN:HB2	2.34	0.54
1:A:451:VAL:HG11	1:A:474:ILE:HA	1.90	0.54
1:A:82:PRO:HG2	1:A:109:PHE:CE2	2.42	0.54
1:C:128:ALA:O	1:C:132:GLY:N	2.40	0.54
1:C:422:ASN:O	1:C:429:LEU:HD22	2.08	0.54
1:D:499:PRO:O	1:D:502:THR:CG2	2.55	0.54
1:F:477:TYR:O	1:F:481:LEU:HB2	2.07	0.54
1:A:88:VAL:HB	1:A:103:SER:HB3	1.90	0.54
1:B:339:ASN:HD21	1:B:424:MET:HE2	1.72	0.54
1:C:414:ARG:O	1:C:440:ALA:HA	2.08	0.54
1:E:433:LEU:HA	1:E:494:ASP:OD2	2.07	0.54
1:A:298:MET:HG2	1:A:338:ALA:HB1	1.90	0.54
1:A:480:ALA:O	1:A:481:LEU:HD13	2.08	0.54
1:C:68:ALA:HA	1:A:489:GLU:HA	1.90	0.54
1:B:350:ILE:CG2	1:B:393:ARG:NH1	2.71	0.54
1:B:520:LEU:CG	1:B:521:PRO:HD2	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:HIS:ND1	1:B:70:HIS:C	2.60	0.54
1:D:499:PRO:O	1:D:502:THR:HG23	2.08	0.54
1:F:437:TRP:CZ2	1:F:502:THR:HG21	2.42	0.54
1:D:514:ARG:HH11	1:D:514:ARG:HG3	1.72	0.54
1:B:489:GLU:CB	1:E:69:ARG:HB2	2.38	0.54
1:B:456:ARG:HG2	1:B:459:ILE:CD1	2.38	0.54
1:B:75:PHE:HD1	1:B:76:GLY:H	1.56	0.54
1:C:205:ILE:HD11	1:F:390:ILE:HG21	1.90	0.54
1:D:422:ASN:O	1:D:429:LEU:HD22	2.07	0.54
1:F:206:THR:OG1	1:F:211:ILE:HD11	2.08	0.54
1:F:375:ASP:OD1	1:F:415:LYS:HG2	2.08	0.54
1:F:393:ARG:HA	1:F:396:LYS:HE3	1.90	0.54
1:B:140:ASP:OD1	1:B:141:SER:N	2.37	0.53
1:B:343:GLN:OE1	1:B:344:PHE:CE2	2.61	0.53
1:F:441:GLN:CG	1:F:482:LEU:HB3	2.38	0.53
1:A:69:ARG:NH1	1:A:81:ARG:O	2.39	0.53
1:B:196:MET:HE2	1:B:230:HIS:HB2	1.89	0.53
1:B:72:SER:OG	1:B:77:LEU:HD12	2.08	0.53
1:D:70:HIS:CE1	1:D:77:LEU:HB3	2.43	0.53
1:F:35:ARG:NH2	1:F:38:GLU:OE1	2.41	0.53
1:A:163:ASN:HA	1:A:172:GLN:HE22	1.73	0.53
1:B:456:ARG:HD2	1:B:456:ARG:O	2.09	0.53
1:B:442:ILE:HD12	1:B:484:PRO:HA	1.90	0.53
1:C:474:ILE:O	1:C:475:GLN:CB	2.55	0.53
1:A:104:GLN:O	1:A:140:ASP:HB3	2.08	0.53
1:A:70:HIS:CE1	1:A:115:GLU:HG2	2.43	0.53
1:B:61:PHE:CZ	1:B:63:GLU:HG3	2.43	0.53
1:C:103:SER:HA	1:C:138:ILE:HB	1.90	0.53
1:F:175:LEU:HD11	1:F:247:ALA:HB1	1.91	0.53
1:B:302:ILE:O	1:B:305:VAL:O	2.26	0.53
1:B:305:VAL:O	1:B:306:LEU:CG	2.54	0.53
1:B:415:LYS:HD2	1:B:417:PHE:HE1	1.65	0.53
1:B:65:ASP:HB2	1:B:120:LYS:HE2	1.91	0.53
1:C:374:VAL:HG21	1:C:412:ILE:HG12	1.90	0.53
1:D:514:ARG:HG3	1:D:514:ARG:NH1	2.23	0.53
1:E:231:ASN:HD21	1:E:239:HIS:CA	2.22	0.53
1:E:444:VAL:HG23	1:E:445:MET:HG2	1.88	0.53
1:E:70:HIS:O	1:E:81:ARG:HD2	2.09	0.53
1:C:146:ILE:HD12	1:F:445:MET:CE	2.38	0.53
1:A:451:VAL:HA	1:A:454:LEU:HD12	1.90	0.53
1:B:380:LEU:HD23	1:B:385:GLN:CD	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:447:ALA:HB2	1:D:482:LEU:HD11	1.90	0.53
1:F:26:GLU:O	1:F:30:HIS:HD2	1.91	0.53
1:F:486:THR:HA	1:F:489:GLU:OE1	2.08	0.53
1:D:295:PRO:HB2	1:D:342:MET:HE3	1.90	0.53
1:D:490:ARG:CZ	1:E:151:ALA:HB2	2.39	0.53
1:E:245:LYS:HG2	1:E:246:ASP:N	2.24	0.53
1:F:284:LEU:HD22	1:F:437:TRP:CH2	2.44	0.53
1:F:350:ILE:HD12	1:F:390:ILE:HD13	1.90	0.53
1:D:196:MET:CE	1:D:237:ALA:HB2	2.38	0.53
1:F:89:THR:HB	1:F:124:VAL:HG11	1.91	0.53
1:F:285:ASP:HB3	1:B:18:LEU:CD1	2.39	0.53
1:A:30:HIS:O	1:A:32:GLY:N	2.42	0.53
1:B:47:THR:HG22	1:B:50:GLU:CD	2.29	0.53
1:C:374:VAL:HG22	1:C:412:ILE:HG12	1.91	0.53
1:D:319:ALA:HB2	1:D:351:THR:HB	1.91	0.53
1:D:47:THR:O	1:D:51:ARG:HG3	2.09	0.53
1:B:284:LEU:O	1:B:287:ILE:HG22	2.09	0.53
1:D:275:LEU:HD22	1:D:508:ARG:NH1	2.24	0.53
1:A:528:ILE:C	1:B:358:ARG:HH12	2.12	0.52
1:C:467:GLU:O	1:C:468:ALA:C	2.48	0.52
1:E:33:SER:HB3	1:E:36:ALA:HB3	1.91	0.52
1:D:399:PHE:CD2	1:E:164:THR:HG23	2.43	0.52
1:A:361:ARG:HH21	1:B:528:ILE:HG12	1.74	0.52
1:A:234:SER:O	1:B:392:ARG:HD3	2.08	0.52
1:D:417:PHE:O	1:D:420:ALA:HB3	2.08	0.52
1:C:164:THR:HG23	1:F:399:PHE:CD2	2.44	0.52
1:A:380:LEU:HD11	1:A:385:GLN:CD	2.30	0.52
1:A:350:ILE:CD1	1:A:393:ARG:HH11	2.11	0.52
1:A:483:ASN:HB2	1:A:484:PRO:HD2	1.91	0.52
1:A:520:LEU:CD1	1:A:521:PRO:HD2	2.39	0.52
1:B:187:SER:HB3	1:B:188:PRO:HD3	1.90	0.52
1:C:315:GLN:OE1	1:C:355:LYS:HG3	2.09	0.52
1:E:339:ASN:CG	1:E:376:VAL:HG23	2.29	0.52
1:E:39:LYS:CD	1:E:39:LYS:N	2.71	0.52
1:F:406:VAL:C	1:F:516:LYS:HE3	2.30	0.52
1:B:72:SER:CB	1:B:148:GLU:OE1	2.57	0.52
1:D:297:ASP:OD1	1:D:299:HIS:CD2	2.63	0.52
1:E:156:TYR:CE1	1:E:184:ALA:HB2	2.44	0.52
1:F:291:SER:HB3	1:F:294:GLN:CD	2.30	0.52
1:C:52:ILE:HG23	1:C:56:LEU:HD22	1.91	0.52
1:D:353:SER:CB	1:D:394:GLY:HA2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:405:THR:O	1:F:516:LYS:HE3	2.10	0.52
1:E:375:ASP:OD2	1:E:414:ARG:HD2	2.10	0.52
1:E:70:HIS:HA	1:E:116:VAL:HG11	1.90	0.52
1:F:470:ARG:NH1	1:F:474:ILE:HG13	2.25	0.52
1:C:212:LYS:HE2	1:C:218:ASP:HB3	1.92	0.52
1:D:443:ALA:HB2	1:D:482:LEU:HD23	1.92	0.52
1:F:445:MET:HE3	1:F:450:ALA:HA	1.91	0.52
1:B:456:ARG:HG2	1:B:459:ILE:HD11	1.91	0.52
1:C:111:GLY:HA3	1:C:141:SER:HA	1.91	0.52
1:C:49:ARG:NH2	1:C:63:GLU:OE2	2.42	0.52
1:F:411:VAL:HG12	1:F:435:LEU:HB2	1.91	0.52
1:A:153:LEU:HD21	1:B:444:VAL:HA	1.92	0.52
1:C:396:LYS:HE2	1:C:529:PRO:O	2.10	0.52
1:E:520:LEU:CD2	1:E:521:PRO:HD2	2.36	0.52
1:A:112:ALA:HB1	1:A:145:ARG:CA	2.41	0.51
1:C:153:LEU:HD11	1:F:444:VAL:HA	1.91	0.51
1:D:196:MET:HE3	1:D:237:ALA:HB2	1.91	0.51
1:F:489:GLU:HA	1:B:68:ALA:HA	1.93	0.51
1:A:70:HIS:HB2	1:A:85:ASP:OD1	2.10	0.51
1:B:140:ASP:O	1:B:179:PRO:HG2	2.11	0.51
1:C:175:LEU:HD11	1:C:247:ALA:HB1	1.92	0.51
1:D:35:ARG:N	1:D:35:ARG:CD	2.72	0.51
1:E:456:ARG:HA	1:E:459:ILE:HG22	1.92	0.51
1:B:61:PHE:HZ	1:B:63:GLU:HG3	1.75	0.51
1:C:104:GLN:HB3	1:C:117:TYR:OH	2.11	0.51
1:D:408:LEU:N	1:D:432:ASP:OD2	2.39	0.51
1:D:497:ILE:HD12	1:D:498:MET:H	1.75	0.51
1:E:39:LYS:H	1:E:39:LYS:HD2	1.73	0.51
1:A:336:ILE:N	1:A:336:ILE:HD12	2.24	0.51
1:B:344:PHE:N	1:B:344:PHE:CD2	2.77	0.51
1:C:177:VAL:HA	1:C:201:SER:OG	2.11	0.51
1:D:520:LEU:HD12	1:D:521:PRO:HD2	1.92	0.51
1:A:418:GLY:HA2	1:B:153:LEU:HD21	1.91	0.51
1:B:483:ASN:HB2	1:B:485:TYR:CD1	2.46	0.51
1:C:218:ASP:O	1:C:219:VAL:HG13	2.10	0.51
1:C:454:LEU:HD21	1:F:75:PHE:CE2	2.46	0.51
1:F:356:ALA:O	1:F:360:VAL:HG23	2.11	0.51
1:F:451:VAL:CG1	1:F:455:HIS:HB2	2.39	0.51
1:A:18:LEU:CD1	1:D:285:ASP:HB3	2.40	0.51
1:B:230:HIS:HA	1:B:234:SER:OG	2.11	0.51
1:A:529:PRO:CA	1:B:358:ARG:NH1	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:ASN:HD21	1:D:352:ALA:HB2	1.74	0.51
1:D:486:THR:O	1:D:489:GLU:HG2	2.10	0.51
1:C:339:ASN:ND2	1:C:374:VAL:HA	2.24	0.51
1:B:432:ASP:OD1	1:E:130:LYS:HE3	2.11	0.51
1:E:48:ALA:HA	1:E:51:ARG:HD2	1.93	0.51
1:F:138:ILE:HG12	1:F:175:LEU:HD23	1.93	0.51
1:A:112:ALA:HB1	1:A:145:ARG:HA	1.93	0.51
1:A:332:ARG:NE	1:A:514:ARG:HH12	2.08	0.51
1:A:391:ILE:HG23	1:B:185:VAL:CG2	2.41	0.51
1:D:45:LYS:HB2	1:D:244:GLU:OE2	2.10	0.51
1:D:49:ARG:HH22	1:D:63:GLU:CD	2.14	0.51
1:F:213:THR:HG22	1:F:213:THR:O	2.10	0.51
1:B:45:LYS:HD2	1:B:200:THR:HG22	1.93	0.51
1:C:19:ALA:HA	1:C:22:ARG:HH11	1.75	0.51
1:E:374:VAL:HB	1:E:412:ILE:HD13	1.93	0.51
1:E:39:LYS:CD	1:E:39:LYS:H	2.22	0.51
1:F:472:ARG:HG2	1:F:476:GLU:HG2	1.93	0.51
1:B:432:ASP:OD1	1:E:130:LYS:CE	2.59	0.51
1:C:475:GLN:H	1:C:477:TYR:H	1.59	0.51
1:D:329:VAL:HG11	1:D:510:LEU:HD12	1.93	0.51
1:E:51:ARG:HD3	1:E:138:ILE:HG21	1.92	0.51
1:E:456:ARG:O	1:E:459:ILE:HG22	2.11	0.51
1:F:45:LYS:HD3	1:F:200:THR:HG21	1.93	0.51
1:F:475:GLN:O	1:F:479:ASP:HB2	2.11	0.51
1:A:118:GLY:HA3	1:A:155:ALA:HB1	1.92	0.50
1:A:207:GLY:O	1:A:211:ILE:HD12	2.10	0.50
1:C:397:LEU:CD1	1:C:401:TYR:CD2	2.93	0.50
1:C:519:SER:O	1:C:520:LEU:HB2	2.11	0.50
1:D:280:GLU:HG3	1:D:281:ASP:H	1.76	0.50
1:B:459:ILE:HG13	1:B:460:ALA:H	1.75	0.50
1:A:528:ILE:HG21	1:B:528:ILE:HD11	1.92	0.50
1:C:14:THR:O	1:C:18:LEU:HD13	2.12	0.50
1:D:194:THR:N	1:D:238:HIS:HD2	1.99	0.50
1:F:238:HIS:HA	1:F:315:GLN:HG2	1.93	0.50
1:A:446:GLY:C	1:A:448:GLN:H	2.14	0.50
1:B:196:MET:HE1	1:B:227:ALA:HA	1.93	0.50
1:B:21:LEU:HG	1:B:25:ILE:HD11	1.94	0.50
1:A:153:LEU:HD22	1:B:418:GLY:O	2.12	0.50
1:E:187:SER:HB3	1:E:188:PRO:HD3	1.94	0.50
1:E:203:MET:O	1:E:230:HIS:HE1	1.93	0.50
1:E:461:ASP:C	1:E:463:GLY:N	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:105:ASP:C	1:F:107:THR:H	2.13	0.50
1:A:82:PRO:HG2	1:A:109:PHE:HE2	1.77	0.50
1:A:22:ARG:O	1:A:26:GLU:OE1	2.30	0.50
1:A:341:PRO:HG3	1:A:375:ASP:HB3	1.93	0.50
1:C:71:ARG:NH2	1:A:490:ARG:HG2	2.26	0.50
1:B:353:SER:HB3	1:B:394:GLY:HA2	1.94	0.50
1:B:457:ARG:CG	1:B:457:ARG:O	2.59	0.50
1:E:141:SER:O	1:E:179:PRO:HG2	2.11	0.50
1:F:441:GLN:HG2	1:F:482:LEU:HB3	1.94	0.50
1:B:74:ASN:HB2	1:B:77:LEU:HD12	1.94	0.50
1:D:145:ARG:HG2	1:D:147:GLN:HG2	1.93	0.50
1:D:353:SER:OG	1:D:394:GLY:HA2	2.12	0.50
1:D:465:ASP:OD1	1:D:466:ALA:N	2.45	0.50
1:E:474:ILE:O	1:E:475:GLN:HG3	2.11	0.50
1:A:213:THR:O	1:A:213:THR:HG22	2.12	0.50
1:B:377:PRO:O	1:B:417:PHE:HD1	1.95	0.50
1:F:215:THR:HG21	1:F:217:GLU:OE2	2.12	0.50
1:A:177:VAL:HG12	1:A:197:VAL:HG23	1.93	0.50
1:B:419:GLY:O	1:B:423:VAL:HG23	2.12	0.50
1:B:456:ARG:HG2	1:B:459:ILE:CG1	2.42	0.50
1:C:69:ARG:NH1	1:C:81:ARG:HB2	2.25	0.50
1:A:251:VAL:O	1:A:255:LEU:HD22	2.12	0.49
1:A:69:ARG:HH12	1:A:81:ARG:HB3	1.76	0.49
1:B:496:VAL:CG1	1:E:67:PHE:HD2	2.24	0.49
1:D:507:VAL:O	1:D:511:ARG:HG3	2.12	0.49
1:F:45:LYS:HE2	1:F:200:THR:HB	1.92	0.49
1:A:205:ILE:HD13	1:B:390:ILE:HG12	1.94	0.49
1:B:410:THR:HG21	1:B:425:GLY:O	2.12	0.49
1:C:106:PHE:O	1:C:106:PHE:CD2	2.65	0.49
1:D:104:GLN:HG3	1:D:138:ILE:O	2.12	0.49
1:F:437:TRP:HE1	1:F:502:THR:HG21	1.77	0.49
1:F:285:ASP:HB3	1:B:18:LEU:HD11	1.94	0.49
1:C:48:ALA:C	1:C:49:ARG:O	2.48	0.49
1:C:396:LYS:HD3	1:F:530:LEU:HG	1.94	0.49
1:A:75:PHE:CE2	1:B:454:LEU:HD13	2.47	0.49
1:E:376:VAL:CG1	1:E:420:ALA:HB1	2.25	0.49
1:F:163:ASN:HA	1:F:172:GLN:HE22	1.75	0.49
1:F:321:ASN:HA	1:F:343:GLN:HB2	1.94	0.49
1:A:326:PHE:HB3	1:A:334:VAL:O	2.12	0.49
1:D:146:ILE:HG23	1:E:444:VAL:HG21	1.94	0.49
1:F:281:ASP:O	1:F:284:LEU:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:GLU:HG2	1:E:69:ARG:HB2	1.95	0.49
1:B:517:ARG:HG3	1:B:517:ARG:NH1	2.27	0.49
1:E:447:ALA:HB1	1:E:474:ILE:HG23	1.95	0.49
1:E:47:THR:HG23	1:E:49:ARG:H	1.77	0.49
1:A:163:ASN:HB3	1:A:190:ILE:CG1	2.43	0.49
1:A:49:ARG:HG3	1:A:88:VAL:HG21	1.94	0.49
1:F:290:ASP:OD1	1:B:13:THR:HG22	2.13	0.49
1:C:208:PRO:HG3	1:C:221:PHE:CE2	2.47	0.49
1:C:350:ILE:HD13	1:C:393:ARG:NH1	2.27	0.49
1:A:161:ARG:HD3	1:B:428:HIS:O	2.12	0.49
1:A:176:VAL:O	1:A:196:MET:HA	2.13	0.49
1:A:393:ARG:HH22	1:B:393:ARG:NH1	2.11	0.49
1:B:89:THR:HB	1:B:124:VAL:HG11	1.95	0.49
1:B:397:LEU:HD23	1:B:423:VAL:CG1	2.43	0.49
1:B:498:MET:CE	1:E:18:LEU:HG	2.43	0.49
1:E:520:LEU:HD13	1:E:521:PRO:HD2	1.94	0.49
1:A:377:PRO:HA	1:A:417:PHE:HD2	1.78	0.49
1:D:410:THR:HB	1:D:434:ASN:ND2	2.27	0.49
1:F:496:VAL:HB	1:B:67:PHE:HE2	1.76	0.49
1:A:40:GLN:NE2	1:A:41:HIS:N	2.59	0.49
1:B:46:LEU:HB3	1:B:50:GLU:HB2	1.94	0.49
1:C:208:PRO:HD3	1:C:221:PHE:CE2	2.47	0.49
1:D:337:VAL:O	1:D:372:THR:HA	2.12	0.49
1:E:175:LEU:HD11	1:E:247:ALA:HB1	1.95	0.49
1:E:214:VAL:HG23	1:E:215:THR:N	2.28	0.49
1:C:208:PRO:HD3	1:C:221:PHE:HE2	1.75	0.48
1:C:482:LEU:HD23	1:C:482:LEU:N	2.28	0.48
1:D:121:ILE:O	1:D:125:MET:HG3	2.13	0.48
1:E:356:ALA:O	1:E:360:VAL:HG23	2.12	0.48
1:B:343:GLN:C	1:B:344:PHE:HD2	2.16	0.48
1:D:302:ILE:HD13	1:D:336:ILE:HG21	1.95	0.48
1:F:21:LEU:HD22	1:E:438:PRO:HG3	1.95	0.48
1:B:350:ILE:HG21	1:B:393:ARG:NH1	2.29	0.48
1:B:455:HIS:CD2	1:B:455:HIS:N	2.81	0.48
1:E:302:ILE:HG22	1:E:306:LEU:HD22	1.94	0.48
1:E:303:GLU:HG2	1:E:309:ALA:O	2.13	0.48
1:F:18:LEU:CG	1:E:498:MET:HE1	2.41	0.48
1:C:391:ILE:HG23	1:F:185:VAL:HG22	1.96	0.48
1:A:457:ARG:HH22	1:A:461:ASP:CG	2.16	0.48
1:B:494:ASP:HB3	1:E:64:LEU:HD12	1.95	0.48
1:C:208:PRO:CD	1:C:221:PHE:CE2	2.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:51:ARG:CG	1:E:51:ARG:NH1	2.66	0.48
1:C:234:SER:O	1:F:392:ARG:NH1	2.46	0.48
1:E:21:LEU:O	1:E:25:ILE:HG13	2.13	0.48
1:E:234:SER:CB	1:E:236:VAL:HG23	2.43	0.48
1:F:289:PRO:HB2	1:F:294:GLN:HG3	1.96	0.48
1:F:77:LEU:HD13	1:F:147:GLN:HG3	1.94	0.48
1:A:40:GLN:HB2	1:A:45:LYS:HD2	1.96	0.48
1:B:89:THR:HG22	1:B:102:PHE:HB2	1.95	0.48
1:C:202:HIS:HE1	1:C:222:GLU:HA	1.78	0.48
1:C:285:ASP:OD2	1:C:500:SER:HB3	2.14	0.48
1:A:459:ILE:CG1	1:A:460:ALA:N	2.77	0.48
1:B:496:VAL:CG1	1:E:67:PHE:CD2	2.97	0.48
1:B:357:ALA:O	1:B:361:ARG:HG3	2.14	0.48
1:C:106:PHE:HD2	1:C:106:PHE:O	1.97	0.48
1:D:65:ASP:HB2	1:D:120:LYS:HE3	1.94	0.48
1:F:297:ASP:OD1	1:F:299:HIS:HD2	1.97	0.48
1:A:442:ILE:HD11	1:A:487:ALA:H	1.79	0.48
1:C:243:ASP:OD2	1:C:244:GLU:N	2.47	0.48
1:D:302:ILE:O	1:D:305:VAL:HG22	2.13	0.48
1:E:350:ILE:HG13	1:E:390:ILE:HD13	1.95	0.48
1:A:391:ILE:HG23	1:B:185:VAL:HG23	1.95	0.48
1:B:370:VAL:HB	1:B:408:LEU:HD23	1.95	0.48
1:C:126:ASP:OD1	1:C:162:ARG:HD3	2.14	0.48
1:C:469:THR:O	1:C:473:LEU:HG	2.13	0.48
1:D:104:GLN:HE21	1:D:140:ASP:H	1.62	0.48
1:E:211:ILE:HG13	1:E:212:LYS:H	1.79	0.48
1:E:47:THR:HG23	1:E:49:ARG:N	2.29	0.48
1:F:357:ALA:O	1:F:361:ARG:HG3	2.14	0.48
1:F:458:THR:HA	1:F:461:ASP:HB2	1.96	0.48
1:A:322:ILE:CG2	1:A:355:LYS:HD3	2.44	0.47
1:A:517:ARG:HG2	1:A:517:ARG:HH11	1.77	0.47
1:C:51:ARG:HH12	1:C:140:ASP:HB2	1.78	0.47
1:E:245:LYS:HG2	1:E:246:ASP:H	1.77	0.47
1:F:10:ASP:O	1:F:16:GLY:HA3	2.14	0.47
1:F:138:ILE:HA	1:F:175:LEU:O	2.14	0.47
1:A:369:PRO:HA	1:A:406:VAL:CG1	2.40	0.47
1:A:454:LEU:HD21	1:B:146:ILE:HG21	1.95	0.47
1:C:158:GLU:OE2	1:C:161:ARG:NH2	2.46	0.47
1:E:103:SER:HB2	1:E:138:ILE:HD12	1.95	0.47
1:B:496:VAL:HG13	1:E:67:PHE:CD2	2.49	0.47
1:E:74:ASN:HB3	1:E:75:PHE:CD1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLN:HB2	1:A:140:ASP:H	1.78	0.47
1:A:332:ARG:CZ	1:A:514:ARG:NH1	2.78	0.47
1:B:21:LEU:HG	1:B:25:ILE:CD1	2.44	0.47
1:B:374:VAL:HG23	1:B:376:VAL:HG12	1.96	0.47
1:B:73:THR:O	1:B:75:PHE:N	2.47	0.47
1:C:110:GLY:O	1:C:142:GLY:N	2.40	0.47
1:D:173:ILE:HD13	1:D:254:LEU:HD23	1.95	0.47
1:A:238:HIS:CE1	1:A:315:GLN:HE21	2.32	0.47
1:A:410:THR:OG1	1:A:434:ASN:ND2	2.47	0.47
1:A:527:ASN:O	1:B:358:ARG:NH1	2.47	0.47
1:B:77:LEU:HD21	1:B:147:GLN:HB3	1.97	0.47
1:C:517:ARG:O	1:C:517:ARG:HG3	2.14	0.47
1:A:18:LEU:HD11	1:D:285:ASP:HB3	1.96	0.47
1:E:112:ALA:HA	1:E:143:GLY:O	2.15	0.47
1:A:141:SER:O	1:A:179:PRO:O	2.33	0.47
1:B:451:VAL:O	1:B:455:HIS:HD2	1.98	0.47
1:E:414:ARG:O	1:E:440:ALA:HA	2.14	0.47
1:A:371:LEU:CD2	1:A:409:ILE:HB	2.45	0.47
1:B:375:ASP:OD2	1:B:414:ARG:HD2	2.14	0.47
1:B:530:LEU:HA	1:B:530:LEU:HD23	1.58	0.47
1:D:161:ARG:HD3	1:E:428:HIS:O	2.14	0.47
1:E:14:THR:O	1:E:18:LEU:HD13	2.14	0.47
1:F:217:GLU:O	1:F:217:GLU:HG2	2.14	0.47
1:A:393:ARG:NH2	1:B:393:ARG:NH1	2.62	0.47
1:C:381:PRO:HG2	1:F:214:VAL:HG21	1.95	0.47
1:C:433:LEU:HA	1:C:494:ASP:OD2	2.14	0.47
1:A:401:TYR:CD1	1:A:425:GLY:HA2	2.49	0.47
1:A:459:ILE:HG13	1:A:460:ALA:N	2.30	0.47
1:B:527:ASN:O	1:B:528:ILE:C	2.53	0.47
1:C:512:GLN:HG3	1:D:91:TYR:CE1	2.49	0.47
1:E:470:ARG:O	1:E:474:ILE:HG13	2.14	0.47
1:F:177:VAL:HA	1:F:201:SER:OG	2.14	0.47
1:A:218:ASP:O	1:A:219:VAL:HG23	2.14	0.47
1:A:35:ARG:NH2	1:A:39:LYS:CE	2.78	0.47
1:B:198:ASP:OD1	1:B:199:GLN:HG2	2.15	0.47
1:C:99:VAL:HG12	1:C:100:ALA:N	2.30	0.47
1:D:350:ILE:HD13	1:D:390:ILE:HD13	1.96	0.47
1:F:45:LYS:HD3	1:F:200:THR:CG2	2.45	0.47
1:E:299:HIS:HE1	1:E:313:GLU:OE1	1.97	0.47
1:A:18:LEU:HD13	1:D:498:MET:HE3	1.96	0.47
1:A:386:GLU:OE2	1:B:204:PHE:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:NH2	1:A:39:LYS:NZ	2.63	0.47
1:A:361:ARG:CD	1:A:403:GLU:OE2	2.61	0.47
1:A:447:ALA:O	1:A:474:ILE:HG23	2.15	0.47
1:B:451:VAL:C	1:B:453:ILE:H	2.18	0.47
1:C:202:HIS:ND1	1:C:226:GLY:HA2	2.29	0.47
1:D:262:ASN:ND2	1:E:523:LYS:HA	2.29	0.47
1:D:296:TYR:O	1:D:342:MET:HG2	2.15	0.47
1:D:319:ALA:N	1:D:320:PRO:HD3	2.30	0.47
1:E:87:VAL:HG23	1:E:104:GLN:HA	1.97	0.47
1:E:472:ARG:O	1:E:476:GLU:HB2	2.15	0.47
1:F:441:GLN:HG3	1:F:482:LEU:O	2.15	0.47
1:F:483:ASN:HB2	1:F:484:PRO:HD2	1.97	0.47
1:A:449:GLY:HA2	1:A:452:ASN:ND2	2.29	0.46
1:A:445:MET:SD	1:A:450:ALA:HA	2.55	0.46
1:A:517:ARG:HG2	1:A:517:ARG:NH1	2.31	0.46
1:E:320:PRO:HB2	1:E:343:GLN:HG3	1.96	0.46
1:F:25:ILE:O	1:F:29:THR:HG23	2.14	0.46
1:D:51:ARG:HG2	1:D:51:ARG:HH11	1.80	0.46
1:A:47:THR:O	1:A:48:ALA:HB3	2.15	0.46
1:B:86:GLY:HA2	1:B:108:VAL:HB	1.96	0.46
1:B:337:VAL:CG2	1:B:372:THR:HG22	2.45	0.46
1:B:281:ASP:O	1:B:500:SER:HA	2.16	0.46
1:C:10:ASP:CG	1:C:11:ILE:H	2.19	0.46
1:D:21:LEU:HD12	1:D:21:LEU:O	2.15	0.46
1:F:457:ARG:NH1	1:F:458:THR:OG1	2.45	0.46
1:A:70:HIS:NE2	1:A:148:GLU:CD	2.67	0.46
1:A:153:LEU:HG	1:B:444:VAL:HG12	1.97	0.46
1:B:490:ARG:HD3	1:B:492:TYR:CZ	2.50	0.46
1:D:286:THR:O	1:D:287:ILE:CG2	2.56	0.46
1:A:67:PHE:CE2	1:D:496:VAL:HG13	2.50	0.46
1:C:153:LEU:HD21	1:F:418:GLY:HA2	1.97	0.46
1:B:455:HIS:HE1	1:B:477:TYR:CE2	2.33	0.46
1:B:77:LEU:O	1:B:79:ALA:N	2.49	0.46
1:B:80:ASN:O	1:B:80:ASN:ND2	2.49	0.46
1:C:209:ASP:N	1:C:209:ASP:OD1	2.47	0.46
1:D:107:THR:O	1:D:107:THR:CG2	2.62	0.46
1:D:441:GLN:HG2	1:D:482:LEU:O	2.16	0.46
1:A:334:VAL:CG2	1:A:371:LEU:HG	2.45	0.46
1:B:111:GLY:C	1:B:141:SER:HB2	2.35	0.46
1:B:496:VAL:HG13	1:E:67:PHE:HE2	1.80	0.46
1:C:285:ASP:OD1	1:C:499:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:ILE:HG21	1:D:393:ARG:NH1	2.31	0.46
1:D:458:THR:HG22	1:D:458:THR:O	2.16	0.46
1:D:513:LEU:HD12	1:D:513:LEU:HA	1.64	0.46
1:A:47:THR:HG22	1:A:47:THR:O	2.16	0.46
1:A:442:ILE:CD1	1:A:487:ALA:H	2.28	0.46
1:B:305:VAL:O	1:B:306:LEU:CB	2.63	0.46
1:C:382:GLY:O	1:C:385:GLN:HB2	2.15	0.46
1:D:354:GLU:OE2	1:D:393:ARG:CD	2.59	0.46
1:E:51:ARG:NH2	1:E:177:VAL:HG21	2.31	0.46
1:A:175:LEU:HA	1:A:195:VAL:HG13	1.98	0.46
1:B:280:GLU:O	1:B:283:GLU:HG3	2.16	0.46
1:C:145:ARG:HG3	1:C:148:GLU:HG3	1.98	0.46
1:D:197:VAL:HG12	1:D:247:ALA:HB2	1.96	0.46
1:E:36:ALA:HA	1:E:39:LYS:CD	2.41	0.46
1:E:47:THR:HG22	1:E:50:GLU:N	2.29	0.46
1:F:517:ARG:O	1:F:518:GLU:HB3	2.15	0.46
1:A:372:THR:HG21	1:A:401:TYR:HE1	1.79	0.46
1:A:350:ILE:HG13	1:A:393:ARG:HD2	1.96	0.46
1:B:69:ARG:NE	1:B:81:ARG:O	2.48	0.46
1:C:146:ILE:HD12	1:F:445:MET:HE1	1.97	0.46
1:C:363:CYS:HB3	1:C:368:VAL:HG22	1.98	0.46
1:D:211:ILE:HG21	1:E:383:VAL:HG23	1.97	0.46
1:D:381:PRO:HB2	1:E:214:VAL:CG2	2.45	0.46
1:A:376:VAL:HG21	1:A:420:ALA:HB1	1.98	0.46
1:A:443:ALA:O	1:B:153:LEU:HD11	2.16	0.46
1:B:350:ILE:HG21	1:B:393:ARG:HH12	1.81	0.46
1:E:69:ARG:NH1	1:E:69:ARG:CG	2.60	0.46
1:F:458:THR:CG2	1:F:469:THR:HG21	2.41	0.46
1:F:493:VAL:HG12	1:F:495:ALA:H	1.80	0.46
1:A:113:LEU:HD23	1:A:113:LEU:O	2.15	0.45
1:A:393:ARG:HH12	1:B:393:ARG:NH2	2.14	0.45
1:A:437:TRP:CE2	1:A:499:PRO:HA	2.50	0.45
1:A:459:ILE:HD12	1:A:460:ALA:N	2.32	0.45
1:B:108:VAL:HG12	1:B:109:PHE:CD1	2.50	0.45
1:D:480:ALA:O	1:D:481:LEU:HD23	2.16	0.45
1:D:47:THR:O	1:D:49:ARG:O	2.34	0.45
1:E:459:ILE:HD11	1:E:470:ARG:HB2	1.98	0.45
1:D:303:GLU:O	1:D:309:ALA:HA	2.16	0.45
1:E:156:TYR:HE1	1:E:184:ALA:HB2	1.81	0.45
1:E:68:ALA:HB3	1:E:85:ASP:OD2	2.17	0.45
1:A:374:VAL:HB	1:A:412:ILE:HG12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:ILE:O	1:C:474:ILE:HG22	2.16	0.45
1:D:198:ASP:HA	1:D:240:MET:SD	2.57	0.45
1:E:36:ALA:CA	1:E:39:LYS:HD3	2.41	0.45
1:A:138:ILE:HG22	1:A:175:LEU:CB	2.39	0.45
1:A:288:VAL:O	1:A:288:VAL:HG22	2.16	0.45
1:A:516:LYS:HB2	1:A:516:LYS:HE2	1.78	0.45
1:B:184:ALA:C	1:B:186:TYR:H	2.20	0.45
1:D:10:ASP:CG	1:D:11:ILE:H	2.20	0.45
1:D:311:PHE:CE2	1:D:313:GLU:HB2	2.51	0.45
1:E:436:ALA:O	1:E:496:VAL:HA	2.16	0.45
1:A:517:ARG:CG	1:A:517:ARG:NH1	2.68	0.45
1:E:461:ASP:C	1:E:463:GLY:H	2.20	0.45
1:A:475:GLN:HA	1:A:475:GLN:NE2	2.31	0.45
1:B:296:TYR:O	1:B:342:MET:HG2	2.17	0.45
1:F:187:SER:HB3	1:F:188:PRO:CD	2.45	0.45
1:A:104:GLN:HB3	1:A:117:TYR:OH	2.16	0.45
1:A:116:VAL:HA	1:A:119:GLN:OE1	2.16	0.45
1:A:77:LEU:HD21	1:A:147:GLN:HG3	1.98	0.45
1:D:113:LEU:HD21	1:D:155:ALA:HB3	1.98	0.45
1:D:253:GLN:NE2	1:D:257:TYR:HE2	2.15	0.45
1:D:286:THR:C	1:D:288:VAL:N	2.64	0.45
1:E:485:TYR:O	1:E:489:GLU:HG3	2.17	0.45
1:E:27:GLU:OE1	1:E:83:TYR:HE2	1.99	0.45
1:F:70:HIS:O	1:F:81:ARG:NH1	2.49	0.45
1:A:372:THR:CG2	1:A:401:TYR:OH	2.64	0.45
1:D:103:SER:HA	1:D:138:ILE:HB	1.99	0.45
1:D:280:GLU:HG3	1:D:281:ASP:N	2.32	0.45
1:D:414:ARG:HA	1:D:439:THR:O	2.17	0.45
1:E:87:VAL:O	1:E:120:LYS:NZ	2.43	0.45
1:F:298:MET:O	1:F:301:VAL:HG13	2.17	0.45
1:B:31:ALA:HB1	1:B:108:VAL:HG22	1.99	0.45
1:A:418:GLY:HA2	1:B:153:LEU:CD2	2.45	0.45
1:B:322:ILE:HD13	1:B:356:ALA:HB2	1.98	0.45
1:B:451:VAL:HG13	1:B:455:HIS:NE2	2.32	0.45
1:D:48:ALA:HA	1:D:51:ARG:HD2	1.99	0.45
1:E:182:GLY:O	1:E:185:VAL:CG1	2.61	0.45
1:F:180:CYS:SG	1:F:185:VAL:HA	2.57	0.45
1:F:411:VAL:HG12	1:F:435:LEU:HD12	1.98	0.45
1:B:87:VAL:HG13	1:B:120:LYS:CD	2.45	0.45
1:C:67:PHE:CD2	1:A:496:VAL:CG2	3.00	0.45
1:E:422:ASN:O	1:E:429:LEU:HD22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:472:ARG:O	1:E:474:ILE:O	2.35	0.45
1:A:43:LYS:HE3	1:A:45:LYS:CE	2.45	0.44
1:B:238:HIS:HA	1:B:315:GLN:HG3	1.99	0.44
1:C:319:ALA:N	1:C:320:PRO:HD3	2.33	0.44
1:D:520:LEU:CB	1:D:521:PRO:CD	2.92	0.44
1:B:32:GLY:H	1:B:107:THR:CG2	2.29	0.44
1:D:108:VAL:HG12	1:D:109:PHE:CD1	2.52	0.44
1:D:447:ALA:HB2	1:D:478:GLU:HG3	2.00	0.44
1:F:141:SER:O	1:F:179:PRO:HG2	2.18	0.44
1:F:476:GLU:OE1	1:F:476:GLU:HA	2.17	0.44
1:A:196:MET:HB3	1:A:201:SER:OG	2.17	0.44
1:A:70:HIS:ND1	1:A:71:ARG:N	2.59	0.44
1:B:14:THR:O	1:B:18:LEU:HG	2.17	0.44
1:D:298:MET:SD	1:D:301:VAL:HG11	2.57	0.44
1:E:455:HIS:ND1	1:E:455:HIS:N	2.64	0.44
1:F:478:GLU:HB3	1:F:482:LEU:HD22	1.99	0.44
1:A:115:GLU:HG3	1:A:116:VAL:N	2.33	0.44
1:D:107:THR:O	1:D:107:THR:HG23	2.16	0.44
1:D:321:ASN:ND2	1:D:352:ALA:HB2	2.33	0.44
1:D:422:ASN:HA	1:D:426:SER:CB	2.46	0.44
1:E:467:GLU:C	1:E:469:THR:N	2.68	0.44
1:F:510:LEU:O	1:F:514:ARG:HG3	2.18	0.44
1:F:70:HIS:HE1	1:F:72:SER:O	2.00	0.44
1:A:347:CYS:SG	1:A:380:LEU:HB3	2.58	0.44
1:A:70:HIS:HE1	1:A:115:GLU:HG2	1.80	0.44
1:B:109:PHE:C	1:B:111:GLY:H	2.21	0.44
1:B:230:HIS:CD2	1:B:234:SER:OG	2.63	0.44
1:B:253:GLN:HG2	1:B:312:PHE:CE1	2.53	0.44
1:B:368:VAL:HA	1:B:369:PRO:HD3	1.88	0.44
1:B:77:LEU:HD21	1:B:147:GLN:CB	2.48	0.44
1:D:483:ASN:HB2	1:D:484:PRO:CD	2.47	0.44
1:A:71:ARG:HH21	1:D:490:ARG:HE	1.65	0.44
1:E:473:LEU:HD13	1:E:473:LEU:HA	1.87	0.44
1:F:45:LYS:CE	1:F:200:THR:HB	2.48	0.44
1:C:438:PRO:HG3	1:D:21:LEU:HD22	1.99	0.44
1:D:51:ARG:HG2	1:D:51:ARG:NH1	2.33	0.44
1:D:398:ILE:HG21	1:E:160:PHE:HB3	1.99	0.44
1:A:40:GLN:CD	1:A:41:HIS:H	2.20	0.44
1:B:196:MET:HE2	1:B:230:HIS:CB	2.47	0.44
1:E:109:PHE:C	1:E:111:GLY:H	2.21	0.44
1:D:399:PHE:CE2	1:E:164:THR:HG23	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:437:TRP:NE1	1:F:502:THR:HG21	2.32	0.44
1:B:113:LEU:HD21	1:B:155:ALA:HB3	2.00	0.44
1:C:70:HIS:C	1:C:70:HIS:ND1	2.68	0.44
1:D:447:ALA:HB1	1:D:474:ILE:HG23	1.99	0.44
1:D:506:ILE:O	1:D:510:LEU:HG	2.18	0.44
1:E:187:SER:O	1:E:191:THR:HG23	2.18	0.44
1:E:414:ARG:O	1:E:441:GLN:N	2.39	0.44
1:F:106:PHE:O	1:F:106:PHE:CD2	2.70	0.44
1:F:370:VAL:HB	1:F:408:LEU:HD23	1.99	0.44
1:A:302:ILE:HD13	1:A:336:ILE:HG21	1.99	0.44
1:B:417:PHE:HA	1:B:443:ALA:O	2.18	0.44
1:B:75:PHE:HD1	1:B:76:GLY:N	2.16	0.44
1:C:181:ALA:O	1:C:184:ALA:HB3	2.18	0.44
1:C:397:LEU:HD11	1:C:401:TYR:HE2	1.82	0.44
1:D:342:MET:HA	1:D:342:MET:CE	2.47	0.44
1:E:78:ASP:N	1:E:78:ASP:OD1	2.50	0.44
1:F:319:ALA:N	1:F:320:PRO:HD3	2.32	0.44
1:F:375:ASP:CG	1:F:414:ARG:HB3	2.38	0.44
1:A:487:ALA:HB1	1:A:492:TYR:HB2	2.00	0.43
1:B:89:THR:HG22	1:B:102:PHE:CB	2.48	0.43
1:B:377:PRO:HB3	1:B:415:LYS:HE3	1.99	0.43
1:C:254:LEU:HD13	1:C:312:PHE:HE2	1.82	0.43
1:C:482:LEU:N	1:C:482:LEU:CD2	2.81	0.43
1:D:24:ARG:NH1	1:D:83:TYR:OH	2.43	0.43
1:A:102:PHE:CE2	1:A:137:GLY:HA3	2.53	0.43
1:A:51:ARG:NH1	1:A:138:ILE:HD12	2.33	0.43
1:A:238:HIS:HA	1:A:315:GLN:HG3	2.00	0.43
1:A:459:ILE:HG21	1:A:470:ARG:HE	1.83	0.43
1:A:529:PRO:HG3	1:B:190:ILE:HA	1.99	0.43
1:C:449:GLY:O	1:C:453:ILE:HD13	2.19	0.43
1:D:196:MET:HE3	1:D:237:ALA:CB	2.48	0.43
1:D:440:ALA:HB3	1:D:484:PRO:HG3	2.00	0.43
1:F:11:ILE:HD12	1:F:11:ILE:N	2.33	0.43
1:F:163:ASN:ND2	1:F:187:SER:OG	2.46	0.43
1:A:350:ILE:HG13	1:A:393:ARG:CD	2.49	0.43
1:A:35:ARG:NH2	1:A:39:LYS:HE2	2.33	0.43
1:A:419:GLY:O	1:A:423:VAL:HG23	2.18	0.43
1:A:449:GLY:HA2	1:A:452:ASN:HD21	1.83	0.43
1:D:141:SER:O	1:D:179:PRO:HG2	2.17	0.43
1:D:294:GLN:OE1	1:D:295:PRO:HD2	2.18	0.43
1:F:46:LEU:HB2	1:F:244:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:483:ASN:HB2	1:F:485:TYR:HD2	1.83	0.43
1:A:51:ARG:HH11	1:A:138:ILE:HD13	1.82	0.43
1:A:374:VAL:CG1	1:A:376:VAL:HG12	2.48	0.43
1:B:405:THR:HA	1:B:518:GLU:OE1	2.17	0.43
1:C:230:HIS:HA	1:C:234:SER:OG	2.19	0.43
1:C:288:VAL:HG12	1:C:289:PRO:O	2.19	0.43
1:E:86:GLY:HA2	1:E:108:VAL:HB	1.99	0.43
1:A:126:ASP:O	1:A:130:LYS:HB3	2.18	0.43
1:A:153:LEU:CD2	1:B:444:VAL:HG12	2.49	0.43
1:B:448:GLN:O	1:B:452:ASN:OD1	2.36	0.43
1:E:47:THR:HG22	1:E:50:GLU:CB	2.48	0.43
1:C:392:ARG:NH1	1:F:234:SER:O	2.52	0.43
1:F:445:MET:CE	1:F:450:ALA:HA	2.48	0.43
1:F:485:TYR:HE2	1:B:17:LYS:NZ	2.16	0.43
1:A:10:ASP:CG	1:A:11:ILE:N	2.70	0.43
1:B:372:THR:OG1	1:B:410:THR:HG22	2.18	0.43
1:C:135:VAL:HG23	1:C:170:ILE:HD12	2.00	0.43
1:C:324:THR:HA	1:C:336:ILE:O	2.18	0.43
1:C:461:ASP:C	1:C:463:GLY:N	2.71	0.43
1:C:472:ARG:HD3	1:C:472:ARG:HA	1.61	0.43
1:C:63:GLU:OE2	1:C:88:VAL:HG23	2.17	0.43
1:F:105:ASP:C	1:F:107:THR:N	2.72	0.43
1:F:210:VAL:O	1:F:214:VAL:HG23	2.18	0.43
1:F:338:ALA:HB1	1:F:373:PHE:HB2	2.00	0.43
1:A:156:TYR:CE1	1:A:184:ALA:HB2	2.54	0.43
1:A:465:ASP:O	1:A:466:ALA:C	2.57	0.43
1:A:478:GLU:O	1:A:482:LEU:HB2	2.18	0.43
1:B:135:VAL:HG12	1:B:172:GLN:HA	2.00	0.43
1:B:177:VAL:HG23	1:B:178:GLY:H	1.83	0.43
1:B:212:LYS:HG3	1:B:213:THR:N	2.34	0.43
1:A:205:ILE:CD1	1:B:390:ILE:HG12	2.49	0.43
1:B:477:TYR:O	1:B:481:LEU:HB2	2.19	0.43
1:B:78:ASP:OD1	1:B:78:ASP:N	2.51	0.43
1:C:461:ASP:O	1:C:462:ALA:C	2.57	0.43
1:D:286:THR:O	1:D:288:VAL:N	2.47	0.43
1:B:498:MET:HE1	1:E:18:LEU:HG	1.98	0.43
1:E:23:ARG:HG3	1:E:24:ARG:H	1.83	0.43
1:E:340:GLN:O	1:E:340:GLN:HG3	2.18	0.43
1:E:474:ILE:O	1:E:476:GLU:N	2.46	0.43
1:B:290:ASP:N	1:B:290:ASP:OD2	2.51	0.43
1:B:275:LEU:HD11	1:B:508:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ILE:H	1:C:146:ILE:HG12	1.30	0.43
1:D:193:PHE:HA	1:D:238:HIS:CD2	2.54	0.43
1:E:483:ASN:HB2	1:E:484:PRO:CD	2.49	0.43
1:F:45:LYS:CD	1:F:200:THR:HB	2.49	0.43
1:F:437:TRP:NE1	1:F:502:THR:CG2	2.78	0.43
1:A:52:ILE:HG23	1:A:56:LEU:HD12	2.01	0.43
1:C:350:ILE:HG22	1:C:390:ILE:CD1	2.48	0.43
1:D:288:VAL:O	1:D:288:VAL:HG22	2.18	0.43
1:E:185:VAL:C	1:E:188:PRO:HD2	2.40	0.43
1:E:451:VAL:HA	1:E:454:LEU:HB2	2.00	0.43
1:A:399:PHE:CG	1:A:528:ILE:HG13	2.54	0.43
1:A:451:VAL:HG13	1:A:477:TYR:CD1	2.54	0.43
1:B:437:TRP:NE1	1:B:502:THR:CG2	2.76	0.43
1:C:113:LEU:HD12	1:C:117:TYR:CE2	2.53	0.43
1:C:238:HIS:HA	1:C:315:GLN:HG2	2.00	0.43
1:C:472:ARG:CD	1:C:475:GLN:HE21	2.31	0.43
1:E:118:GLY:HA3	1:E:155:ALA:HB1	2.01	0.43
1:A:121:ILE:O	1:A:125:MET:HG3	2.20	0.42
1:A:374:VAL:HG22	1:A:424:MET:HB3	2.01	0.42
1:B:74:ASN:H	1:B:77:LEU:HD12	1.84	0.42
1:E:141:SER:O	1:E:179:PRO:O	2.36	0.42
1:E:129:LEU:HA	1:E:170:ILE:HD13	2.00	0.42
1:F:141:SER:O	1:F:179:PRO:O	2.37	0.42
1:F:451:VAL:HG13	1:F:455:HIS:CB	2.47	0.42
1:A:528:ILE:O	1:B:358:ARG:NH1	2.52	0.42
1:B:477:TYR:O	1:B:481:LEU:N	2.52	0.42
1:C:337:VAL:O	1:C:372:THR:HA	2.19	0.42
1:E:246:ASP:O	1:E:249:GLU:N	2.51	0.42
1:F:320:PRO:HB2	1:F:343:GLN:HG3	2.01	0.42
1:A:438:PRO:HD3	1:A:497:ILE:O	2.19	0.42
1:A:398:ILE:HD13	1:B:160:PHE:CD2	2.54	0.42
1:B:290:ASP:HB3	1:E:13:THR:HA	2.00	0.42
1:B:77:LEU:HD21	1:B:147:GLN:CG	2.48	0.42
1:C:180:CYS:HB3	1:C:203:MET:HG2	2.01	0.42
1:D:437:TRP:CE2	1:D:499:PRO:HA	2.54	0.42
1:D:523:LYS:HA	1:E:262:ASN:ND2	2.33	0.42
1:E:98:PRO:O	1:E:134:PRO:HD2	2.19	0.42
1:F:45:LYS:HE3	1:F:177:VAL:O	2.19	0.42
1:F:456:ARG:HG3	1:F:457:ARG:N	2.34	0.42
1:A:204:PHE:HA	1:B:386:GLU:OE2	2.19	0.42
1:A:199:GLN:HG3	1:A:222:GLU:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:HIS:CE1	1:A:315:GLN:NE2	2.87	0.42
1:A:459:ILE:CG1	1:A:460:ALA:H	2.32	0.42
1:B:483:ASN:HB2	1:B:485:TYR:HD1	1.83	0.42
1:D:262:ASN:HD21	1:E:523:LYS:HA	1.85	0.42
1:F:475:GLN:HG2	1:F:475:GLN:O	2.18	0.42
1:A:176:VAL:HG12	1:A:201:SER:HB2	2.02	0.42
1:A:40:GLN:H	1:A:40:GLN:CD	2.22	0.42
1:A:76:GLY:O	1:A:78:ASP:N	2.52	0.42
1:C:108:VAL:O	1:C:109:PHE:CG	2.73	0.42
1:C:414:ARG:HA	1:C:440:ALA:HA	2.02	0.42
1:C:83:TYR:C	1:C:85:ASP:H	2.23	0.42
1:D:35:ARG:N	1:D:35:ARG:HD2	2.33	0.42
1:D:391:ILE:HG21	1:E:185:VAL:HG21	2.01	0.42
1:E:113:LEU:CD1	1:E:117:TYR:CD2	2.95	0.42
1:C:164:THR:HG23	1:F:399:PHE:CE2	2.54	0.42
1:F:305:VAL:HG11	1:F:506:ILE:CD1	2.49	0.42
1:A:367:ASN:HA	1:A:406:VAL:CG2	2.50	0.42
1:B:111:GLY:O	1:B:141:SER:HB2	2.19	0.42
1:B:148:GLU:HB2	1:B:152:SER:OG	2.19	0.42
1:C:170:ILE:O	1:C:170:ILE:HG13	2.18	0.42
1:D:342:MET:HA	1:D:342:MET:HE2	2.01	0.42
1:D:520:LEU:CB	1:D:521:PRO:HD2	2.42	0.42
1:B:489:GLU:CG	1:E:69:ARG:HB2	2.49	0.42
1:F:451:VAL:HG13	1:F:455:HIS:HD2	1.83	0.42
1:A:337:VAL:O	1:A:372:THR:HA	2.19	0.42
1:B:32:GLY:H	1:B:107:THR:HG21	1.85	0.42
1:C:339:ASN:HD22	1:C:375:ASP:H	1.68	0.42
1:C:454:LEU:O	1:C:455:HIS:HD2	2.03	0.42
1:E:121:ILE:O	1:E:125:MET:HG3	2.20	0.42
1:E:447:ALA:HB2	1:E:478:GLU:HG3	2.01	0.42
1:D:454:LEU:HD21	1:E:75:PHE:CZ	2.53	0.42
1:F:472:ARG:O	1:F:476:GLU:HG2	2.19	0.42
1:A:108:VAL:O	1:A:110:GLY:O	2.38	0.42
1:B:163:ASN:HD22	1:B:172:GLN:HE22	1.68	0.42
1:B:372:THR:CG2	1:B:410:THR:HG22	2.49	0.42
1:B:488:ALA:O	1:E:68:ALA:HA	2.19	0.42
1:C:519:SER:O	1:C:520:LEU:HB3	2.20	0.42
1:E:254:LEU:HD12	1:E:254:LEU:HA	1.74	0.42
1:F:89:THR:HG22	1:F:102:PHE:HB2	2.02	0.42
1:A:193:PHE:HA	1:A:238:HIS:CD2	2.55	0.42
1:A:21:LEU:O	1:A:21:LEU:HD12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLN:N	1:B:316:PRO:HD3	2.34	0.42
1:B:324:THR:HA	1:B:336:ILE:O	2.20	0.42
1:B:482:LEU:CD2	1:B:482:LEU:N	2.83	0.42
1:C:372:THR:HB	1:C:410:THR:HB	2.02	0.42
1:C:445:MET:HG3	1:C:450:ALA:HB2	2.01	0.42
1:D:287:ILE:O	1:D:289:PRO:HD3	2.19	0.42
1:F:307:ASP:O	1:F:308:ASP:HB2	2.20	0.42
1:F:427:LYS:CD	1:F:431:ALA:O	2.68	0.42
1:A:65:ASP:OD2	1:A:123:LYS:HD3	2.20	0.42
1:A:405:THR:O	1:A:516:LYS:CD	2.68	0.42
1:C:240:MET:O	1:C:240:MET:HG3	2.18	0.42
1:C:397:LEU:HG	1:C:423:VAL:HG12	1.97	0.42
1:C:459:ILE:HD13	1:C:459:ILE:C	2.41	0.42
1:F:122:VAL:HG13	1:F:162:ARG:NE	2.35	0.42
1:F:349:ASP:H	1:F:352:ALA:HB3	1.85	0.42
1:F:458:THR:HA	1:F:461:ASP:CB	2.50	0.42
1:A:340:GLN:HG3	1:A:340:GLN:O	2.19	0.41
1:B:265:GLU:HB2	1:B:266:PRO:CD	2.50	0.41
1:C:33:SER:OG	1:C:35:ARG:HG3	2.20	0.41
1:E:66:GLU:HG2	1:E:67:PHE:CE1	2.55	0.41
1:C:278:THR:O	1:C:281:ASP:HB2	2.20	0.41
1:C:397:LEU:HD11	1:C:401:TYR:CD2	2.55	0.41
1:C:70:HIS:CE1	1:C:81:ARG:HG2	2.55	0.41
1:D:346:GLY:O	1:D:377:PRO:HD2	2.20	0.41
1:E:146:ILE:H	1:E:146:ILE:HG13	1.50	0.41
1:A:177:VAL:HG12	1:A:197:VAL:CG2	2.51	0.41
1:A:455:HIS:ND1	1:A:455:HIS:N	2.67	0.41
1:A:466:ALA:O	1:A:467:GLU:C	2.59	0.41
1:A:87:VAL:HG23	1:A:104:GLN:HA	2.02	0.41
1:B:241:ALA:HB1	1:B:246:ASP:HB2	2.03	0.41
1:A:529:PRO:N	1:B:358:ARG:HH12	2.19	0.41
1:C:299:HIS:O	1:C:303:GLU:HG3	2.21	0.41
1:C:397:LEU:CD1	1:C:401:TYR:CE2	3.03	0.41
1:D:182:GLY:C	1:D:205:ILE:HD12	2.40	0.41
1:D:380:LEU:O	1:D:385:GLN:HG3	2.21	0.41
1:D:478:GLU:HG3	1:D:482:LEU:HD12	2.02	0.41
1:F:433:LEU:HA	1:F:433:LEU:HD12	1.89	0.41
1:A:442:ILE:CD1	1:A:487:ALA:HB2	2.50	0.41
1:A:74:ASN:O	1:A:75:PHE:CD1	2.74	0.41
1:B:215:THR:OG1	1:B:217:GLU:OE1	2.38	0.41
1:B:238:HIS:HA	1:B:315:GLN:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ARG:CZ	1:B:39:LYS:HZ2	2.33	0.41
1:D:193:PHE:CB	1:D:254:LEU:HD21	2.50	0.41
1:E:214:VAL:CG2	1:E:215:THR:N	2.84	0.41
1:F:319:ALA:HB2	1:F:351:THR:HB	2.02	0.41
1:A:153:LEU:HD21	1:B:418:GLY:HA2	2.02	0.41
1:F:438:PRO:O	1:B:17:LYS:HG3	2.20	0.41
1:C:106:PHE:O	1:C:109:PHE:O	2.39	0.41
1:D:196:MET:HE2	1:D:230:HIS:HB2	2.01	0.41
1:E:103:SER:HA	1:E:138:ILE:HB	2.03	0.41
1:F:203:MET:HE3	1:F:236:VAL:HG11	2.02	0.41
1:F:300:SER:O	1:F:304:HIS:ND1	2.53	0.41
1:A:442:ILE:HG13	1:A:442:ILE:O	2.19	0.41
1:A:483:ASN:HB2	1:A:484:PRO:CD	2.51	0.41
1:A:77:LEU:HD11	1:A:147:GLN:CG	2.50	0.41
1:B:181:ALA:HA	1:B:204:PHE:O	2.21	0.41
1:D:70:HIS:HA	1:D:116:VAL:HG21	2.01	0.41
1:D:180:CYS:SG	1:D:185:VAL:HA	2.60	0.41
1:F:102:PHE:CD1	1:F:102:PHE:C	2.93	0.41
1:F:372:THR:HG21	1:F:401:TYR:CE1	2.55	0.41
1:A:440:ALA:HB3	1:A:484:PRO:HB3	2.02	0.41
1:A:70:HIS:HA	1:A:116:VAL:HG21	2.02	0.41
1:B:241:ALA:HB1	1:B:246:ASP:CB	2.49	0.41
1:B:442:ILE:HG21	1:B:487:ALA:HB2	2.03	0.41
1:B:29:THR:HA	1:B:49:ARG:CZ	2.51	0.41
1:B:70:HIS:O	1:B:81:ARG:HD2	2.21	0.41
1:F:45:LYS:NZ	1:F:244:GLU:OE2	2.49	0.41
1:F:473:LEU:HA	1:F:476:GLU:HB2	2.01	0.41
1:B:122:VAL:HG13	1:B:162:ARG:NE	2.36	0.41
1:B:354:GLU:OE2	1:B:393:ARG:HD2	2.20	0.41
1:C:156:TYR:CE1	1:C:184:ALA:HB2	2.56	0.41
1:E:32:GLY:HA3	1:E:107:THR:OG1	2.20	0.41
1:F:427:LYS:HD3	1:F:427:LYS:HA	1.66	0.41
1:F:464:ASP:C	1:F:466:ALA:H	2.24	0.41
1:A:103:SER:HA	1:A:138:ILE:CG1	2.47	0.41
1:A:180:CYS:SG	1:A:185:VAL:HA	2.60	0.41
1:A:372:THR:HG21	1:A:401:TYR:CZ	2.55	0.41
1:B:348:LEU:HD11	1:B:424:MET:HE2	2.02	0.41
1:B:414:ARG:HD2	1:B:414:ARG:HH11	1.72	0.41
1:C:266:PRO:HB2	1:C:333:PRO:HG2	2.02	0.41
1:D:20:ASP:O	1:D:24:ARG:HG2	2.21	0.41
1:B:88:VAL:CG1	1:B:103:SER:HB3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ARG:HB3	1:B:39:LYS:NZ	2.35	0.41
1:B:513:LEU:HD21	1:E:127:PHE:HE1	1.86	0.41
1:E:414:ARG:HA	1:E:440:ALA:HA	2.02	0.41
1:F:461:ASP:O	1:F:462:ALA:C	2.58	0.41
1:A:205:ILE:CD1	1:B:390:ILE:HG21	2.51	0.41
1:C:397:LEU:CD1	1:C:397:LEU:C	2.89	0.41
1:D:163:ASN:HA	1:D:172:GLN:HE22	1.85	0.41
1:E:10:ASP:O	1:E:11:ILE:HB	2.21	0.41
1:E:209:ASP:O	1:E:213:THR:HG23	2.20	0.41
1:E:296:TYR:O	1:E:342:MET:HG2	2.21	0.41
1:F:451:VAL:C	1:F:453:ILE:N	2.73	0.41
1:F:70:HIS:ND1	1:F:71:ARG:N	2.69	0.41
1:A:170:ILE:HG13	1:A:170:ILE:O	2.20	0.40
1:A:298:MET:CE	1:A:301:VAL:HG11	2.51	0.40
1:A:390:ILE:HG13	1:A:390:ILE:O	2.21	0.40
1:C:275:LEU:O	1:C:504:ARG:HD2	2.20	0.40
1:C:393:ARG:HA	1:C:393:ARG:HD3	1.82	0.40
1:F:77:LEU:CD1	1:F:147:GLN:HG3	2.50	0.40
1:A:280:GLU:HG3	1:A:280:GLU:H	1.50	0.40
1:A:457:ARG:HG3	1:A:457:ARG:O	2.20	0.40
1:A:70:HIS:CD2	1:A:72:SER:HB3	2.57	0.40
1:B:35:ARG:NH1	1:B:38:GLU:OE1	2.54	0.40
1:D:108:VAL:HG12	1:D:109:PHE:N	2.35	0.40
1:D:197:VAL:CG1	1:D:247:ALA:HB2	2.50	0.40
1:D:278:THR:OG1	1:D:280:GLU:HG3	2.22	0.40
1:D:49:ARG:NH2	1:D:63:GLU:OE1	2.51	0.40
1:E:208:PRO:CA	1:E:211:ILE:HG12	2.35	0.40
1:E:338:ALA:HA	1:E:373:PHE:O	2.21	0.40
1:E:516:LYS:O	1:E:516:LYS:HG3	2.20	0.40
1:E:87:VAL:CG1	1:E:120:LYS:HD3	2.51	0.40
1:F:10:ASP:OD1	1:F:11:ILE:N	2.43	0.40
1:F:74:ASN:HB3	1:F:75:PHE:CD1	2.57	0.40
1:A:108:VAL:HG12	1:A:109:PHE:HD2	1.87	0.40
1:A:65:ASP:HB3	1:A:68:ALA:HB2	2.03	0.40
1:B:35:ARG:HB3	1:B:39:LYS:HZ1	1.86	0.40
1:B:458:THR:HG22	1:B:458:THR:O	2.21	0.40
1:D:113:LEU:HD13	1:D:156:TYR:CE1	2.55	0.40
1:A:91:TYR:CE1	1:D:512:GLN:HG3	2.55	0.40
1:E:47:THR:H	1:E:50:GLU:CD	2.25	0.40
1:E:84:GLY:C	1:E:86:GLY:H	2.24	0.40
1:F:370:VAL:HG12	1:F:372:THR:HG22	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:375:ASP:OD2	1:F:414:ARG:HB3	2.20	0.40
1:A:397:LEU:HD22	1:A:401:TYR:CE2	2.56	0.40
1:B:350:ILE:HD13	1:B:390:ILE:CD1	2.50	0.40
1:B:75:PHE:CD1	1:B:76:GLY:N	2.89	0.40
1:D:174:SER:OG	1:D:191:THR:HG21	2.21	0.40
1:E:65:ASP:OD2	1:E:123:LYS:HD2	2.21	0.40
1:B:438:PRO:HG3	1:E:21:LEU:HD22	2.02	0.40
1:E:481:LEU:C	1:E:483:ASN:H	2.24	0.40
1:F:68:ALA:HA	1:E:489:GLU:HA	2.02	0.40
1:A:457:ARG:CZ	1:A:461:ASP:HB2	2.51	0.40
1:A:282:ALA:HA	1:A:500:SER:OG	2.21	0.40
1:B:140:ASP:O	1:B:179:PRO:CD	2.69	0.40
1:B:344:PHE:C	1:B:346:GLY:H	2.23	0.40
1:C:111:GLY:O	1:C:141:SER:HB2	2.20	0.40
1:C:464:ASP:CG	1:C:465:ASP:N	2.74	0.40
1:F:193:PHE:HA	1:F:238:HIS:CE1	2.56	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	519/530 (98%)	470 (91%)	38 (7%)	11 (2%)	7	7
1	B	519/530 (98%)	455 (88%)	52 (10%)	12 (2%)	6	6
1	C	519/530 (98%)	475 (92%)	37 (7%)	7 (1%)	12	15
1	D	519/530 (98%)	472 (91%)	41 (8%)	6 (1%)	13	17
1	E	519/530 (98%)	476 (92%)	39 (8%)	4 (1%)	19	27
1	F	519/530 (98%)	479 (92%)	33 (6%)	7 (1%)	12	15
All	All	3114/3180 (98%)	2827 (91%)	240 (8%)	47 (2%)	10	12

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	520	LEU
1	F	480	ALA
1	B	75	PHE
1	B	306	LEU
1	D	198	ASP
1	E	11	ILE
1	E	520	LEU
1	C	110	GLY
1	C	455	HIS
1	C	464	ASP
1	C	468	ALA
1	C	475	GLN
1	F	198	ASP
1	A	31	ALA
1	A	451	VAL
1	B	141	SER
1	B	183	GLY
1	D	11	ILE
1	D	50	GLU
1	D	287	ILE
1	D	289	PRO
1	D	414	ARG
1	F	106	PHE
1	A	78	ASP
1	A	112	ALA
1	A	466	ALA
1	B	74	ASN
1	B	78	ASP
1	B	414	ARG
1	E	414	ARG
1	F	289	PRO
1	A	11	ILE
1	A	77	LEU
1	A	406	VAL
1	A	447	ALA
1	A	465	ASP
1	B	70	HIS
1	B	109	PHE
1	E	109	PHE
1	F	145	ARG
1	F	465	ASP
1	A	467	GLU

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Mol	Chain	Res	Type
1	B	345	ALA
1	B	520	LEU
1	C	414	ARG
1	F	463	GLY
1	B	528	ILE

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	412/421 (98%)	361 (88%)	51 (12%)	4	5
1	B	412/421 (98%)	371 (90%)	41 (10%)	7	10
1	C	412/421 (98%)	383 (93%)	29 (7%)	15	21
1	D	412/421 (98%)	377 (92%)	35 (8%)	10	14
1	E	412/421 (98%)	370 (90%)	42 (10%)	7	9
1	F	412/421 (98%)	376 (91%)	36 (9%)	10	14
All	All	2472/2526 (98%)	2238 (90%)	234 (10%)	8	11

All (234) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	21	LEU
1	C	49	ARG
1	C	70	HIS
1	C	75	PHE
1	C	117	TYR
1	C	124	VAL
1	C	146	ILE
1	C	162	ARG
1	C	177	VAL
1	C	205	ILE
1	C	222	GLU
1	C	223	GLU
1	C	229	THR

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Mol	Chain	Res	Type
1	C	236	VAL
1	C	240	MET
1	C	264	SER
1	C	310	GLU
1	C	349	ASP
1	C	350	ILE
1	C	397	LEU
1	C	429	LEU
1	C	448	GLN
1	C	451	VAL
1	C	455	HIS
1	C	457	ARG
1	C	459	ILE
1	C	472	ARG
1	C	482	LEU
1	C	489	GLU
1	F	11	ILE
1	F	35	ARG
1	F	77	LEU
1	F	107	THR
1	F	113	LEU
1	F	117	TYR
1	F	147	GLN
1	F	177	VAL
1	F	199	GLN
1	F	209	ASP
1	F	215	THR
1	F	217	GLU
1	F	219	VAL
1	F	246	ASP
1	F	251	VAL
1	F	264	SER
1	F	294	GLN
1	F	301	VAL
1	F	332	ARG
1	F	358	ARG
1	F	372	THR
1	F	374	VAL
1	F	383	VAL
1	F	386	GLU
1	F	433	LEU
1	F	453	ILE

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Mol	Chain	Res	Type
1	F	457	ARG
1	F	458	THR
1	F	461	ASP
1	F	467	GLU
1	F	475	GLN
1	F	505	HIS
1	F	512	GLN
1	F	513	LEU
1	F	516	LYS
1	F	520	LEU
1	A	21	LEU
1	A	40	GLN
1	A	54	LEU
1	A	63	GLU
1	A	69	ARG
1	A	70	HIS
1	A	71	ARG
1	A	81	ARG
1	A	99	VAL
1	A	103	SER
1	A	117	TYR
1	A	122	VAL
1	A	124	VAL
1	A	147	GLN
1	A	150	VAL
1	A	185	VAL
1	A	200	THR
1	A	215	THR
1	A	233	THR
1	A	255	LEU
1	A	256	SER
1	A	280	GLU
1	A	288	VAL
1	A	301	VAL
1	A	308	ASP
1	A	310	GLU
1	A	317	LEU
1	A	326	PHE
1	A	332	ARG
1	A	350	ILE
1	A	358	ARG
1	A	380	LEU

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Mol	Chain	Res	Type
1	A	397	LEU
1	A	406	VAL
1	A	415	LYS
1	A	427	LYS
1	A	433	LEU
1	A	444	VAL
1	A	455	HIS
1	A	458	THR
1	A	461	ASP
1	A	472	ARG
1	A	473	LEU
1	A	475	GLN
1	A	481	LEU
1	A	486	THR
1	A	496	VAL
1	A	512	GLN
1	A	516	LYS
1	A	517	ARG
1	A	519	SER
1	B	13	THR
1	B	17	LYS
1	B	35	ARG
1	B	39	LYS
1	B	46	LEU
1	B	47	THR
1	B	70	HIS
1	B	80	ASN
1	B	117	TYR
1	B	173	ILE
1	B	177	VAL
1	B	200	THR
1	B	205	ILE
1	B	210	VAL
1	B	217	GLU
1	B	229	THR
1	B	244	GLU
1	B	245	LYS
1	B	260	SER
1	B	275	LEU
1	B	290	ASP
1	B	303	GLU
1	B	304	HIS

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Mol	Chain	Res	Type
1	B	310	GLU
1	B	334	VAL
1	B	374	VAL
1	B	387	HIS
1	B	392	ARG
1	B	414	ARG
1	B	433	LEU
1	B	439	THR
1	B	448	GLN
1	B	455	HIS
1	B	457	ARG
1	B	469	THR
1	B	472	ARG
1	B	481	LEU
1	B	482	LEU
1	B	490	ARG
1	B	493	VAL
1	B	496	VAL
1	D	35	ARG
1	D	40	GLN
1	D	107	THR
1	D	115	GLU
1	D	117	TYR
1	D	147	GLN
1	D	218	ASP
1	D	219	VAL
1	D	236	VAL
1	D	265	GLU
1	D	280	GLU
1	D	286	THR
1	D	301	VAL
1	D	310	GLU
1	D	337	VAL
1	D	342	MET
1	D	358	ARG
1	D	372	THR
1	D	384	ASP
1	D	387	HIS
1	D	392	ARG
1	D	403	GLU
1	D	427	LYS
1	D	429	LEU

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Mol	Chain	Res	Type
1	D	433	LEU
1	D	439	THR
1	D	470	ARG
1	D	493	VAL
1	D	494	ASP
1	D	496	VAL
1	D	502	THR
1	D	505	HIS
1	D	513	LEU
1	D	517	ARG
1	D	520	LEU
1	E	39	LYS
1	E	40	GLN
1	E	43	LYS
1	E	47	THR
1	E	58	GLU
1	E	64	LEU
1	E	69	ARG
1	E	70	HIS
1	E	71	ARG
1	E	78	ASP
1	E	116	VAL
1	E	117	TYR
1	E	124	VAL
1	E	145	ARG
1	E	152	SER
1	E	153	LEU
1	E	174	SER
1	E	177	VAL
1	E	180	CYS
1	E	209	ASP
1	E	213	THR
1	E	215	THR
1	E	219	VAL
1	E	245	LYS
1	E	264	SER
1	E	265	GLU
1	E	306	LEU
1	E	317	LEU
1	E	429	LEU
1	E	448	GLN
1	E	451	VAL

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Mol	Chain	Res	Type
1	E	452	ASN
1	E	454	LEU
1	E	455	HIS
1	E	461	ASP
1	E	473	LEU
1	E	475	GLN
1	E	481	LEU
1	E	493	VAL
1	E	516	LYS
1	E	519	SER
1	E	520	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	230	HIS
1	C	239	HIS
1	C	293	ASN
1	C	299	HIS
1	C	339	ASN
1	C	448	GLN
1	C	455	HIS
1	C	475	GLN
1	F	30	HIS
1	F	172	GLN
1	F	199	GLN
1	F	253	GLN
1	F	299	HIS
1	F	339	ASN
1	F	505	HIS
1	F	512	GLN
1	A	30	HIS
1	A	104	GLN
1	A	172	GLN
1	A	238	HIS
1	A	315	GLN
1	A	422	ASN
1	A	475	GLN
1	A	512	GLN
1	B	30	HIS
1	B	80	ASN
1	B	172	GLN

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Mol	Chain	Res	Type
1	B	230	HIS
1	B	299	HIS
1	B	339	ASN
1	B	422	ASN
1	B	434	ASN
1	B	448	GLN
1	B	455	HIS
1	B	475	GLN
1	B	512	GLN
1	D	104	GLN
1	D	172	GLN
1	D	238	HIS
1	D	253	GLN
1	D	299	HIS
1	D	343	GLN
1	D	527	ASN
1	E	80	ASN
1	E	172	GLN
1	E	199	GLN
1	E	230	HIS
1	E	231	ASN
1	E	239	HIS
1	E	299	HIS
1	E	343	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [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	521/530 (98%)	0.61	50 (9%) 8 9	39, 81, 153, 270	0
1	B	521/530 (98%)	0.63	53 (10%) 6 7	35, 81, 154, 242	0
1	C	521/530 (98%)	0.43	31 (5%) 21 24	25, 64, 134, 204	0
1	D	521/530 (98%)	0.50	40 (7%) 13 14	23, 63, 139, 258	0
1	E	521/530 (98%)	0.47	28 (5%) 25 28	26, 65, 137, 192	0
1	F	521/530 (98%)	0.52	41 (7%) 12 13	25, 64, 138, 266	0
All	All	3126/3180 (98%)	0.53	243 (7%) 13 14	23, 70, 143, 270	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	459	ILE	8.3
1	F	460	ALA	7.7
1	D	459	ILE	7.3
1	E	466	ALA	7.3
1	F	383	VAL	7.2
1	B	466	ALA	7.0
1	F	470	ARG	6.7
1	D	462	ALA	6.0
1	E	462	ALA	5.9
1	E	44	GLY	5.8
1	B	477	TYR	5.7
1	B	462	ALA	5.7
1	C	466	ALA	5.5
1	A	447	ALA	5.4
1	A	462	ALA	5.3
1	F	469	THR	5.3
1	C	459	ILE	5.1
1	D	472	ARG	5.0
1	F	451	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	468	ALA	4.9
1	F	466	ALA	4.8
1	A	142	GLY	4.8
1	D	455	HIS	4.8
1	E	383	VAL	4.8
1	B	208	PRO	4.8
1	F	462	ALA	4.7
1	B	77	LEU	4.7
1	B	469	THR	4.7
1	E	468	ALA	4.7
1	D	460	ALA	4.6
1	B	456	ARG	4.5
1	B	473	LEU	4.5
1	A	417	PHE	4.4
1	F	453	ILE	4.4
1	A	473	LEU	4.4
1	F	477	TYR	4.4
1	C	465	ASP	4.4
1	E	460	ALA	4.4
1	D	465	ASP	4.3
1	D	469	THR	4.3
1	D	519	SER	4.2
1	F	464	ASP	4.1
1	D	466	ALA	4.1
1	A	477	TYR	4.0
1	F	463	GLY	4.0
1	A	317	LEU	4.0
1	A	225	GLY	4.0
1	B	519	SER	4.0
1	A	468	ALA	4.0
1	F	465	ASP	4.0
1	A	451	VAL	4.0
1	B	465	ASP	3.9
1	B	470	ARG	3.8
1	F	219	VAL	3.8
1	B	291	SER	3.7
1	E	35	ARG	3.7
1	F	519	SER	3.7
1	F	473	LEU	3.6
1	D	457	ARG	3.6
1	E	36	ALA	3.6
1	C	76	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	218	ASP	3.6
1	D	454	LEU	3.6
1	D	490	ARG	3.5
1	C	462	ALA	3.5
1	A	459	ILE	3.5
1	A	463	GLY	3.4
1	B	468	ALA	3.4
1	A	224	LEU	3.4
1	C	77	LEU	3.3
1	A	200	THR	3.3
1	F	10	ASP	3.2
1	D	461	ASP	3.2
1	F	282	ALA	3.2
1	C	469	THR	3.2
1	B	40	GLN	3.2
1	B	142	GLY	3.1
1	D	287	ILE	3.1
1	E	76	GLY	3.1
1	A	218	ASP	3.1
1	B	460	ALA	3.1
1	D	456	ARG	3.0
1	B	459	ILE	3.0
1	F	35	ARG	3.0
1	E	242	GLY	3.0
1	F	467	GLU	3.0
1	B	518	GLU	3.0
1	B	11	ILE	3.0
1	A	37	VAL	3.0
1	A	284	LEU	3.0
1	A	469	THR	2.9
1	A	530	LEU	2.9
1	B	464	ASP	2.9
1	D	451	VAL	2.9
1	A	461	ASP	2.9
1	A	35	ARG	2.9
1	A	207	GLY	2.9
1	E	183	GLY	2.9
1	A	457	ARG	2.9
1	C	460	ALA	2.8
1	A	241	ALA	2.8
1	A	475	GLN	2.8
1	B	467	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	33	SER	2.8
1	A	44	GLY	2.8
1	A	456	ARG	2.8
1	B	233	THR	2.8
1	A	474	ILE	2.8
1	F	457	ARG	2.8
1	A	293	ASN	2.8
1	A	466	ALA	2.8
1	D	473	LEU	2.8
1	B	452	ASN	2.8
1	C	461	ASP	2.7
1	D	471	ALA	2.7
1	D	421	TYR	2.7
1	A	154	GLY	2.7
1	E	463	GLY	2.7
1	A	470	ARG	2.7
1	D	474	ILE	2.7
1	A	45	LYS	2.7
1	B	140	ASP	2.7
1	B	448	GLN	2.7
1	D	159	ILE	2.7
1	E	142	GLY	2.7
1	B	281	ASP	2.7
1	E	155	ALA	2.7
1	B	293	ASN	2.7
1	E	473	LEU	2.7
1	A	471	ALA	2.6
1	A	197	VAL	2.6
1	A	464	ASP	2.6
1	E	519	SER	2.6
1	D	383	VAL	2.6
1	A	32	GLY	2.6
1	A	287	ILE	2.6
1	D	44	GLY	2.6
1	F	454	LEU	2.5
1	B	530	LEU	2.5
1	F	44	GLY	2.5
1	E	459	ILE	2.5
1	D	218	ASP	2.5
1	F	398	ILE	2.5
1	B	44	GLY	2.5
1	E	212	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	211	ILE	2.5
1	C	108	VAL	2.5
1	F	450	ALA	2.4
1	B	79	ALA	2.4
1	F	154	GLY	2.4
1	B	296	TYR	2.4
1	F	420	ALA	2.4
1	B	219	VAL	2.4
1	B	395	ALA	2.4
1	A	34	ALA	2.4
1	D	31	ALA	2.4
1	D	470	ARG	2.4
1	B	418	GLY	2.4
1	A	476	GLU	2.4
1	B	446	GLY	2.4
1	D	491	GLY	2.4
1	C	227	ALA	2.4
1	A	79	ALA	2.4
1	B	13	THR	2.4
1	C	12	HIS	2.3
1	F	421	TYR	2.3
1	E	154	GLY	2.3
1	A	216	GLY	2.3
1	F	518	GLU	2.3
1	F	492	TYR	2.3
1	C	219	VAL	2.3
1	A	219	VAL	2.3
1	C	35	ARG	2.3
1	B	304	HIS	2.3
1	D	37	VAL	2.3
1	C	472	ARG	2.3
1	B	269	PHE	2.3
1	F	395	ALA	2.3
1	B	292	ALA	2.3
1	E	469	THR	2.2
1	C	492	TYR	2.2
1	A	465	ASP	2.2
1	B	461	ASP	2.2
1	F	288	VAL	2.2
1	C	457	ARG	2.2
1	D	151	ALA	2.2
1	C	226	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	473	LEU	2.2
1	B	10	ASP	2.2
1	E	156	TYR	2.2
1	E	221	PHE	2.2
1	F	76	GLY	2.2
1	A	11	ILE	2.2
1	E	80	ASN	2.2
1	A	467	GLU	2.2
1	C	456	ARG	2.2
1	C	383	VAL	2.2
1	B	311	PHE	2.2
1	B	225	GLY	2.2
1	D	76	GLY	2.2
1	A	77	LEU	2.2
1	D	492	TYR	2.2
1	F	461	ASP	2.2
1	B	80	ASN	2.2
1	F	458	THR	2.2
1	F	479	ASP	2.2
1	E	186	TYR	2.2
1	C	197	VAL	2.2
1	B	286	THR	2.2
1	C	530	LEU	2.2
1	E	465	ASP	2.2
1	C	40	GLN	2.2
1	D	475	GLN	2.2
1	B	383	VAL	2.1
1	D	417	PHE	2.1
1	B	450	ALA	2.1
1	D	395	ALA	2.1
1	D	419	GLY	2.1
1	B	447	ALA	2.1
1	C	431	ALA	2.1
1	E	464	ASP	2.1
1	A	472	ARG	2.1
1	D	284	LEU	2.1
1	C	421	TYR	2.1
1	A	383	VAL	2.1
1	E	292	ALA	2.1
1	C	153	LEU	2.1
1	F	468	ALA	2.1
1	B	42	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	463	GLY	2.1
1	C	72	SER	2.1
1	A	428	HIS	2.0
1	F	293	ASN	2.0
1	C	200	THR	2.0
1	B	282	ALA	2.0
1	B	431	ALA	2.0
1	D	282	ALA	2.0
1	F	490	ARG	2.0
1	C	43	LYS	2.0
1	B	82	PRO	2.0
1	F	382	GLY	2.0
1	C	10	ASP	2.0
1	D	35	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.