



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:33 PM GMT

PDB ID : 1XO6
Title : Acyl-CoA Carboxylase Beta Subunit from *S. coelicolor* (PccB), apo form #3
Authors : Diacovich, L.; Mitchell, D.L.; Pham, H.; Gago, G.; Melgar, M.M.; Khosla, C.; Gramajo, H.; Tsai, S.-C.
Deposited on : 2004-10-05
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

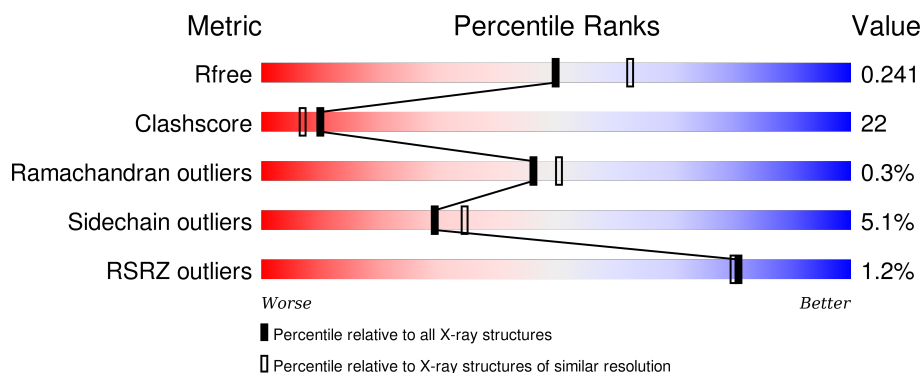
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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>0%</div> <div> <div></div> <div>64%</div> <div>31%</div> <div>..</div> </div> </div>
1	B	530	<div> <div>0%</div> <div> <div></div> <div>68%</div> <div>27%</div> <div>..</div> </div> </div>
1	C	530	<div> <div>0%</div> <div> <div></div> <div>64%</div> <div>30%</div> <div>..</div> </div> </div>
1	D	530	<div> <div>2%</div> <div> <div></div> <div>65%</div> <div>30%</div> <div>..</div> </div> </div>
1	E	530	<div> <div>0%</div> <div> <div></div> <div>65%</div> <div>31%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	530	<div><div></div><div>2%</div><div>68%</div><div>27%</div><div></div><div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25641 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	A	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			
1	B	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			
1	C	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			
1	D	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			
1	E	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			
1	F	521	Total	C	N	O	S	0	0	0
			3953	2481	698	761	13			

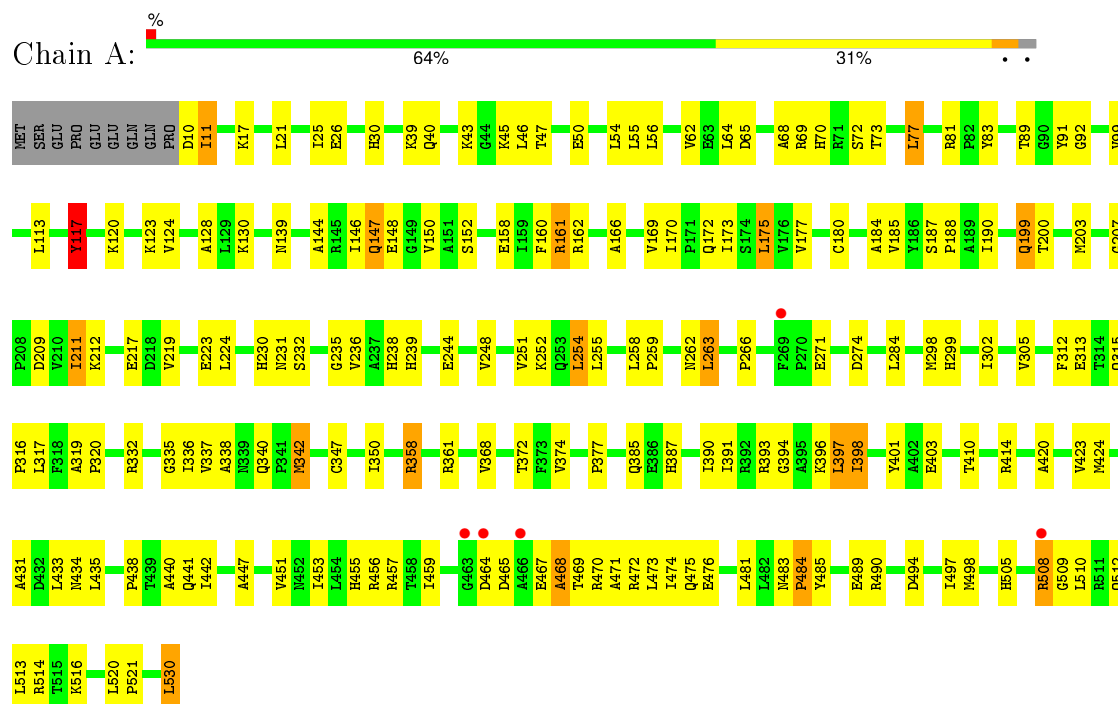
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	326	Total	O	0	0
			326	326		
2	B	320	Total	O	0	0
			320	320		
2	C	338	Total	O	0	0
			338	338		
2	D	332	Total	O	0	0
			332	332		
2	E	291	Total	O	0	0
			291	291		
2	F	316	Total	O	0	0
			316	316		

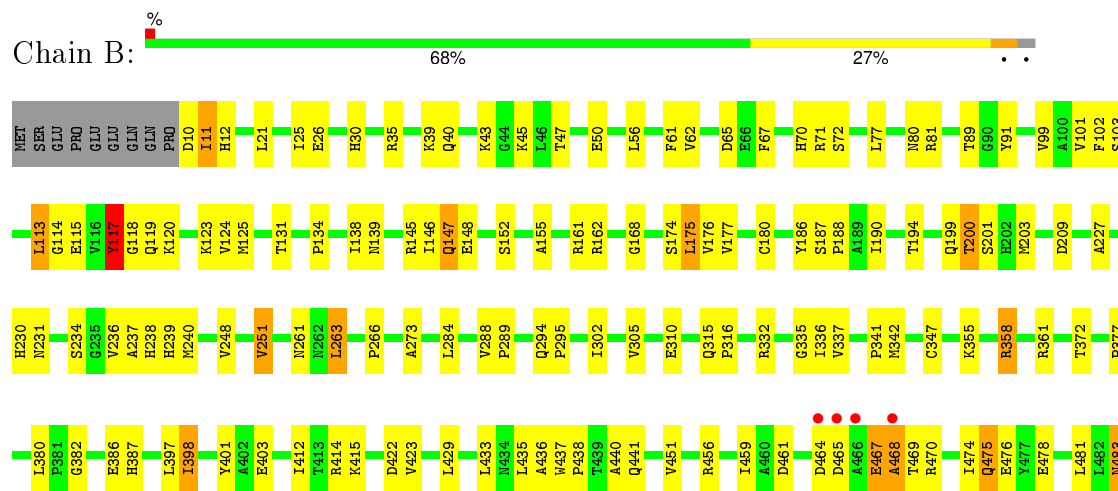
3 Residue-property plots

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

- Molecule 1: propionyl-CoA carboxylase complex B subunit

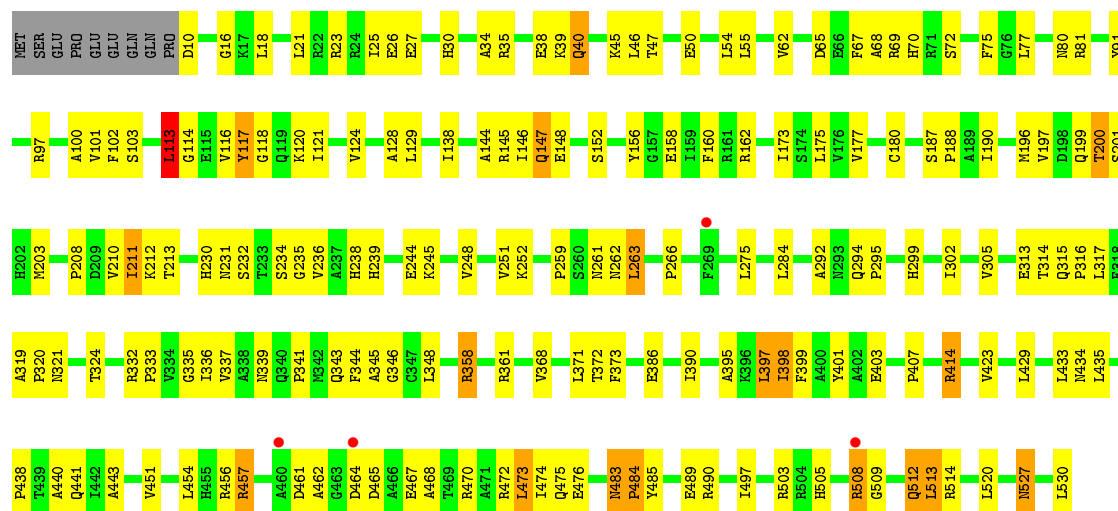


- Molecule 1: propionyl-CoA carboxylase complex B subunit

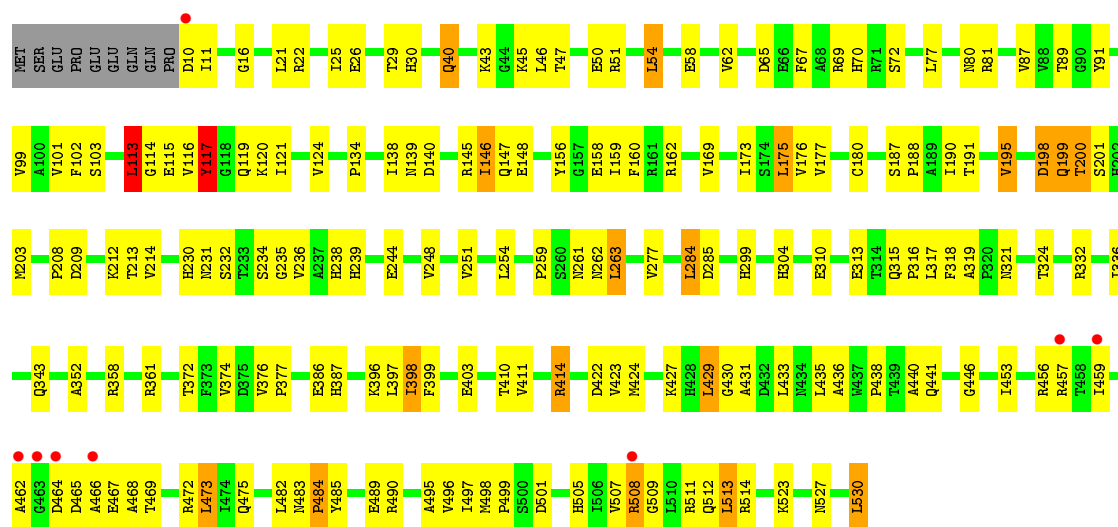




- Molecule 1: propionyl-CoA carboxylase complex B subunit

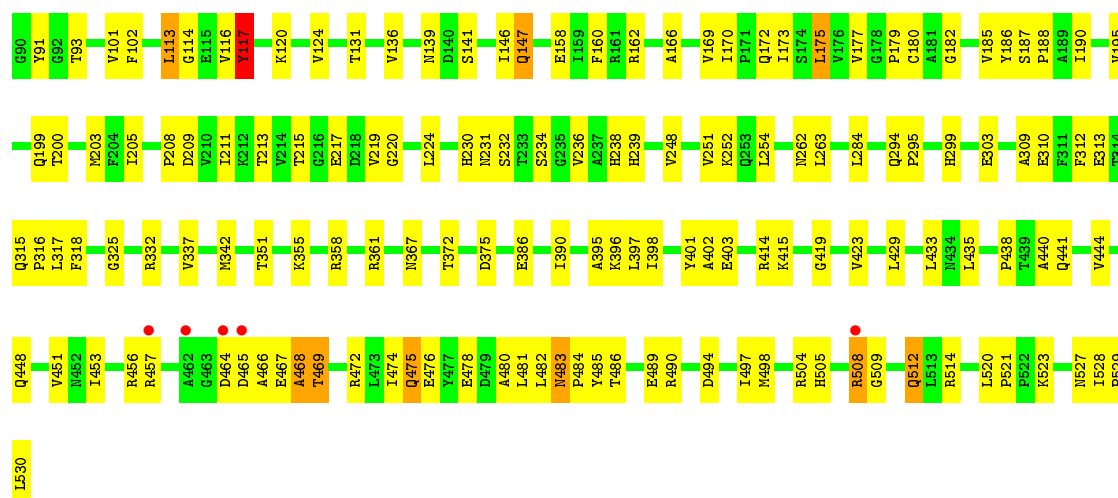


- Molecule 1: propionyl-CoA carboxylase complex B subunit

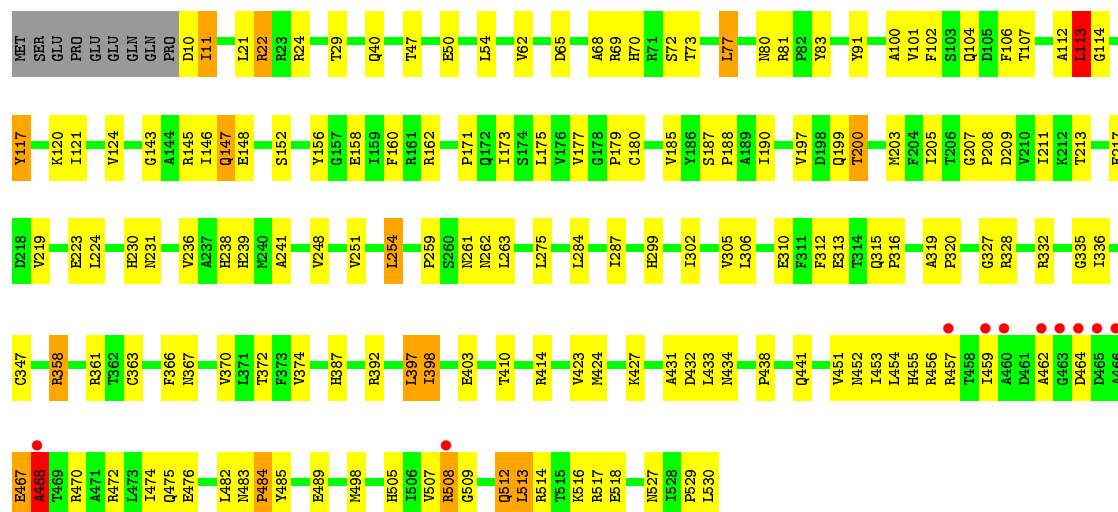


- Molecule 1: propionyl-CoA carboxylase complex B subunit





- Molecule 1: propionyl-CoA carboxylase complex B subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.77Å 178.95Å 296.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 2.20 76.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.0 (49.41-2.20) 83.4 (76.60-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.246 0.203 , 0.241	Depositor DCC
R_{free} test set	8903 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.947	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 286988 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25641	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/4033	0.70	4/5478 (0.1%)
1	B	0.34	0/4033	0.76	9/5478 (0.2%)
1	C	0.34	0/4033	0.71	7/5478 (0.1%)
1	D	0.35	0/4033	0.73	9/5478 (0.2%)
1	E	0.34	0/4033	0.64	4/5478 (0.1%)
1	F	0.33	0/4033	0.69	7/5478 (0.1%)
All	All	0.34	0/24198	0.71	40/32868 (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	A	0	1
1	B	0	1
1	D	0	1
1	E	0	1
All	All	0	4

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	468	ALA	CB-CA-C	-19.45	80.93	110.10
1	D	468	ALA	N-CA-CB	-18.62	84.04	110.10
1	B	467	GLU	CB-CA-C	-17.35	75.70	110.40
1	C	468	ALA	N-CA-CB	-16.60	86.86	110.10
1	A	468	ALA	N-CA-CB	-15.68	88.14	110.10
1	F	467	GLU	CB-CA-C	-15.65	79.09	110.40
1	A	467	GLU	N-CA-C	12.68	145.22	111.00
1	F	468	ALA	N-CA-C	-11.71	79.40	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	467	GLU	N-CA-C	11.16	141.13	111.00
1	C	199	GLN	CB-CA-C	-10.24	89.92	110.40
1	D	467	GLU	N-CA-C	9.91	137.75	111.00
1	D	199	GLN	CB-CA-C	-9.40	91.60	110.40
1	D	467	GLU	CB-CA-C	-9.32	91.76	110.40
1	A	467	GLU	CB-CA-C	-9.29	91.81	110.40
1	B	469	THR	N-CA-CB	9.12	127.63	110.30
1	C	467	GLU	CB-CA-C	-9.05	92.30	110.40
1	F	199	GLN	CB-CA-C	-9.03	92.35	110.40
1	B	469	THR	N-CA-C	-8.75	87.38	111.00
1	B	468	ALA	N-CA-C	-8.51	88.03	111.00
1	F	468	ALA	CB-CA-C	8.50	122.85	110.10
1	A	199	GLN	CB-CA-C	-8.48	93.44	110.40
1	E	468	ALA	CB-CA-C	-8.30	97.64	110.10
1	E	199	GLN	CB-CA-C	-8.24	93.92	110.40
1	E	200	THR	N-CA-CB	8.00	125.51	110.30
1	B	199	GLN	CB-CA-C	-7.80	94.81	110.40
1	B	467	GLU	CA-CB-CG	-7.63	96.61	113.40
1	B	468	ALA	N-CA-CB	-7.49	99.61	110.10
1	B	200	THR	N-CA-CB	7.13	123.85	110.30
1	D	200	THR	N-CA-CB	7.07	123.73	110.30
1	F	467	GLU	N-CA-C	6.90	129.63	111.00
1	C	113	LEU	CA-CB-CG	6.49	130.24	115.30
1	C	200	THR	N-CA-CB	6.34	122.34	110.30
1	F	200	THR	N-CA-CB	6.19	122.06	110.30
1	C	414	ARG	N-CA-C	5.97	127.11	111.00
1	E	469	THR	N-CA-C	-5.93	94.99	111.00
1	D	113	LEU	CA-CB-CG	5.74	128.51	115.30
1	D	414	ARG	N-CA-C	5.51	125.88	111.00
1	D	200	THR	N-CA-C	-5.37	96.51	111.00
1	F	113	LEU	CA-CB-CG	5.30	127.50	115.30
1	D	198	ASP	CB-CA-C	5.25	120.91	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	TYR	Sidechain
1	B	117	TYR	Sidechain
1	D	117	TYR	Sidechain
1	E	117	TYR	Sidechain

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	3953	0	3880	197	0
1	B	3953	0	3880	179	0
1	C	3953	0	3880	193	0
1	D	3953	0	3880	201	0
1	E	3953	0	3880	190	0
1	F	3953	0	3880	179	0
2	A	326	0	0	52	0
2	B	320	0	0	43	0
2	C	338	0	0	68	0
2	D	332	0	0	77	0
2	E	291	0	0	50	0
2	F	316	0	0	46	0
All	All	25641	0	23280	1034	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1034) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:99:VAL:HA	2:D:778:HOH:O	1.54	1.04
1:B:99:VAL:HA	2:B:833:HOH:O	1.55	1.03
1:D:62:VAL:HG21	1:E:508:ARG:HG3	1.42	1.02
1:D:414:ARG:O	2:D:851:HOH:O	1.79	1.01
1:D:89:THR:HG23	2:D:723:HOH:O	1.65	0.96
1:A:147:GLN:H	1:A:147:GLN:HE21	1.13	0.95
1:B:147:GLN:H	1:B:147:GLN:HE21	0.97	0.95
1:C:160:PHE:HB3	1:F:398:ILE:HD13	1.47	0.93
1:A:358:ARG:HG2	2:D:725:HOH:O	1.68	0.92
1:B:147:GLN:H	1:B:147:GLN:NE2	1.65	0.92
1:D:262:ASN:HB3	2:D:832:HOH:O	1.69	0.92
1:D:483:ASN:HD22	1:D:485:TYR:H	1.18	0.91
1:C:70:HIS:HD2	1:C:72:SER:H	1.18	0.91
1:E:187:SER:HB3	1:E:188:PRO:HD3	1.53	0.90
1:D:177:VAL:HG23	2:D:838:HOH:O	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:PRO:HB2	1:E:342:MET:HE3	1.53	0.90
1:B:194:THR:HB	2:B:746:HOH:O	1.74	0.88
1:F:372:THR:HG23	1:F:410:THR:HG23	1.56	0.87
1:E:62:VAL:HG21	1:F:508:ARG:HG3	1.53	0.87
1:E:483:ASN:HD22	1:E:485:TYR:H	1.18	0.85
1:E:435:LEU:HD13	2:E:773:HOH:O	1.75	0.85
1:A:393:ARG:HB2	2:A:625:HOH:O	1.76	0.85
1:F:147:GLN:H	1:F:147:GLN:HE21	1.22	0.85
1:E:55:LEU:HA	2:E:600:HOH:O	1.76	0.85
1:D:70:HIS:HD2	1:D:72:SER:H	1.23	0.84
1:C:483:ASN:HD22	1:C:485:TYR:H	1.26	0.84
1:B:71:ARG:HH22	1:B:119:GLN:HE22	1.24	0.84
1:E:147:GLN:H	1:E:147:GLN:NE2	1.75	0.83
1:A:483:ASN:HD22	1:A:485:TYR:H	1.24	0.83
1:B:508:ARG:NE	1:C:91:TYR:OH	2.13	0.82
1:F:77:LEU:HB3	2:F:809:HOH:O	1.78	0.82
1:D:508:ARG:HG3	1:F:62:VAL:HG21	1.61	0.82
1:B:147:GLN:N	1:B:147:GLN:HE21	1.78	0.81
1:F:70:HIS:HD2	1:F:72:SER:H	1.27	0.81
2:C:754:HOH:O	1:F:529:PRO:HG2	1.79	0.81
1:B:65:ASP:HB2	1:B:120:LYS:HE3	1.63	0.81
1:C:187:SER:HB3	1:C:188:PRO:HD3	1.61	0.81
1:B:295:PRO:HB2	1:B:342:MET:CE	2.11	0.80
1:D:140:ASP:HB2	2:D:838:HOH:O	1.81	0.80
1:E:295:PRO:HB2	1:E:342:MET:CE	2.11	0.80
1:E:147:GLN:H	1:E:147:GLN:HE21	1.27	0.80
1:A:62:VAL:HG21	1:C:508:ARG:HG3	1.61	0.80
1:A:508:ARG:HG3	1:B:62:VAL:HG21	1.61	0.80
1:B:508:ARG:HG3	1:C:62:VAL:HG21	1.63	0.80
1:A:398:ILE:HD13	1:D:160:PHE:HB3	1.63	0.80
1:B:295:PRO:HB2	1:B:342:MET:HE1	1.62	0.79
1:A:484:PRO:HD3	2:A:856:HOH:O	1.83	0.79
1:C:147:GLN:HE21	1:C:147:GLN:H	1.29	0.79
1:F:508:ARG:HD3	1:F:509:GLY:N	1.97	0.79
1:F:261:ASN:HA	2:F:819:HOH:O	1.83	0.79
1:C:138:ILE:HD12	1:C:175:LEU:HD23	1.65	0.79
1:F:187:SER:HB3	1:F:188:PRO:HD3	1.62	0.78
1:A:128:ALA:HA	2:A:794:HOH:O	1.83	0.78
1:C:197:VAL:HB	2:C:786:HOH:O	1.84	0.78
1:B:187:SER:HB3	1:B:188:PRO:HD3	1.64	0.78
1:A:332:ARG:CZ	1:A:514:ARG:HH21	1.97	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:MET:HE1	2:C:722:HOH:O	1.83	0.78
1:E:505:HIS:HA	1:E:508:ARG:HD2	1.65	0.78
1:A:70:HIS:HD2	1:A:72:SER:H	1.32	0.78
1:E:367:ASN:HA	2:E:768:HOH:O	1.83	0.77
1:D:498:MET:HE3	1:F:22:ARG:HD3	1.65	0.77
1:D:187:SER:HB3	1:D:188:PRO:HD3	1.65	0.77
1:D:121:ILE:HA	2:D:801:HOH:O	1.85	0.77
1:F:451:VAL:HG21	1:F:474:ILE:HG12	1.66	0.77
1:A:266:PRO:HG3	2:A:731:HOH:O	1.85	0.77
1:A:187:SER:HB3	1:A:188:PRO:HD3	1.68	0.76
1:C:368:VAL:HG13	2:C:839:HOH:O	1.85	0.76
1:D:508:ARG:NE	1:F:91:TYR:OH	2.18	0.76
1:B:99:VAL:HB	2:B:846:HOH:O	1.84	0.76
1:C:147:GLN:NE2	1:C:147:GLN:H	1.82	0.76
1:F:171:PRO:HD3	2:F:819:HOH:O	1.85	0.76
1:A:248:VAL:O	1:A:251:VAL:HG22	1.84	0.76
1:C:177:VAL:HA	2:C:786:HOH:O	1.86	0.75
1:D:159:ILE:HG12	2:D:788:HOH:O	1.86	0.75
1:F:50:GLU:O	1:F:54:LEU:HD13	1.85	0.75
1:A:258:LEU:HD12	2:A:669:HOH:O	1.87	0.75
1:E:175:LEU:HD22	1:E:177:VAL:HG13	1.67	0.75
1:C:252:LYS:HD2	2:C:775:HOH:O	1.86	0.75
1:A:508:ARG:HE	1:B:62:VAL:HG11	1.52	0.74
1:A:332:ARG:NE	1:A:514:ARG:HH21	1.86	0.74
1:A:147:GLN:NE2	1:A:147:GLN:H	1.84	0.74
1:C:398:ILE:HG13	2:F:721:HOH:O	1.85	0.74
1:C:128:ALA:HA	2:C:832:HOH:O	1.85	0.74
1:D:361:ARG:HD2	1:D:403:GLU:OE2	1.88	0.74
1:F:483:ASN:HD22	1:F:485:TYR:H	1.34	0.74
1:C:314:THR:HG23	2:C:678:HOH:O	1.87	0.74
1:F:457:ARG:HD2	1:F:457:ARG:N	2.02	0.73
1:E:248:VAL:O	1:E:251:VAL:HG22	1.87	0.73
1:F:254:LEU:HD13	1:F:312:PHE:HE2	1.53	0.73
1:F:147:GLN:H	1:F:147:GLN:NE2	1.86	0.73
1:D:457:ARG:H	1:D:457:ARG:HD2	1.52	0.73
1:D:462:ALA:HB3	2:D:685:HOH:O	1.87	0.73
1:D:508:ARG:HE	1:F:62:VAL:HG11	1.52	0.73
1:C:336:ILE:HG23	2:C:856:HOH:O	1.89	0.73
1:C:34:ALA:O	1:C:38:GLU:HG3	1.87	0.73
1:A:91:TYR:OH	1:C:508:ARG:NE	2.22	0.73
1:D:62:VAL:HG11	1:E:508:ARG:HE	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ALA:HA	2:B:746:HOH:O	1.88	0.72
1:C:485:TYR:O	1:C:489:GLU:HG3	1.89	0.72
1:A:433:LEU:HD21	1:A:508:ARG:NH1	2.03	0.72
1:E:45:LYS:HG2	2:E:801:HOH:O	1.89	0.72
1:C:275:LEU:HD23	2:C:771:HOH:O	1.89	0.72
1:C:508:ARG:HD3	1:C:509:GLY:N	2.05	0.71
1:C:230:HIS:HB3	1:C:236:VAL:HG22	1.71	0.71
1:C:23:ARG:HH11	1:C:23:ARG:HB3	1.53	0.71
1:C:292:ALA:HB1	2:C:599:HOH:O	1.90	0.71
1:B:398:ILE:HD13	1:E:160:PHE:HB3	1.73	0.71
1:C:113:LEU:HD22	2:C:843:HOH:O	1.91	0.71
1:E:504:ARG:HD3	2:E:570:HOH:O	1.90	0.71
1:D:473:LEU:HD13	2:D:655:HOH:O	1.90	0.71
1:E:508:ARG:HD3	1:E:509:GLY:N	2.06	0.71
1:D:457:ARG:N	1:D:457:ARG:HD2	2.05	0.71
1:A:65:ASP:HB2	1:A:120:LYS:HE3	1.73	0.71
1:D:482:LEU:HD21	2:D:690:HOH:O	1.91	0.70
1:B:438:PRO:HG3	1:C:21:LEU:HD22	1.72	0.70
1:D:45:LYS:HE2	2:D:824:HOH:O	1.89	0.70
1:D:65:ASP:HB2	1:D:120:LYS:HE3	1.72	0.70
1:D:508:ARG:HD3	1:D:509:GLY:N	2.06	0.70
1:A:451:VAL:HG21	1:A:474:ILE:HG12	1.73	0.70
1:D:456:ARG:HH11	1:D:457:ARG:NH1	1.90	0.70
1:A:62:VAL:HG11	1:C:508:ARG:HE	1.56	0.70
1:A:508:ARG:HD3	1:A:509:GLY:N	2.06	0.70
1:A:438:PRO:HG3	1:B:21:LEU:HD22	1.72	0.70
1:B:288:VAL:HG13	2:B:743:HOH:O	1.91	0.69
1:C:372:THR:HG23	2:C:606:HOH:O	1.92	0.69
1:D:508:ARG:HH21	1:F:62:VAL:HG11	1.56	0.69
1:B:113:LEU:HD22	1:B:117:TYR:CD1	2.28	0.69
1:E:117:TYR:HA	2:E:785:HOH:O	1.93	0.69
1:C:152:SER:HB2	2:C:854:HOH:O	1.93	0.69
1:A:62:VAL:HG11	1:C:508:ARG:HH21	1.57	0.69
1:E:89:THR:HB	1:E:124:VAL:HG21	1.75	0.69
1:F:121:ILE:O	1:F:124:VAL:HG12	1.92	0.69
1:D:40:GLN:HA	2:D:824:HOH:O	1.93	0.69
1:A:175:LEU:HD22	1:A:177:VAL:HG13	1.72	0.69
1:F:457:ARG:HD2	1:F:457:ARG:H	1.57	0.69
1:D:433:LEU:HD21	1:D:508:ARG:NH1	2.09	0.68
1:E:62:VAL:HG11	1:F:508:ARG:HE	1.57	0.68
1:D:446:GLY:HA2	2:D:690:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:HIS:HA	1:A:508:ARG:HD2	1.76	0.68
1:D:91:TYR:OH	1:E:508:ARG:NE	2.27	0.68
1:A:390:ILE:HA	2:A:625:HOH:O	1.94	0.68
1:B:341:PRO:HD2	2:B:745:HOH:O	1.92	0.68
1:E:91:TYR:OH	1:F:508:ARG:NE	2.27	0.68
1:C:208:PRO:HA	1:C:211:ILE:HD12	1.74	0.68
1:A:431:ALA:HB1	2:A:623:HOH:O	1.94	0.67
1:C:341:PRO:HD2	2:C:851:HOH:O	1.94	0.67
1:F:372:THR:HG22	2:F:532:HOH:O	1.94	0.67
1:A:459:ILE:HG21	1:A:470:ARG:HH21	1.58	0.67
1:D:87:VAL:HG13	2:D:723:HOH:O	1.95	0.67
1:B:161:ARG:CZ	2:E:758:HOH:O	2.41	0.67
1:F:431:ALA:HB1	2:F:823:HOH:O	1.93	0.67
1:D:148:GLU:HG3	2:D:786:HOH:O	1.95	0.67
1:A:451:VAL:HG21	1:A:474:ILE:CG1	2.25	0.66
1:E:185:VAL:HG21	1:E:205:ILE:HG12	1.78	0.66
1:D:469:THR:O	1:D:473:LEU:HD22	1.96	0.66
1:B:152:SER:HB3	2:B:669:HOH:O	1.96	0.66
1:F:361:ARG:HD2	1:F:403:GLU:OE2	1.95	0.66
1:C:505:HIS:HA	1:C:508:ARG:HD2	1.77	0.66
1:B:398:ILE:HG22	1:B:423:VAL:HG22	1.77	0.66
1:F:113:LEU:HD22	1:F:117:TYR:CD1	2.29	0.66
1:E:433:LEU:HD21	1:E:508:ARG:NH1	2.11	0.66
1:D:501:ASP:HB2	2:D:779:HOH:O	1.95	0.66
1:A:508:ARG:HH21	1:B:62:VAL:HG11	1.59	0.66
1:C:23:ARG:HB3	1:C:23:ARG:NH1	2.11	0.66
1:A:170:ILE:HG13	2:A:760:HOH:O	1.95	0.66
1:D:113:LEU:HD22	1:D:117:TYR:CD1	2.31	0.65
1:E:47:THR:OG1	1:E:50:GLU:HG3	1.96	0.65
1:A:508:ARG:NE	1:B:91:TYR:OH	2.29	0.65
1:D:410:THR:HG22	2:D:814:HOH:O	1.94	0.65
1:D:230:HIS:HB3	1:D:236:VAL:HG22	1.79	0.65
1:D:43:LYS:HD2	2:D:824:HOH:O	1.95	0.65
1:A:394:GLY:N	2:A:843:HOH:O	2.28	0.65
1:D:508:ARG:NE	1:F:62:VAL:HG11	2.12	0.65
1:D:497:ILE:HD12	2:D:779:HOH:O	1.97	0.65
1:A:259:PRO:HG2	2:A:807:HOH:O	1.95	0.65
1:C:433:LEU:HD21	1:C:508:ARG:NH1	2.11	0.65
1:D:497:ILE:HB	2:D:779:HOH:O	1.96	0.65
1:E:65:ASP:HB2	1:E:120:LYS:HE3	1.77	0.65
1:E:70:HIS:HD2	1:E:72:SER:H	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:315:GLN:N	1:F:316:PRO:HD3	2.12	0.65
1:A:184:ALA:HB3	2:A:842:HOH:O	1.97	0.64
1:F:65:ASP:HB2	1:F:120:LYS:HE3	1.79	0.64
1:C:65:ASP:HB2	1:C:120:LYS:HE3	1.79	0.64
1:E:395:ALA:O	1:E:398:ILE:HG12	1.97	0.64
1:A:494:ASP:HA	2:A:782:HOH:O	1.97	0.64
1:B:315:GLN:N	1:B:316:PRO:HD3	2.13	0.64
1:B:508:ARG:HD3	1:B:509:GLY:N	2.13	0.64
1:D:231:ASN:HD21	1:D:239:HIS:N	1.96	0.64
1:B:433:LEU:HD21	1:B:508:ARG:NH1	2.13	0.64
1:D:70:HIS:CD2	1:D:72:SER:H	2.12	0.64
1:D:508:ARG:NH2	1:F:62:VAL:HG11	2.13	0.64
1:C:395:ALA:O	1:C:398:ILE:HG23	1.98	0.64
1:A:469:THR:O	1:A:473:LEU:HD13	1.98	0.64
2:C:801:HOH:O	1:F:146:ILE:HG22	1.97	0.64
1:C:248:VAL:O	1:C:251:VAL:HG22	1.98	0.64
1:C:372:THR:HG21	1:C:401:TYR:OH	1.97	0.63
1:B:70:HIS:HD2	1:B:72:SER:H	1.44	0.63
1:D:438:PRO:HG3	1:F:21:LEU:HD22	1.80	0.63
1:F:512:GLN:HB3	2:F:707:HOH:O	1.98	0.63
1:F:197:VAL:HG13	2:F:829:HOH:O	1.96	0.63
1:B:175:LEU:HD22	1:B:177:VAL:HG13	1.80	0.63
1:E:325:GLY:HA2	2:E:700:HOH:O	1.98	0.63
1:D:505:HIS:HA	1:D:508:ARG:HD2	1.81	0.63
1:C:266:PRO:HG3	2:C:839:HOH:O	1.98	0.63
1:F:179:PRO:HD2	2:F:818:HOH:O	1.98	0.63
1:C:457:ARG:N	1:C:457:ARG:HD2	2.12	0.63
1:D:120:LYS:HE2	2:D:723:HOH:O	1.99	0.63
1:D:212:LYS:HG3	2:D:598:HOH:O	1.98	0.62
1:D:21:LEU:HD22	1:E:438:PRO:HG3	1.80	0.62
1:E:81:ARG:HB3	2:E:777:HOH:O	1.99	0.62
1:D:436:ALA:HB3	2:D:834:HOH:O	1.98	0.62
1:B:512:GLN:HG3	1:C:91:TYR:CE1	2.34	0.62
1:B:437:TRP:HB3	2:B:834:HOH:O	1.98	0.62
1:A:158:GLU:O	1:A:162:ARG:HG2	2.00	0.62
1:A:160:PHE:HB3	1:D:398:ILE:HD13	1.80	0.62
1:E:332:ARG:HD3	1:E:514:ARG:NH2	2.15	0.62
1:D:198:ASP:O	1:D:199:GLN:HB2	1.99	0.62
1:F:284:LEU:O	1:F:287:ILE:HG22	1.99	0.62
1:C:259:PRO:HD3	2:C:571:HOH:O	2.00	0.62
1:E:170:ILE:HG13	2:E:691:HOH:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ARG:O	1:B:459:ILE:HG22	2.00	0.62
1:A:147:GLN:N	1:A:147:GLN:HE21	1.94	0.62
1:C:160:PHE:HB3	1:F:398:ILE:CD1	2.24	0.62
1:E:113:LEU:HD22	1:E:117:TYR:CD1	2.35	0.62
1:F:453:ILE:HB	2:F:775:HOH:O	2.00	0.61
1:F:433:LEU:HD21	1:F:508:ARG:CZ	2.30	0.61
1:B:415:LYS:HE2	2:B:666:HOH:O	1.99	0.61
1:B:524:LYS:NZ	2:E:768:HOH:O	2.32	0.61
1:A:368:VAL:HG13	2:A:731:HOH:O	2.00	0.61
1:D:485:TYR:O	1:D:489:GLU:HG3	2.01	0.61
1:F:328:ARG:NH2	2:F:846:HOH:O	2.33	0.61
1:A:440:ALA:N	2:A:856:HOH:O	2.33	0.61
1:E:456:ARG:HD2	1:E:457:ARG:NH1	2.15	0.61
1:A:271:GLU:HB3	2:A:736:HOH:O	2.00	0.61
1:A:54:LEU:HD13	2:A:604:HOH:O	2.01	0.61
1:A:361:ARG:HD2	1:A:403:GLU:OE2	2.00	0.61
1:A:47:THR:OG1	1:A:50:GLU:HG3	2.01	0.61
1:D:459:ILE:HD11	1:D:466:ALA:O	2.01	0.61
1:E:361:ARG:HD3	2:E:739:HOH:O	2.01	0.61
1:C:465:ASP:HB3	2:C:688:HOH:O	2.01	0.61
1:C:232:SER:HB3	1:C:317:LEU:HB3	1.83	0.60
1:A:485:TYR:O	1:A:489:GLU:HG3	2.01	0.60
1:F:366:PHE:HB2	2:F:753:HOH:O	2.01	0.60
1:B:39:LYS:NZ	1:B:39:LYS:HB3	2.16	0.60
1:C:262:ASN:HA	2:C:850:HOH:O	2.01	0.60
1:C:113:LEU:HD13	2:C:843:HOH:O	2.01	0.60
1:A:530:LEU:HG	1:D:396:LYS:HD3	1.83	0.60
1:D:259:PRO:HG2	2:D:854:HOH:O	2.00	0.60
1:B:238:HIS:ND1	2:B:746:HOH:O	2.32	0.60
1:C:25:ILE:HD13	1:C:67:PHE:HZ	1.67	0.60
1:D:483:ASN:HB2	1:D:484:PRO:HD2	1.82	0.60
1:C:266:PRO:HB3	2:C:571:HOH:O	2.02	0.60
1:C:399:PHE:HA	2:F:721:HOH:O	2.00	0.60
1:C:10:ASP:O	1:C:16:GLY:HA3	2.02	0.60
1:A:254:LEU:HD13	1:A:312:PHE:HE2	1.66	0.60
1:B:21:LEU:O	1:B:25:ILE:HG23	2.02	0.60
1:D:147:GLN:HB2	2:D:786:HOH:O	2.00	0.60
1:E:523:LYS:HB2	2:E:797:HOH:O	2.01	0.59
1:A:113:LEU:HD22	1:A:117:TYR:CD1	2.37	0.59
1:B:490:ARG:HG3	2:B:698:HOH:O	2.00	0.59
1:E:21:LEU:HD22	1:F:438:PRO:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:ARG:HD2	2:D:536:HOH:O	2.02	0.59
1:D:530:LEU:HD22	2:D:725:HOH:O	2.01	0.59
1:F:231:ASN:HD21	1:F:239:HIS:N	2.00	0.59
1:A:508:ARG:NE	1:B:62:VAL:HG11	2.17	0.59
1:A:508:ARG:CG	1:B:62:VAL:HG21	2.33	0.59
1:A:70:HIS:CD2	1:A:72:SER:H	2.16	0.59
1:D:248:VAL:O	1:D:251:VAL:HG22	2.02	0.59
1:D:62:VAL:HG11	1:E:508:ARG:NE	2.16	0.59
1:E:483:ASN:HD22	1:E:485:TYR:N	1.95	0.59
1:E:68:ALA:HB3	2:E:735:HOH:O	2.03	0.59
1:E:451:VAL:HG21	1:E:474:ILE:CG1	2.32	0.59
1:E:215:THR:HB	2:E:659:HOH:O	2.03	0.59
1:F:77:LEU:N	2:F:724:HOH:O	2.34	0.59
1:B:47:THR:OG1	1:B:50:GLU:HG3	2.03	0.59
1:D:62:VAL:HG21	1:E:508:ARG:CG	2.26	0.59
1:F:433:LEU:HD21	1:F:508:ARG:NH2	2.17	0.59
1:A:332:ARG:HE	1:A:514:ARG:HE	1.49	0.59
1:A:266:PRO:HB3	2:A:815:HOH:O	2.02	0.59
1:C:40:GLN:HA	1:C:40:GLN:HE21	1.65	0.59
1:D:399:PHE:HB2	2:D:857:HOH:O	2.02	0.58
1:E:361:ARG:HD2	1:E:403:GLU:OE2	2.03	0.58
1:A:315:GLN:N	1:A:316:PRO:HD3	2.18	0.58
1:A:148:GLU:HG3	2:A:712:HOH:O	2.03	0.58
1:A:459:ILE:HD11	1:A:473:LEU:HD22	1.86	0.58
1:A:483:ASN:HB2	1:A:484:PRO:HD2	1.85	0.58
1:D:433:LEU:HD21	1:D:508:ARG:HH12	1.68	0.58
1:E:21:LEU:O	1:E:25:ILE:HG22	2.03	0.58
1:E:372:THR:HG21	1:E:401:TYR:OH	2.03	0.58
1:A:505:HIS:O	1:A:508:ARG:HD3	2.03	0.58
1:A:298:MET:HE3	2:A:749:HOH:O	2.03	0.58
1:B:56:LEU:HD22	2:B:846:HOH:O	2.02	0.58
1:E:429:LEU:C	2:E:758:HOH:O	2.42	0.58
1:D:315:GLN:N	1:D:316:PRO:HD3	2.19	0.58
1:C:472:ARG:O	1:C:476:GLU:HG3	2.02	0.58
1:D:433:LEU:HD13	2:D:858:HOH:O	2.03	0.58
1:C:316:PRO:HD2	2:C:639:HOH:O	2.03	0.58
1:C:505:HIS:O	1:C:508:ARG:HD3	2.02	0.58
1:C:138:ILE:HG13	2:C:865:HOH:O	2.03	0.58
1:D:209:ASP:HB2	2:D:840:HOH:O	2.03	0.58
1:B:248:VAL:O	1:B:251:VAL:HG13	2.04	0.58
1:F:72:SER:HB3	2:F:809:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:GLN:HE21	1:C:147:GLN:N	2.01	0.58
1:B:186:TYR:O	1:B:190:ILE:HG12	2.04	0.58
1:D:10:ASP:CG	1:D:11:ILE:H	2.07	0.58
1:C:371:LEU:HB2	2:C:856:HOH:O	2.03	0.57
1:E:456:ARG:HH11	1:E:457:ARG:NH1	2.02	0.57
1:E:215:THR:HG21	2:E:770:HOH:O	2.02	0.57
1:C:520:LEU:HD13	2:C:692:HOH:O	2.03	0.57
1:A:139:ASN:HB3	2:A:685:HOH:O	2.03	0.57
1:A:70:HIS:CE1	1:A:81:ARG:HG2	2.39	0.57
1:F:483:ASN:HB2	1:F:484:PRO:HD2	1.85	0.57
1:E:456:ARG:HD2	1:E:457:ARG:CZ	2.34	0.57
1:F:262:ASN:OD1	1:F:263:LEU:HD22	2.03	0.57
1:C:145:ARG:HD2	1:C:148:GLU:OE2	2.05	0.57
1:B:505:HIS:O	1:B:508:ARG:HD3	2.04	0.57
1:A:433:LEU:HD21	1:A:508:ARG:HH12	1.67	0.57
1:C:230:HIS:HD2	2:C:722:HOH:O	1.86	0.57
1:B:230:HIS:HB3	1:B:236:VAL:HG22	1.85	0.57
1:D:254:LEU:HG	2:D:856:HOH:O	2.04	0.57
1:B:436:ALA:HB3	2:B:839:HOH:O	2.04	0.57
1:B:125:MET:HG3	2:B:711:HOH:O	2.05	0.57
1:D:134:PRO:HD2	2:D:778:HOH:O	2.04	0.57
1:D:121:ILE:HG22	2:D:788:HOH:O	2.04	0.57
1:E:451:VAL:HG21	1:E:474:ILE:HG13	1.86	0.57
1:E:230:HIS:HB3	1:E:236:VAL:HG22	1.84	0.57
1:A:508:ARG:NH2	1:B:62:VAL:HG11	2.20	0.57
1:C:201:SER:HB3	2:C:786:HOH:O	2.05	0.57
1:B:438:PRO:HD2	2:B:834:HOH:O	2.03	0.57
1:A:335:GLY:C	1:A:336:ILE:HD12	2.24	0.57
1:B:273:ALA:HB3	2:B:841:HOH:O	2.05	0.57
1:F:505:HIS:C	1:F:508:ARG:HH11	2.07	0.57
1:E:89:THR:HB	1:E:124:VAL:CG2	2.34	0.57
1:C:47:THR:OG1	1:C:50:GLU:HG3	2.04	0.57
1:B:174:SER:HB3	2:B:811:HOH:O	2.04	0.57
1:E:55:LEU:HD12	2:E:600:HOH:O	2.04	0.57
1:E:474:ILE:O	1:E:478:GLU:HG2	2.04	0.57
1:A:64:LEU:HB3	2:C:829:HOH:O	2.04	0.57
1:B:147:GLN:N	1:B:147:GLN:NE2	2.45	0.57
1:C:113:LEU:HD22	1:C:117:TYR:CD1	2.40	0.57
1:A:10:ASP:OD1	1:A:11:ILE:N	2.37	0.57
1:B:113:LEU:HD13	1:B:114:GLY:N	2.20	0.57
1:F:175:LEU:HD22	1:F:177:VAL:HG13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:472:ARG:O	1:E:476:GLU:HG3	2.05	0.57
1:E:62:VAL:HG21	1:F:508:ARG:CG	2.29	0.56
1:A:62:VAL:HG11	1:C:508:ARG:NH2	2.20	0.56
1:A:173:ILE:HD11	2:A:669:HOH:O	2.03	0.56
1:F:175:LEU:CD2	1:F:177:VAL:HG13	2.35	0.56
1:F:262:ASN:HA	2:F:828:HOH:O	2.04	0.56
2:D:803:HOH:O	1:F:21:LEU:HA	2.04	0.56
1:E:523:LYS:HD3	2:E:797:HOH:O	2.05	0.56
1:F:173:ILE:HG21	1:F:251:VAL:HG23	1.87	0.56
1:C:35:ARG:O	1:C:39:LYS:HG3	2.05	0.56
1:D:173:ILE:HA	2:D:835:HOH:O	2.05	0.56
1:F:397:LEU:HD13	1:F:423:VAL:CG1	2.34	0.56
1:D:456:ARG:O	1:D:459:ILE:HG22	2.04	0.56
1:E:85:ASP:HB3	2:E:785:HOH:O	2.04	0.56
1:F:10:ASP:CG	1:F:11:ILE:H	2.08	0.56
1:B:467:GLU:HB3	2:B:656:HOH:O	2.05	0.56
1:F:230:HIS:HB3	1:F:236:VAL:HG22	1.87	0.56
1:A:161:ARG:NH2	1:D:430:GLY:HA2	2.21	0.56
1:F:374:VAL:HG22	1:F:424:MET:HB3	1.86	0.56
1:C:55:LEU:HA	2:C:775:HOH:O	2.06	0.56
1:E:172:GLN:C	1:E:173:ILE:HD12	2.26	0.56
1:E:217:GLU:HB3	2:E:659:HOH:O	2.04	0.56
1:E:482:LEU:HD11	2:E:804:HOH:O	2.04	0.56
1:C:190:ILE:CD1	1:F:398:ILE:HD11	2.35	0.56
1:A:190:ILE:HG12	2:D:857:HOH:O	2.05	0.56
1:E:315:GLN:N	1:E:316:PRO:HD3	2.20	0.56
1:F:433:LEU:HD21	1:F:508:ARG:NH1	2.20	0.56
1:A:350:ILE:HG12	2:A:625:HOH:O	2.05	0.56
1:C:23:ARG:O	1:C:27:GLU:HG3	2.04	0.56
1:E:315:GLN:HB2	1:E:355:LYS:HE3	1.87	0.56
1:A:219:VAL:HG23	1:A:223:GLU:OE1	2.05	0.56
1:C:438:PRO:HG3	2:C:811:HOH:O	2.05	0.56
1:D:508:ARG:CG	1:F:62:VAL:HG21	2.35	0.56
1:A:397:LEU:HD13	1:A:423:VAL:HG12	1.87	0.56
1:B:361:ARG:HD2	1:B:403:GLU:OE2	2.06	0.56
1:B:10:ASP:OD1	1:B:11:ILE:N	2.39	0.56
1:A:45:LYS:HG2	1:A:200:THR:HG23	1.88	0.56
1:E:62:VAL:HG11	1:F:508:ARG:HH21	1.71	0.56
1:E:414:ARG:O	1:E:441:GLN:N	2.38	0.55
1:E:208:PRO:HA	1:E:211:ILE:HD11	1.88	0.55
1:D:62:VAL:CG2	1:E:508:ARG:HG3	2.29	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:485:TYR:O	1:E:489:GLU:HG3	2.07	0.55
1:B:56:LEU:HD12	1:B:61:PHE:HB2	1.88	0.55
1:F:398:ILE:HG22	1:F:423:VAL:HG22	1.88	0.55
1:E:131:THR:HG21	2:F:707:HOH:O	2.05	0.55
1:A:17:LYS:HE2	2:C:730:HOH:O	2.06	0.55
1:D:102:PHE:HB3	2:D:801:HOH:O	2.05	0.55
1:A:211:ILE:HG13	1:A:212:LYS:N	2.20	0.55
1:C:211:ILE:HD13	1:C:212:LYS:N	2.22	0.55
1:F:248:VAL:O	1:F:251:VAL:HG12	2.06	0.55
1:B:489:GLU:HG2	1:C:69:ARG:HG3	1.88	0.55
1:D:483:ASN:HD22	1:D:485:TYR:N	1.97	0.55
2:A:782:HOH:O	1:B:123:LYS:NZ	2.38	0.55
1:B:332:ARG:HD3	1:B:514:ARG:NH2	2.22	0.55
1:A:332:ARG:HH22	1:A:510:LEU:HB3	1.72	0.55
1:E:69:ARG:HD3	1:E:83:TYR:CD2	2.42	0.55
1:C:117:TYR:HB3	2:C:843:HOH:O	2.05	0.55
1:B:148:GLU:HB2	2:B:669:HOH:O	2.06	0.55
1:B:70:HIS:HE1	1:B:80:ASN:O	1.90	0.55
1:D:208:PRO:HD2	2:D:836:HOH:O	2.07	0.55
1:C:333:PRO:HB2	2:C:839:HOH:O	2.07	0.55
1:B:433:LEU:HD21	1:B:508:ARG:HH12	1.71	0.54
1:B:412:ILE:HG23	2:B:732:HOH:O	2.07	0.54
1:B:231:ASN:HD21	1:B:239:HIS:N	2.04	0.54
1:B:530:LEU:HG	1:E:396:LYS:HD3	1.89	0.54
1:A:232:SER:HB3	1:A:317:LEU:HB3	1.89	0.54
1:D:101:VAL:HG13	2:D:837:HOH:O	2.07	0.54
1:A:490:ARG:HH22	1:D:115:GLU:CD	2.10	0.54
1:E:262:ASN:OD1	1:E:263:LEU:HD22	2.07	0.54
1:C:483:ASN:ND2	1:C:485:TYR:H	2.01	0.54
1:A:512:GLN:HG3	1:B:91:TYR:CE1	2.42	0.54
1:E:70:HIS:HA	1:E:116:VAL:HG21	1.90	0.54
1:B:414:ARG:O	1:B:441:GLN:N	2.39	0.54
1:B:81:ARG:HD3	2:B:632:HOH:O	2.06	0.54
1:B:451:VAL:HG21	1:B:474:ILE:CG1	2.38	0.54
1:E:231:ASN:HD21	1:E:239:HIS:N	2.06	0.54
1:D:441:GLN:HG3	2:D:851:HOH:O	2.07	0.54
1:F:24:ARG:HG2	2:F:835:HOH:O	2.05	0.54
1:A:459:ILE:HD12	1:A:470:ARG:HB3	1.88	0.54
1:C:69:ARG:HD3	1:C:81:ARG:O	2.07	0.54
1:E:173:ILE:N	1:E:173:ILE:HD12	2.23	0.54
1:C:121:ILE:O	1:C:124:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:ASN:HB2	1:C:484:PRO:HD2	1.88	0.54
1:A:332:ARG:NE	1:A:514:ARG:HE	2.06	0.54
1:C:398:ILE:HD12	1:C:398:ILE:O	2.07	0.54
1:F:254:LEU:CD1	1:F:312:PHE:HE2	2.20	0.54
1:C:361:ARG:HD2	1:C:403:GLU:OE2	2.08	0.54
1:B:451:VAL:HG21	1:B:474:ILE:HG12	1.89	0.54
1:B:89:THR:HB	1:B:124:VAL:HG21	1.89	0.54
1:B:508:ARG:NE	1:C:62:VAL:HG11	2.24	0.53
1:D:277:VAL:HG22	2:D:780:HOH:O	2.08	0.53
1:B:39:LYS:O	1:B:43:LYS:HG3	2.08	0.53
1:B:261:ASN:OD1	1:B:263:LEU:HB2	2.08	0.53
1:B:475:GLN:HE22	1:B:476:GLU:HG3	1.74	0.53
1:D:45:LYS:CD	1:D:200:THR:HG23	2.37	0.53
1:F:472:ARG:O	1:F:476:GLU:HG3	2.08	0.53
1:F:498:MET:HE2	2:F:729:HOH:O	2.08	0.53
1:E:505:HIS:O	1:E:508:ARG:HD3	2.08	0.53
1:F:147:GLN:N	1:F:147:GLN:HE21	2.00	0.53
1:A:259:PRO:HD3	2:A:815:HOH:O	2.07	0.53
1:D:25:ILE:O	1:D:29:THR:HG23	2.08	0.53
1:E:254:LEU:HD13	1:E:312:PHE:HE2	1.74	0.53
1:D:46:LEU:HD13	1:D:244:GLU:OE2	2.07	0.53
1:F:70:HIS:HE1	1:F:80:ASN:O	1.91	0.53
1:E:120:LYS:HD2	2:E:735:HOH:O	2.07	0.53
1:B:25:ILE:HG22	1:B:67:PHE:HZ	1.73	0.53
1:A:21:LEU:HD22	1:C:438:PRO:HG3	1.90	0.53
1:B:89:THR:HB	1:B:124:VAL:CG2	2.39	0.53
1:C:315:GLN:N	1:C:316:PRO:HD3	2.23	0.53
1:E:316:PRO:HD2	2:E:699:HOH:O	2.09	0.53
1:A:21:LEU:HB2	2:C:811:HOH:O	2.08	0.53
1:C:97:ARG:HB2	2:C:721:HOH:O	2.09	0.53
1:D:414:ARG:O	1:D:441:GLN:N	2.39	0.53
1:E:87:VAL:HG12	2:E:785:HOH:O	2.07	0.53
1:B:134:PRO:HD2	2:B:833:HOH:O	2.08	0.53
1:B:335:GLY:C	1:B:336:ILE:HD12	2.30	0.53
1:E:433:LEU:HD21	1:E:508:ARG:CZ	2.39	0.53
1:D:70:HIS:HA	1:D:116:VAL:HG21	1.91	0.53
1:D:398:ILE:HG22	1:D:423:VAL:HG22	1.91	0.53
1:D:427:LYS:HA	1:D:431:ALA:HB3	1.90	0.53
1:E:62:VAL:HG11	1:F:508:ARG:NE	2.23	0.52
1:B:295:PRO:HB2	1:B:342:MET:HE2	1.89	0.52
1:C:373:PHE:HE1	2:C:856:HOH:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:212:LYS:HD2	2:D:795:HOH:O	2.09	0.52
1:E:372:THR:HG23	2:E:545:HOH:O	2.08	0.52
1:A:414:ARG:O	1:A:441:GLN:N	2.42	0.52
1:A:372:THR:OG1	1:A:410:THR:HG23	2.09	0.52
1:B:508:ARG:CG	1:C:62:VAL:HG21	2.34	0.52
1:A:62:VAL:HG11	1:C:508:ARG:NE	2.22	0.52
1:E:70:HIS:N	2:E:777:HOH:O	2.41	0.52
1:C:324:THR:HA	1:C:336:ILE:O	2.10	0.52
1:B:114:GLY:HA2	2:B:669:HOH:O	2.09	0.52
1:B:161:ARG:HG3	2:E:758:HOH:O	2.07	0.52
2:D:641:HOH:O	1:F:65:ASP:HA	2.10	0.52
1:E:139:ASN:HB3	2:E:702:HOH:O	2.09	0.52
1:D:377:PRO:HD3	2:D:806:HOH:O	2.09	0.52
1:D:456:ARG:HH11	1:D:457:ARG:HH12	1.57	0.52
1:E:166:ALA:HB1	2:E:691:HOH:O	2.09	0.52
1:C:414:ARG:O	1:C:441:GLN:N	2.41	0.52
1:F:485:TYR:O	1:F:489:GLU:HG3	2.10	0.52
1:A:207:GLY:O	1:A:211:ILE:HG23	2.10	0.52
1:B:464:ASP:O	1:B:465:ASP:HB2	2.08	0.52
1:B:134:PRO:N	2:B:833:HOH:O	2.42	0.52
1:E:263:LEU:HD22	1:E:263:LEU:N	2.24	0.52
1:E:231:ASN:HD21	1:E:239:HIS:C	2.13	0.52
1:E:299:HIS:HE1	1:E:313:GLU:OE2	1.93	0.52
1:C:433:LEU:HD21	1:C:508:ARG:CZ	2.39	0.52
1:F:414:ARG:O	1:F:441:GLN:N	2.40	0.52
1:C:230:HIS:HA	1:C:234:SER:OG	2.10	0.52
1:F:470:ARG:O	1:F:474:ILE:HG13	2.10	0.52
1:A:438:PRO:HD3	1:A:497:ILE:O	2.08	0.52
1:F:197:VAL:HG22	2:F:829:HOH:O	2.09	0.52
1:E:457:ARG:HD2	1:E:457:ARG:N	2.24	0.52
1:F:363:CYS:HA	2:F:753:HOH:O	2.09	0.52
1:B:505:HIS:HA	1:B:508:ARG:HD2	1.91	0.52
1:D:508:ARG:CZ	1:F:62:VAL:HG11	2.40	0.52
1:A:62:VAL:HG21	1:C:508:ARG:CG	2.37	0.52
2:B:792:HOH:O	1:E:444:VAL:HG21	2.09	0.52
1:D:124:VAL:HB	2:D:801:HOH:O	2.09	0.51
1:C:505:HIS:C	1:C:508:ARG:HH11	2.14	0.51
1:A:455:HIS:O	1:A:459:ILE:HG12	2.10	0.51
1:C:343:GLN:N	2:C:810:HOH:O	2.43	0.51
1:B:168:GLY:HA3	2:E:797:HOH:O	2.09	0.51
1:C:336:ILE:HD12	2:C:856:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:505:HIS:ND1	1:E:508:ARG:CZ	2.74	0.51
1:A:211:ILE:CD1	1:A:217:GLU:HB2	2.40	0.51
1:B:139:ASN:HB3	2:B:554:HOH:O	2.10	0.51
1:C:158:GLU:O	1:C:162:ARG:HG2	2.09	0.51
1:E:62:VAL:CG2	1:F:508:ARG:HG3	2.33	0.51
1:C:25:ILE:HD13	1:C:67:PHE:CZ	2.46	0.51
1:A:262:ASN:OD1	1:A:263:LEU:HD13	2.11	0.51
1:A:472:ARG:O	1:A:476:GLU:HG3	2.10	0.51
1:E:175:LEU:HD23	1:E:195:VAL:HG13	1.92	0.51
1:E:70:HIS:HE1	1:E:80:ASN:O	1.94	0.51
1:F:259:PRO:HG3	2:F:828:HOH:O	2.11	0.51
1:A:457:ARG:HB2	2:A:675:HOH:O	2.09	0.51
1:C:261:ASN:OD1	1:C:263:LEU:HB2	2.10	0.51
1:D:235:GLY:HA2	2:D:783:HOH:O	2.11	0.51
1:F:238:HIS:HA	1:F:315:GLN:HG2	1.93	0.51
1:C:129:LEU:HD23	2:C:862:HOH:O	2.10	0.51
1:E:147:GLN:N	1:E:147:GLN:HE21	2.03	0.51
1:A:505:HIS:C	1:A:508:ARG:HH11	2.14	0.51
1:E:68:ALA:HA	1:F:489:GLU:HA	1.93	0.51
1:A:447:ALA:O	1:A:451:VAL:HG22	2.11	0.51
1:E:113:LEU:C	1:E:113:LEU:HD13	2.32	0.50
1:C:238:HIS:HA	1:C:315:GLN:HG2	1.92	0.50
1:B:336:ILE:N	1:B:336:ILE:HD12	2.25	0.50
1:A:424:MET:HE3	2:A:691:HOH:O	2.11	0.50
1:E:475:GLN:HA	1:E:478:GLU:OE1	2.10	0.50
1:A:230:HIS:HB3	1:A:236:VAL:HG22	1.91	0.50
1:B:26:GLU:O	1:B:30:HIS:HD2	1.94	0.50
1:A:271:GLU:HG3	1:A:271:GLU:O	2.12	0.50
1:E:337:VAL:O	1:E:372:THR:HA	2.11	0.50
1:F:332:ARG:HD3	1:F:514:ARG:NH2	2.26	0.50
2:C:714:HOH:O	1:F:392:ARG:HG2	2.11	0.50
1:B:35:ARG:O	1:B:39:LYS:HG3	2.11	0.50
1:E:505:HIS:HB3	1:E:508:ARG:NH1	2.27	0.50
1:C:203:MET:N	2:C:722:HOH:O	2.45	0.50
1:C:470:ARG:O	1:C:474:ILE:HG13	2.11	0.50
1:F:505:HIS:O	1:F:508:ARG:HD3	2.12	0.50
1:E:231:ASN:HD21	1:E:239:HIS:CA	2.24	0.50
1:D:176:VAL:HG22	2:D:855:HOH:O	2.11	0.50
1:C:101:VAL:HG22	1:C:102:PHE:N	2.27	0.50
1:E:481:LEU:N	1:E:481:LEU:HD22	2.27	0.50
1:F:451:VAL:HG21	1:F:474:ILE:CG1	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PHE:HB3	1:D:398:ILE:CD1	2.40	0.50
1:C:438:PRO:HD3	1:C:497:ILE:O	2.12	0.50
1:B:414:ARG:HG2	2:B:823:HOH:O	2.12	0.50
1:C:100:ALA:HB1	1:C:124:VAL:HG22	1.94	0.50
1:F:211:ILE:HD11	2:F:531:HOH:O	2.12	0.50
1:B:505:HIS:C	1:B:508:ARG:HH11	2.15	0.49
1:A:255:LEU:HA	2:A:669:HOH:O	2.12	0.49
1:F:106:PHE:HB3	2:F:815:HOH:O	2.12	0.49
1:F:336:ILE:HD12	1:F:336:ILE:N	2.27	0.49
1:C:70:HIS:HA	1:C:116:VAL:HG21	1.93	0.49
1:C:113:LEU:HG	1:C:156:TYR:CE1	2.47	0.49
1:C:345:ALA:N	2:C:810:HOH:O	2.45	0.49
1:D:191:THR:HB	2:D:835:HOH:O	2.11	0.49
1:E:169:VAL:HA	1:E:262:ASN:ND2	2.26	0.49
1:A:224:LEU:HD11	1:D:386:GLU:HG3	1.93	0.49
1:D:119:GLN:HG3	2:D:729:HOH:O	2.10	0.49
1:A:180:CYS:HB3	1:A:203:MET:HG2	1.94	0.49
1:F:397:LEU:HD13	1:F:423:VAL:HG12	1.94	0.49
1:C:266:PRO:HG2	2:C:543:HOH:O	2.12	0.49
1:F:241:ALA:HB3	2:F:829:HOH:O	2.12	0.49
1:E:93:THR:HG23	2:E:771:HOH:O	2.11	0.49
1:B:481:LEU:HD22	1:B:481:LEU:N	2.27	0.49
1:D:180:CYS:HB3	1:D:203:MET:HG2	1.93	0.49
1:D:505:HIS:O	1:D:508:ARG:HD3	2.12	0.49
1:A:62:VAL:CG1	1:C:508:ARG:HH21	2.24	0.49
1:B:289:PRO:HD2	2:B:743:HOH:O	2.11	0.49
1:D:169:VAL:HA	1:D:262:ASN:ND2	2.28	0.49
1:F:24:ARG:HA	2:F:835:HOH:O	2.11	0.49
1:B:113:LEU:HD22	1:B:117:TYR:CE1	2.48	0.49
1:F:302:ILE:O	1:F:305:VAL:HG22	2.12	0.49
1:A:147:GLN:HB2	2:A:712:HOH:O	2.11	0.49
1:F:100:ALA:HB1	1:F:124:VAL:HG22	1.94	0.49
1:B:11:ILE:HG23	1:B:12:HIS:ND1	2.28	0.49
1:A:340:GLN:CD	1:A:342:MET:HB2	2.33	0.49
1:A:99:VAL:HB	2:A:830:HOH:O	2.12	0.49
1:A:398:ILE:HG22	1:A:423:VAL:HG22	1.94	0.49
1:C:332:ARG:HD3	1:C:514:ARG:HH21	1.78	0.49
1:D:464:ASP:O	1:D:465:ASP:HB2	2.12	0.49
1:F:505:HIS:HA	1:F:508:ARG:HD2	1.95	0.49
1:A:231:ASN:HD21	1:A:239:HIS:CA	2.25	0.49
1:F:69:ARG:HD2	1:F:81:ARG:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ARG:HG2	2:D:786:HOH:O	2.13	0.49
1:A:238:HIS:HA	1:A:315:GLN:HG2	1.95	0.49
1:A:481:LEU:N	1:A:481:LEU:HD22	2.28	0.49
1:C:236:VAL:HG12	2:C:714:HOH:O	2.12	0.49
1:D:456:ARG:NH1	1:D:457:ARG:HH12	2.11	0.49
1:E:186:TYR:O	1:E:190:ILE:HG12	2.13	0.49
1:E:101:VAL:HG23	1:E:136:VAL:O	2.13	0.49
1:E:483:ASN:HB2	1:E:484:PRO:HD2	1.94	0.48
1:E:451:VAL:HB	2:E:703:HOH:O	2.12	0.48
1:B:231:ASN:HD21	1:B:239:HIS:CA	2.26	0.48
1:A:231:ASN:HD21	1:A:239:HIS:N	2.11	0.48
1:A:498:MET:HE2	2:B:810:HOH:O	2.13	0.48
1:D:508:ARG:HH21	1:F:62:VAL:CG1	2.24	0.48
1:C:490:ARG:HG3	2:C:824:HOH:O	2.12	0.48
1:A:299:HIS:HE1	1:A:313:GLU:OE2	1.95	0.48
1:A:169:VAL:CG2	1:D:523:LYS:HE2	2.43	0.48
1:B:162:ARG:HH11	1:B:162:ARG:HG2	1.78	0.48
1:B:101:VAL:HG22	1:B:102:PHE:N	2.28	0.48
1:A:219:VAL:HG12	2:A:576:HOH:O	2.12	0.48
1:F:107:THR:HG23	2:F:815:HOH:O	2.12	0.48
1:F:306:LEU:HD13	1:F:327:GLY:HA3	1.95	0.48
1:B:433:LEU:HD21	1:B:508:ARG:CZ	2.44	0.48
1:E:70:HIS:CE1	1:E:77:LEU:HD22	2.47	0.48
1:A:211:ILE:HD12	1:A:217:GLU:HB2	1.94	0.48
1:C:527:ASN:HD21	1:F:358:ARG:HD3	1.78	0.48
1:C:434:ASN:HB3	2:C:825:HOH:O	2.13	0.48
1:A:483:ASN:HB2	1:A:484:PRO:CD	2.43	0.48
1:B:190:ILE:HD11	1:E:398:ILE:HD11	1.94	0.48
1:D:158:GLU:O	1:D:162:ARG:HG2	2.13	0.48
1:D:501:ASP:CB	2:D:779:HOH:O	2.59	0.48
1:C:180:CYS:HB3	1:C:203:MET:HG2	1.96	0.48
1:D:398:ILE:HD12	1:D:398:ILE:C	2.34	0.48
1:F:454:LEU:HG	2:F:775:HOH:O	2.13	0.48
1:F:114:GLY:HA2	2:F:685:HOH:O	2.13	0.48
1:E:505:HIS:C	1:E:508:ARG:HH11	2.16	0.48
1:A:396:LYS:HD3	1:D:530:LEU:HG	1.96	0.48
1:B:176:VAL:HG12	1:B:201:SER:HB2	1.95	0.48
1:C:259:PRO:HG3	2:C:850:HOH:O	2.13	0.48
1:C:503:ARG:NH1	2:C:771:HOH:O	2.47	0.48
1:A:336:ILE:N	1:A:336:ILE:HD12	2.29	0.48
1:A:340:GLN:OE1	1:A:342:MET:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:LEU:HD13	2:D:608:HOH:O	2.13	0.48
1:E:317:LEU:HD13	2:E:748:HOH:O	2.13	0.48
1:B:508:ARG:CZ	1:C:62:VAL:HG11	2.43	0.48
1:D:496:VAL:HG22	2:D:834:HOH:O	2.14	0.48
1:C:464:ASP:O	1:C:465:ASP:HB3	2.14	0.48
1:A:372:THR:HG21	1:A:401:TYR:OH	2.14	0.48
1:C:337:VAL:O	1:C:372:THR:HA	2.13	0.48
1:E:438:PRO:HD3	1:E:497:ILE:O	2.14	0.48
1:A:113:LEU:HD13	1:A:113:LEU:C	2.34	0.48
1:B:146:ILE:HA	2:B:792:HOH:O	2.14	0.48
1:D:47:THR:OG1	1:D:50:GLU:HG3	2.13	0.48
1:C:299:HIS:HE1	1:C:313:GLU:OE2	1.97	0.48
1:C:397:LEU:HD13	1:C:423:VAL:HG12	1.96	0.48
1:D:483:ASN:HB2	1:D:484:PRO:CD	2.44	0.47
1:C:70:HIS:CD2	1:C:72:SER:H	2.11	0.47
1:B:508:ARG:NH2	1:C:62:VAL:HG11	2.29	0.47
1:E:230:HIS:HA	1:E:234:SER:OG	2.14	0.47
1:B:113:LEU:C	1:B:113:LEU:HD13	2.34	0.47
1:B:459:ILE:HD11	1:B:470:ARG:HB2	1.96	0.47
1:B:496:VAL:HG22	2:B:839:HOH:O	2.14	0.47
1:E:209:ASP:O	1:E:213:THR:HG23	2.14	0.47
1:A:89:THR:HB	1:A:124:VAL:HG21	1.95	0.47
1:A:56:LEU:HD13	1:A:92:GLY:HA3	1.96	0.47
1:D:321:ASN:ND2	1:D:352:ALA:HB2	2.29	0.47
1:F:319:ALA:N	1:F:320:PRO:HD3	2.29	0.47
1:A:391:ILE:O	2:A:843:HOH:O	2.19	0.47
1:D:398:ILE:HG13	1:D:399:PHE:N	2.28	0.47
1:E:238:HIS:HA	1:E:315:GLN:HG2	1.95	0.47
1:D:58:GLU:HG3	2:D:745:HOH:O	2.14	0.47
1:C:70:HIS:HE1	1:C:80:ASN:O	1.96	0.47
1:D:70:HIS:HE1	1:D:80:ASN:O	1.96	0.47
1:B:230:HIS:HA	1:B:234:SER:OG	2.15	0.47
1:B:45:LYS:HG2	1:B:200:THR:CG2	2.45	0.47
1:D:101:VAL:HG22	1:D:102:PHE:N	2.29	0.47
1:F:456:ARG:HB3	1:F:457:ARG:NH1	2.30	0.47
1:E:113:LEU:HD13	1:E:114:GLY:N	2.29	0.47
1:E:50:GLU:O	1:E:54:LEU:HD13	2.15	0.47
1:F:512:GLN:HB3	1:F:512:GLN:HE21	1.57	0.47
1:A:338:ALA:HB1	2:A:749:HOH:O	2.14	0.47
1:C:512:GLN:HB3	1:C:512:GLN:HE21	1.54	0.47
1:F:209:ASP:O	1:F:213:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:PRO:CD	2:B:833:HOH:O	2.63	0.47
1:C:346:GLY:N	2:C:810:HOH:O	2.46	0.47
1:F:516:LYS:HE2	1:F:518:GLU:HG3	1.97	0.47
1:B:302:ILE:O	1:B:305:VAL:HG22	2.15	0.47
1:F:70:HIS:CE1	1:F:81:ARG:HG2	2.50	0.47
1:A:391:ILE:C	2:A:843:HOH:O	2.53	0.47
1:B:372:THR:HG21	1:B:401:TYR:OH	2.15	0.47
1:B:522:PRO:HG2	2:B:793:HOH:O	2.15	0.47
1:F:101:VAL:HG22	1:F:102:PHE:N	2.30	0.47
1:E:187:SER:HB3	1:E:188:PRO:CD	2.34	0.46
1:A:393:ARG:HD3	2:A:625:HOH:O	2.14	0.46
1:B:505:HIS:CA	1:B:508:ARG:HH11	2.27	0.46
1:C:433:LEU:HD21	1:C:508:ARG:HH12	1.80	0.46
1:C:118:GLY:N	2:C:843:HOH:O	2.47	0.46
1:D:238:HIS:HA	1:D:315:GLN:HG2	1.97	0.46
1:C:451:VAL:HG21	1:C:474:ILE:CG1	2.45	0.46
1:D:422:ASP:O	1:D:429:LEU:HD22	2.15	0.46
1:C:386:GLU:HG3	1:F:224:LEU:HD11	1.96	0.46
1:A:89:THR:HB	1:A:124:VAL:CG2	2.46	0.46
1:E:69:ARG:HG3	1:F:489:GLU:HG2	1.96	0.46
1:A:146:ILE:HD12	1:D:453:ILE:HG21	1.98	0.46
1:B:386:GLU:HG3	1:E:224:LEU:HD11	1.97	0.46
1:A:77:LEU:HB3	2:A:723:HOH:O	2.14	0.46
1:F:508:ARG:HD3	1:F:509:GLY:H	1.75	0.46
1:A:508:ARG:HH21	1:B:62:VAL:CG1	2.27	0.46
1:B:398:ILE:C	1:B:398:ILE:HD12	2.36	0.46
1:C:208:PRO:O	1:C:211:ILE:HD13	2.15	0.46
1:D:191:THR:CB	2:D:835:HOH:O	2.63	0.46
1:E:35:ARG:NH1	1:E:39:LYS:NZ	2.64	0.46
1:D:299:HIS:HE1	1:D:313:GLU:OE2	1.97	0.46
1:D:139:ASN:HB3	2:D:720:HOH:O	2.15	0.46
1:B:358:ARG:HD3	1:E:527:ASN:HD21	1.80	0.46
1:B:435:LEU:HD22	1:B:435:LEU:N	2.31	0.46
1:A:10:ASP:N	2:A:823:HOH:O	2.47	0.46
1:E:62:VAL:HG11	1:F:508:ARG:NH2	2.31	0.46
1:B:507:VAL:HG11	2:B:841:HOH:O	2.16	0.46
1:C:302:ILE:O	1:C:305:VAL:HG22	2.15	0.46
1:D:261:ASN:OD1	1:D:263:LEU:HB2	2.16	0.46
1:E:69:ARG:HD2	1:E:81:ARG:O	2.15	0.46
1:E:101:VAL:HG22	1:E:102:PHE:N	2.31	0.46
1:E:466:ALA:O	1:E:469:THR:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:498:MET:HE2	2:E:708:HOH:O	2.16	0.46
1:F:219:VAL:CG2	1:F:223:GLU:HB3	2.45	0.46
1:D:134:PRO:CD	2:D:778:HOH:O	2.63	0.46
1:D:62:VAL:HG11	1:E:508:ARG:HH21	1.81	0.46
1:F:190:ILE:HD13	2:F:721:HOH:O	2.16	0.46
1:A:166:ALA:HB1	2:A:760:HOH:O	2.16	0.46
1:F:231:ASN:HD21	1:F:239:HIS:CA	2.29	0.46
1:F:158:GLU:O	1:F:162:ARG:HG2	2.16	0.46
1:A:358:ARG:HD3	1:D:527:ASN:HD21	1.81	0.46
1:F:483:ASN:HB2	1:F:484:PRO:CD	2.45	0.46
1:C:457:ARG:H	1:C:457:ARG:HD2	1.80	0.46
1:F:10:ASP:HB2	2:F:834:HOH:O	2.16	0.46
1:E:172:GLN:HG3	2:E:691:HOH:O	2.14	0.45
1:E:482:LEU:HD21	2:E:804:HOH:O	2.15	0.45
1:B:294:GLN:HA	1:B:295:PRO:HD3	1.83	0.45
1:D:438:PRO:HD3	1:D:497:ILE:O	2.17	0.45
1:C:173:ILE:HD12	1:C:173:ILE:N	2.31	0.45
1:D:65:ASP:HA	2:E:604:HOH:O	2.16	0.45
2:A:845:HOH:O	1:B:131:THR:HG22	2.15	0.45
1:F:275:LEU:HD21	1:F:507:VAL:HG11	1.98	0.45
1:E:520:LEU:HB3	1:E:521:PRO:CD	2.46	0.45
1:E:419:GLY:O	1:E:423:VAL:HG23	2.16	0.45
1:B:315:GLN:HB2	1:B:355:LYS:HE3	1.99	0.45
1:B:337:VAL:O	1:B:372:THR:HA	2.17	0.45
1:A:453:ILE:HG23	1:A:456:ARG:HH22	1.80	0.45
1:A:468:ALA:HA	1:A:471:ALA:HB3	1.99	0.45
1:D:175:LEU:HD22	1:D:177:VAL:HG13	1.98	0.45
1:F:47:THR:OG1	1:F:50:GLU:HG3	2.16	0.45
1:F:468:ALA:O	1:F:472:ARG:N	2.48	0.45
1:D:530:LEU:HB2	2:D:725:HOH:O	2.16	0.45
1:A:68:ALA:HA	1:C:489:GLU:HA	1.98	0.45
1:C:398:ILE:HD11	1:F:160:PHE:HB3	1.98	0.45
1:F:148:GLU:HB2	2:F:685:HOH:O	2.17	0.45
1:C:144:ALA:HA	2:C:854:HOH:O	2.17	0.45
1:D:25:ILE:HG22	1:D:67:PHE:HZ	1.81	0.45
1:B:489:GLU:HG3	2:C:728:HOH:O	2.17	0.45
1:E:180:CYS:HB3	1:E:203:MET:HG2	1.98	0.45
1:F:335:GLY:C	1:F:336:ILE:HD12	2.37	0.45
1:F:455:HIS:O	1:F:459:ILE:HG22	2.17	0.45
1:E:303:GLU:O	1:E:309:ALA:HA	2.17	0.45
1:F:432:ASP:HB2	1:F:513:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:483:ASN:ND2	2:E:654:HOH:O	2.44	0.45
1:D:176:VAL:HG12	1:D:201:SER:HB2	1.97	0.45
1:E:464:ASP:O	1:E:465:ASP:HB3	2.16	0.45
1:D:483:ASN:ND2	1:D:485:TYR:H	2.00	0.45
1:B:231:ASN:HD21	1:B:239:HIS:C	2.20	0.45
1:C:358:ARG:HD3	1:F:527:ASN:HD21	1.82	0.45
1:C:245:LYS:NZ	1:C:245:LYS:HB2	2.31	0.45
1:D:134:PRO:N	2:D:778:HOH:O	2.50	0.44
1:C:440:ALA:HB3	1:C:484:PRO:HB3	1.98	0.44
1:A:398:ILE:HD11	1:D:190:ILE:CD1	2.47	0.44
1:B:398:ILE:CD1	1:E:160:PHE:HB3	2.42	0.44
1:C:146:ILE:HG21	2:F:775:HOH:O	2.17	0.44
1:A:21:LEU:O	1:A:25:ILE:HG13	2.16	0.44
1:D:321:ASN:HD21	1:D:352:ALA:HB2	1.81	0.44
1:E:415:LYS:HD2	2:E:620:HOH:O	2.17	0.44
1:A:508:ARG:HG3	1:B:62:VAL:CG2	2.38	0.44
1:D:318:PHE:O	1:D:319:ALA:C	2.56	0.44
1:E:402:ALA:HA	1:E:429:LEU:O	2.17	0.44
1:A:254:LEU:CD1	1:A:312:PHE:HE2	2.31	0.44
1:F:162:ARG:HG2	1:F:162:ARG:HH11	1.83	0.44
1:F:475:GLN:NE2	2:F:652:HOH:O	2.50	0.44
1:C:339:ASN:ND2	2:C:724:HOH:O	2.50	0.44
1:E:10:ASP:N	2:E:634:HOH:O	2.49	0.44
1:E:26:GLU:O	1:E:30:HIS:HD2	2.01	0.44
1:E:494:ASP:HB2	2:E:773:HOH:O	2.17	0.44
1:B:433:LEU:HD21	1:B:508:ARG:NH2	2.32	0.44
1:D:43:LYS:HB2	2:D:824:HOH:O	2.18	0.44
1:D:11:ILE:N	2:D:581:HOH:O	2.50	0.44
1:D:46:LEU:N	1:D:46:LEU:HD12	2.32	0.44
1:B:483:ASN:HD22	1:B:485:TYR:H	1.65	0.44
1:F:434:ASN:HB3	2:F:747:HOH:O	2.17	0.44
1:D:414:ARG:C	2:D:851:HOH:O	2.44	0.44
1:E:483:ASN:ND2	1:E:485:TYR:H	1.99	0.44
1:D:70:HIS:CE1	1:D:81:ARG:HG2	2.53	0.44
1:A:505:HIS:O	1:A:508:ARG:CD	2.66	0.44
1:C:336:ILE:CD1	2:C:856:HOH:O	2.66	0.44
1:B:161:ARG:NE	2:E:758:HOH:O	2.50	0.44
1:A:516:LYS:N	2:A:845:HOH:O	2.49	0.44
1:C:483:ASN:ND2	2:C:831:HOH:O	2.49	0.44
1:A:398:ILE:HD12	1:A:398:ILE:C	2.37	0.44
1:D:498:MET:HE1	1:F:21:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:LEU:O	1:D:25:ILE:HG23	2.17	0.44
1:D:489:GLU:HA	1:F:68:ALA:HA	2.00	0.44
1:A:512:GLN:NE2	2:A:715:HOH:O	2.50	0.44
1:E:70:HIS:HD2	1:E:72:SER:N	2.12	0.44
1:E:113:LEU:C	1:E:113:LEU:CD1	2.86	0.44
1:D:212:LYS:C	1:D:214:VAL:H	2.21	0.44
1:B:474:ILE:O	1:B:478:GLU:HG2	2.17	0.44
1:E:480:ALA:HB3	1:E:481:LEU:HD22	1.98	0.44
2:B:549:HOH:O	1:E:386:GLU:HG2	2.18	0.44
1:A:464:ASP:O	1:A:465:ASP:HB3	2.17	0.44
1:B:113:LEU:C	1:B:113:LEU:CD1	2.86	0.44
1:B:145:ARG:HD2	1:B:148:GLU:OE2	2.18	0.44
1:A:235:GLY:HA2	2:A:642:HOH:O	2.17	0.44
1:D:505:HIS:C	1:D:508:ARG:HH11	2.16	0.44
1:D:230:HIS:HA	1:D:234:SER:OG	2.18	0.44
1:E:332:ARG:HD3	1:E:514:ARG:CZ	2.48	0.44
1:F:208:PRO:O	1:F:211:ILE:HG13	2.17	0.44
1:C:210:VAL:HA	1:C:213:THR:HG22	1.99	0.44
1:B:422:ASP:O	1:B:429:LEU:HD22	2.17	0.44
1:E:56:LEU:HD12	1:E:61:PHE:HB2	2.00	0.44
1:D:232:SER:HB3	1:D:317:LEU:HB3	1.99	0.44
1:B:227:ALA:HB1	1:B:240:MET:HG3	2.00	0.43
1:F:29:THR:HG21	2:F:795:HOH:O	2.16	0.43
1:B:176:VAL:HG22	2:B:741:HOH:O	2.16	0.43
1:F:427:LYS:HA	1:F:431:ALA:HB3	2.00	0.43
1:F:248:VAL:O	1:F:251:VAL:CG1	2.66	0.43
1:D:507:VAL:O	1:D:511:ARG:HG3	2.18	0.43
1:C:438:PRO:HD3	2:C:806:HOH:O	2.19	0.43
1:E:60:SER:HB2	2:E:771:HOH:O	2.18	0.43
1:E:467:GLU:O	1:E:468:ALA:HB3	2.18	0.43
1:F:452:ASN:ND2	1:F:470:ARG:HH11	2.16	0.43
1:E:332:ARG:HD2	2:E:629:HOH:O	2.19	0.43
1:A:319:ALA:N	1:A:320:PRO:HD3	2.32	0.43
1:C:483:ASN:HB2	1:C:484:PRO:CD	2.49	0.43
1:C:483:ASN:HD22	1:C:485:TYR:N	2.04	0.43
1:C:103:SER:HA	1:C:138:ILE:HB	2.00	0.43
1:B:200:THR:O	1:B:200:THR:HG22	2.17	0.43
1:A:73:THR:C	2:A:723:HOH:O	2.57	0.43
1:E:486:THR:O	1:E:490:ARG:HG2	2.18	0.43
1:C:231:ASN:HD21	1:C:239:HIS:CA	2.32	0.43
1:A:350:ILE:HG13	1:A:385:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:LEU:HD22	1:E:117:TYR:CE1	2.53	0.43
1:F:29:THR:O	1:F:29:THR:HG22	2.17	0.43
1:A:302:ILE:O	1:A:305:VAL:HG22	2.19	0.43
1:D:495:ALA:HB2	2:D:554:HOH:O	2.19	0.43
1:C:45:LYS:HG2	1:C:200:THR:HG23	1.99	0.43
1:A:442:ILE:HD12	1:A:484:PRO:HA	2.00	0.43
1:F:254:LEU:HD13	1:F:312:PHE:CE2	2.41	0.43
1:D:411:VAL:C	2:D:814:HOH:O	2.57	0.43
1:C:454:LEU:HD11	2:C:801:HOH:O	2.18	0.43
1:B:39:LYS:HZ3	1:B:39:LYS:HB3	1.82	0.43
1:A:144:ALA:HB1	1:A:152:SER:OG	2.19	0.43
1:F:70:HIS:CD2	1:F:72:SER:H	2.19	0.43
1:D:456:ARG:NH1	1:D:457:ARG:NH1	2.64	0.43
1:D:473:LEU:HA	2:D:655:HOH:O	2.18	0.43
1:C:75:PHE:CZ	1:F:454:LEU:HD13	2.54	0.43
1:A:146:ILE:HG13	1:A:146:ILE:H	1.62	0.43
1:F:112:ALA:HA	1:F:143:GLY:O	2.19	0.43
1:A:69:ARG:HD3	1:A:83:TYR:CD2	2.53	0.43
1:A:398:ILE:CG1	1:D:190:ILE:HD11	2.48	0.43
1:D:374:VAL:HG23	2:D:814:HOH:O	2.19	0.43
1:B:361:ARG:NH2	1:E:528:ILE:HG22	2.33	0.43
1:C:294:GLN:HA	1:C:295:PRO:HD3	1.82	0.43
1:D:472:ARG:NH1	2:D:655:HOH:O	2.51	0.43
1:E:414:ARG:O	1:E:440:ALA:HA	2.19	0.43
1:F:299:HIS:HE1	1:F:313:GLU:OE2	2.01	0.43
1:E:512:GLN:HE21	1:E:512:GLN:HB3	1.56	0.43
1:D:101:VAL:CG2	1:D:102:PHE:N	2.81	0.42
1:E:147:GLN:N	1:E:147:GLN:NE2	2.57	0.42
1:A:266:PRO:HG2	2:A:593:HOH:O	2.19	0.42
1:D:40:GLN:CD	1:D:45:LYS:HE3	2.39	0.42
1:A:172:GLN:HG3	2:A:760:HOH:O	2.18	0.42
1:E:453:ILE:HG23	1:E:456:ARG:HH22	1.84	0.42
1:B:209:ASP:HB2	2:B:803:HOH:O	2.19	0.42
1:D:483:ASN:ND2	1:D:485:TYR:HB2	2.34	0.42
1:B:512:GLN:HE21	1:B:512:GLN:HB3	1.66	0.42
1:C:508:ARG:HD3	1:C:509:GLY:H	1.80	0.42
1:A:508:ARG:CZ	1:B:62:VAL:HG11	2.49	0.42
1:C:21:LEU:O	1:C:25:ILE:HG12	2.18	0.42
1:D:16:GLY:HA3	2:D:581:HOH:O	2.18	0.42
1:C:231:ASN:HD21	1:C:239:HIS:N	2.17	0.42
1:C:407:PRO:HB3	1:C:513:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:SER:O	1:E:179:PRO:HB2	2.19	0.42
1:A:372:THR:HB	2:A:763:HOH:O	2.19	0.42
1:F:370:VAL:HG22	2:F:675:HOH:O	2.18	0.42
1:D:69:ARG:HH21	1:D:81:ARG:HB2	1.85	0.42
1:B:508:ARG:HG3	1:C:62:VAL:CG2	2.41	0.42
1:F:73:THR:C	2:F:724:HOH:O	2.58	0.42
1:C:429:LEU:HG	2:F:730:HOH:O	2.18	0.42
1:A:347:CYS:SG	1:A:377:PRO:HG2	2.59	0.42
1:F:180:CYS:HB3	1:F:203:MET:HG2	2.01	0.42
1:D:514:ARG:HD2	2:D:808:HOH:O	2.18	0.42
1:B:505:HIS:O	1:B:508:ARG:NH1	2.48	0.42
1:C:114:GLY:H	1:C:117:TYR:HB3	1.85	0.42
1:D:113:LEU:HD22	1:D:117:TYR:CE1	2.54	0.42
1:B:382:GLY:N	1:E:211:ILE:HG22	2.35	0.42
1:B:414:ARG:O	1:B:440:ALA:HA	2.20	0.42
1:C:45:LYS:HG2	1:C:200:THR:CG2	2.49	0.42
1:A:420:ALA:HB3	2:A:707:HOH:O	2.20	0.42
1:A:46:LEU:HD13	1:A:244:GLU:OE2	2.18	0.42
1:A:332:ARG:CZ	1:A:514:ARG:NH2	2.75	0.42
1:D:114:GLY:H	1:D:117:TYR:HB3	1.84	0.42
1:D:374:VAL:HG22	1:D:424:MET:HB3	2.01	0.42
1:F:207:GLY:O	1:F:211:ILE:HG23	2.19	0.42
1:F:152:SER:HB2	2:F:685:HOH:O	2.19	0.42
1:E:527:ASN:HB2	2:E:745:HOH:O	2.19	0.42
1:A:55:LEU:O	1:A:252:LYS:HE2	2.20	0.42
1:C:235:GLY:HA2	2:C:638:HOH:O	2.20	0.42
1:D:324:THR:HA	1:D:336:ILE:O	2.19	0.42
1:B:103:SER:HA	1:B:138:ILE:HB	2.01	0.42
1:C:190:ILE:HD11	1:F:398:ILE:HD11	2.00	0.42
1:A:505:HIS:HB3	1:A:508:ARG:NH1	2.34	0.42
1:D:361:ARG:NH2	2:D:533:HOH:O	2.40	0.42
1:E:70:HIS:HA	1:E:116:VAL:CG2	2.49	0.42
1:F:177:VAL:HG12	1:F:197:VAL:CG2	2.49	0.42
1:A:374:VAL:HG22	1:A:424:MET:HB3	2.02	0.42
1:C:46:LEU:HB2	1:C:244:GLU:OE2	2.19	0.42
1:C:319:ALA:N	1:C:320:PRO:HD3	2.33	0.42
1:C:26:GLU:O	1:C:30:HIS:HD2	2.02	0.42
1:F:77:LEU:HD12	2:F:809:HOH:O	2.20	0.42
1:F:185:VAL:O	1:F:188:PRO:HD2	2.19	0.42
1:C:341:PRO:C	2:C:810:HOH:O	2.57	0.42
1:A:520:LEU:HB3	1:A:521:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:GLU:O	1:A:30:HIS:HD2	2.03	0.42
1:E:182:GLY:O	1:E:185:VAL:HG22	2.19	0.42
1:C:315:GLN:NE2	2:C:559:HOH:O	2.42	0.42
1:B:489:GLU:HA	1:C:68:ALA:HA	2.00	0.42
1:B:483:ASN:HB2	1:B:484:PRO:HD2	2.01	0.42
1:A:130:LYS:HE2	2:C:807:HOH:O	2.19	0.42
1:B:498:MET:HE3	1:C:18:LEU:HD13	2.02	0.42
1:D:89:THR:HB	1:D:124:VAL:CG2	2.50	0.42
1:E:295:PRO:HB2	1:E:342:MET:HE1	1.98	0.42
1:E:195:VAL:HG13	1:E:195:VAL:O	2.20	0.42
1:E:448:GLN:O	1:E:451:VAL:HG22	2.20	0.42
1:F:230:HIS:HB2	2:F:831:HOH:O	2.19	0.42
1:B:115:GLU:HG3	2:B:760:HOH:O	2.19	0.42
1:F:104:GLN:HB3	2:F:630:HOH:O	2.20	0.41
1:B:361:ARG:HH21	1:E:528:ILE:HG22	1.85	0.41
1:A:490:ARG:HD3	2:A:659:HOH:O	2.20	0.41
1:C:390:ILE:HG13	1:F:205:ILE:CD1	2.50	0.41
1:F:69:ARG:HD3	1:F:83:TYR:CD2	2.55	0.41
1:B:188:PRO:HG2	2:B:741:HOH:O	2.19	0.41
1:A:530:LEU:HA	1:A:530:LEU:HD12	1.85	0.41
1:F:441:GLN:HG2	1:F:482:LEU:O	2.19	0.41
1:B:508:ARG:HE	1:C:62:VAL:HG11	1.86	0.41
1:C:456:ARG:HD2	1:C:457:ARG:NH2	2.36	0.41
1:A:200:THR:HG21	2:A:620:HOH:O	2.20	0.41
1:D:285:ASP:OD1	1:D:499:PRO:HD2	2.19	0.41
1:B:118:GLY:HA3	1:B:155:ALA:HB1	2.02	0.41
1:B:347:CYS:SG	1:B:377:PRO:HG2	2.61	0.41
1:B:238:HIS:HA	1:B:315:GLN:HG2	2.03	0.41
1:B:26:GLU:O	1:B:30:HIS:CD2	2.72	0.41
1:B:498:MET:CE	1:C:18:LEU:HD13	2.50	0.41
1:C:443:ALA:HB1	2:C:834:HOH:O	2.20	0.41
1:D:376:VAL:HG13	1:D:376:VAL:O	2.20	0.41
1:A:332:ARG:CD	1:A:514:ARG:HH21	2.34	0.41
1:C:473:LEU:HD12	1:C:473:LEU:HA	1.92	0.41
1:B:414:ARG:HA	1:B:440:ALA:HA	2.03	0.41
1:A:337:VAL:O	1:A:372:THR:HA	2.20	0.41
1:B:266:PRO:HG2	2:B:583:HOH:O	2.19	0.41
1:D:146:ILE:H	1:D:146:ILE:HG13	1.69	0.41
1:D:62:VAL:HG11	1:E:508:ARG:NH2	2.35	0.41
1:B:71:ARG:NH2	1:B:119:GLN:HE22	2.05	0.41
1:D:508:ARG:HB3	2:D:797:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:VAL:HG13	2:A:842:HOH:O	2.20	0.41
1:A:77:LEU:N	2:A:723:HOH:O	2.54	0.41
1:C:348:LEU:HG	2:C:724:HOH:O	2.19	0.41
1:B:70:HIS:O	1:B:81:ARG:HD2	2.21	0.41
1:E:528:ILE:HD12	2:E:739:HOH:O	2.20	0.41
1:E:375:ASP:CG	1:E:414:ARG:HB3	2.40	0.41
1:A:434:ASN:HB3	2:A:670:HOH:O	2.20	0.41
1:D:509:GLY:O	1:D:513:LEU:HB2	2.21	0.41
1:A:62:VAL:CG2	1:C:508:ARG:HG3	2.43	0.41
1:F:145:ARG:HD2	1:F:148:GLU:OE2	2.20	0.41
1:B:517:ARG:NH2	2:B:629:HOH:O	2.46	0.41
1:B:315:GLN:N	1:B:316:PRO:CD	2.82	0.41
1:D:81:ARG:HD3	2:D:656:HOH:O	2.21	0.41
1:D:508:ARG:HG3	1:F:62:VAL:CG2	2.41	0.41
1:A:508:ARG:HD3	1:A:509:GLY:H	1.85	0.41
1:D:498:MET:CE	1:F:21:LEU:HD23	2.51	0.41
1:E:74:ASN:O	1:E:77:LEU:HB2	2.21	0.41
1:E:68:ALA:C	1:E:69:ARG:HG2	2.41	0.41
1:C:114:GLY:O	2:C:843:HOH:O	2.22	0.41
1:D:321:ASN:HA	1:D:343:GLN:HB2	2.01	0.41
1:A:150:VAL:HG23	2:D:706:HOH:O	2.20	0.41
1:D:284:LEU:HD13	1:D:304:HIS:CD2	2.55	0.41
1:E:219:VAL:HG22	1:E:220:GLY:N	2.36	0.41
1:B:180:CYS:HB3	1:B:203:MET:HG2	2.01	0.41
1:D:505:HIS:HB3	1:D:508:ARG:NH1	2.36	0.41
1:E:69:ARG:HB3	2:E:777:HOH:O	2.21	0.41
1:C:321:ASN:HA	1:C:343:GLN:HB2	2.03	0.41
1:C:344:PHE:O	1:C:345:ALA:HB3	2.21	0.41
1:D:231:ASN:HD21	1:D:239:HIS:CA	2.34	0.41
1:F:177:VAL:HG12	1:F:197:VAL:HG21	2.03	0.41
1:D:195:VAL:HG11	1:D:251:VAL:HG12	2.03	0.41
1:E:318:PHE:CZ	1:E:351:THR:HB	2.56	0.41
1:D:440:ALA:HB3	1:D:484:PRO:HB3	2.02	0.40
1:D:51:ARG:NH1	2:D:838:HOH:O	2.52	0.40
1:E:483:ASN:HB2	1:E:484:PRO:CD	2.51	0.40
1:E:252:LYS:HE2	2:E:600:HOH:O	2.20	0.40
1:F:24:ARG:HD3	1:F:83:TYR:OH	2.21	0.40
1:F:104:GLN:HB3	1:F:117:TYR:OH	2.21	0.40
1:C:473:LEU:HD12	1:C:476:GLU:OE1	2.21	0.40
1:B:517:ARG:HH11	1:B:517:ARG:HG3	1.86	0.40
1:D:490:ARG:HG3	2:D:706:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LYS:O	1:A:43:LYS:HG3	2.21	0.40
1:E:158:GLU:O	1:E:162:ARG:HG2	2.21	0.40
1:F:113:LEU:HG	1:F:156:TYR:CE1	2.56	0.40
1:A:172:GLN:CG	2:A:760:HOH:O	2.69	0.40
1:F:367:ASN:ND2	2:F:828:HOH:O	2.54	0.40
1:B:230:HIS:HB3	1:B:236:VAL:CG2	2.51	0.40
1:F:248:VAL:HA	1:F:251:VAL:HG12	2.03	0.40
1:F:370:VAL:HG13	2:F:675:HOH:O	2.19	0.40
1:F:200:THR:O	1:F:200:THR:CG2	2.69	0.40
1:A:433:LEU:HD21	1:A:508:ARG:CZ	2.50	0.40
1:A:455:HIS:CB	1:A:473:LEU:HD23	2.51	0.40
1:F:113:LEU:C	1:F:113:LEU:HD13	2.41	0.40
1:F:315:GLN:N	1:F:316:PRO:CD	2.82	0.40
1:C:332:ARG:HD3	1:C:514:ARG:NH2	2.36	0.40
1:E:232:SER:HB3	1:E:317:LEU:HB3	2.02	0.40
1:E:520:LEU:N	1:E:520:LEU:HD12	2.36	0.40
1:A:123:LYS:HD2	2:C:569:HOH:O	2.21	0.40
1:F:462:ALA:O	1:F:464:ASP:O	2.40	0.40
1:D:26:GLU:O	1:D:30:HIS:HD2	2.03	0.40
1:E:294:GLN:HA	1:E:295:PRO:HD3	1.87	0.40
1:B:398:ILE:HD12	1:B:398:ILE:O	2.21	0.40
1:C:343:GLN:C	2:C:810:HOH:O	2.60	0.40
1:D:113:LEU:HG	1:D:156:TYR:CE1	2.57	0.40
1:F:211:ILE:CD1	1:F:217:GLU:HB2	2.51	0.40
1:E:386:GLU:HA	1:E:390:ILE:HG22	2.03	0.40
1:D:103:SER:HA	1:D:138:ILE:HB	2.04	0.40
1:B:316:PRO:HG2	2:B:683:HOH:O	2.21	0.40
1:A:332:ARG:NE	1:A:514:ARG:NH2	2.62	0.40
1:D:40:GLN:OE1	1:D:45:LYS:HE3	2.20	0.40
1:B:43:LYS:HE2	2:B:686:HOH:O	2.22	0.40
1:A:146:ILE:CD1	1:D:453:ILE:HG21	2.52	0.40
1:C:335:GLY:HA3	2:C:777:HOH:O	2.22	0.40
1:E:529:PRO:HD3	2:E:766:HOH:O	2.22	0.40
1:F:517:ARG:NH2	2:F:718:HOH:O	2.54	0.40
1:C:461:ASP:O	1:C:462:ALA:HB3	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	519/530 (98%)	499 (96%)	18 (4%)	2 (0%)	39	42
1	B	519/530 (98%)	496 (96%)	21 (4%)	2 (0%)	39	42
1	C	519/530 (98%)	501 (96%)	18 (4%)	0	100	100
1	D	519/530 (98%)	499 (96%)	18 (4%)	2 (0%)	39	42
1	E	519/530 (98%)	500 (96%)	17 (3%)	2 (0%)	39	42
1	F	519/530 (98%)	497 (96%)	20 (4%)	2 (0%)	39	42
All	All	3114/3180 (98%)	2992 (96%)	112 (4%)	10 (0%)	46	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ILE
1	E	11	ILE
1	A	199	GLN
1	B	11	ILE
1	B	468	ALA
1	F	468	ALA
1	D	146	ILE
1	D	213	THR
1	E	146	ILE
1	F	11	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%)	389 (94%)	23 (6%)	26	29
1	B	412/421 (98%)	392 (95%)	20 (5%)	31	36
1	C	412/421 (98%)	389 (94%)	23 (6%)	26	29
1	D	412/421 (98%)	387 (94%)	25 (6%)	23	26
1	E	412/421 (98%)	397 (96%)	15 (4%)	42	52
1	F	412/421 (98%)	393 (95%)	19 (5%)	33	40
All	All	2472/2526 (98%)	2347 (95%)	125 (5%)	29	34

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	77	LEU
1	A	117	TYR
1	A	147	GLN
1	A	161	ARG
1	A	175	LEU
1	A	209	ASP
1	A	211	ILE
1	A	254	LEU
1	A	263	LEU
1	A	274	ASP
1	A	284	LEU
1	A	342	MET
1	A	358	ARG
1	A	387	HIS
1	A	397	LEU
1	A	398	ILE
1	A	435	LEU
1	A	475	GLN
1	A	484	PRO
1	A	508	ARG
1	A	513	LEU
1	A	530	LEU
1	B	40	GLN
1	B	77	LEU
1	B	113	LEU
1	B	117	TYR
1	B	147	GLN
1	B	175	LEU
1	B	251	VAL

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Mol	Chain	Res	Type
1	B	263	LEU
1	B	284	LEU
1	B	310	GLU
1	B	358	ARG
1	B	380	LEU
1	B	387	HIS
1	B	397	LEU
1	B	398	ILE
1	B	461	ASP
1	B	475	GLN
1	B	483	ASN
1	B	508	ARG
1	B	530	LEU
1	C	40	GLN
1	C	54	LEU
1	C	77	LEU
1	C	113	LEU
1	C	117	TYR
1	C	147	GLN
1	C	211	ILE
1	C	263	LEU
1	C	284	LEU
1	C	358	ARG
1	C	397	LEU
1	C	398	ILE
1	C	435	LEU
1	C	457	ARG
1	C	473	LEU
1	C	475	GLN
1	C	483	ASN
1	C	484	PRO
1	C	508	ARG
1	C	512	GLN
1	C	513	LEU
1	C	527	ASN
1	C	530	LEU
1	D	22	ARG
1	D	40	GLN
1	D	54	LEU
1	D	77	LEU
1	D	113	LEU
1	D	117	TYR

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Mol	Chain	Res	Type
1	D	175	LEU
1	D	195	VAL
1	D	263	LEU
1	D	284	LEU
1	D	310	GLU
1	D	358	ARG
1	D	372	THR
1	D	387	HIS
1	D	397	LEU
1	D	398	ILE
1	D	429	LEU
1	D	435	LEU
1	D	473	LEU
1	D	475	GLN
1	D	484	PRO
1	D	508	ARG
1	D	512	GLN
1	D	513	LEU
1	D	530	LEU
1	E	40	GLN
1	E	77	LEU
1	E	113	LEU
1	E	117	TYR
1	E	147	GLN
1	E	175	LEU
1	E	284	LEU
1	E	310	GLU
1	E	358	ARG
1	E	397	LEU
1	E	475	GLN
1	E	483	ASN
1	E	508	ARG
1	E	512	GLN
1	E	530	LEU
1	F	22	ARG
1	F	40	GLN
1	F	77	LEU
1	F	113	LEU
1	F	117	TYR
1	F	147	GLN
1	F	254	LEU
1	F	310	GLU

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Mol	Chain	Res	Type
1	F	347	CYS
1	F	358	ARG
1	F	387	HIS
1	F	397	LEU
1	F	398	ILE
1	F	467	GLU
1	F	484	PRO
1	F	508	ARG
1	F	512	GLN
1	F	513	LEU
1	F	530	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	40	GLN
1	A	70	HIS
1	A	74	ASN
1	A	147	GLN
1	A	199	GLN
1	A	231	ASN
1	A	294	GLN
1	A	299	HIS
1	A	315	GLN
1	A	387	HIS
1	A	475	GLN
1	A	483	ASN
1	A	512	GLN
1	A	527	ASN
1	B	30	HIS
1	B	40	GLN
1	B	70	HIS
1	B	119	GLN
1	B	147	GLN
1	B	231	ASN
1	B	299	HIS
1	B	475	GLN
1	B	483	ASN
1	B	512	GLN
1	B	527	ASN
1	C	30	HIS

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Mol	Chain	Res	Type
1	C	40	GLN
1	C	70	HIS
1	C	74	ASN
1	C	119	GLN
1	C	147	GLN
1	C	163	ASN
1	C	231	ASN
1	C	299	HIS
1	C	387	HIS
1	C	448	GLN
1	C	455	HIS
1	C	475	GLN
1	C	483	ASN
1	C	512	GLN
1	C	527	ASN
1	D	30	HIS
1	D	40	GLN
1	D	70	HIS
1	D	74	ASN
1	D	119	GLN
1	D	231	ASN
1	D	299	HIS
1	D	448	GLN
1	D	455	HIS
1	D	483	ASN
1	D	512	GLN
1	D	527	ASN
1	E	30	HIS
1	E	40	GLN
1	E	70	HIS
1	E	74	ASN
1	E	147	GLN
1	E	163	ASN
1	E	199	GLN
1	E	231	ASN
1	E	299	HIS
1	E	387	HIS
1	E	475	GLN
1	E	483	ASN
1	E	512	GLN
1	E	527	ASN
1	F	40	GLN

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Mol	Chain	Res	Type
1	F	70	HIS
1	F	74	ASN
1	F	147	GLN
1	F	199	GLN
1	F	231	ASN
1	F	299	HIS
1	F	387	HIS
1	F	448	GLN
1	F	452	ASN
1	F	483	ASN
1	F	512	GLN
1	F	527	ASN

5.3.3 RNA [i](#)

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 carbohydrates 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	521/530 (98%)	-0.38	5 (0%) 84 83	20, 32, 51, 98	0
1	B	521/530 (98%)	-0.33	5 (0%) 84 83	23, 34, 54, 100	0
1	C	521/530 (98%)	-0.22	4 (0%) 87 87	21, 32, 51, 84	0
1	D	521/530 (98%)	-0.28	8 (1%) 76 75	19, 31, 50, 86	0
1	E	521/530 (98%)	-0.32	6 (1%) 81 80	22, 35, 53, 99	0
1	F	521/530 (98%)	-0.29	10 (1%) 70 68	18, 34, 55, 100	0
All	All	3126/3180 (98%)	-0.30	38 (1%) 81 80	18, 33, 53, 100	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	464	ASP	5.0
1	B	464	ASP	4.5
1	F	464	ASP	4.4
1	F	508	ARG	4.4
1	C	464	ASP	4.1
1	E	508	ARG	4.0
1	F	468	ALA	3.9
1	F	466	ALA	3.9
1	D	457	ARG	3.8
1	B	466	ALA	3.7
1	D	464	ASP	3.7
1	F	463	GLY	3.7
1	C	508	ARG	3.3
1	A	508	ARG	3.2
1	D	462	ALA	3.2
1	E	464	ASP	2.9
1	F	459	ILE	2.9
1	F	457	ARG	2.7
1	B	508	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	463	GLY	2.6
1	B	465	ASP	2.6
1	F	465	ASP	2.5
1	A	466	ALA	2.5
1	C	269	PHE	2.4
1	C	460	ALA	2.4
1	D	463	GLY	2.4
1	E	10	ASP	2.3
1	F	460	ALA	2.3
1	D	508	ARG	2.3
1	B	468	ALA	2.3
1	E	457	ARG	2.3
1	E	462	ALA	2.2
1	D	10	ASP	2.2
1	E	465	ASP	2.2
1	F	462	ALA	2.2
1	D	459	ILE	2.1
1	A	269	PHE	2.1
1	D	466	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.