Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 10:12 am BST

PDB ID	:	2B7M
Title	:	Crystal Structure of the S. cerevisiae Exocyst Component Exo70p
Authors	:	Hamburger, Z.A.; Hamburger, A.E.; West, A.P.; Weis, W.I.
Deposited on	:	2005-10-04
Resolution	:	3.50 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

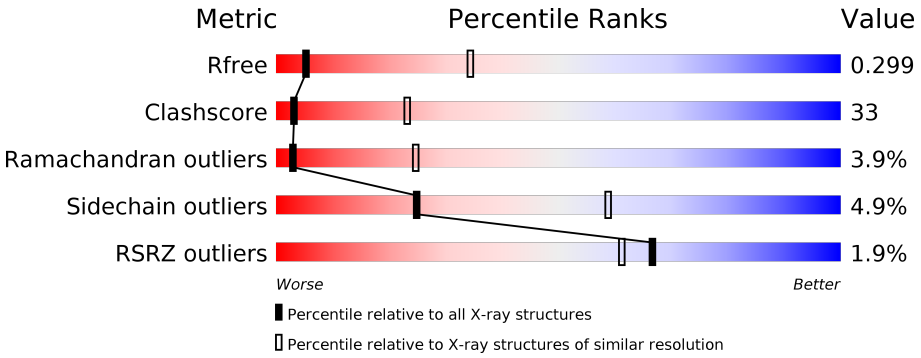
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	566	2% 36% 50% • 9%
1	B	566	2% 38% 49% 5% 8%
1	C	566	% 41% 46% 5% 8%
1	D	566	% 41% 47% • 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 16823 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 Exocyst complex component EXO70.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	513	Total	C	N	O	S	Se	0	0	0
			4153	2637	703	795	5	13			
1	B	523	Total	C	N	O	S	Se	0	0	0
			4247	2699	721	809	5	13			
1	C	518	Total	C	N	O	S	Se	0	0	0
			4205	2676	712	799	5	13			
1	D	520	Total	C	N	O	S	Se	0	0	0
			4218	2683	715	802	5	13			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	GLY	-	CLONING ARTIFACT	UNP P19658
A	59	ALA	-	CLONING ARTIFACT	UNP P19658
A	60	MSE	-	CLONING ARTIFACT	UNP P19658
A	61	GLY	-	CLONING ARTIFACT	UNP P19658
A	62	SER	-	CLONING ARTIFACT	UNP P19658
A	110	MSE	MET	MODIFIED RESIDUE	UNP P19658
A	169	MSE	MET	MODIFIED RESIDUE	UNP P19658
A	214	MSE	MET	MODIFIED RESIDUE	UNP P19658
A	239	MSE	MET	MODIFIED RESIDUE	UNP P19658
A	376	MSE	MET	MODIFIED RESIDUE	UNP P19658
A	393	MSE	MET	MODIFIED RESIDUE	UNP P19658
A	451	MSE	MET	MODIFIED RESIDUE	UNP P19658
A	478	MSE	MET	MODIFIED RESIDUE	UNP P19658
A	495	MSE	MET	MODIFIED RESIDUE	UNP P19658
A	515	MSE	MET	MODIFIED RESIDUE	UNP P19658
A	527	MSE	MET	MODIFIED RESIDUE	UNP P19658
A	586	MSE	MET	MODIFIED RESIDUE	UNP P19658
A	588	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	58	GLY	-	CLONING ARTIFACT	UNP P19658
B	59	ALA	-	CLONING ARTIFACT	UNP P19658
B	60	MSE	-	CLONING ARTIFACT	UNP P19658

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Chain	Residue	Modelled	Actual	Comment	Reference
B	61	GLY	-	CLONING ARTIFACT	UNP P19658
B	62	SER	-	CLONING ARTIFACT	UNP P19658
B	110	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	169	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	214	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	239	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	376	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	393	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	451	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	478	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	495	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	515	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	527	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	586	MSE	MET	MODIFIED RESIDUE	UNP P19658
B	588	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	58	GLY	-	CLONING ARTIFACT	UNP P19658
C	59	ALA	-	CLONING ARTIFACT	UNP P19658
C	60	MSE	-	CLONING ARTIFACT	UNP P19658
C	61	GLY	-	CLONING ARTIFACT	UNP P19658
C	62	SER	-	CLONING ARTIFACT	UNP P19658
C	110	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	169	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	214	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	239	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	376	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	393	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	451	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	478	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	495	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	515	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	527	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	586	MSE	MET	MODIFIED RESIDUE	UNP P19658
C	588	MSE	MET	MODIFIED RESIDUE	UNP P19658
D	58	GLY	-	CLONING ARTIFACT	UNP P19658
D	59	ALA	-	CLONING ARTIFACT	UNP P19658
D	60	MSE	-	CLONING ARTIFACT	UNP P19658
D	61	GLY	-	CLONING ARTIFACT	UNP P19658
D	62	SER	-	CLONING ARTIFACT	UNP P19658
D	110	MSE	MET	MODIFIED RESIDUE	UNP P19658
D	169	MSE	MET	MODIFIED RESIDUE	UNP P19658
D	214	MSE	MET	MODIFIED RESIDUE	UNP P19658
D	239	MSE	MET	MODIFIED RESIDUE	UNP P19658

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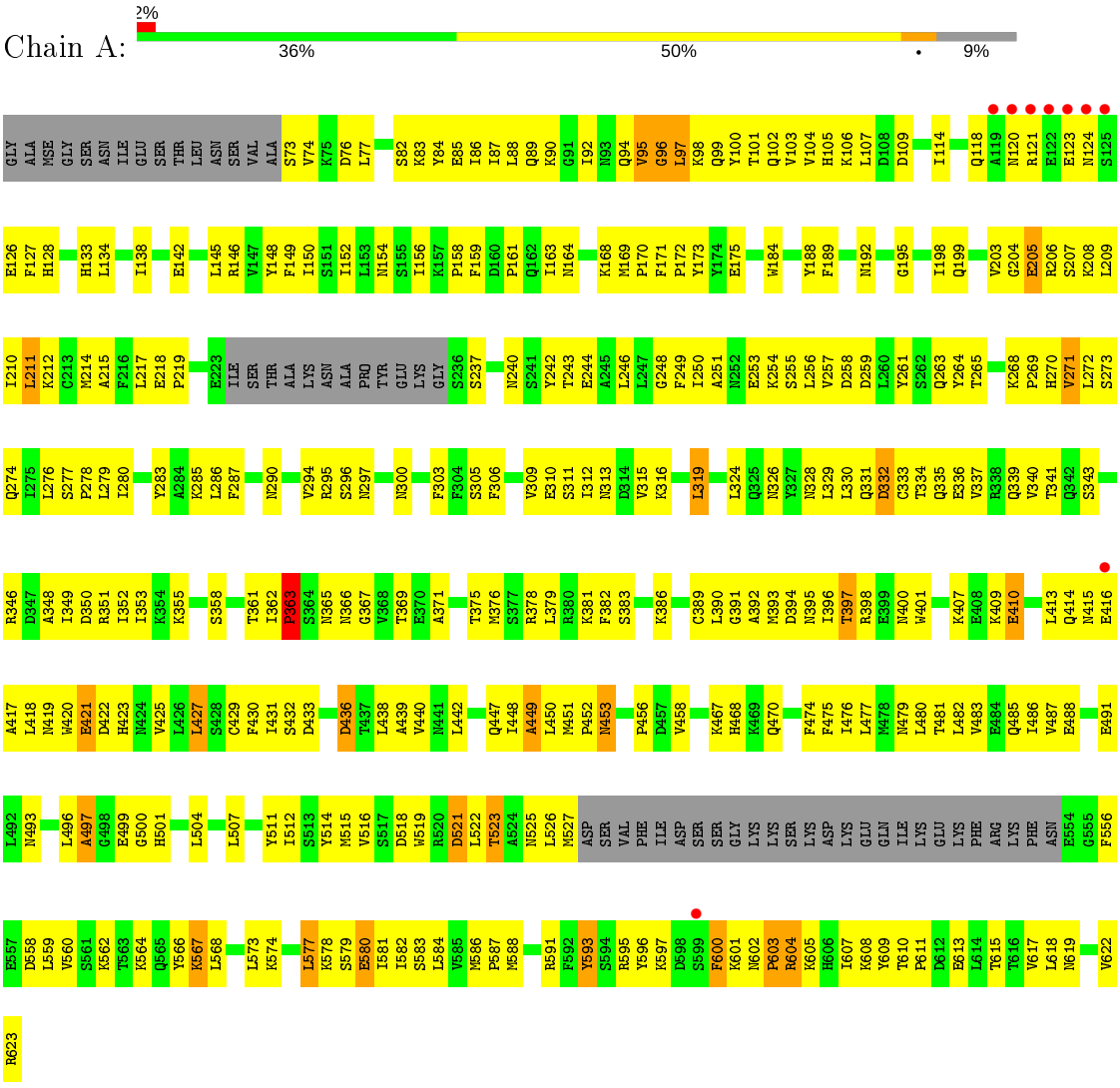
Chain	Residue	Modelled	Actual	Comment	Reference
D	376	MSE	MET	MODIFIED RESIDUE	UNP P19658
D	393	MSE	MET	MODIFIED RESIDUE	UNP P19658
D	451	MSE	MET	MODIFIED RESIDUE	UNP P19658
D	478	MSE	MET	MODIFIED RESIDUE	UNP P19658
D	495	MSE	MET	MODIFIED RESIDUE	UNP P19658
D	515	MSE	MET	MODIFIED RESIDUE	UNP P19658
D	527	MSE	MET	MODIFIED RESIDUE	UNP P19658
D	586	MSE	MET	MODIFIED RESIDUE	UNP P19658
D	588	MSE	MET	MODIFIED RESIDUE	UNP P19658

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

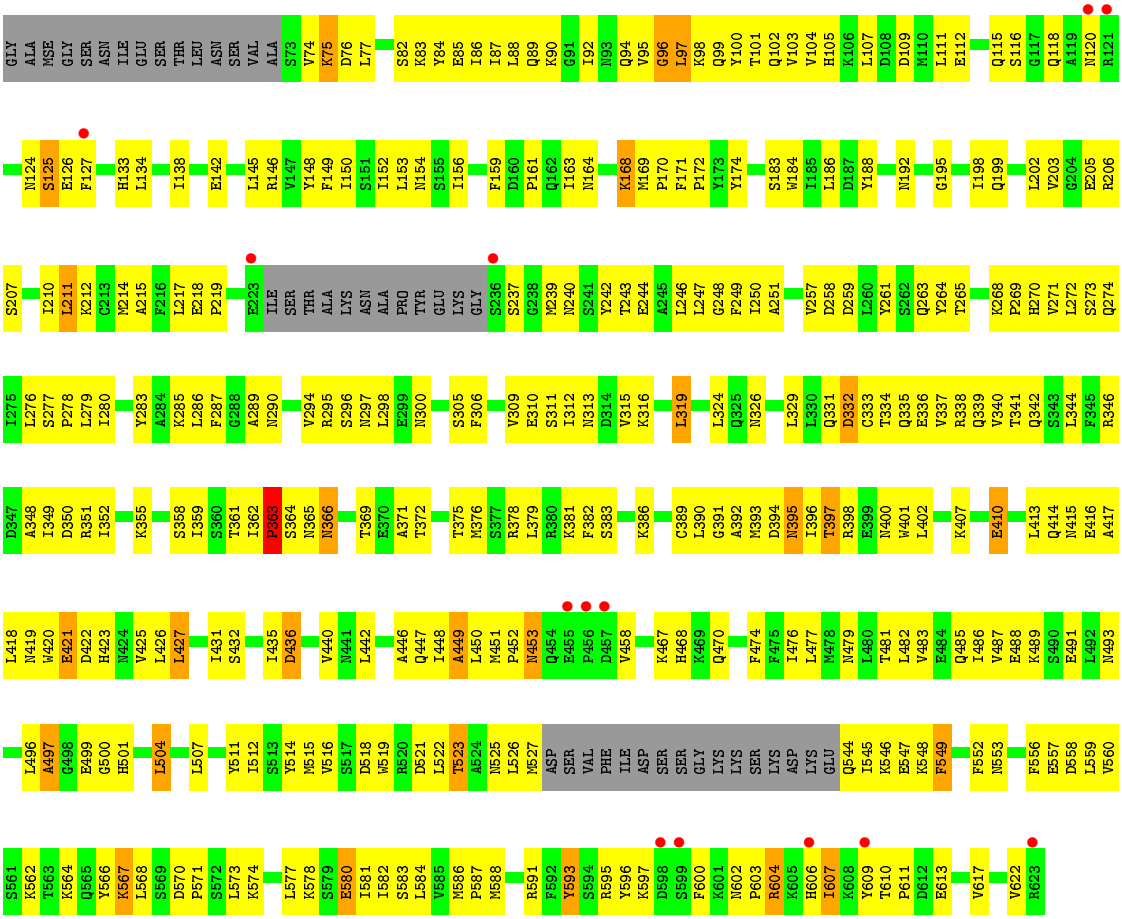
- Molecule 1: Exocyst complex component EXO70

Chain A:



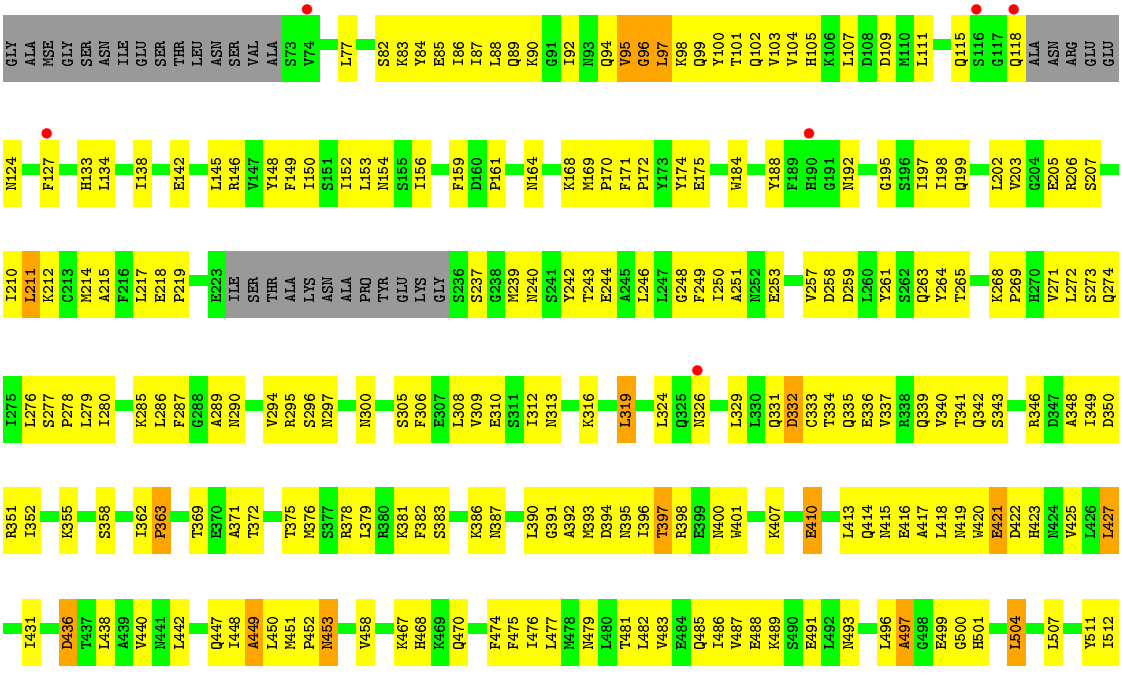
- Molecule 1: Exocyst complex component EXO70

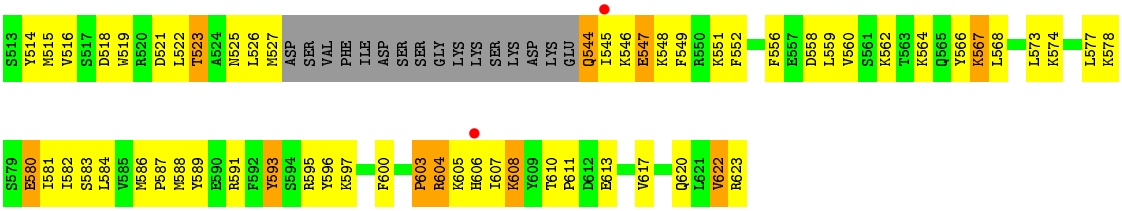
Chain B:

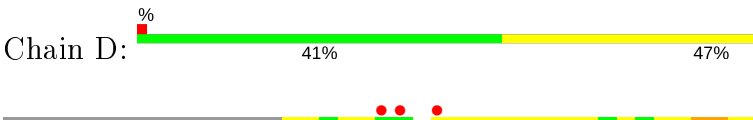


• Molecule 1: Exocyst complex component EXO70

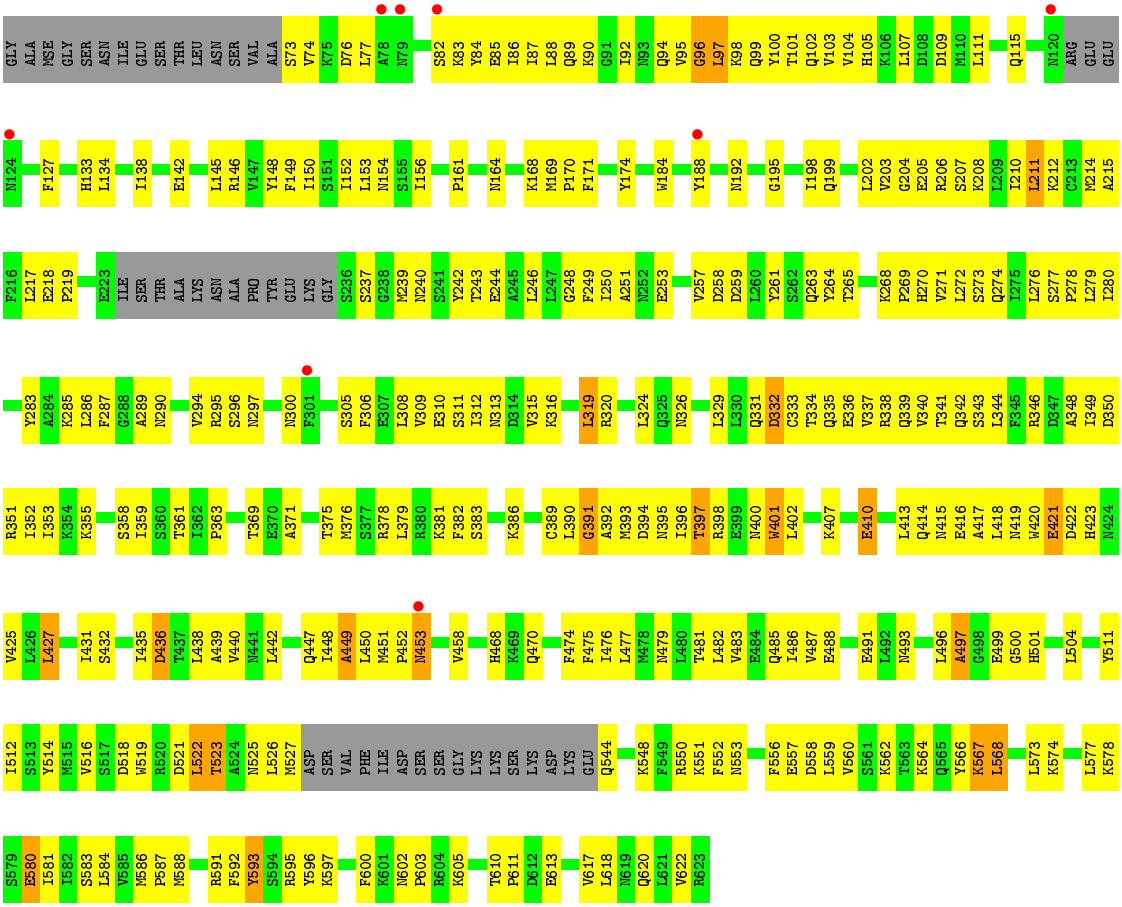
Chain C:







• Molecule 1: Exocyst complex component EXO70



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	415.73Å 55.13Å 132.93Å 90.00° 104.05° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 29.93 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.5 (20.00-3.50) 95.3 (29.93-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 3.47Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.254 , 0.305 0.243 , 0.299	Depositor DCC
R_{free} test set	2175 reflections (6.03%)	wwPDB-VP
Wilson B-factor (Å^2)	102.1	Xtriage
Anisotropy	0.363	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 122.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16823	wwPDB-VP
Average B, all atoms (Å^2)	129.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.44	0/4212	0.62	0/5654
1	B	0.33	0/4308	0.58	1/5779 (0.0%)
1	C	0.34	0/4265	0.57	0/5720
1	D	0.37	0/4278	0.59	0/5738
All	All	0.37	0/17063	0.59	1/22891 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	125	SER	N-CA-C	5.53	125.94	111.00

There are no chirality outliers.

There are no planarity outliers.

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	4153	0	4177	295	0
1	B	4247	0	4278	287	0
1	C	4205	0	4241	272	0
1	D	4218	0	4252	295	0
All	All	16823	0	16948	1130	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 33.

All (1130) 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:398:ARG:HB2	1:B:401:TRP:CZ2	1.58	1.37
1:A:120:ASN:HB3	1:D:320:ARG:HH22	1.01	1.10
1:C:526:LEU:HD12	1:C:552:PHE:HB2	1.28	1.10
1:A:476:ILE:HG21	1:A:511:TYR:CZ	1.86	1.10
1:D:398:ARG:HB2	1:D:401:TRP:CZ2	1.89	1.08
1:D:338:ARG:O	1:D:342:GLN:HG2	1.53	1.07
1:A:476:ILE:HG21	1:A:511:TYR:CE2	1.90	1.07
1:D:476:ILE:HG21	1:D:511:TYR:CE2	1.91	1.05
1:D:476:ILE:HG21	1:D:511:TYR:CZ	1.91	1.05
1:B:398:ARG:HB2	1:B:401:TRP:CE2	1.94	1.02
1:B:398:ARG:CB	1:B:401:TRP:CZ2	2.43	1.01
1:C:552:PHE:CE2	1:C:589:TYR:CD2	2.52	0.98
1:D:526:LEU:HD12	1:D:552:PHE:HB2	1.45	0.97
1:A:120:ASN:HB3	1:D:320:ARG:NH2	1.80	0.96
1:B:526:LEU:HD12	1:B:552:PHE:HB2	1.46	0.94
1:A:285:LYS:HE2	1:A:285:LYS:HA	1.49	0.93
1:C:285:LYS:HA	1:C:285:LYS:HE2	1.51	0.92
1:B:285:LYS:HA	1:B:285:LYS:HE2	1.52	0.92
1:A:474:PHE:CD1	1:A:566:TYR:HB3	2.06	0.91
1:D:285:LYS:HA	1:D:285:LYS:HE2	1.50	0.90
1:A:488:GLU:HA	1:A:493:ASN:HD22	1.38	0.89
1:D:276:LEU:HA	1:D:279:LEU:HD12	1.54	0.89
1:B:116:SER:HB2	1:B:120:ASN:HD21	1.38	0.88
1:D:169:MSE:HG3	1:D:170:PRO:HD2	1.57	0.86
1:B:169:MSE:HG3	1:B:170:PRO:HD2	1.56	0.86
1:C:276:LEU:HA	1:C:279:LEU:HD12	1.58	0.86
1:A:169:MSE:HG3	1:A:170:PRO:HD2	1.58	0.85
1:C:552:PHE:CE2	1:C:589:TYR:HD2	1.94	0.85
1:B:488:GLU:HA	1:B:493:ASN:HD22	1.42	0.84
1:C:169:MSE:HG3	1:C:170:PRO:HD2	1.59	0.84
1:A:352:ILE:HG12	1:A:375:THR:HG22	1.59	0.83
1:B:276:LEU:HA	1:B:279:LEU:HD12	1.59	0.83
1:C:488:GLU:HA	1:C:493:ASN:HD22	1.41	0.83
1:C:526:LEU:HD12	1:C:552:PHE:CB	2.07	0.83
1:B:352:ILE:HG12	1:B:375:THR:HG22	1.60	0.83
1:B:298:LEU:HD22	1:B:344:LEU:HD23	1.61	0.82
1:A:272:LEU:O	1:A:276:LEU:HD23	1.80	0.82
1:D:560:VAL:HG12	1:D:564:LYS:HE3	1.61	0.82
1:B:526:LEU:CD1	1:B:552:PHE:HB2	2.10	0.82
1:A:276:LEU:HA	1:A:279:LEU:HD12	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:352:ILE:HG12	1:C:375:THR:HG22	1.60	0.81
1:D:352:ILE:HG12	1:D:375:THR:HG22	1.62	0.81
1:D:488:GLU:HA	1:D:493:ASN:HD22	1.44	0.81
1:B:74:VAL:HG23	1:B:75:LYS:H	1.44	0.81
1:C:87:ILE:HA	1:C:90:LYS:HE2	1.63	0.81
1:B:560:VAL:HG12	1:B:564:LYS:HE3	1.63	0.80
1:B:87:ILE:HA	1:B:90:LYS:HE2	1.63	0.80
1:B:272:LEU:O	1:B:276:LEU:HD23	1.82	0.80
1:C:319:LEU:HG	1:C:324:LEU:HD11	1.64	0.80
1:D:87:ILE:HA	1:D:90:LYS:HE2	1.63	0.79
1:D:602:ASN:HD22	1:D:605:LYS:HE3	1.47	0.79
1:D:319:LEU:HG	1:D:324:LEU:HD11	1.64	0.79
1:B:116:SER:HB2	1:B:120:ASN:ND2	1.97	0.79
1:C:526:LEU:CD1	1:C:552:PHE:HB2	2.11	0.79
1:D:393:MSE:HE3	1:D:427:LEU:HB2	1.64	0.79
1:A:87:ILE:HA	1:A:90:LYS:HE2	1.65	0.79
1:D:398:ARG:HB2	1:D:401:TRP:CE2	2.17	0.78
1:D:453:ASN:N	1:D:453:ASN:HD22	1.81	0.78
1:C:272:LEU:O	1:C:276:LEU:HD23	1.82	0.78
1:B:453:ASN:N	1:B:453:ASN:HD22	1.81	0.78
1:A:453:ASN:HD22	1:A:453:ASN:N	1.81	0.78
1:A:319:LEU:HG	1:A:324:LEU:HD11	1.66	0.77
1:A:560:VAL:HG12	1:A:564:LYS:HE3	1.64	0.77
1:B:118:GLN:NE2	1:B:127:PHE:HB2	1.99	0.77
1:D:602:ASN:ND2	1:D:605:LYS:HE3	2.00	0.77
1:D:272:LEU:O	1:D:276:LEU:HD23	1.85	0.77
1:B:319:LEU:HG	1:B:324:LEU:HD11	1.67	0.77
1:C:453:ASN:HD22	1:C:453:ASN:N	1.81	0.77
1:C:560:VAL:HG12	1:C:564:LYS:HE3	1.65	0.76
1:B:393:MSE:HE3	1:B:427:LEU:HB2	1.68	0.76
1:A:567:LYS:O	1:A:567:LYS:HD2	1.85	0.76
1:D:526:LEU:HD13	1:D:548:LYS:O	1.85	0.76
1:D:567:LYS:HD2	1:D:567:LYS:O	1.86	0.75
1:B:567:LYS:O	1:B:567:LYS:HD2	1.87	0.75
1:D:283:TYR:OH	1:D:311:SER:OG	2.02	0.75
1:A:351:ARG:NH1	1:A:378:ARG:HD2	2.01	0.74
1:B:283:TYR:OH	1:B:311:SER:OG	2.05	0.74
1:D:73:SER:HB3	1:D:76:ASP:HB2	1.67	0.74
1:C:111:LEU:O	1:C:115:GLN:HG3	1.88	0.74
1:B:82:SER:O	1:B:86:ILE:HG13	1.88	0.73
1:C:351:ARG:NH1	1:C:378:ARG:HD2	2.03	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:LYS:O	1:C:567:LYS:HD2	1.86	0.73
1:D:246:LEU:O	1:D:250:ILE:HG13	1.88	0.73
1:D:351:ARG:NH1	1:D:378:ARG:HD2	2.03	0.73
1:C:393:MSE:HE3	1:C:427:LEU:HB2	1.71	0.73
1:D:369:THR:HG22	1:D:371:ALA:H	1.54	0.72
1:A:476:ILE:CG2	1:A:511:TYR:CE2	2.71	0.72
1:A:496:LEU:HB3	1:A:500:GLY:HA3	1.71	0.72
1:C:246:LEU:O	1:C:250:ILE:HG13	1.89	0.72
1:D:476:ILE:CG2	1:D:511:TYR:CE2	2.71	0.72
1:D:359:ILE:CG2	1:D:361:THR:HG22	2.19	0.71
1:C:206:ARG:O	1:C:210:ILE:HG13	1.90	0.71
1:B:351:ARG:NH1	1:B:378:ARG:HD2	2.05	0.71
1:A:290:ASN:O	1:A:294:VAL:HG23	1.91	0.71
1:C:419:ASN:O	1:C:421:GLU:N	2.24	0.71
1:A:369:THR:HG22	1:A:371:ALA:H	1.56	0.71
1:B:246:LEU:O	1:B:250:ILE:HG13	1.90	0.71
1:A:431:ILE:CG2	1:A:496:LEU:HD21	2.21	0.71
1:C:164:ASN:HD21	1:D:89:GLN:HE22	1.39	0.70
1:C:522:LEU:HD11	1:C:556:PHE:HA	1.73	0.70
1:C:82:SER:O	1:C:86:ILE:HG13	1.92	0.70
1:D:206:ARG:O	1:D:210:ILE:HG13	1.90	0.70
1:D:584:LEU:O	1:D:584:LEU:HD12	1.91	0.70
1:C:172:PRO:CG	1:D:89:GLN:HG2	2.20	0.70
1:A:121:ARG:HD3	1:A:124:ASN:ND2	2.06	0.70
1:B:206:ARG:O	1:B:210:ILE:HG13	1.91	0.70
1:B:369:THR:HG22	1:B:371:ALA:H	1.55	0.70
1:B:522:LEU:HD11	1:B:556:PHE:HA	1.72	0.70
1:B:74:VAL:HG23	1:B:75:LYS:N	2.06	0.70
1:C:369:THR:HG22	1:C:371:ALA:H	1.55	0.70
1:B:101:THR:HG23	1:B:188:TYR:CD1	2.28	0.69
1:A:206:ARG:O	1:A:210:ILE:HG13	1.92	0.69
1:C:431:ILE:CG2	1:C:496:LEU:HD21	2.22	0.69
1:A:427:LEU:O	1:A:427:LEU:HD12	1.93	0.69
1:A:246:LEU:O	1:A:250:ILE:HG13	1.92	0.69
1:D:101:THR:HG23	1:D:188:TYR:CD1	2.28	0.69
1:D:338:ARG:O	1:D:342:GLN:CG	2.39	0.68
1:D:522:LEU:HD11	1:D:556:PHE:HA	1.74	0.68
1:A:365:ASN:ND2	1:A:367:GLY:HA3	2.08	0.68
1:B:283:TYR:CZ	1:B:315:VAL:HG21	2.27	0.68
1:A:415:ASN:O	1:A:417:ALA:N	2.26	0.68
1:C:268:LYS:HB2	1:C:269:PRO:HD3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:526:LEU:HD11	1:C:552:PHE:N	2.06	0.68
1:D:82:SER:O	1:D:86:ILE:HG13	1.94	0.68
1:A:82:SER:O	1:A:86:ILE:HG13	1.93	0.68
1:C:118:GLN:HG2	1:C:124:ASN:ND2	2.07	0.68
1:C:172:PRO:HG2	1:D:89:GLN:HG2	1.74	0.68
1:B:268:LYS:HB2	1:B:269:PRO:HD3	1.75	0.68
1:D:556:PHE:O	1:D:560:VAL:HG23	1.94	0.68
1:A:352:ILE:HG12	1:A:375:THR:CG2	2.23	0.67
1:B:556:PHE:O	1:B:560:VAL:HG23	1.94	0.67
1:D:290:ASN:O	1:D:294:VAL:HG23	1.94	0.67
1:A:283:TYR:CZ	1:A:315:VAL:HG21	2.29	0.67
1:A:474:PHE:CE1	1:A:566:TYR:HB3	2.29	0.67
1:A:393:MSE:HE3	1:A:427:LEU:HB2	1.75	0.67
1:C:101:THR:HG23	1:C:188:TYR:CD1	2.29	0.67
1:B:74:VAL:HG12	1:B:127:PHE:CZ	2.30	0.67
1:B:134:LEU:O	1:B:138:ILE:HG13	1.94	0.66
1:D:268:LYS:HB2	1:D:269:PRO:HD3	1.76	0.66
1:A:522:LEU:HD11	1:A:556:PHE:HA	1.75	0.66
1:A:285:LYS:HE2	1:A:285:LYS:CA	2.25	0.66
1:D:273:SER:O	1:D:277:SER:HB2	1.96	0.66
1:A:268:LYS:HB2	1:A:269:PRO:HD3	1.78	0.66
1:B:431:ILE:CG2	1:B:496:LEU:HD21	2.25	0.66
1:C:352:ILE:HG12	1:C:375:THR:CG2	2.25	0.66
1:D:74:VAL:HG22	1:D:127:PHE:CE2	2.30	0.66
1:A:273:SER:O	1:A:277:SER:HB2	1.95	0.66
1:B:419:ASN:O	1:B:421:GLU:N	2.28	0.66
1:C:164:ASN:HD21	1:D:89:GLN:NE2	1.92	0.66
1:B:578:LYS:HE2	1:B:622:VAL:HA	1.78	0.66
1:C:450:LEU:HB3	1:C:468:HIS:HD2	1.61	0.66
1:D:496:LEU:HB3	1:D:500:GLY:HA3	1.78	0.66
1:A:526:LEU:O	1:A:527:MSE:HG3	1.96	0.66
1:B:92:ILE:HG12	1:B:100:TYR:CD1	2.30	0.66
1:C:290:ASN:O	1:C:294:VAL:HG23	1.96	0.66
1:C:526:LEU:O	1:C:527:MSE:HG3	1.95	0.66
1:A:450:LEU:HB3	1:A:468:HIS:HD2	1.62	0.65
1:D:341:THR:HG21	1:D:392:ALA:HB3	1.77	0.65
1:B:526:LEU:O	1:B:527:MSE:HG3	1.96	0.65
1:C:481:THR:O	1:C:485:GLN:HG3	1.96	0.65
1:A:101:THR:HG23	1:A:188:TYR:CD1	2.31	0.65
1:D:111:LEU:O	1:D:115:GLN:HG3	1.97	0.65
1:B:553:ASN:O	1:B:557:GLU:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:LEU:HB3	1:D:468:HIS:HD2	1.62	0.65
1:C:584:LEU:O	1:C:584:LEU:HD12	1.97	0.65
1:D:359:ILE:HG22	1:D:361:THR:HG22	1.79	0.65
1:B:290:ASN:O	1:B:294:VAL:HG23	1.97	0.65
1:B:285:LYS:CA	1:B:285:LYS:HE2	2.26	0.65
1:D:526:LEU:O	1:D:527:MSE:HG3	1.97	0.65
1:B:352:ILE:HG12	1:B:375:THR:CG2	2.26	0.64
1:C:552:PHE:CZ	1:C:589:TYR:HD2	2.14	0.64
1:A:394:ASP:HB3	1:A:423:HIS:CE1	2.32	0.64
1:A:556:PHE:O	1:A:560:VAL:HG23	1.96	0.64
1:C:415:ASN:O	1:C:417:ALA:N	2.30	0.64
1:C:544:GLN:HA	1:C:547:GLU:CD	2.18	0.64
1:D:333:CYS:O	1:D:337:VAL:HG23	1.97	0.64
1:D:283:TYR:CZ	1:D:315:VAL:HG21	2.32	0.64
1:D:305:SER:O	1:D:309:VAL:HG23	1.97	0.64
1:D:415:ASN:O	1:D:417:ALA:N	2.31	0.64
1:A:381:LYS:HA	1:A:381:LYS:HE3	1.80	0.64
1:B:273:SER:O	1:B:277:SER:HB2	1.98	0.64
1:B:341:THR:CG2	1:B:392:ALA:HB3	2.27	0.64
1:B:305:SER:O	1:B:309:VAL:HG23	1.97	0.64
1:C:285:LYS:CA	1:C:285:LYS:HE2	2.26	0.64
1:B:394:ASP:HB3	1:B:423:HIS:CE1	2.32	0.63
1:D:550:ARG:HH11	1:D:550:ARG:HB3	1.62	0.63
1:A:92:ILE:HG12	1:A:100:TYR:CD1	2.34	0.63
1:B:333:CYS:O	1:B:337:VAL:HG23	1.98	0.63
1:D:394:ASP:HB3	1:D:423:HIS:CE1	2.32	0.63
1:A:207:SER:O	1:A:211:LEU:HB2	1.99	0.63
1:D:481:THR:O	1:D:485:GLN:HG3	1.98	0.63
1:C:394:ASP:HB3	1:C:423:HIS:CE1	2.34	0.63
1:B:481:THR:O	1:B:485:GLN:HG3	1.99	0.63
1:C:218:GLU:HB3	1:C:219:PRO:HD3	1.81	0.63
1:A:74:VAL:HG22	1:A:127:PHE:CE2	2.34	0.63
1:B:218:GLU:HB3	1:B:219:PRO:HD3	1.81	0.63
1:B:427:LEU:O	1:B:427:LEU:HD12	1.99	0.63
1:B:450:LEU:HB3	1:B:468:HIS:HD2	1.63	0.63
1:C:398:ARG:HB2	1:C:401:TRP:CZ2	2.34	0.63
1:D:352:ILE:HG12	1:D:375:THR:CG2	2.27	0.63
1:B:415:ASN:O	1:B:417:ALA:N	2.31	0.63
1:D:218:GLU:HB3	1:D:219:PRO:HD3	1.81	0.63
1:C:92:ILE:HG12	1:C:100:TYR:CD1	2.34	0.62
1:C:148:TYR:O	1:C:152:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:SER:O	1:C:309:VAL:HG23	1.99	0.62
1:D:431:ILE:CG2	1:D:496:LEU:HD21	2.29	0.62
1:A:218:GLU:HB3	1:A:219:PRO:HD3	1.81	0.62
1:A:271:VAL:HG12	1:A:272:LEU:N	2.14	0.62
1:B:512:ILE:HD11	1:B:573:LEU:HD22	1.81	0.62
1:C:273:SER:O	1:C:277:SER:HB2	1.99	0.62
1:C:522:LEU:HD12	1:C:559:LEU:HD12	1.80	0.62
1:B:393:MSE:HE3	1:B:427:LEU:CB	2.30	0.62
1:A:114:ILE:HG23	1:A:118:GLN:OE1	2.00	0.62
1:D:393:MSE:HE3	1:D:427:LEU:CB	2.29	0.62
1:B:522:LEU:HD12	1:B:559:LEU:HD12	1.82	0.62
1:C:511:TYR:O	1:C:514:TYR:HB2	1.99	0.62
1:A:512:ILE:HD11	1:A:573:LEU:HD22	1.82	0.62
1:B:118:GLN:HE22	1:B:127:PHE:HB2	1.63	0.62
1:B:584:LEU:O	1:B:584:LEU:HD12	1.99	0.62
1:C:134:LEU:O	1:C:138:ILE:HG13	2.00	0.62
1:D:381:LYS:HE3	1:D:381:LYS:HA	1.82	0.62
1:C:175:GLU:CG	1:D:94:GLN:HE21	2.12	0.62
1:A:481:THR:O	1:A:485:GLN:HG3	1.99	0.62
1:B:111:LEU:O	1:B:115:GLN:HG3	1.99	0.62
1:D:340:VAL:O	1:D:343:SER:N	2.33	0.62
1:A:584:LEU:O	1:A:584:LEU:HD12	2.00	0.62
1:D:92:ILE:HG12	1:D:100:TYR:CD1	2.35	0.62
1:D:148:TYR:O	1:D:152:ILE:HG13	2.00	0.62
1:D:522:LEU:HD22	1:D:552:PHE:CE1	2.35	0.62
1:A:431:ILE:HG21	1:A:496:LEU:HD21	1.80	0.62
1:B:349:ILE:HG21	1:B:401:TRP:O	2.00	0.61
1:B:496:LEU:HB3	1:B:500:GLY:HA3	1.81	0.61
1:D:340:VAL:O	1:D:343:SER:HB3	2.00	0.61
1:D:419:ASN:O	1:D:421:GLU:N	2.32	0.61
1:A:101:THR:HG23	1:A:188:TYR:HD1	1.65	0.61
1:A:419:ASN:O	1:A:421:GLU:N	2.33	0.61
1:C:195:GLY:O	1:C:198:ILE:HG22	2.01	0.61
1:D:285:LYS:CA	1:D:285:LYS:HE2	2.25	0.61
1:C:381:LYS:HA	1:C:381:LYS:HE3	1.82	0.61
1:D:101:THR:HG23	1:D:188:TYR:HD1	1.65	0.61
1:A:351:ARG:HH12	1:A:378:ARG:HD2	1.65	0.61
1:A:148:TYR:O	1:A:152:ILE:HG13	2.00	0.61
1:C:393:MSE:HE3	1:C:427:LEU:CB	2.31	0.61
1:C:496:LEU:HB3	1:C:500:GLY:HA3	1.82	0.61
1:A:600:PHE:C	1:A:601:LYS:HD2	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:ILE:HD11	1:C:573:LEU:HD22	1.83	0.60
1:D:349:ILE:HG21	1:D:401:TRP:O	2.01	0.60
1:D:522:LEU:HD12	1:D:559:LEU:HD12	1.82	0.60
1:A:195:GLY:O	1:A:198:ILE:HG22	2.02	0.60
1:B:595:ARG:HG2	1:B:596:TYR:CD2	2.37	0.60
1:C:470:GLN:HB2	1:C:518:ASP:OD2	2.02	0.60
1:A:134:LEU:O	1:A:138:ILE:HG13	2.01	0.60
1:B:470:GLN:HB2	1:B:518:ASP:OD2	2.01	0.60
1:B:148:TYR:O	1:B:152:ILE:HG13	2.01	0.60
1:B:381:LYS:HA	1:B:381:LYS:HE3	1.83	0.60
1:D:195:GLY:O	1:D:198:ILE:HG22	2.02	0.60
1:D:339:GLN:HA	1:D:342:GLN:CD	2.21	0.60
1:D:470:GLN:HB2	1:D:518:ASP:OD2	2.01	0.60
1:A:203:VAL:HG11	1:A:274:GLN:HB3	1.84	0.60
1:A:610:THR:HG23	1:A:611:PRO:HD2	1.83	0.60
1:B:306:PHE:CE2	1:B:341:THR:HG23	2.37	0.60
1:C:101:THR:HG23	1:C:188:TYR:HD1	1.65	0.60
1:D:522:LEU:CD2	1:D:552:PHE:CD1	2.84	0.60
1:C:526:LEU:CD1	1:C:552:PHE:N	2.65	0.60
1:A:73:SER:HB2	1:A:76:ASP:OD2	2.02	0.59
1:B:142:GLU:O	1:B:145:LEU:HB2	2.01	0.59
1:D:401:TRP:C	1:D:401:TRP:CD1	2.75	0.59
1:A:142:GLU:O	1:A:145:LEU:HB2	2.01	0.59
1:A:379:LEU:O	1:A:382:PHE:HB2	2.02	0.59
1:A:511:TYR:O	1:A:514:TYR:HB2	2.02	0.59
1:A:95:VAL:O	1:A:96:GLY:C	2.39	0.59
1:B:95:VAL:O	1:B:96:GLY:C	2.40	0.59
1:C:175:GLU:HG2	1:D:94:GLN:HE21	1.65	0.59
1:A:398:ARG:HB2	1:A:401:TRP:CZ2	2.38	0.59
1:A:522:LEU:HD12	1:A:559:LEU:HD12	1.84	0.59
1:A:349:ILE:HG21	1:A:401:TRP:O	2.02	0.59
1:A:439:ALA:HB1	1:A:511:TYR:OH	2.02	0.59
1:B:101:THR:HG23	1:B:188:TYR:HD1	1.65	0.59
1:C:556:PHE:O	1:C:560:VAL:HG23	2.01	0.59
1:D:134:LEU:O	1:D:138:ILE:HG13	2.01	0.59
1:D:351:ARG:HH12	1:D:378:ARG:HD2	1.67	0.59
1:A:101:THR:HG21	1:A:184:TRP:HE1	1.67	0.59
1:C:526:LEU:HD11	1:C:551:LYS:HB2	1.84	0.59
1:D:306:PHE:CE2	1:D:341:THR:HG23	2.37	0.59
1:A:393:MSE:HE3	1:A:427:LEU:CB	2.33	0.59
1:C:142:GLU:O	1:C:145:LEU:HB2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:GLN:O	1:D:105:HIS:HB2	2.03	0.59
1:B:195:GLY:O	1:B:198:ILE:HG22	2.02	0.59
1:A:333:CYS:O	1:A:337:VAL:HG23	2.03	0.59
1:C:340:VAL:O	1:C:343:SER:HB3	2.02	0.59
1:C:95:VAL:O	1:C:96:GLY:C	2.41	0.59
1:D:451:MSE:HE3	1:D:468:HIS:CD2	2.37	0.59
1:A:586:MSE:HB2	1:A:587:PRO:HD3	1.85	0.58
1:B:511:TYR:O	1:B:514:TYR:HB2	2.03	0.58
1:C:333:CYS:O	1:C:337:VAL:HG23	2.03	0.58
1:C:351:ARG:HH12	1:C:378:ARG:HD2	1.67	0.58
1:D:101:THR:HG21	1:D:184:TRP:HE1	1.69	0.58
1:C:431:ILE:HG21	1:C:496:LEU:HD21	1.83	0.58
1:C:586:MSE:HB2	1:C:587:PRO:HD3	1.85	0.58
1:D:142:GLU:O	1:D:145:LEU:HB2	2.03	0.58
1:B:607:ILE:N	1:B:607:ILE:HD12	2.18	0.58
1:C:595:ARG:HG2	1:C:596:TYR:CD2	2.39	0.58
1:A:602:ASN:HD22	1:A:605:LYS:HB2	1.69	0.58
1:B:74:VAL:O	1:B:76:ASP:N	2.36	0.58
1:C:622:VAL:HG12	1:C:623:ARG:HH21	1.68	0.58
1:D:427:LEU:HD12	1:D:427:LEU:O	2.04	0.58
1:B:203:VAL:HG11	1:B:274:GLN:HB3	1.85	0.58
1:C:102:GLN:O	1:C:105:HIS:HB2	2.04	0.58
1:D:512:ILE:HD11	1:D:573:LEU:HD22	1.84	0.58
1:B:102:GLN:O	1:B:105:HIS:HB2	2.03	0.58
1:A:476:ILE:HB	1:A:511:TYR:CD2	2.38	0.58
1:B:265:THR:HA	1:B:268:LYS:HE3	1.86	0.58
1:D:580:GLU:OE1	1:D:580:GLU:HA	2.03	0.58
1:D:586:MSE:HB2	1:D:587:PRO:HD3	1.86	0.58
1:D:95:VAL:O	1:D:96:GLY:C	2.42	0.58
1:C:101:THR:HG21	1:C:184:TRP:HE1	1.68	0.57
1:D:346:ARG:HH21	1:D:400:ASN:HA	1.70	0.57
1:C:203:VAL:HG11	1:C:274:GLN:HB3	1.85	0.57
1:D:203:VAL:HG11	1:D:274:GLN:HB3	1.85	0.57
1:A:305:SER:O	1:A:309:VAL:HG23	2.04	0.57
1:B:431:ILE:HG21	1:B:496:LEU:HD21	1.85	0.57
1:D:439:ALA:HB1	1:D:511:TYR:OH	2.04	0.57
1:A:453:ASN:ND2	1:A:453:ASN:N	2.52	0.57
1:C:552:PHE:CE2	1:C:589:TYR:CE2	2.92	0.57
1:D:512:ILE:O	1:D:516:VAL:HG23	2.05	0.57
1:A:242:TYR:CE2	1:A:286:LEU:HD23	2.39	0.57
1:A:394:ASP:HB3	1:A:423:HIS:HE1	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:LYS:HG3	1:A:609:TYR:CD1	2.39	0.57
1:A:102:GLN:O	1:A:105:HIS:HB2	2.05	0.57
1:A:470:GLN:HB2	1:A:518:ASP:OD2	2.04	0.57
1:A:595:ARG:HG2	1:A:596:TYR:CD2	2.39	0.57
1:B:362:ILE:HD11	1:B:446:ALA:HA	1.87	0.57
1:C:453:ASN:N	1:C:453:ASN:ND2	2.53	0.57
1:D:394:ASP:HB3	1:D:423:HIS:HE1	1.70	0.57
1:B:341:THR:HG21	1:B:392:ALA:HB3	1.86	0.57
1:B:586:MSE:HB2	1:B:587:PRO:HD3	1.85	0.57
1:D:271:VAL:HG12	1:D:272:LEU:N	2.19	0.57
1:D:595:ARG:HG2	1:D:596:TYR:CD2	2.40	0.57
1:C:349:ILE:HG21	1:C:401:TRP:O	2.05	0.57
1:A:214:MSE:HE3	1:A:242:TYR:CZ	2.40	0.56
1:A:521:ASP:O	1:A:525:ASN:HB2	2.05	0.56
1:B:207:SER:O	1:B:211:LEU:HB2	2.05	0.56
1:B:161:PRO:HG2	1:B:217:LEU:HD11	1.87	0.56
1:B:74:VAL:CG2	1:B:75:LYS:H	2.17	0.56
1:D:207:SER:O	1:D:211:LEU:HB2	2.06	0.56
1:A:436:ASP:O	1:A:440:VAL:HG23	2.06	0.56
1:A:476:ILE:HG13	1:A:511:TYR:CE2	2.40	0.56
1:B:101:THR:HG21	1:B:184:TRP:HE1	1.71	0.56
1:C:512:ILE:O	1:C:516:VAL:HG23	2.06	0.56
1:D:340:VAL:C	1:D:343:SER:H	2.09	0.56
1:D:476:ILE:HB	1:D:511:TYR:CD2	2.39	0.56
1:B:578:LYS:NZ	1:B:622:VAL:HG23	2.21	0.56
1:D:453:ASN:N	1:D:453:ASN:ND2	2.53	0.56
1:A:331:GLN:O	1:A:335:GLN:HG2	2.06	0.56
1:A:346:ARG:HH21	1:A:400:ASN:HA	1.71	0.56
1:B:394:ASP:HB3	1:B:423:HIS:HE1	1.70	0.56
1:C:207:SER:O	1:C:211:LEU:HB2	2.04	0.56
1:B:346:ARG:HH21	1:B:400:ASN:HA	1.70	0.56
1:B:398:ARG:CB	1:B:401:TRP:CE2	2.82	0.56
1:B:512:ILE:O	1:B:516:VAL:HG23	2.06	0.56
1:B:580:GLU:HA	1:B:580:GLU:OE1	2.06	0.56
1:D:521:ASP:O	1:D:525:ASN:HB2	2.06	0.56
1:A:482:LEU:HD13	1:A:486:ILE:HD13	1.87	0.56
1:A:518:ASP:HB3	1:A:559:LEU:HD21	1.88	0.56
1:A:512:ILE:HD11	1:A:573:LEU:CD2	2.36	0.56
1:D:497:ALA:HA	1:D:501:HIS:HD2	1.71	0.56
1:D:83:LYS:O	1:D:87:ILE:HG12	2.05	0.56
1:C:521:ASP:O	1:C:525:ASN:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:ASP:O	1:B:525:ASN:HB2	2.05	0.55
1:C:346:ARG:HH21	1:C:400:ASN:HA	1.71	0.55
1:A:580:GLU:OE1	1:A:580:GLU:HA	2.06	0.55
1:B:257:VAL:HG21	1:B:272:LEU:HD13	1.87	0.55
1:D:474:PHE:CD1	1:D:566:TYR:HB3	2.40	0.55
1:B:83:LYS:O	1:B:87:ILE:HG12	2.06	0.55
1:A:99:GLN:O	1:A:103:VAL:HG23	2.06	0.55
1:C:610:THR:HG23	1:C:611:PRO:HD2	1.87	0.55
1:C:83:LYS:O	1:C:87:ILE:HG12	2.06	0.55
1:A:265:THR:HA	1:A:268:LYS:HE3	1.88	0.55
1:B:453:ASN:ND2	1:B:453:ASN:N	2.53	0.55
1:B:518:ASP:HB3	1:B:559:LEU:HD21	1.87	0.55
1:C:306:PHE:CE2	1:C:341:THR:HG23	2.40	0.55
1:B:99:GLN:O	1:B:103:VAL:HG23	2.07	0.55
1:B:355:LYS:HA	1:B:358:SER:HB2	1.88	0.55
1:D:553:ASN:O	1:D:557:GLU:HG3	2.07	0.55
1:A:355:LYS:HA	1:A:358:SER:HB2	1.89	0.55
1:B:331:GLN:O	1:B:335:GLN:HG2	2.07	0.55
1:C:355:LYS:HA	1:C:358:SER:HB2	1.89	0.55
1:B:341:THR:CG2	1:B:392:ALA:CB	2.85	0.55
1:B:351:ARG:HH12	1:B:378:ARG:HD2	1.68	0.55
1:B:451:MSE:HE3	1:B:468:HIS:CD2	2.41	0.55
1:C:497:ALA:HA	1:C:501:HIS:HD2	1.72	0.55
1:D:161:PRO:HG2	1:D:217:LEU:HD11	1.88	0.55
1:D:265:THR:HA	1:D:268:LYS:HE3	1.87	0.55
1:D:341:THR:HG21	1:D:392:ALA:CB	2.37	0.55
1:A:161:PRO:HG2	1:A:217:LEU:HD11	1.87	0.55
1:B:339:GLN:O	1:B:339:GLN:HG2	2.06	0.54
1:B:512:ILE:HD11	1:B:573:LEU:CD2	2.36	0.54
1:C:265:THR:HA	1:C:268:LYS:HE3	1.88	0.54
1:D:486:ILE:HD12	1:D:486:ILE:H	1.72	0.54
1:A:497:ALA:HA	1:A:501:HIS:HD2	1.71	0.54
1:C:394:ASP:HB3	1:C:423:HIS:HE1	1.72	0.54
1:B:341:THR:HB	1:B:392:ALA:CB	2.38	0.54
1:B:497:ALA:HA	1:B:501:HIS:HD2	1.72	0.54
1:C:474:PHE:CD1	1:C:566:TYR:HB3	2.43	0.54
1:A:593:TYR:HE1	1:A:607:ILE:HG21	1.70	0.54
1:A:77:LEU:H	1:A:77:LEU:HD22	1.73	0.54
1:D:242:TYR:CE2	1:D:286:LEU:HD23	2.43	0.54
1:C:164:ASN:ND2	1:D:89:GLN:HE22	2.06	0.54
1:A:242:TYR:CD2	1:A:286:LEU:HD23	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LEU:HG	1:A:276:LEU:HD23	1.89	0.54
1:A:277:SER:HB3	1:A:278:PRO:CD	2.38	0.54
1:B:257:VAL:CG2	1:B:272:LEU:HD13	2.38	0.54
1:B:298:LEU:HD22	1:B:344:LEU:CD2	2.35	0.54
1:C:580:GLU:HA	1:C:580:GLU:OE1	2.07	0.54
1:D:574:LYS:O	1:D:578:LYS:HG3	2.08	0.54
1:B:210:ILE:HB	1:B:279:LEU:HD21	1.90	0.54
1:A:83:LYS:O	1:A:87:ILE:HG12	2.07	0.54
1:B:361:THR:O	1:B:363:PRO:HD3	2.08	0.54
1:B:379:LEU:O	1:B:382:PHE:HB2	2.07	0.54
1:C:574:LYS:O	1:C:578:LYS:HG3	2.08	0.54
1:A:287:PHE:HZ	1:A:337:VAL:HG21	1.73	0.54
1:D:523:THR:HG21	1:D:588:MSE:HG3	1.90	0.54
1:A:306:PHE:CE2	1:A:341:THR:HG23	2.43	0.54
1:A:339:GLN:O	1:A:339:GLN:HG2	2.08	0.54
1:B:214:MSE:HE3	1:B:242:TYR:CZ	2.43	0.54
1:B:77:LEU:H	1:B:77:LEU:HD22	1.73	0.54
1:C:271:VAL:HG12	1:C:272:LEU:N	2.22	0.54
1:D:272:LEU:HG	1:D:276:LEU:HD23	1.91	0.54
1:D:519:TRP:CE2	1:D:581:ILE:HD13	2.43	0.54
1:D:401:TRP:CD1	1:D:402:LEU:HG	2.43	0.53
1:D:511:TYR:O	1:D:514:TYR:HB2	2.08	0.53
1:D:518:ASP:HB3	1:D:559:LEU:HD21	1.90	0.53
1:A:210:ILE:HB	1:A:279:LEU:HD21	1.89	0.53
1:B:474:PHE:CD1	1:B:566:TYR:HB3	2.43	0.53
1:C:242:TYR:CE2	1:C:286:LEU:HD23	2.43	0.53
1:C:518:ASP:HB3	1:C:559:LEU:HD21	1.91	0.53
1:D:338:ARG:C	1:D:342:GLN:HE21	2.12	0.53
1:B:169:MSE:CG	1:B:170:PRO:HD2	2.36	0.53
1:D:332:ASP:O	1:D:335:GLN:HB2	2.09	0.53
1:B:610:THR:HG23	1:B:611:PRO:HD2	1.90	0.53
1:C:331:GLN:O	1:C:335:GLN:HG2	2.07	0.53
1:C:379:LEU:O	1:C:382:PHE:HB2	2.08	0.53
1:D:355:LYS:HA	1:D:358:SER:HB2	1.89	0.53
1:D:379:LEU:O	1:D:382:PHE:HB2	2.09	0.53
1:D:99:GLN:O	1:D:103:VAL:HG23	2.07	0.53
1:A:212:LYS:O	1:A:215:ALA:HB3	2.09	0.53
1:B:94:GLN:O	1:B:94:GLN:HG2	2.09	0.53
1:D:214:MSE:HE3	1:D:242:TYR:CZ	2.44	0.53
1:D:331:GLN:O	1:D:335:GLN:HG2	2.08	0.53
1:A:127:PHE:N	1:A:127:PHE:CD1	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:TYR:O	1:A:597:LYS:HB2	2.08	0.53
1:B:593:TYR:O	1:B:597:LYS:HB2	2.08	0.53
1:A:121:ARG:CB	1:A:124:ASN:HB2	2.39	0.53
1:A:210:ILE:HG23	1:A:249:PHE:CD2	2.44	0.53
1:A:250:ILE:HG23	1:A:276:LEU:HD11	1.91	0.53
1:B:574:LYS:O	1:B:578:LYS:HG3	2.09	0.53
1:C:88:LEU:HD11	1:C:107:LEU:CD1	2.39	0.53
1:C:545:ILE:HG21	1:C:596:TYR:HB3	1.90	0.53
1:D:341:THR:O	1:D:344:LEU:HB2	2.09	0.53
1:A:523:THR:HG21	1:A:588:MSE:HG3	1.90	0.52
1:B:287:PHE:HZ	1:B:337:VAL:HG21	1.74	0.52
1:C:397:THR:N	1:C:400:ASN:HD22	2.07	0.52
1:C:100:TYR:O	1:C:104:VAL:HG23	2.08	0.52
1:D:593:TYR:O	1:D:597:LYS:HB2	2.10	0.52
1:D:77:LEU:HD22	1:D:77:LEU:H	1.74	0.52
1:B:210:ILE:HG23	1:B:249:PHE:CD2	2.45	0.52
1:C:277:SER:HB3	1:C:278:PRO:CD	2.40	0.52
1:C:427:LEU:HD12	1:C:427:LEU:O	2.08	0.52
1:C:99:GLN:O	1:C:103:VAL:HG23	2.09	0.52
1:D:339:GLN:O	1:D:339:GLN:HG2	2.07	0.52
1:A:100:TYR:O	1:A:104:VAL:HG23	2.10	0.52
1:A:309:VAL:HA	1:A:312:ILE:HG22	1.92	0.52
1:B:523:THR:HG21	1:B:588:MSE:HG3	1.90	0.52
1:D:210:ILE:HB	1:D:279:LEU:HD21	1.91	0.52
1:B:271:VAL:HG12	1:B:272:LEU:N	2.23	0.52
1:C:339:GLN:HG2	1:C:339:GLN:O	2.08	0.52
1:A:332:ASP:O	1:A:335:GLN:HB2	2.09	0.52
1:B:92:ILE:HG12	1:B:100:TYR:CG	2.45	0.52
1:B:272:LEU:HG	1:B:276:LEU:HD23	1.92	0.52
1:B:340:VAL:C	1:B:342:GLN:N	2.62	0.52
1:C:161:PRO:HG2	1:C:217:LEU:HD11	1.92	0.52
1:C:272:LEU:HG	1:C:276:LEU:HD23	1.91	0.52
1:C:287:PHE:HZ	1:C:337:VAL:HG21	1.74	0.52
1:C:523:THR:HG21	1:C:588:MSE:HG3	1.90	0.52
1:C:512:ILE:HD11	1:C:573:LEU:CD2	2.39	0.52
1:D:518:ASP:O	1:D:559:LEU:HD11	2.09	0.52
1:A:622:VAL:HG22	1:A:622:VAL:O	2.09	0.52
1:A:88:LEU:HD11	1:A:107:LEU:CD1	2.40	0.52
1:B:332:ASP:O	1:B:335:GLN:HB2	2.10	0.52
1:D:169:MSE:CG	1:D:170:PRO:HD2	2.36	0.52
1:A:602:ASN:HD22	1:A:605:LYS:CB	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:MSE:CG	1:C:170:PRO:HD2	2.38	0.52
1:C:332:ASP:O	1:C:335:GLN:HB2	2.10	0.52
1:D:316:LYS:NZ	1:D:334:THR:HG21	2.25	0.52
1:A:295:ARG:NH2	1:A:336:GLU:HB3	2.25	0.51
1:A:479:ASN:O	1:A:482:LEU:HB3	2.11	0.51
1:A:574:LYS:O	1:A:578:LYS:HG3	2.09	0.51
1:B:519:TRP:CE2	1:B:581:ILE:HD13	2.45	0.51
1:C:479:ASN:O	1:C:482:LEU:HB3	2.10	0.51
1:A:346:ARG:O	1:A:349:ILE:HG22	2.10	0.51
1:A:175:GLU:CG	1:B:94:GLN:HE21	2.23	0.51
1:B:96:GLY:O	1:B:98:LYS:N	2.43	0.51
1:C:346:ARG:O	1:C:349:ILE:HG22	2.10	0.51
1:C:94:GLN:O	1:C:94:GLN:HG2	2.11	0.51
1:D:483:VAL:O	1:D:487:VAL:HG23	2.11	0.51
1:A:283:TYR:OH	1:A:311:SER:OG	2.28	0.51
1:A:512:ILE:O	1:A:516:VAL:HG23	2.09	0.51
1:B:242:TYR:CE2	1:B:286:LEU:HD23	2.46	0.51
1:C:77:LEU:H	1:C:77:LEU:HD22	1.75	0.51
1:D:309:VAL:HA	1:D:312:ILE:HG22	1.92	0.51
1:B:100:TYR:O	1:B:104:VAL:HG23	2.11	0.51
1:B:346:ARG:O	1:B:349:ILE:HG22	2.11	0.51
1:C:210:ILE:HB	1:C:279:LEU:HD21	1.92	0.51
1:D:512:ILE:HD11	1:D:573:LEU:CD2	2.40	0.51
1:A:394:ASP:CB	1:A:423:HIS:HE1	2.23	0.51
1:B:568:LEU:N	1:B:568:LEU:HD12	2.25	0.51
1:C:436:ASP:O	1:C:440:VAL:HG23	2.11	0.51
1:D:287:PHE:HZ	1:D:337:VAL:HG21	1.74	0.51
1:D:431:ILE:HG21	1:D:496:LEU:HD21	1.91	0.51
1:C:544:GLN:HA	1:C:547:GLU:OE1	2.11	0.51
1:D:88:LEU:HD11	1:D:107:LEU:CD1	2.41	0.51
1:D:603:PRO:C	1:D:605:LYS:H	2.13	0.51
1:B:394:ASP:CB	1:B:423:HIS:HE1	2.24	0.51
1:C:210:ILE:HG23	1:C:249:PHE:CD2	2.46	0.51
1:D:210:ILE:HG23	1:D:249:PHE:CD2	2.46	0.51
1:D:257:VAL:HG21	1:D:272:LEU:HD13	1.93	0.51
1:D:397:THR:N	1:D:400:ASN:HD22	2.09	0.51
1:A:169:MSE:CG	1:A:170:PRO:HD2	2.37	0.51
1:D:261:TYR:C	1:D:263:GLN:H	2.14	0.51
1:D:452:PRO:O	1:D:453:ASN:HB2	2.10	0.51
1:B:341:THR:HG21	1:B:392:ALA:CB	2.40	0.51
1:C:622:VAL:O	1:C:622:VAL:HG22	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:LEU:HB3	1:D:468:HIS:CD2	2.46	0.51
1:D:96:GLY:O	1:D:98:LYS:N	2.44	0.51
1:D:338:ARG:O	1:D:342:GLN:NE2	2.40	0.51
1:D:610:THR:HG23	1:D:611:PRO:HD2	1.92	0.51
1:B:341:THR:HB	1:B:392:ALA:HB1	1.92	0.50
1:D:100:TYR:O	1:D:104:VAL:HG23	2.10	0.50
1:D:394:ASP:CB	1:D:423:HIS:HE1	2.24	0.50
1:A:121:ARG:HD3	1:A:124:ASN:HD22	1.75	0.50
1:B:316:LYS:NZ	1:B:334:THR:HG21	2.26	0.50
1:A:261:TYR:C	1:A:263:GLN:H	2.14	0.50
1:A:92:ILE:HG12	1:A:100:TYR:CG	2.46	0.50
1:A:303:PHE:CD1	1:A:381:LYS:HG2	2.45	0.50
1:A:586:MSE:O	1:A:587:PRO:C	2.50	0.50
1:A:94:GLN:O	1:A:94:GLN:HG2	2.11	0.50
1:B:306:PHE:HE2	1:B:341:THR:CG2	2.24	0.50
1:B:397:THR:N	1:B:400:ASN:HD22	2.09	0.50
1:C:295:ARG:NH2	1:C:336:GLU:HB3	2.27	0.50
1:B:116:SER:O	1:B:120:ASN:ND2	2.44	0.50
1:C:451:MSE:HE3	1:C:468:HIS:CD2	2.47	0.50
1:A:476:ILE:CB	1:A:511:TYR:CE2	2.95	0.50
1:A:610:THR:CG2	1:A:611:PRO:HD2	2.42	0.50
1:C:568:LEU:HD12	1:C:568:LEU:N	2.27	0.50
1:D:277:SER:HB3	1:D:278:PRO:CD	2.42	0.50
1:B:309:VAL:HA	1:B:312:ILE:HG22	1.93	0.50
1:C:309:VAL:HA	1:C:312:ILE:HG22	1.93	0.50
1:C:316:LYS:NZ	1:C:334:THR:HG21	2.26	0.50
1:A:261:TYR:HD2	1:A:264:TYR:HB2	1.76	0.50
1:D:94:GLN:O	1:D:94:GLN:HG2	2.11	0.50
1:A:608:LYS:HE2	1:A:609:TYR:CE1	2.46	0.50
1:B:146:ARG:O	1:B:150:ILE:HG13	2.12	0.50
1:B:398:ARG:HB2	1:B:401:TRP:HZ2	1.57	0.50
1:B:486:ILE:H	1:B:486:ILE:HD12	1.77	0.50
1:C:261:TYR:C	1:C:263:GLN:H	2.14	0.50
1:C:450:LEU:HB3	1:C:468:HIS:CD2	2.45	0.50
1:C:477:LEU:O	1:C:481:THR:HG23	2.11	0.50
1:C:85:GLU:OE1	1:C:133:HIS:NE2	2.43	0.50
1:A:277:SER:HB3	1:A:278:PRO:HD3	1.93	0.49
1:A:448:ILE:HG22	1:A:449:ALA:N	2.26	0.49
1:C:242:TYR:CD2	1:C:286:LEU:HD23	2.47	0.49
1:C:544:GLN:CD	1:C:544:GLN:N	2.65	0.49
1:D:340:VAL:HA	1:D:343:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:TYR:C	1:B:263:GLN:H	2.15	0.49
1:C:394:ASP:CB	1:C:423:HIS:HE1	2.25	0.49
1:D:482:LEU:HD13	1:D:486:ILE:HD13	1.95	0.49
1:A:303:PHE:HE2	1:A:382:PHE:CG	2.30	0.49
1:B:277:SER:HB3	1:B:278:PRO:CD	2.41	0.49
1:C:257:VAL:HG21	1:C:272:LEU:HD13	1.93	0.49
1:A:475:PHE:O	1:A:479:ASN:ND2	2.46	0.49
1:C:96:GLY:O	1:C:98:LYS:N	2.45	0.49
1:D:295:ARG:NH2	1:D:336:GLU:HB3	2.27	0.49
1:D:448:ILE:HG22	1:D:449:ALA:N	2.26	0.49
1:A:249:PHE:O	1:A:253:GLU:HG2	2.13	0.49
1:A:518:ASP:O	1:A:559:LEU:HD11	2.13	0.49
1:B:88:LEU:HD11	1:B:107:LEU:CD1	2.41	0.49
1:B:154:ASN:C	1:B:156:ILE:H	2.16	0.49
1:B:87:ILE:HA	1:B:90:LYS:CE	2.40	0.49
1:D:378:ARG:O	1:D:381:LYS:HB3	2.12	0.49
1:D:578:LYS:HE2	1:D:622:VAL:HA	1.93	0.49
1:A:243:THR:O	1:A:246:LEU:N	2.46	0.49
1:A:568:LEU:N	1:A:568:LEU:HD12	2.28	0.49
1:B:203:VAL:HG11	1:B:274:GLN:CB	2.43	0.49
1:C:486:ILE:H	1:C:486:ILE:HD12	1.76	0.49
1:D:257:VAL:CG2	1:D:272:LEU:HD13	2.43	0.49
1:D:242:TYR:CD2	1:D:286:LEU:HD23	2.47	0.49
1:A:85:GLU:OE1	1:A:133:HIS:NE2	2.43	0.49
1:A:207:SER:HA	1:A:210:ILE:HD12	1.95	0.49
1:B:261:TYR:HD2	1:B:264:TYR:HB2	1.77	0.49
1:B:394:ASP:O	1:B:396:ILE:HG13	2.13	0.49
1:B:593:TYR:CG	1:B:611:PRO:HD3	2.48	0.49
1:C:482:LEU:HD13	1:C:486:ILE:HD13	1.95	0.49
1:D:203:VAL:HG11	1:D:274:GLN:CB	2.42	0.49
1:A:173:TYR:OH	1:A:256:LEU:HA	2.12	0.49
1:C:261:TYR:HD2	1:C:264:TYR:HB2	1.78	0.49
1:A:418:LEU:HB3	1:A:425:VAL:HG11	1.94	0.48
1:A:96:GLY:O	1:A:98:LYS:N	2.46	0.48
1:B:295:ARG:NH2	1:B:336:GLU:HB3	2.27	0.48
1:C:214:MSE:HE3	1:C:242:TYR:CZ	2.48	0.48
1:C:483:VAL:O	1:C:487:VAL:HG23	2.12	0.48
1:A:243:THR:O	1:A:244:GLU:C	2.51	0.48
1:A:324:LEU:O	1:A:326:ASN:N	2.46	0.48
1:B:483:VAL:O	1:B:487:VAL:HG23	2.14	0.48
1:B:560:VAL:O	1:B:564:LYS:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:350:ASP:O	1:C:351:ARG:C	2.51	0.48
1:A:146:ARG:O	1:A:150:ILE:HG13	2.12	0.48
1:A:568:LEU:O	1:A:574:LYS:HE3	2.13	0.48
1:B:207:SER:HA	1:B:210:ILE:HD12	1.95	0.48
1:B:309:VAL:O	1:B:310:GLU:C	2.52	0.48
1:B:482:LEU:HD13	1:B:486:ILE:HD13	1.95	0.48
1:B:518:ASP:O	1:B:559:LEU:HD11	2.12	0.48
1:C:567:LYS:HA	1:C:623:ARG:OXT	2.14	0.48
1:D:250:ILE:HG23	1:D:276:LEU:HD11	1.95	0.48
1:D:390:LEU:HD12	1:D:423:HIS:HB3	1.96	0.48
1:A:257:VAL:HG21	1:A:272:LEU:HD13	1.95	0.48
1:B:202:LEU:HD12	1:B:202:LEU:O	2.12	0.48
1:B:568:LEU:O	1:B:574:LYS:HE3	2.13	0.48
1:B:553:ASN:OD1	1:B:609:TYR:HB2	2.14	0.48
1:C:519:TRP:CE2	1:C:581:ILE:HD13	2.48	0.48
1:D:593:TYR:CG	1:D:611:PRO:HD3	2.48	0.48
1:A:350:ASP:O	1:A:351:ARG:C	2.51	0.48
1:C:203:VAL:HG11	1:C:274:GLN:CB	2.43	0.48
1:C:378:ARG:O	1:C:381:LYS:HB3	2.12	0.48
1:C:552:PHE:CD2	1:C:589:TYR:CE2	3.02	0.48
1:B:450:LEU:HB3	1:B:468:HIS:CD2	2.47	0.48
1:C:593:TYR:O	1:C:597:LYS:HB2	2.13	0.48
1:D:127:PHE:CD1	1:D:127:PHE:N	2.82	0.48
1:A:287:PHE:CZ	1:A:337:VAL:HG21	2.48	0.48
1:B:250:ILE:HG23	1:B:276:LEU:HD11	1.95	0.48
1:B:242:TYR:CD2	1:B:286:LEU:HD23	2.48	0.48
1:D:383:SER:HB2	1:D:491:GLU:HB2	1.96	0.48
1:D:526:LEU:HD11	1:D:551:LYS:HB2	1.96	0.48
1:D:568:LEU:HD12	1:D:568:LEU:N	2.29	0.48
1:A:476:ILE:HG13	1:A:511:TYR:HE2	1.77	0.48
1:A:519:TRP:CE2	1:A:581:ILE:HD13	2.48	0.48
1:A:73:SER:O	1:A:76:ASP:HB2	2.14	0.48
1:C:476:ILE:HG21	1:C:511:TYR:CE1	2.49	0.48
1:C:610:THR:CG2	1:C:611:PRO:HD2	2.44	0.48
1:D:486:ILE:HD12	1:D:486:ILE:N	2.29	0.48
1:A:365:ASN:HD21	1:A:367:GLY:HA3	1.78	0.48
1:A:451:MSE:HE3	1:A:468:HIS:CD2	2.49	0.48
1:B:479:ASN:O	1:B:482:LEU:HB3	2.13	0.48
1:C:526:LEU:HD12	1:C:552:PHE:CA	2.43	0.48
1:D:85:GLU:OE1	1:D:133:HIS:NE2	2.42	0.48
1:C:277:SER:HB3	1:C:278:PRO:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ASP:O	1:B:440:VAL:HG23	2.14	0.47
1:C:568:LEU:O	1:C:574:LYS:HE3	2.13	0.47
1:A:348:ALA:O	1:A:352:ILE:HG13	2.14	0.47
1:A:175:GLU:HG2	1:B:94:GLN:HE21	1.79	0.47
1:C:376:MSE:SE	1:C:483:VAL:HG13	2.64	0.47
1:A:593:TYR:CG	1:A:611:PRO:HD3	2.50	0.47
1:C:545:ILE:HG23	1:C:596:TYR:HD1	1.78	0.47
1:D:306:PHE:HE2	1:D:341:THR:CG2	2.27	0.47
1:D:550:ARG:HB3	1:D:550:ARG:NH1	2.27	0.47
1:A:118:GLN:NE2	1:A:127:PHE:CZ	2.83	0.47
1:A:483:VAL:O	1:A:487:VAL:HG23	2.12	0.47
1:A:578:LYS:HE2	1:A:622:VAL:HA	1.96	0.47
1:B:447:GLN:HE22	1:B:458:VAL:HA	1.79	0.47
1:A:272:LEU:HG	1:A:276:LEU:CD2	2.44	0.47
1:B:526:LEU:HD12	1:B:552:PHE:CB	2.33	0.47
1:B:84:TYR:O	1:B:87:ILE:HB	2.13	0.47
1:C:603:PRO:HG2	1:C:604:ARG:H	1.80	0.47
1:D:447:GLN:HE22	1:D:458:VAL:HA	1.79	0.47
1:A:309:VAL:O	1:A:310:GLU:C	2.51	0.47
1:B:287:PHE:CZ	1:B:337:VAL:HG21	2.49	0.47
1:B:448:ILE:HG22	1:B:449:ALA:N	2.30	0.47
1:C:257:VAL:CG2	1:C:272:LEU:HD13	2.44	0.47
1:C:309:VAL:O	1:C:310:GLU:C	2.53	0.47
1:D:479:ASN:O	1:D:482:LEU:HB3	2.15	0.47
1:B:295:ARG:HH21	1:B:336:GLU:HB3	1.80	0.47
1:B:558:ASP:OD1	1:B:562:LYS:HE3	2.15	0.47
1:C:287:PHE:CZ	1:C:337:VAL:HG21	2.49	0.47
1:C:448:ILE:HG22	1:C:449:ALA:N	2.30	0.47
1:A:397:THR:N	1:A:400:ASN:HD22	2.12	0.47
1:C:383:SER:HB2	1:C:491:GLU:HB2	1.97	0.47
1:D:212:LYS:O	1:D:215:ALA:HB3	2.15	0.47
1:D:295:ARG:HH21	1:D:336:GLU:HB3	1.80	0.47
1:D:348:ALA:O	1:D:352:ILE:HG13	2.15	0.47
1:A:324:LEU:C	1:A:326:ASN:N	2.67	0.47
1:B:277:SER:HB3	1:B:278:PRO:HD3	1.97	0.47
1:B:359:ILE:HG22	1:B:361:THR:H	1.78	0.47
1:C:188:TYR:O	1:C:192:ASN:ND2	2.48	0.47
1:C:212:LYS:O	1:C:215:ALA:HB3	2.15	0.47
1:C:620:GLN:C	1:C:622:VAL:H	2.18	0.47
1:C:84:TYR:O	1:C:87:ILE:HB	2.14	0.47
1:A:376:MSE:SE	1:A:483:VAL:HG13	2.65	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ILE:H	1:B:210:ILE:HG13	1.52	0.47
1:B:306:PHE:CE2	1:B:341:THR:CG2	2.98	0.47
1:B:378:ARG:O	1:B:381:LYS:HB3	2.15	0.47
1:C:164:ASN:ND2	1:C:171:PHE:HD2	2.13	0.47
1:C:526:LEU:HD22	1:C:548:LYS:HB3	1.97	0.47
1:C:606:HIS:O	1:C:608:LYS:N	2.48	0.47
1:D:84:TYR:O	1:D:87:ILE:HB	2.15	0.47
1:A:295:ARG:HH21	1:A:336:GLU:HB3	1.79	0.46
1:A:516:VAL:O	1:A:516:VAL:HG12	2.14	0.46
1:C:341:THR:HG21	1:C:392:ALA:CB	2.45	0.46
1:D:401:TRP:C	1:D:401:TRP:HD1	2.19	0.46
1:D:558:ASP:OD1	1:D:562:LYS:HE3	2.14	0.46
1:A:107:LEU:C	1:A:109:ASP:N	2.67	0.46
1:B:188:TYR:O	1:B:192:ASN:ND2	2.49	0.46
1:B:237:SER:OG	1:B:240:ASN:HB2	2.15	0.46
1:B:350:ASP:O	1:B:351:ARG:C	2.53	0.46
1:B:586:MSE:O	1:B:587:PRO:C	2.54	0.46
1:D:261:TYR:HD2	1:D:264:TYR:HB2	1.80	0.46
1:D:600:PHE:CD1	1:D:600:PHE:N	2.83	0.46
1:A:375:THR:OG1	1:A:438:LEU:HD22	2.15	0.46
1:A:84:TYR:O	1:A:87:ILE:HB	2.14	0.46
1:B:365:ASN:O	1:B:366:ASN:C	2.53	0.46
1:C:548:LYS:O	1:C:549:PHE:C	2.53	0.46
1:D:346:ARG:O	1:D:349:ILE:HG22	2.15	0.46
1:A:248:GLY:O	1:A:251:ALA:HB3	2.15	0.46
1:A:413:LEU:O	1:A:414:GLN:HG3	2.16	0.46
1:B:401:TRP:CD1	1:B:401:TRP:C	2.89	0.46
1:C:146:ARG:O	1:C:150:ILE:HG13	2.16	0.46
1:C:578:LYS:HE2	1:C:622:VAL:HA	1.98	0.46
1:D:476:ILE:CB	1:D:511:TYR:CE2	2.98	0.46
1:A:398:ARG:NH1	1:A:433:ASP:OD1	2.49	0.46
1:B:401:TRP:CD1	1:B:402:LEU:HG	2.50	0.46
1:B:418:LEU:HB3	1:B:425:VAL:HG11	1.97	0.46
1:B:90:LYS:HB3	1:B:94:GLN:OE1	2.15	0.46
1:C:295:ARG:HH21	1:C:336:GLU:HB3	1.79	0.46
1:C:390:LEU:HD22	1:C:390:LEU:N	2.30	0.46
1:D:92:ILE:HG12	1:D:100:TYR:CG	2.50	0.46
1:B:390:LEU:O	1:B:392:ALA:N	2.48	0.46
1:B:407:LYS:HD2	1:B:410:GLU:OE2	2.16	0.46
1:B:622:VAL:HG22	1:B:622:VAL:O	2.15	0.46
1:D:350:ASP:O	1:D:351:ARG:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:438:LEU:O	1:D:438:LEU:HD12	2.15	0.46
1:D:548:LYS:HG2	1:D:592:PHE:CZ	2.51	0.46
1:D:522:LEU:HD22	1:D:552:PHE:CD1	2.49	0.46
1:A:378:ARG:O	1:A:381:LYS:HB3	2.15	0.46
1:A:390:LEU:O	1:A:392:ALA:N	2.49	0.46
1:A:607:ILE:HG22	1:A:609:TYR:O	2.15	0.46
1:B:376:MSE:SE	1:B:483:VAL:HG13	2.66	0.46
1:C:475:PHE:O	1:C:479:ASN:ND2	2.49	0.46
1:D:394:ASP:O	1:D:396:ILE:HG13	2.14	0.46
1:D:526:LEU:CD1	1:D:552:PHE:HB2	2.31	0.46
1:A:560:VAL:O	1:A:564:LYS:HG3	2.15	0.46
1:C:398:ARG:HB2	1:C:401:TRP:CE2	2.50	0.46
1:C:593:TYR:CG	1:C:611:PRO:HD3	2.51	0.46
1:C:85:GLU:O	1:C:89:GLN:HB2	2.15	0.46
1:D:146:ARG:O	1:D:150:ILE:HG13	2.16	0.46
1:A:154:ASN:C	1:A:156:ILE:H	2.19	0.46
1:A:383:SER:HB2	1:A:491:GLU:HB2	1.98	0.46
1:B:212:LYS:O	1:B:215:ALA:HB3	2.16	0.46
1:B:248:GLY:O	1:B:251:ALA:HB3	2.16	0.46
1:B:383:SER:HB2	1:B:491:GLU:HB2	1.96	0.46
1:B:77:LEU:N	1:B:77:LEU:HD22	2.30	0.46
1:C:154:ASN:C	1:C:156:ILE:H	2.19	0.46
1:D:154:ASN:C	1:D:156:ILE:H	2.19	0.46
1:D:390:LEU:O	1:D:392:ALA:N	2.49	0.46
1:A:394:ASP:O	1:A:396:ILE:HG13	2.16	0.46
1:A:558:ASP:OD1	1:A:562:LYS:HE3	2.15	0.46
1:C:447:GLN:HE22	1:C:458:VAL:HA	1.81	0.46
1:C:526:LEU:HD22	1:C:548:LYS:CB	2.46	0.46
1:D:431:ILE:O	1:D:435:ILE:HG13	2.16	0.46
1:D:603:PRO:C	1:D:605:LYS:N	2.68	0.46
1:A:257:VAL:CG2	1:A:272:LEU:HD13	2.46	0.45
1:A:389:CYS:O	1:A:393:MSE:HB2	2.15	0.45
1:B:557:GLU:HG2	1:B:609:TYR:OH	2.17	0.45
1:D:287:PHE:CZ	1:D:337:VAL:HG21	2.49	0.45
1:A:77:LEU:HD22	1:A:77:LEU:N	2.31	0.45
1:C:153:LEU:HA	1:C:174:TYR:HE2	1.82	0.45
1:C:243:THR:O	1:C:244:GLU:C	2.54	0.45
1:C:372:THR:HG22	1:C:482:LEU:HD12	1.98	0.45
1:C:558:ASP:OD1	1:C:562:LYS:HE3	2.16	0.45
1:C:92:ILE:HG12	1:C:100:TYR:CG	2.51	0.45
1:D:164:ASN:ND2	1:D:171:PHE:HD2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:LEU:HA	1:B:174:TYR:HE2	1.82	0.45
1:B:164:ASN:ND2	1:B:171:PHE:HD2	2.14	0.45
1:B:297:ASN:ND2	1:B:300:ASN:HB2	2.31	0.45
1:C:159:PHE:CZ	1:C:172:PRO:HD2	2.52	0.45
1:A:121:ARG:HB3	1:A:124:ASN:HB2	1.99	0.45
1:C:394:ASP:O	1:C:396:ILE:HG13	2.16	0.45
1:A:452:PRO:O	1:A:453:ASN:HB2	2.16	0.45
1:A:603:PRO:C	1:A:605:LYS:H	2.19	0.45
1:B:243:THR:O	1:B:244:GLU:C	2.55	0.45
1:B:431:ILE:O	1:B:435:ILE:HG13	2.16	0.45
1:B:476:ILE:HG21	1:B:511:TYR:CE1	2.52	0.45
1:C:107:LEU:C	1:C:109:ASP:N	2.70	0.45
1:D:248:GLY:O	1:D:251:ALA:HB3	2.16	0.45
1:D:277:SER:HB3	1:D:278:PRO:HD3	1.98	0.45
1:A:297:ASN:ND2	1:A:300:ASN:HB2	2.32	0.45
1:A:340:VAL:O	1:A:343:SER:HB3	2.16	0.45
1:A:447:GLN:HE22	1:A:458:VAL:HA	1.81	0.45
1:B:283:TYR:CE2	1:B:315:VAL:HG21	2.52	0.45
1:D:586:MSE:O	1:D:587:PRO:C	2.55	0.45
1:B:544:GLN:O	1:B:547:GLU:HG3	2.17	0.45
1:C:276:LEU:HD13	1:C:279:LEU:HD12	1.99	0.45
1:A:188:TYR:O	1:A:192:ASN:ND2	2.50	0.45
1:B:390:LEU:HD12	1:B:423:HIS:HB3	1.98	0.45
1:B:477:LEU:O	1:B:481:THR:HG23	2.17	0.45
1:C:342:GLN:HG2	1:C:342:GLN:H	1.57	0.45
1:C:397:THR:O	1:C:400:ASN:HB2	2.17	0.45
1:C:545:ILE:HD12	1:C:596:TYR:CE1	2.52	0.45
1:D:286:LEU:O	1:D:289:ALA:HB3	2.16	0.45
1:D:309:VAL:O	1:D:310:GLU:C	2.53	0.45
1:D:477:LEU:O	1:D:481:THR:HG23	2.17	0.45
1:D:584:LEU:C	1:D:584:LEU:HD12	2.37	0.45
1:A:146:ARG:HH11	1:A:146:ARG:HG3	1.82	0.45
1:A:324:LEU:C	1:A:326:ASN:H	2.20	0.45
1:A:90:LYS:HB3	1:A:94:GLN:OE1	2.16	0.45
1:B:390:LEU:N	1:B:390:LEU:HD22	2.31	0.45
1:B:549:PHE:CE1	1:B:607:ILE:HG12	2.52	0.45
1:B:85:GLU:OE1	1:B:133:HIS:NE2	2.41	0.45
1:A:203:VAL:HG11	1:A:274:GLN:CB	2.46	0.45
1:A:211:LEU:HD13	1:A:211:LEU:HA	1.77	0.45
1:A:306:PHE:HE2	1:A:341:THR:CG2	2.29	0.45
1:A:450:LEU:HB3	1:A:468:HIS:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:PHE:CZ	1:B:172:PRO:HD2	2.52	0.45
1:B:451:MSE:HE1	1:B:467:LYS:H	1.82	0.45
1:C:527:MSE:HA	1:C:548:LYS:NZ	2.32	0.45
1:D:376:MSE:SE	1:D:483:VAL:HG13	2.66	0.45
1:B:326:ASN:HD21	1:B:329:LEU:HD11	1.81	0.44
1:B:306:PHE:CD2	1:B:341:THR:HG23	2.52	0.44
1:C:248:GLY:O	1:C:251:ALA:HB3	2.16	0.44
1:C:504:LEU:O	1:C:507:LEU:HB3	2.17	0.44
1:C:518:ASP:O	1:C:559:LEU:HD11	2.17	0.44
1:D:188:TYR:O	1:D:192:ASN:ND2	2.50	0.44
1:B:107:LEU:C	1:B:109:ASP:N	2.69	0.44
1:B:239:MSE:O	1:B:239:MSE:HE3	2.17	0.44
1:B:77:LEU:H	1:B:77:LEU:CD2	2.30	0.44
1:C:237:SER:OG	1:C:240:ASN:HB2	2.17	0.44
1:D:476:ILE:HG13	1:D:511:TYR:CE2	2.52	0.44
1:A:164:ASN:ND2	1:A:171:PHE:HD2	2.16	0.44
1:A:237:SER:OG	1:A:240:ASN:HB2	2.17	0.44
1:A:390:LEU:HD22	1:A:390:LEU:N	2.32	0.44
1:A:451:MSE:HE1	1:A:467:LYS:H	1.83	0.44
1:C:309:VAL:HG12	1:C:313:ASN:ND2	2.32	0.44
1:D:568:LEU:O	1:D:574:LYS:HE3	2.18	0.44
1:B:470:GLN:HA	1:B:515:MSE:HA	1.98	0.44
1:C:211:LEU:HD13	1:C:211:LEU:HA	1.84	0.44
1:C:560:VAL:O	1:C:564:LYS:HG3	2.17	0.44
1:D:578:LYS:NZ	1:D:622:VAL:HG23	2.31	0.44
1:A:477:LEU:O	1:A:481:THR:HG23	2.17	0.44
1:C:548:LYS:O	1:C:551:LYS:N	2.50	0.44
1:D:560:VAL:O	1:D:564:LYS:HG3	2.17	0.44
1:C:172:PRO:HG3	1:D:89:GLN:HG2	1.98	0.44
1:D:90:LYS:HB3	1:D:94:GLN:OE1	2.17	0.44
1:A:172:PRO:HG2	1:B:89:GLN:HG2	2.00	0.44
1:A:390:LEU:HD12	1:A:423:HIS:HB3	1.99	0.44
1:B:111:LEU:HG	1:B:115:GLN:HE21	1.83	0.44
1:C:207:SER:HA	1:C:210:ILE:HD12	2.00	0.44
1:C:297:ASN:ND2	1:C:300:ASN:HB2	2.32	0.44
1:C:418:LEU:HB3	1:C:425:VAL:HG11	1.98	0.44
1:C:497:ALA:HA	1:C:501:HIS:CD2	2.53	0.44
1:D:207:SER:HA	1:D:210:ILE:HD12	2.00	0.44
1:D:324:LEU:C	1:D:326:ASN:N	2.71	0.44
1:D:397:THR:O	1:D:400:ASN:HB2	2.17	0.44
1:D:620:GLN:C	1:D:622:VAL:H	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:LEU:HD22	1:D:77:LEU:N	2.31	0.44
1:D:87:ILE:HA	1:D:90:LYS:CE	2.40	0.44
1:A:285:LYS:HA	1:A:285:LYS:CE	2.31	0.44
1:A:381:LYS:CE	1:A:381:LYS:HA	2.46	0.44
1:A:85:GLU:O	1:A:89:GLN:HB2	2.18	0.44
1:B:184:TRP:C	1:B:184:TRP:CD1	2.90	0.44
1:C:390:LEU:O	1:C:392:ALA:N	2.51	0.44
1:C:452:PRO:O	1:C:453:ASN:HB2	2.17	0.44
1:C:586:MSE:O	1:C:587:PRO:C	2.55	0.44
1:D:243:THR:O	1:D:246:LEU:N	2.51	0.44
1:A:184:TRP:CD1	1:A:184:TRP:C	2.91	0.44
1:A:427:LEU:HD12	1:A:427:LEU:C	2.38	0.44
1:A:603:PRO:O	1:A:605:LYS:N	2.51	0.44
1:B:518:ASP:HB3	1:B:559:LEU:CD2	2.48	0.44
1:C:272:LEU:HG	1:C:276:LEU:CD2	2.48	0.44
1:C:250:ILE:HG23	1:C:276:LEU:HD11	1.98	0.44
1:C:326:ASN:HD21	1:C:329:LEU:HD11	1.82	0.44
1:D:272:LEU:HG	1:D:276:LEU:CD2	2.48	0.44
1:A:350:ASP:O	1:A:353:ILE:N	2.51	0.44
1:A:365:ASN:O	1:A:366:ASN:HB2	2.17	0.44
1:C:451:MSE:HE1	1:C:467:LYS:H	1.81	0.44
1:D:243:THR:O	1:D:244:GLU:C	2.55	0.44
1:B:610:THR:CG2	1:B:611:PRO:HD2	2.47	0.43
1:C:306:PHE:HE2	1:C:341:THR:CG2	2.31	0.43
1:D:211:LEU:HA	1:D:211:LEU:HD13	1.83	0.43
1:D:381:LYS:HA	1:D:381:LYS:CE	2.48	0.43
1:A:303:PHE:CE2	1:A:382:PHE:CD1	3.06	0.43
1:B:324:LEU:C	1:B:326:ASN:N	2.71	0.43
1:D:184:TRP:CD1	1:D:184:TRP:C	2.92	0.43
1:A:407:LYS:HD2	1:A:410:GLU:OE2	2.18	0.43
1:B:276:LEU:HD13	1:B:279:LEU:HD12	2.00	0.43
1:C:280:ILE:HD13	1:C:324:LEU:HD13	2.01	0.43
1:C:324:LEU:C	1:C:326:ASN:N	2.71	0.43
1:D:239:MSE:HE3	1:D:239:MSE:O	2.18	0.43
1:D:326:ASN:HD21	1:D:329:LEU:HD11	1.82	0.43
1:D:351:ARG:O	1:D:355:LYS:CB	2.67	0.43
1:D:389:CYS:O	1:D:393:MSE:HB2	2.18	0.43
1:D:407:LYS:HD2	1:D:410:GLU:OE2	2.17	0.43
1:D:85:GLU:O	1:D:89:GLN:HB2	2.18	0.43
1:A:250:ILE:HG23	1:A:276:LEU:CD1	2.48	0.43
1:A:497:ALA:HA	1:A:501:HIS:CD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LEU:O	1:B:289:ALA:HB3	2.18	0.43
1:B:364:SER:C	1:B:366:ASN:H	2.22	0.43
1:B:378:ARG:HA	1:B:378:ARG:HD3	1.87	0.43
1:B:604:ARG:HD3	1:B:604:ARG:N	2.32	0.43
1:C:486:ILE:N	1:C:486:ILE:HD12	2.33	0.43
1:C:77:LEU:N	1:C:77:LEU:HD22	2.33	0.43
1:D:107:LEU:C	1:D:109:ASP:N	2.69	0.43
1:D:249:PHE:O	1:D:253:GLU:HG2	2.18	0.43
1:D:297:ASN:ND2	1:D:300:ASN:HB2	2.32	0.43
1:D:306:PHE:CD2	1:D:341:THR:HG23	2.52	0.43
1:D:418:LEU:HB3	1:D:425:VAL:HG11	2.00	0.43
1:D:497:ALA:HA	1:D:501:HIS:CD2	2.51	0.43
1:A:309:VAL:HG12	1:A:313:ASN:ND2	2.33	0.43
1:A:326:ASN:HD21	1:A:329:LEU:HD11	1.83	0.43
1:A:603:PRO:HB2	1:A:604:ARG:CZ	2.48	0.43
1:A:77:LEU:H	1:A:77:LEU:CD2	2.30	0.43
1:B:348:ALA:O	1:B:352:ILE:HG13	2.18	0.43
1:B:372:THR:HG22	1:B:482:LEU:HD12	2.00	0.43
1:C:603:PRO:O	1:C:605:LYS:N	2.51	0.43
1:B:112:GLU:HA	1:B:115:GLN:CD	2.39	0.43
1:B:613:GLU:O	1:B:617:VAL:HG23	2.19	0.43
1:A:105:HIS:O	1:A:107:LEU:N	2.52	0.43
1:A:361:THR:O	1:A:363:PRO:HD3	2.18	0.43
1:B:146:ARG:HH11	1:B:146:ARG:HG3	1.84	0.43
1:C:249:PHE:O	1:C:253:GLU:HG2	2.19	0.43
1:C:378:ARG:HD3	1:C:378:ARG:HA	1.86	0.43
1:C:90:LYS:HB3	1:C:94:GLN:OE1	2.18	0.43
1:A:601:LYS:N	1:A:601:LYS:HD2	2.33	0.43
1:B:164:ASN:O	1:B:168:LYS:HA	2.19	0.43
1:B:272:LEU:HG	1:B:276:LEU:CD2	2.48	0.43
1:A:164:ASN:HD21	1:B:89:GLN:NE2	2.17	0.43
1:D:276:LEU:HD13	1:D:279:LEU:HD12	2.00	0.43
1:D:526:LEU:HD22	1:D:548:LYS:HE2	2.00	0.43
1:A:189:PHE:CD1	1:A:198:ILE:HD13	2.54	0.43
1:A:158:PRO:HG3	1:A:209:LEU:HD23	2.01	0.43
1:B:280:ILE:HD13	1:B:324:LEU:HD13	2.01	0.43
1:B:74:VAL:C	1:B:76:ASP:H	2.22	0.43
1:C:326:ASN:HD21	1:C:329:LEU:CD1	2.32	0.43
1:D:153:LEU:HA	1:D:174:TYR:HE2	1.83	0.43
1:D:378:ARG:HD3	1:D:378:ARG:HA	1.87	0.43
1:A:246:LEU:HG	1:A:250:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:GLU:HA	1:A:499:GLU:OE1	2.19	0.43
1:C:87:ILE:HA	1:C:90:LYS:CE	2.40	0.43
1:D:246:LEU:HG	1:D:250:ILE:HD11	1.99	0.43
1:A:163:ILE:HD13	1:A:163:ILE:HA	1.91	0.42
1:B:545:ILE:HB	1:B:600:PHE:CE1	2.54	0.42
1:A:172:PRO:CG	1:B:89:GLN:HG2	2.49	0.42
1:C:184:TRP:CD1	1:C:184:TRP:C	2.92	0.42
1:C:393:MSE:HE3	1:C:427:LEU:CA	2.49	0.42
1:C:470:GLN:HA	1:C:515:MSE:HA	2.00	0.42
1:C:485:GLN:O	1:C:489:LYS:HG3	2.19	0.42
1:A:328:ASN:N	1:A:328:ASN:OD1	2.52	0.42
1:B:96:GLY:O	1:B:97:LEU:C	2.58	0.42
1:C:521:ASP:O	1:C:522:LEU:C	2.57	0.42
1:D:111:LEU:HG	1:D:115:GLN:HE21	1.84	0.42
1:D:204:GLY:O	1:D:208:LYS:HG3	2.20	0.42
1:D:436:ASP:O	1:D:440:VAL:HG23	2.18	0.42
1:C:175:GLU:HG3	1:D:94:GLN:HE21	1.83	0.42
1:A:438:LEU:HD12	1:A:438:LEU:O	2.18	0.42
1:B:397:THR:O	1:B:400:ASN:HB2	2.19	0.42
1:C:545:ILE:O	1:C:546:LYS:C	2.57	0.42
1:D:146:ARG:HH11	1:D:146:ARG:HG3	1.83	0.42
1:D:339:GLN:HA	1:D:342:GLN:CG	2.49	0.42
1:D:613:GLU:O	1:D:617:VAL:HG23	2.19	0.42
1:A:390:LEU:O	1:A:391:GLY:C	2.57	0.42
1:A:397:THR:O	1:A:400:ASN:HB2	2.20	0.42
1:A:409:LYS:HD2	1:A:409:LYS:O	2.20	0.42
1:A:470:GLN:HA	1:A:515:MSE:HA	2.01	0.42
1:B:270:HIS:O	1:B:273:SER:HB3	2.20	0.42
1:B:401:TRP:HH2	1:B:426:LEU:CD2	2.33	0.42
1:B:570:ASP:HA	1:B:571:PRO:HD3	1.87	0.42
1:D:309:VAL:HG12	1:D:313:ASN:ND2	2.34	0.42
1:D:77:LEU:H	1:D:77:LEU:CD2	2.32	0.42
1:A:96:GLY:O	1:A:97:LEU:C	2.58	0.42
1:D:96:GLY:O	1:D:97:LEU:C	2.57	0.42
1:A:146:ARG:O	1:A:149:PHE:HB3	2.19	0.42
1:A:486:ILE:H	1:A:486:ILE:HD12	1.84	0.42
1:B:326:ASN:HD21	1:B:329:LEU:CD1	2.32	0.42
1:C:413:LEU:O	1:C:414:GLN:HG3	2.20	0.42
1:C:613:GLU:O	1:C:617:VAL:HG23	2.20	0.42
1:C:175:GLU:CD	1:D:94:GLN:HG3	2.39	0.42
1:A:89:GLN:HE22	1:B:164:ASN:HD21	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:GLU:HA	1:B:499:GLU:OE1	2.20	0.42
1:C:239:MSE:HE3	1:C:239:MSE:O	2.19	0.42
1:C:246:LEU:HG	1:C:250:ILE:HD11	2.01	0.42
1:C:286:LEU:O	1:C:289:ALA:HB3	2.20	0.42
1:C:348:ALA:O	1:C:352:ILE:HG13	2.20	0.42
1:C:526:LEU:HD21	1:C:551:LYS:HB2	2.01	0.42
1:D:237:SER:OG	1:D:240:ASN:HB2	2.19	0.42
1:D:326:ASN:HD21	1:D:329:LEU:CD1	2.33	0.42
1:D:350:ASP:O	1:D:353:ILE:N	2.52	0.42
1:D:413:LEU:O	1:D:414:GLN:HG3	2.19	0.42
1:D:499:GLU:HA	1:D:499:GLU:OE1	2.19	0.42
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.90	0.42
1:B:485:GLN:O	1:B:489:LYS:HG3	2.19	0.42
1:C:419:ASN:C	1:C:421:GLU:H	2.22	0.42
1:D:202:LEU:O	1:D:202:LEU:HD12	2.20	0.42
1:D:401:TRP:CD1	1:D:402:LEU:CD2	3.03	0.42
1:A:393:MSE:HE3	1:A:427:LEU:CA	2.50	0.42
1:B:413:LEU:O	1:B:414:GLN:HG3	2.20	0.42
1:B:452:PRO:O	1:B:453:ASN:HB2	2.19	0.42
1:B:486:ILE:N	1:B:486:ILE:HD12	2.33	0.42
1:B:547:GLU:C	1:B:549:PHE:H	2.23	0.42
1:C:146:ARG:HH11	1:C:146:ARG:HG3	1.85	0.42
1:C:390:LEU:HD12	1:C:423:HIS:HB3	2.02	0.42
1:D:393:MSE:HE3	1:D:427:LEU:CA	2.50	0.42
1:A:603:PRO:HG2	1:A:604:ARG:H	1.84	0.42
1:B:389:CYS:O	1:B:393:MSE:HB2	2.20	0.42
1:C:96:GLY:O	1:C:97:LEU:C	2.58	0.42
1:D:280:ILE:HD13	1:D:324:LEU:HD13	2.02	0.42
1:D:432:SER:O	1:D:436:ASP:OD1	2.38	0.42
1:A:429:CYS:O	1:A:430:PHE:C	2.58	0.41
1:A:521:ASP:O	1:A:522:LEU:C	2.58	0.41
1:B:393:MSE:HE3	1:B:427:LEU:CA	2.50	0.41
1:B:602:ASN:HD22	1:B:606:HIS:CD2	2.38	0.41
1:C:243:THR:O	1:C:246:LEU:N	2.53	0.41
1:C:379:LEU:HD23	1:C:379:LEU:HA	1.92	0.41
1:C:518:ASP:HB3	1:C:559:LEU:CD2	2.49	0.41
1:D:516:VAL:HG12	1:D:516:VAL:O	2.19	0.41
1:A:105:HIS:C	1:A:107:LEU:N	2.73	0.41
1:A:432:SER:O	1:A:436:ASP:OD1	2.38	0.41
1:A:488:GLU:HA	1:A:493:ASN:ND2	2.18	0.41
1:A:578:LYS:NZ	1:A:622:VAL:HG23	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:ILE:C	1:A:584:LEU:H	2.24	0.41
1:B:309:VAL:HG12	1:B:313:ASN:ND2	2.35	0.41
1:B:395:ASN:HD22	1:B:395:ASN:HA	1.67	0.41
1:C:582:ILE:C	1:C:584:LEU:H	2.23	0.41
1:D:210:ILE:HG13	1:D:210:ILE:H	1.55	0.41
1:D:308:LEU:HA	1:D:308:LEU:HD23	1.84	0.41
1:A:362:ILE:O	1:A:363:PRO:C	2.58	0.41
1:A:378:ARG:HD3	1:A:378:ARG:HA	1.89	0.41
1:A:579:SER:O	1:A:580:GLU:C	2.59	0.41
1:B:246:LEU:HG	1:B:250:ILE:HD11	2.01	0.41
1:B:610:THR:HB	1:B:613:GLU:HG3	2.02	0.41
1:C:127:PHE:HD1	1:C:127:PHE:H	1.67	0.41
1:C:261:TYR:C	1:C:263:GLN:N	2.73	0.41
1:C:375:THR:OG1	1:C:438:LEU:HD22	2.21	0.41
1:B:264:TYR:N	1:B:264:TYR:CD1	2.89	0.41
1:C:407:LYS:HD2	1:C:410:GLU:OE2	2.20	0.41
1:C:383:SER:HB2	1:C:491:GLU:CB	2.50	0.41
1:A:159:PHE:CZ	1:A:172:PRO:HD2	2.56	0.41
1:A:261:TYR:C	1:A:263:GLN:N	2.73	0.41
1:A:316:LYS:NZ	1:A:334:THR:HG21	2.35	0.41
1:A:330:LEU:O	1:A:334:THR:HG23	2.19	0.41
1:A:430:PHE:O	1:A:433:ASP:N	2.53	0.41
1:A:518:ASP:HB3	1:A:559:LEU:CD2	2.48	0.41
1:B:419:ASN:C	1:B:421:GLU:H	2.22	0.41
1:B:432:SER:O	1:B:436:ASP:OD1	2.39	0.41
1:B:521:ASP:O	1:B:522:LEU:C	2.58	0.41
1:A:507:LEU:HD11	1:A:511:TYR:HE1	1.85	0.41
1:A:615:THR:O	1:A:619:ASN:ND2	2.53	0.41
1:A:622:VAL:CG1	1:A:623:ARG:NH1	2.83	0.41
1:B:163:ILE:HA	1:B:163:ILE:HD13	1.94	0.41
1:D:341:THR:CG2	1:D:392:ALA:HB3	2.47	0.41
1:D:438:LEU:C	1:D:438:LEU:HD12	2.41	0.41
1:A:577:LEU:O	1:A:581:ILE:HG13	2.20	0.41
1:A:89:GLN:NE2	1:B:164:ASN:HD21	2.18	0.41
1:D:146:ARG:O	1:D:149:PHE:HB3	2.20	0.41
1:D:309:VAL:O	1:D:312:ILE:HG22	2.21	0.41
1:D:475:PHE:O	1:D:479:ASN:ND2	2.54	0.41
1:D:521:ASP:O	1:D:522:LEU:C	2.58	0.41
1:A:254:LYS:O	1:A:255:SER:C	2.58	0.41
1:A:613:GLU:O	1:A:617:VAL:HG23	2.19	0.41
1:C:202:LEU:HD12	1:C:202:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:TYR:N	1:C:264:TYR:CD1	2.89	0.41
1:C:324:LEU:C	1:C:326:ASN:H	2.24	0.41
1:C:362:ILE:O	1:C:363:PRO:C	2.58	0.41
1:C:77:LEU:CD2	1:C:77:LEU:H	2.33	0.41
1:D:283:TYR:CE2	1:D:315:VAL:HG21	2.56	0.41
1:D:324:LEU:C	1:D:326:ASN:H	2.24	0.41
1:A:205:GLU:O	1:A:206:ARG:C	2.60	0.41
1:C:499:GLU:OE1	1:C:499:GLU:HA	2.21	0.41
1:C:610:THR:HB	1:C:613:GLU:HG3	2.02	0.41
1:D:518:ASP:HB3	1:D:559:LEU:CD2	2.50	0.41
1:D:603:PRO:O	1:D:605:LYS:N	2.54	0.41
1:A:126:GLU:C	1:A:128:HIS:H	2.23	0.41
1:A:210:ILE:H	1:A:210:ILE:HG13	1.50	0.41
1:A:379:LEU:O	1:A:382:PHE:N	2.52	0.41
1:A:523:THR:CG2	1:A:588:MSE:HG3	2.51	0.41
1:B:146:ARG:O	1:B:149:PHE:HB3	2.20	0.41
1:B:338:ARG:O	1:B:342:GLN:HG2	2.21	0.41
1:D:340:VAL:C	1:D:342:GLN:N	2.70	0.41
1:D:476:ILE:CG2	1:D:511:TYR:CZ	2.82	0.41
1:D:559:LEU:HD23	1:D:559:LEU:HA	1.88	0.41
1:A:204:GLY:O	1:A:208:LYS:HG3	2.20	0.41
1:A:280:ILE:HD13	1:A:324:LEU:HD13	2.03	0.41
1:C:195:GLY:C	1:C:197:ILE:N	2.74	0.41
1:C:206:ARG:HD2	1:C:206:ARG:HA	1.93	0.41
1:A:264:TYR:CD1	1:A:264:TYR:N	2.89	0.40
1:B:362:ILE:O	1:B:363:PRO:O	2.39	0.40
1:B:381:LYS:CE	1:B:381:LYS:HA	2.49	0.40
1:B:582:ILE:C	1:B:584:LEU:H	2.25	0.40
1:C:419:ASN:C	1:C:421:GLU:N	2.74	0.40
1:C:516:VAL:HG12	1:C:516:VAL:O	2.22	0.40
1:C:527:MSE:HA	1:C:548:LYS:HZ1	1.85	0.40
1:D:390:LEU:O	1:D:391:GLY:C	2.60	0.40
1:D:610:THR:CG2	1:D:611:PRO:HD2	2.50	0.40
1:D:593:TYR:CD1	1:D:611:PRO:HD3	2.56	0.40
1:A:306:PHE:CE2	1:A:341:THR:CG2	3.03	0.40
1:A:303:PHE:HE2	1:A:382:PHE:CD1	2.39	0.40
1:A:476:ILE:CB	1:A:511:TYR:CD2	3.03	0.40
1:B:324:LEU:C	1:B:326:ASN:H	2.24	0.40
1:C:146:ARG:O	1:C:149:PHE:HB3	2.21	0.40
1:C:308:LEU:HD23	1:C:308:LEU:HA	1.84	0.40
1:A:618:LEU:HD23	1:A:618:LEU:HA	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:SER:O	1:B:186:LEU:HB2	2.21	0.40
1:B:211:LEU:HA	1:B:211:LEU:HD13	1.81	0.40
1:B:504:LEU:O	1:B:507:LEU:HB3	2.22	0.40
1:B:523:THR:CG2	1:B:588:MSE:HG3	2.51	0.40
1:C:381:LYS:HA	1:C:381:LYS:CE	2.49	0.40
1:D:306:PHE:CE2	1:D:341:THR:CG2	3.01	0.40
1:D:419:ASN:C	1:D:421:GLU:H	2.25	0.40
1:D:552:PHE:O	1:D:556:PHE:N	2.49	0.40
1:A:270:HIS:O	1:A:273:SER:HB3	2.21	0.40
1:B:124:ASN:O	1:B:126:GLU:N	2.53	0.40
1:B:247:LEU:O	1:B:248:GLY:C	2.60	0.40
1:B:287:PHE:CE1	1:B:312:ILE:HB	2.56	0.40
1:B:383:SER:HB2	1:B:491:GLU:CB	2.52	0.40
1:B:497:ALA:HA	1:B:501:HIS:CD2	2.53	0.40
1:C:306:PHE:CD2	1:C:341:THR:HG23	2.56	0.40
1:D:270:HIS:O	1:D:273:SER:HB3	2.22	0.40
1:D:550:ARG:O	1:D:551:LYS:C	2.58	0.40
1:D:523:THR:CG2	1:D:588:MSE:HG3	2.50	0.40
1:A:121:ARG:HB2	1:A:124:ASN:HB2	2.02	0.40
1:A:398:ARG:HB2	1:A:401:TRP:CE2	2.55	0.40
1:B:154:ASN:C	1:B:156:ILE:N	2.74	0.40
1:D:261:TYR:C	1:D:263:GLN:N	2.74	0.40
1:D:340:VAL:HA	1:D:343:SER:CB	2.50	0.40
1:D:618:LEU:HD23	1:D:618:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	507/566 (90%)	403 (80%)	84 (17%)	20 (4%)	3 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	517/566 (91%)	413 (80%)	82 (16%)	22 (4%)	2 22
1	C	510/566 (90%)	410 (80%)	77 (15%)	23 (4%)	2 21
1	D	512/566 (90%)	418 (82%)	79 (15%)	15 (3%)	4 31
All	All	2046/2264 (90%)	1644 (80%)	322 (16%)	80 (4%)	3 25

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	GLY
1	A	97	LEU
1	A	416	GLU
1	A	420	TRP
1	A	497	ALA
1	A	604	ARG
1	B	75	LYS
1	B	96	GLY
1	B	97	LEU
1	B	125	SER
1	B	416	GLU
1	B	420	TRP
1	B	497	ALA
1	B	603	PRO
1	C	96	GLY
1	C	97	LEU
1	C	416	GLU
1	C	420	TRP
1	C	497	ALA
1	C	603	PRO
1	C	604	ARG
1	C	608	LYS
1	D	96	GLY
1	D	97	LEU
1	D	416	GLU
1	D	420	TRP
1	D	497	ALA
1	A	603	PRO
1	B	548	LYS
1	C	593	TYR
1	C	607	ILE
1	A	168	LYS
1	A	449	ALA

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Mol	Chain	Res	Type
1	A	593	TYR
1	B	363	PRO
1	B	410	GLU
1	B	449	ALA
1	B	593	TYR
1	C	168	LYS
1	C	410	GLU
1	C	449	ALA
1	D	168	LYS
1	D	410	GLU
1	D	449	ALA
1	D	593	TYR
1	A	296	SER
1	A	410	GLU
1	A	583	SER
1	A	591	ARG
1	B	168	LYS
1	B	296	SER
1	B	366	ASN
1	B	386	LYS
1	B	391	GLY
1	B	523	THR
1	B	583	SER
1	B	591	ARG
1	C	296	SER
1	C	386	LYS
1	C	583	SER
1	C	591	ARG
1	D	296	SER
1	D	523	THR
1	D	583	SER
1	D	591	ARG
1	A	106	LYS
1	A	386	LYS
1	A	521	ASP
1	A	523	THR
1	B	546	LYS
1	C	523	THR
1	C	547	GLU
1	A	363	PRO
1	C	387	ASN
1	D	386	LYS

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Mol	Chain	Res	Type
1	D	391	GLY
1	C	622	VAL
1	C	391	GLY
1	A	95	VAL
1	C	95	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	470/501 (94%)	446 (95%)	24 (5%)	24	57
1	B	480/501 (96%)	457 (95%)	23 (5%)	25	60
1	C	476/501 (95%)	454 (95%)	22 (5%)	27	61
1	D	477/501 (95%)	453 (95%)	24 (5%)	24	58
All	All	1903/2004 (95%)	1810 (95%)	93 (5%)	25	59

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	GLU
1	A	199	GLN
1	A	205	GLU
1	A	211	LEU
1	A	258	ASP
1	A	259	ASP
1	A	271	VAL
1	A	319	LEU
1	A	332	ASP
1	A	363	PRO
1	A	395	ASN
1	A	397	THR
1	A	421	GLU
1	A	422	ASP
1	A	427	LEU
1	A	436	ASP

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Mol	Chain	Res	Type
1	A	442	LEU
1	A	453	ASN
1	A	456	PRO
1	A	504	LEU
1	A	567	LYS
1	A	577	LEU
1	A	580	GLU
1	A	600	PHE
1	B	199	GLN
1	B	205	GLU
1	B	211	LEU
1	B	258	ASP
1	B	259	ASP
1	B	319	LEU
1	B	332	ASP
1	B	363	PRO
1	B	395	ASN
1	B	397	THR
1	B	421	GLU
1	B	422	ASP
1	B	427	LEU
1	B	436	ASP
1	B	442	LEU
1	B	453	ASN
1	B	504	LEU
1	B	549	PHE
1	B	567	LYS
1	B	577	LEU
1	B	580	GLU
1	B	604	ARG
1	B	607	ILE
1	C	199	GLN
1	C	205	GLU
1	C	211	LEU
1	C	258	ASP
1	C	259	ASP
1	C	319	LEU
1	C	332	ASP
1	C	363	PRO
1	C	395	ASN
1	C	397	THR
1	C	421	GLU

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Mol	Chain	Res	Type
1	C	422	ASP
1	C	427	LEU
1	C	436	ASP
1	C	442	LEU
1	C	453	ASN
1	C	504	LEU
1	C	544	GLN
1	C	567	LYS
1	C	577	LEU
1	C	580	GLU
1	C	600	PHE
1	D	199	GLN
1	D	205	GLU
1	D	211	LEU
1	D	258	ASP
1	D	259	ASP
1	D	319	LEU
1	D	332	ASP
1	D	363	PRO
1	D	395	ASN
1	D	397	THR
1	D	401	TRP
1	D	421	GLU
1	D	422	ASP
1	D	427	LEU
1	D	436	ASP
1	D	442	LEU
1	D	453	ASN
1	D	504	LEU
1	D	522	LEU
1	D	544	GLN
1	D	567	LYS
1	D	568	LEU
1	D	577	LEU
1	D	580	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	124	ASN
1	A	297	ASN

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Mol	Chain	Res	Type
1	A	313	ASN
1	A	395	ASN
1	A	400	ASN
1	A	423	HIS
1	A	441	ASN
1	A	453	ASN
1	A	454	GLN
1	A	468	HIS
1	A	493	ASN
1	A	501	HIS
1	B	89	GLN
1	B	115	GLN
1	B	118	GLN
1	B	120	ASN
1	B	192	ASN
1	B	297	ASN
1	B	300	ASN
1	B	313	ASN
1	B	395	ASN
1	B	400	ASN
1	B	423	HIS
1	B	441	ASN
1	B	453	ASN
1	B	454	GLN
1	B	468	HIS
1	B	493	ASN
1	B	501	HIS
1	B	553	ASN
1	B	602	ASN
1	B	606	HIS
1	C	89	GLN
1	C	124	ASN
1	C	297	ASN
1	C	313	ASN
1	C	395	ASN
1	C	400	ASN
1	C	423	HIS
1	C	441	ASN
1	C	453	ASN
1	C	454	GLN
1	C	468	HIS
1	C	493	ASN

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Mol	Chain	Res	Type
1	C	501	HIS
1	C	619	ASN
1	D	89	GLN
1	D	94	GLN
1	D	115	GLN
1	D	297	ASN
1	D	313	ASN
1	D	342	GLN
1	D	395	ASN
1	D	400	ASN
1	D	423	HIS
1	D	441	ASN
1	D	453	ASN
1	D	454	GLN
1	D	468	HIS
1	D	493	ASN
1	D	501	HIS
1	D	602	ASN
1	D	619	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	500/566 (88%)	-0.52	9 (1%)	68	62	11, 86, 200, 202	0
1	B	510/566 (90%)	-0.40	13 (2%)	57	51	44, 139, 202, 202	0
1	C	505/566 (89%)	-0.33	8 (1%)	72	66	36, 151, 202, 202	0
1	D	507/566 (89%)	-0.39	8 (1%)	72	66	11, 135, 202, 202	0
All	All	2022/2264 (89%)	-0.41	38 (1%)	66	61	11, 132, 202, 202	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	236	SER	4.8
1	A	599	SER	4.4
1	A	125	SER	4.1
1	A	124	ASN	4.0
1	D	120	ASN	4.0
1	A	123	GLU	3.8
1	A	121	ARG	3.6
1	C	606	HIS	3.2
1	A	119	ALA	3.1
1	B	120	ASN	3.0
1	B	623	ARG	3.0
1	B	457	ASP	2.9
1	B	223	GLU	2.8
1	B	127	PHE	2.8
1	A	122	GLU	2.7
1	B	456	PRO	2.7
1	B	599	SER	2.7
1	C	190	HIS	2.7
1	B	609	TYR	2.6
1	D	79	ASN	2.6
1	A	416	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	455	GLU	2.5
1	C	326	ASN	2.5
1	D	82	SER	2.5
1	B	606	HIS	2.5
1	C	116	SER	2.5
1	D	188	TYR	2.4
1	A	120	ASN	2.4
1	D	453	ASN	2.3
1	D	124	ASN	2.3
1	C	127	PHE	2.3
1	C	545	ILE	2.3
1	D	301	PHE	2.3
1	D	78	ALA	2.3
1	C	74	VAL	2.2
1	B	598	ASP	2.2
1	C	118	GLN	2.2
1	B	121	ARG	2.2

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.