Full wwPDB X-ray Structure Validation Report (i)

Nov 6, 2023 – 03:58 AM EST

PDB ID	:	3DW8
Title	:	Structure of a Protein Phosphatase 2A Holoenzyme with B55 subunit
Authors	:	Xu, Y.; Chen, Y.; Zhang, P.; Jeffrey, P.D.; Shi, Y.
Deposited on	:	2008-07-21
Resolution	:	2.85 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

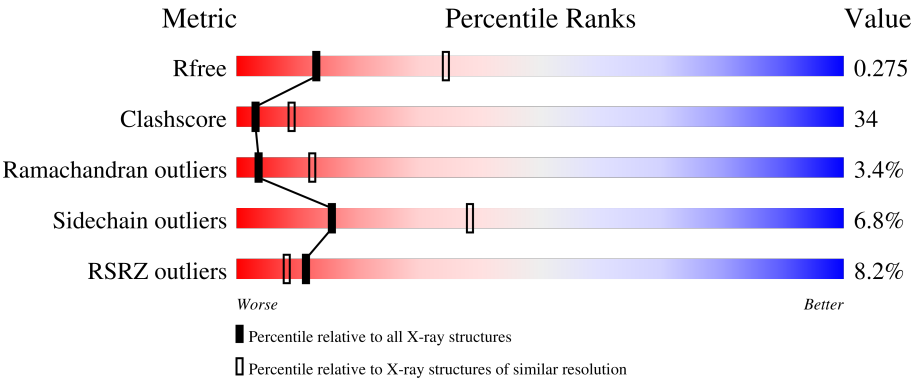
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	582	13% 38% 53% 8%
1	D	582	15% 45% 47% 7%
2	B	447	3% 51% 38% 6%
2	E	447	2% 55% 34% 6%
3	C	309	% 49% 41% 7%

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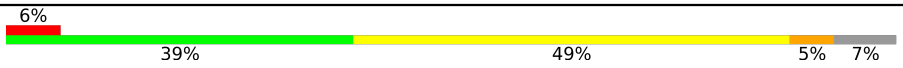
Mol	Chain	Length	Quality of chain
3	F	309	
4	G	7	
4	H	7	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 20717 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 Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	0
			4535	2882	764	861	28			
1	D	582	Total	C	N	O	S	0	0	0
			4535	2882	764	861	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	expression tag	UNP P30153
D	8	MET	-	expression tag	UNP P30153

- Molecule 2 is a protein called Serine/threonine-protein phosphatase 2A 55 kDa regulatory subunit B alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3429	2158	595	658	18			
2	E	421	Total	C	N	O	S	0	0	0
			3428	2157	595	658	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	310	VAL	ILE	engineered mutation	UNP P63151
E	310	VAL	ILE	engineered mutation	UNP P63151

- Molecule 3 is a protein called Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	288	Total	C	N	O	S	0	0	0
			2322	1471	396	440	15			
3	F	288	Total	C	N	O	S	0	0	0
			2322	1471	396	440	15			

- Molecule 4 is a protein called microcystin LR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	0	0	0
			71	49	10	12			
4	H	7	Total	C	N	O	0	0	0
			71	49	10	12			

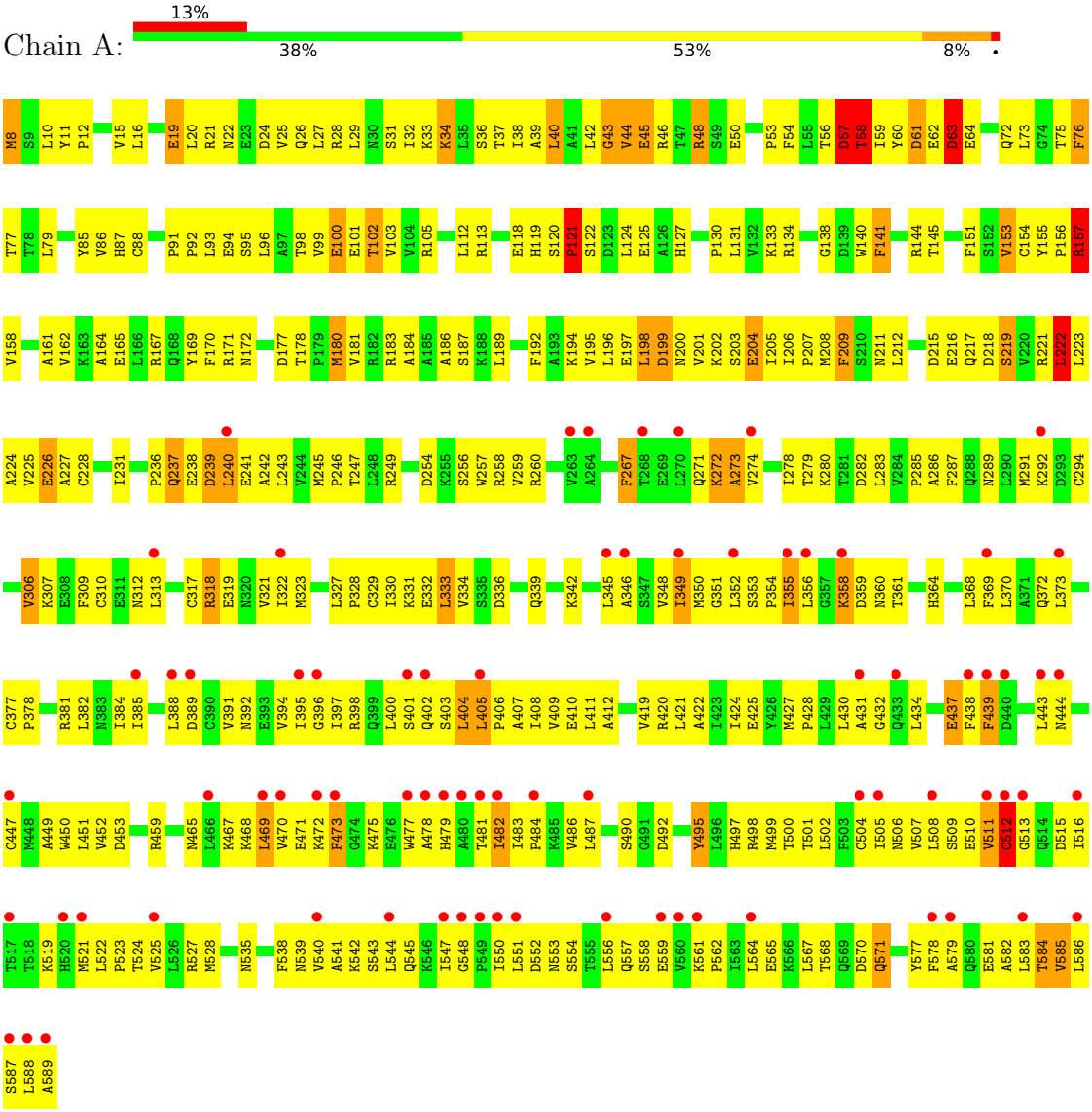
- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	2	Total	Mn	0	0
			2	2		
5	F	2	Total	Mn	0	0
			2	2		

3 Residue-property plots (i)

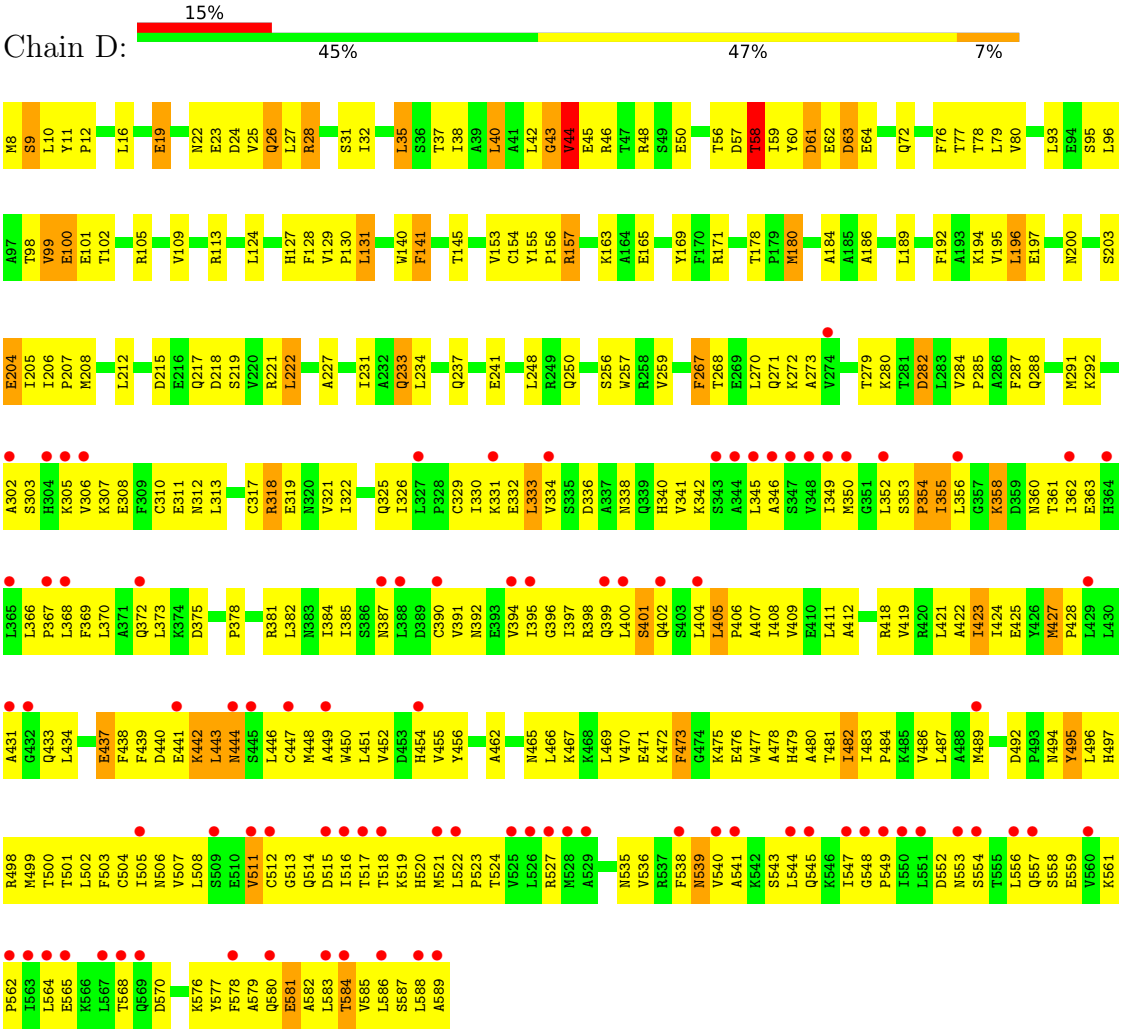
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform



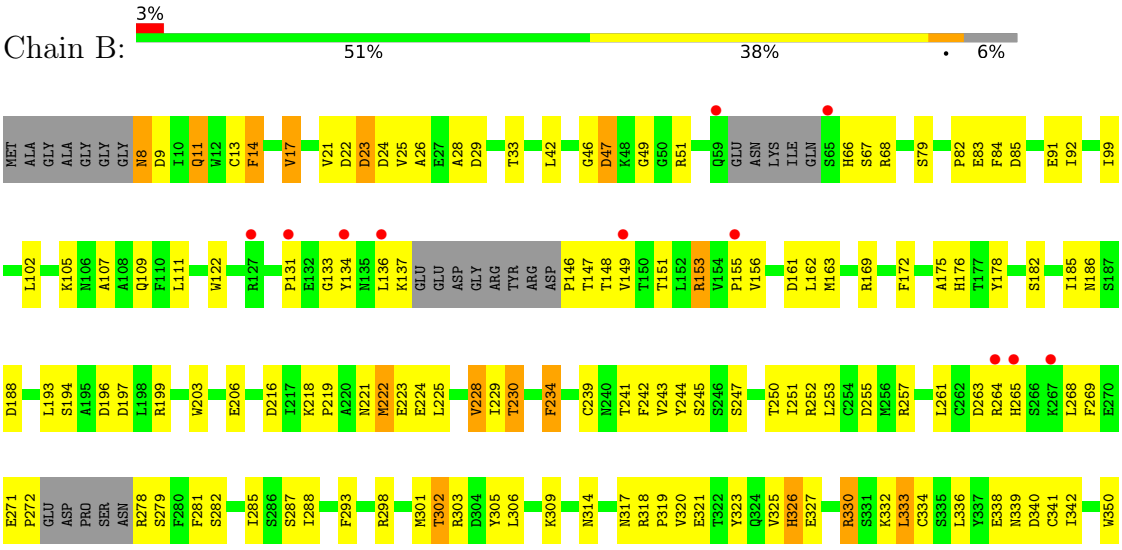
• Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform

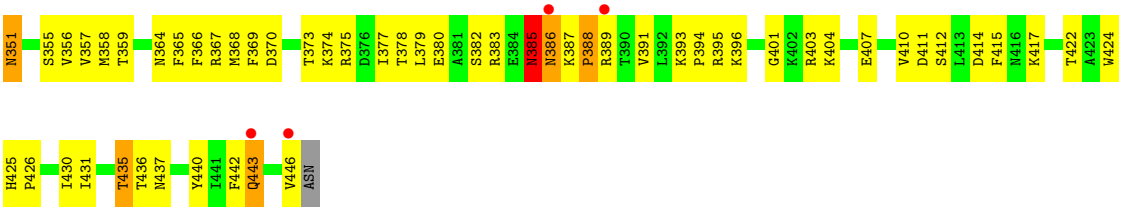
Chain D:



• Molecule 2: Serine/threonine-protein phosphatase 2A 55 kDa regulatory subunit B alpha isoform

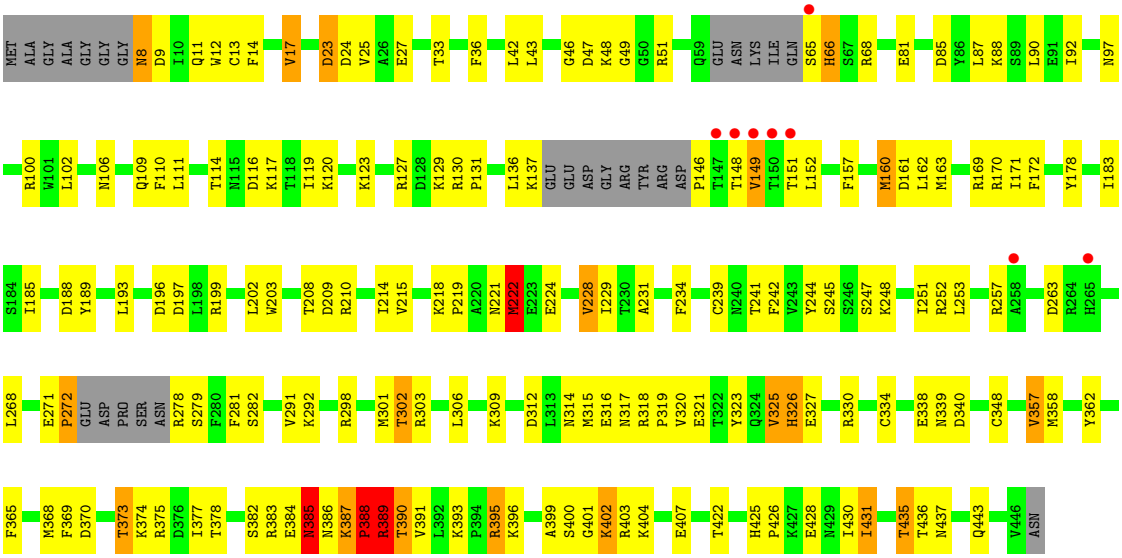
Chain B:





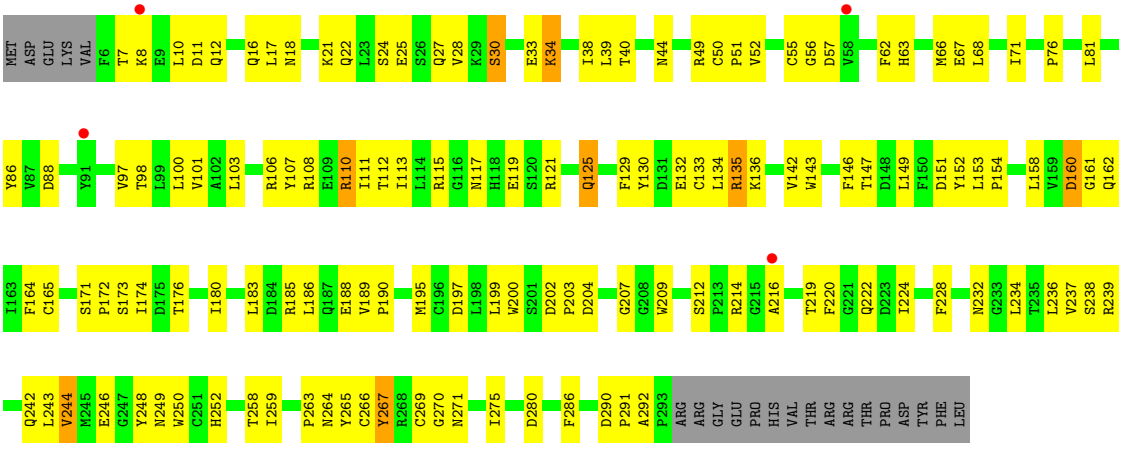
• Molecule 2: Serine/threonine-protein phosphatase 2A 55 kDa regulatory subunit B alpha isoform

Chain E:



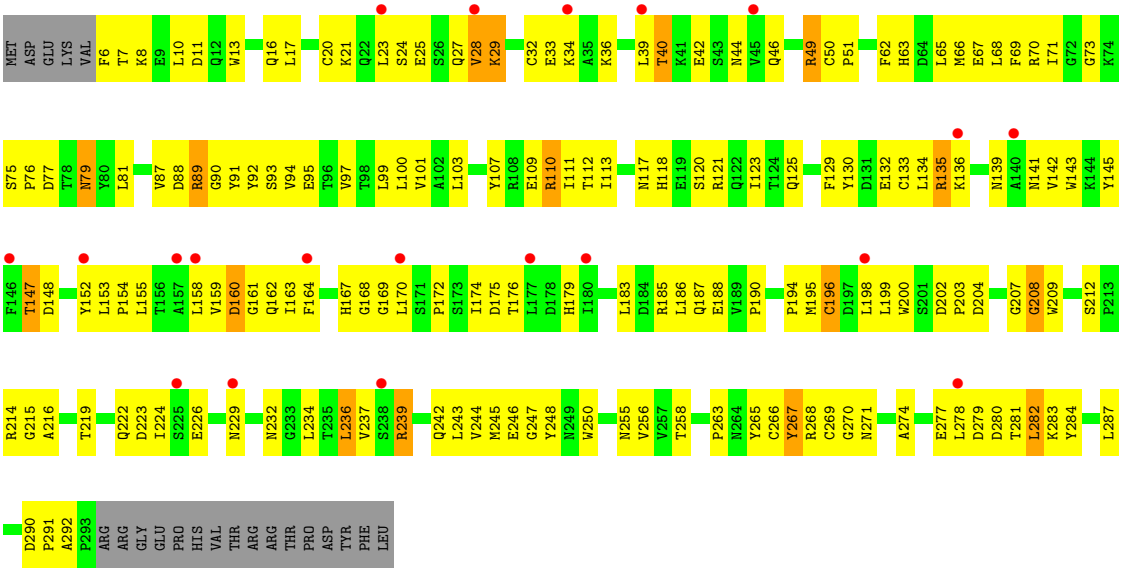
• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain C:



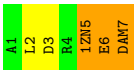
• Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain F:



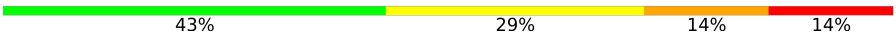
• Molecule 4: microcystin LR

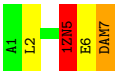
Chain G:



• Molecule 4: microcystin LR

Chain H:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	247.34Å 121.39Å 172.48Å 90.00° 132.60° 90.00°	Depositor
Resolution (Å)	49.63 – 2.85 49.63 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.63-2.85) 99.3 (49.63-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.40 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.285 0.219 , 0.275	Depositor DCC
R_{free} test set	4180 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	78.6	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 72.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	20717	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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

Bond lengths and bond angles in the following residue types are not validated in this section: DAM, ACB, MN, DAL, 1ZN, FGA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.42	0/4609	0.65	1/6256 (0.0%)
1	D	0.44	0/4609	0.66	1/6256 (0.0%)
2	B	0.55	0/3501	0.76	2/4730 (0.0%)
2	E	0.59	1/3500 (0.0%)	0.80	2/4728 (0.0%)
3	C	0.43	0/2379	0.68	0/3227
3	F	0.42	0/2379	0.65	0/3227
4	G	0.43	0/17	0.60	0/19
4	H	0.43	0/17	0.50	0/19
All	All	0.48	1/21011 (0.0%)	0.70	6/28462 (0.0%)

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
4	G	0	2
4	H	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	13	CYS	CB-SG	-6.12	1.71	1.82

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	44	VAL	N-CA-C	-6.37	93.79	111.00
2	B	146	PRO	N-CA-CB	5.70	110.13	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	85	ASP	N-CA-C	-5.68	95.67	111.00
2	E	146	PRO	N-CA-CB	5.65	110.08	103.30
1	A	222	LEU	CA-CB-CG	5.62	128.24	115.30
2	E	100	ARG	NE-CZ-NH1	-5.32	117.64	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	G	5	1ZN	Peptide,Mainchain
4	H	5	1ZN	Peptide,Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4535	0	4642	402	0
1	D	4535	0	4642	368	0
2	B	3429	0	3323	209	0
2	E	3428	0	3322	178	0
3	C	2322	0	2223	113	0
3	F	2322	0	2223	165	0
4	G	71	0	61	4	0
4	H	71	0	61	2	0
5	C	2	0	0	0	0
5	F	2	0	0	0	0
All	All	20717	0	20497	1392	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 34.

All (1392) 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:A:208:MET:SD	1:A:208:MET:CE	2.01	1.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:ILE:HG12	3:C:108:ARG:HH21	1.10	1.11
1:A:478:ALA:HA	1:A:482:ILE:HD12	1.30	1.10
1:D:22:ASN:ND2	1:D:27:LEU:HD12	1.69	1.08
1:A:373:LEU:HD21	1:A:404:LEU:HB3	1.39	1.04
2:E:370:ASP:HB3	2:E:373:THR:HG22	1.37	1.04
2:B:199:ARG:HH21	2:B:218:LYS:HD3	1.24	1.03
1:D:378:PRO:O	1:D:382:LEU:HB2	1.57	1.03
1:D:100:GLU:HG3	2:E:106:ASN:HD21	1.25	1.02
2:E:373:THR:HG23	2:E:375:ARG:H	1.22	1.01
1:D:506:ASN:HD21	1:D:543:SER:HA	1.26	0.99
2:E:25:VAL:HG13	2:E:437:ASN:HB3	1.44	0.99
1:D:59:ILE:HD13	1:D:95:SER:HB3	1.42	0.98
1:A:307:LYS:HE2	1:A:351:GLY:HA3	1.44	0.97
2:B:199:ARG:NH2	2:B:218:LYS:HD3	1.79	0.97
1:D:478:ALA:HA	1:D:482:ILE:HD12	1.46	0.96
1:A:11:TYR:HB3	1:A:12:PRO:HD3	1.47	0.96
3:F:28:VAL:HG11	3:F:142:VAL:HG13	1.45	0.96
2:B:278:ARG:HG3	2:B:279:SER:H	1.29	0.95
1:D:405:LEU:HB2	1:D:406:PRO:HD3	1.49	0.94
1:A:378:PRO:O	1:A:382:LEU:HB2	1.68	0.92
3:C:81:LEU:HD13	3:C:112:THR:HB	1.52	0.92
1:D:178:THR:HG22	1:D:180:MET:H	1.35	0.92
2:E:399:ALA:HB3	2:E:402:LYS:HE2	1.48	0.91
2:B:325:VAL:HG23	2:B:367:ARG:HG3	1.53	0.90
1:A:178:THR:HG22	1:A:180:MET:H	1.36	0.90
2:B:330:ARG:HH11	2:B:330:ARG:HG3	1.35	0.90
1:A:432:GLY:HA3	1:A:472:LYS:HE3	1.51	0.90
1:A:479:HIS:HB2	1:A:516:ILE:HD13	1.53	0.89
3:C:28:VAL:HG11	3:C:142:VAL:HG13	1.55	0.89
3:F:100:LEU:HA	3:F:103:LEU:HD12	1.54	0.89
2:B:21:VAL:HA	2:B:383:ARG:HH12	1.36	0.88
1:A:186:ALA:HB2	1:A:212:LEU:HD13	1.56	0.88
2:B:334:CYS:O	2:B:338:GLU:HG2	1.74	0.88
2:B:251:ILE:H	2:B:251:ILE:HD12	1.39	0.87
1:A:21:ARG:O	1:A:21:ARG:HG2	1.72	0.87
2:B:21:VAL:HA	2:B:383:ARG:NH1	1.88	0.87
1:D:124:LEU:HD11	1:D:154:CYS:HB2	1.57	0.87
3:C:125:GLN:HA	3:C:130:TYR:HB2	1.56	0.86
2:E:393:LYS:HB3	2:E:395:ARG:NH2	1.91	0.86
1:A:404:LEU:HD12	1:A:408:ILE:HD11	1.56	0.86
3:C:34:LYS:HE2	3:C:34:LYS:HA	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:GLY:O	1:D:400:LEU:HD13	1.75	0.86
1:D:141:PHE:HE1	1:D:180:MET:SD	1.98	0.86
1:A:59:ILE:HG12	1:A:95:SER:HB3	1.56	0.85
1:D:452:VAL:HG22	1:D:497:HIS:CE1	2.11	0.85
2:E:395:ARG:NH1	2:E:395:ARG:HA	1.91	0.85
2:B:25:VAL:HG13	2:B:437:ASN:HB3	1.59	0.84
1:A:15:VAL:HG22	2:B:136:LEU:HD21	1.58	0.84
1:D:56:THR:O	1:D:59:ILE:HD12	1.76	0.84
1:D:443:LEU:HD12	1:D:443:LEU:H	1.42	0.84
2:B:351:ASN:HD21	2:B:355:SER:H	1.24	0.84
2:B:25:VAL:HG22	2:B:437:ASN:HD22	1.42	0.84
1:D:318:ARG:HG2	1:D:319:GLU:N	1.92	0.83
2:B:250:THR:HB	2:B:268:LEU:HD11	1.60	0.83
1:A:155:TYR:HB3	1:A:156:PRO:HD3	1.61	0.81
2:E:396:LYS:HB3	2:E:407:GLU:HG2	1.60	0.81
1:A:25:VAL:HG22	1:A:28:ARG:HH12	1.45	0.81
3:C:38:ILE:HG12	3:C:108:ARG:NH2	1.94	0.81
3:C:103:LEU:HB3	3:C:111:ILE:CD1	2.10	0.81
1:A:141:PHE:CE2	2:B:105:LYS:HA	2.16	0.81
1:D:409:VAL:HG22	1:D:446:LEU:HD21	1.63	0.81
3:C:50:CYS:HB2	3:C:51:PRO:HA	1.62	0.80
2:B:8:ASN:N	2:B:8:ASN:HD22	1.75	0.80
3:F:16:GLN:HG2	3:F:21:LYS:HB2	1.62	0.80
3:F:266:CYS:O	3:F:268:ARG:HG2	1.82	0.80
1:A:236:PRO:HG2	1:A:239:ASP:OD2	1.81	0.80
1:A:113:ARG:HG2	1:A:153:VAL:HG11	1.62	0.80
2:E:221:ASN:HD21	2:E:224:GLU:HG3	1.45	0.80
1:D:58:THR:HG23	1:D:59:ILE:H	1.45	0.79
1:D:391:VAL:O	1:D:395:ILE:HG12	1.81	0.79
3:F:125:GLN:HA	3:F:130:TYR:CB	2.13	0.79
3:F:109:GLU:HB2	3:F:110:ARG:HH21	1.47	0.79
2:E:309:LYS:HD3	2:E:319:PRO:HG3	1.65	0.78
1:D:431:ALA:HB1	1:D:473:PHE:HE2	1.48	0.78
1:D:392:ASN:HD21	1:D:397:ILE:HG12	1.49	0.78
1:A:197:GLU:CD	1:A:197:GLU:H	1.88	0.78
1:A:223:LEU:O	1:A:226:GLU:HG3	1.84	0.78
3:F:76:PRO:HB2	3:F:110:ARG:HD2	1.66	0.78
1:A:43:GLY:HA3	1:A:45:GLU:OE1	1.83	0.78
1:A:59:ILE:HG22	1:A:59:ILE:O	1.83	0.78
2:E:8:ASN:N	2:E:8:ASN:HD22	1.80	0.77
1:A:141:PHE:HE1	1:A:180:MET:SD	2.08	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:HH12	2:B:153:ARG:NH1	1.82	0.77
2:E:370:ASP:CB	2:E:373:THR:HG22	2.13	0.77
1:A:392:ASN:OD1	1:A:397:ILE:HG12	1.85	0.77
2:B:387:LYS:HA	2:B:387:LYS:HE2	1.65	0.77
2:B:162:LEU:HD23	2:B:163:MET:N	2.00	0.77
3:C:115:ARG:NH1	3:C:151:ASP:HA	1.99	0.76
3:F:79:ASN:ND2	3:F:110:ARG:HA	1.99	0.76
1:D:543:SER:O	1:D:547:ILE:HG12	1.84	0.76
2:E:393:LYS:HB3	2:E:395:ARG:HH21	1.51	0.76
1:D:439:PHE:HA	1:D:443:LEU:HD13	1.68	0.76
2:E:25:VAL:CG1	2:E:437:ASN:HB3	2.16	0.76
2:E:251:ILE:HD12	2:E:251:ILE:N	2.01	0.76
1:D:577:TYR:O	1:D:581:GLU:HB3	1.86	0.76
3:F:125:GLN:HA	3:F:130:TYR:HB2	1.66	0.76
3:C:125:GLN:HA	3:C:130:TYR:CB	2.15	0.75
1:D:32:ILE:HA	1:D:35:LEU:HD22	1.68	0.75
3:F:237:VAL:HB	3:F:256:VAL:HG22	1.68	0.75
1:D:321:VAL:HA	1:D:325:GLN:HG2	1.69	0.75
1:D:479:HIS:HB2	1:D:516:ILE:HD13	1.68	0.75
1:A:553:ASN:O	1:A:557:GLN:HG2	1.86	0.75
1:A:178:THR:HG22	1:A:180:MET:N	2.01	0.75
3:C:67:GLU:HB2	3:C:292:ALA:HB2	1.69	0.75
1:A:385:ILE:HG21	1:A:430:LEU:HD11	1.68	0.75
2:B:436:THR:HG23	2:B:437:ASN:N	2.02	0.75
1:D:155:TYR:HB3	1:D:156:PRO:HD3	1.69	0.74
1:A:12:PRO:O	1:A:16:LEU:HD13	1.87	0.74
1:A:267:PHE:CE2	1:A:287:PHE:HB2	2.23	0.74
2:B:327:GLU:OE2	2:B:330:ARG:HG3	1.87	0.74
2:B:396:LYS:HD3	2:B:407:GLU:OE2	1.87	0.74
3:F:76:PRO:HB2	3:F:110:ARG:CD	2.17	0.74
1:D:102:THR:HG22	1:D:105:ARG:HH22	1.52	0.74
1:D:561:LYS:HD2	1:D:588:LEU:HD22	1.69	0.74
1:D:192:PHE:O	1:D:196:LEU:HD23	1.88	0.73
2:E:87:LEU:HD12	2:E:87:LEU:H	1.53	0.73
1:A:45:GLU:H	1:A:45:GLU:CD	1.91	0.73
1:D:22:ASN:HD21	1:D:27:LEU:HD12	1.52	0.73
1:D:284:VAL:O	1:D:288:GLN:HG3	1.88	0.73
1:D:544:LEU:HD12	1:D:564:LEU:HD21	1.69	0.73
3:F:117:ASN:HB3	3:F:199:LEU:O	1.89	0.73
3:C:266:CYS:SG	4:G:2:LEU:HD13	2.29	0.72
1:A:571:GLN:CD	1:A:571:GLN:H	1.93	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:395:ARG:HA	2:E:395:ARG:HH11	1.53	0.72
1:D:506:ASN:ND2	1:D:543:SER:HA	2.01	0.72
2:E:271:GLU:HG3	2:E:318:ARG:HG2	1.71	0.72
1:A:561:LYS:O	1:A:565:GLU:HG3	1.90	0.72
1:A:217:GLN:OE1	2:B:239:CYS:HB3	1.90	0.72
1:A:421:LEU:O	1:A:425:GLU:HG2	1.89	0.72
2:B:373:THR:O	2:B:374:LYS:HB2	1.89	0.72
3:F:154:PRO:HA	3:F:185:ARG:NH1	2.04	0.72
1:A:396:GLY:O	1:A:400:LEU:HD13	1.90	0.71
3:C:204:ASP:OD2	3:C:219:THR:HB	1.90	0.71
2:E:251:ILE:HD12	2:E:251:ILE:H	1.55	0.71
1:A:350:MET:HB3	1:A:391:VAL:CG2	2.20	0.71
1:D:349:ILE:HG23	1:D:350:MET:HE2	1.72	0.71
1:D:405:LEU:HD12	1:D:405:LEU:H	1.53	0.71
2:E:178:TYR:HB2	2:E:196:ASP:HB3	1.72	0.71
3:F:121:ARG:O	3:F:125:GLN:HG3	1.90	0.71
2:B:330:ARG:HH11	2:B:330:ARG:CG	2.02	0.71
1:A:141:PHE:CZ	2:B:105:LYS:HG3	2.25	0.71
1:A:543:SER:O	1:A:547:ILE:HG12	1.89	0.71
1:A:127:HIS:C	1:A:130:PRO:HD2	2.11	0.71
3:F:121:ARG:HG2	3:F:147:THR:CG2	2.21	0.71
2:B:21:VAL:CA	2:B:383:ARG:HH12	2.03	0.70
1:D:59:ILE:HD13	1:D:95:SER:CB	2.20	0.70
1:D:392:ASN:ND2	1:D:397:ILE:HG12	2.05	0.70
3:F:121:ARG:NH2	3:F:148:ASP:HA	2.06	0.70
1:A:545:GLN:OE1	1:A:582:ALA:HA	1.90	0.70
1:A:271:GLN:HA	1:A:274:VAL:HG12	1.73	0.70
1:D:178:THR:HG22	1:D:180:MET:N	2.06	0.70
1:D:492:ASP:OD2	1:D:497:HIS:HB2	1.90	0.70
1:D:363:GLU:HG2	1:D:363:GLU:O	1.91	0.70
2:B:25:VAL:HG22	2:B:437:ASN:ND2	2.07	0.70
1:D:346:ALA:HA	1:D:349:ILE:HG22	1.73	0.70
1:A:559:GLU:C	1:A:562:PRO:HD2	2.12	0.69
3:F:174:ILE:HD11	3:F:183:LEU:HD11	1.74	0.69
1:D:24:ASP:HB3	1:D:27:LEU:HG	1.73	0.69
1:D:100:GLU:HG2	2:E:110:PHE:CZ	2.27	0.69
3:C:38:ILE:CG1	3:C:108:ARG:HH21	1.98	0.69
1:D:570:ASP:O	1:D:576:LYS:HE2	1.93	0.69
2:E:271:GLU:HG2	2:E:272:PRO:HD2	1.74	0.69
1:D:19:GLU:HB3	1:D:31:SER:OG	1.93	0.69
2:E:373:THR:CG2	2:E:375:ARG:H	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:81:LEU:CD1	3:C:112:THR:HB	2.23	0.69
1:D:77:THR:O	1:D:80:VAL:HG12	1.93	0.69
1:D:287:PHE:HE1	1:D:291:MET:SD	2.15	0.69
1:A:169:TYR:O	1:A:172:ASN:HB2	1.92	0.69
2:B:11:GLN:HE21	2:B:11:GLN:HA	1.57	0.68
1:D:217:GLN:OE1	2:E:239:CYS:HB3	1.93	0.68
1:A:282:ASP:O	1:A:285:PRO:HD2	1.94	0.68
1:D:59:ILE:HG23	1:D:96:LEU:HD23	1.74	0.68
1:D:366:LEU:HB3	1:D:367:PRO:HD3	1.75	0.68
3:F:172:PRO:HG3	3:F:209:TRP:CD2	2.29	0.68
1:A:46:ARG:HD2	1:A:50:GLU:OE2	1.94	0.68
1:D:11:TYR:HB3	1:D:12:PRO:HD3	1.76	0.68
2:B:197:ASP:HB3	2:B:228:VAL:HG22	1.74	0.68
3:C:24:SER:OG	3:C:27:GLN:HG3	1.93	0.68
2:E:14:PHE:HZ	2:E:17:VAL:HG22	1.57	0.68
2:E:241:THR:HG23	2:E:253:LEU:HD21	1.76	0.68
1:A:402:GLN:O	1:A:405:LEU:HD11	1.93	0.68
1:A:564:LEU:O	1:A:568:THR:HG23	1.93	0.68
1:A:279:THR:HA	1:A:283:LEU:HG	1.74	0.67
1:A:577:TYR:O	1:A:581:GLU:HB3	1.94	0.67
3:C:44:ASN:OD1	3:C:185:ARG:HD3	1.94	0.67
1:D:141:PHE:CE1	1:D:180:MET:SD	2.85	0.67
2:E:14:PHE:CZ	2:E:17:VAL:HG22	2.28	0.67
1:D:381:ARG:O	1:D:385:ILE:HG12	1.93	0.67
1:D:395:ILE:HD12	1:D:400:LEU:HD11	1.77	0.67
2:E:85:ASP:HB3	2:E:90:LEU:HB3	1.75	0.67
1:A:475:LYS:HB2	1:A:512:CYS:HA	1.76	0.67
1:D:545:GLN:OE1	1:D:582:ALA:HA	1.94	0.67
1:A:467:LYS:HB2	1:A:507:VAL:CG1	2.24	0.67
1:A:431:ALA:HB1	1:A:473:PHE:HE2	1.58	0.67
2:B:14:PHE:CD1	2:B:14:PHE:C	2.68	0.67
1:A:382:LEU:HD21	1:A:422:ALA:HB1	1.77	0.67
1:D:22:ASN:HD22	1:D:27:LEU:HD12	1.56	0.67
2:E:25:VAL:HG11	2:E:436:THR:HG22	1.76	0.67
3:F:79:ASN:HD21	3:F:110:ARG:HA	1.58	0.67
3:F:174:ILE:CD1	3:F:194:PRO:HB2	2.25	0.66
1:D:427:MET:N	1:D:428:PRO:HD2	2.10	0.66
2:B:351:ASN:HD21	2:B:355:SER:N	1.93	0.66
1:D:516:ILE:HA	1:D:519:LYS:HD2	1.77	0.66
1:A:8:MET:SD	1:A:8:MET:N	2.69	0.66
1:A:427:MET:N	1:A:428:PRO:HD2	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:214:ARG:NH2	3:C:242:GLN:HG2	2.11	0.66
2:B:234:PHE:CD1	2:B:242:PHE:HB3	2.31	0.66
1:D:405:LEU:HB2	1:D:406:PRO:CD	2.23	0.66
2:B:8:ASN:HD21	2:B:375:ARG:NH2	1.94	0.66
1:A:246:PRO:HA	1:A:249:ARG:NH1	2.11	0.65
1:D:427:MET:HE3	1:D:427:MET:HA	1.77	0.65
1:D:467:LYS:HB2	1:D:507:VAL:HG12	1.76	0.65
3:F:163:ILE:HG23	3:F:236:LEU:HD23	1.78	0.65
1:A:453:ASP:O	1:A:459:ARG:HD3	1.96	0.65
2:B:196:ASP:HB2	2:B:199:ARG:H	1.62	0.65
1:D:23:GLU:HA	1:D:23:GLU:OE1	1.94	0.65
1:D:267:PHE:CE2	1:D:287:PHE:HB2	2.31	0.65
1:A:11:TYR:HB3	1:A:12:PRO:CD	2.26	0.65
2:B:320:VAL:HG12	2:B:321:GLU:HG3	1.79	0.65
1:D:59:ILE:HG22	1:D:59:ILE:O	1.97	0.65
2:E:387:LYS:O	2:E:390:THR:HB	1.97	0.65
1:A:75:THR:O	1:A:76:PHE:HD1	1.80	0.65
1:A:330:ILE:O	1:A:334:VAL:HG23	1.97	0.65
3:C:115:ARG:HH12	3:C:151:ASP:HA	1.62	0.65
3:C:243:LEU:HD11	3:C:271:ASN:CG	2.17	0.65
3:F:222:GLN:O	3:F:226:GLU:HG3	1.96	0.65
1:A:15:VAL:HG22	2:B:136:LEU:CD2	2.27	0.65
1:A:22:ASN:ND2	1:A:27:LEU:HD12	2.12	0.65
1:A:93:LEU:HD13	1:A:112:LEU:HD23	1.78	0.65
1:D:282:ASP:O	1:D:285:PRO:HD2	1.96	0.65
1:A:515:ASP:O	1:A:519:LYS:HB2	1.97	0.65
1:D:441:GLU:O	1:D:442:LYS:HG2	1.97	0.65
2:E:219:PRO:HG2	2:E:222:MET:CE	2.27	0.65
1:A:208:MET:CE	1:A:208:MET:CB	2.75	0.64
1:A:548:GLY:HA3	1:A:586:LEU:HD22	1.79	0.64
1:A:209:PHE:CE1	1:A:247:THR:HG21	2.32	0.64
1:A:405:LEU:H	1:A:405:LEU:HD12	1.61	0.64
3:C:209:TRP:CE2	3:C:224:ILE:HD13	2.32	0.64
2:B:298:ARG:HH21	2:B:314:ASN:HD21	1.46	0.64
1:A:75:THR:O	1:A:75:THR:OG1	2.16	0.64
1:A:192:PHE:O	1:A:195:VAL:HG22	1.97	0.64
1:D:373:LEU:HD21	1:D:404:LEU:HB3	1.80	0.64
2:E:373:THR:O	2:E:374:LYS:HB2	1.96	0.64
2:E:47:ASP:HB2	2:E:51:ARG:H	1.63	0.64
1:D:556:LEU:O	1:D:588:LEU:HD11	1.96	0.64
1:A:19:GLU:HB3	1:A:31:SER:OG	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:336:LEU:HD21	2:B:415:PHE:CE2	2.33	0.63
1:A:391:VAL:HG12	1:A:391:VAL:O	1.98	0.63
1:D:131:LEU:HD12	1:D:131:LEU:O	1.98	0.63
2:E:373:THR:HG23	2:E:375:ARG:N	2.03	0.63
1:A:58:THR:HA	1:A:60:TYR:CD1	2.34	0.63
1:A:204:GLU:O	1:A:207:PRO:HD2	1.99	0.63
1:A:395:ILE:HD12	1:A:400:LEU:HD11	1.80	0.63
2:B:436:THR:CG2	2:B:437:ASN:H	2.12	0.63
1:D:267:PHE:CE2	1:D:287:PHE:HD2	2.17	0.63
3:F:109:GLU:HB2	3:F:110:ARG:NH2	2.14	0.63
1:A:38:ILE:O	1:A:42:LEU:HD23	1.98	0.63
1:A:211:ASN:HA	1:D:8:MET:HE3	1.79	0.63
3:F:87:VAL:O	3:F:88:ASP:HB2	1.96	0.63
1:A:59:ILE:HG12	1:A:95:SER:CB	2.27	0.63
1:A:553:ASN:HA	1:A:556:LEU:HD12	1.79	0.63
2:B:436:THR:CG2	2:B:437:ASN:N	2.62	0.63
2:E:373:THR:HG23	2:E:375:ARG:HG3	1.81	0.63
1:A:127:HIS:O	1:A:130:PRO:HD2	1.99	0.62
1:A:373:LEU:HD11	1:A:385:ILE:HD11	1.81	0.62
2:E:241:THR:CG2	2:E:253:LEU:HD21	2.28	0.62
2:B:272:PRO:HG2	2:B:318:ARG:HE	1.64	0.62
1:A:208:MET:CE	1:A:208:MET:HB2	2.29	0.62
1:A:287:PHE:HE1	1:A:291:MET:SD	2.22	0.62
3:F:103:LEU:HB3	3:F:111:ILE:CD1	2.30	0.62
1:D:57:ASP:HB3	2:E:129:LYS:NZ	2.14	0.62
1:D:127:HIS:C	1:D:130:PRO:HD2	2.20	0.62
1:D:373:LEU:HD11	1:D:385:ILE:HD11	1.81	0.62
1:D:405:LEU:H	1:D:405:LEU:CD1	2.13	0.62
3:F:246:GLU:OE1	3:F:246:GLU:HA	1.98	0.62
1:D:145:THR:HG23	1:D:184:ALA:HB2	1.82	0.62
1:D:318:ARG:O	1:D:321:VAL:HG22	2.00	0.62
1:D:350:MET:HB3	1:D:391:VAL:CG2	2.30	0.62
1:A:59:ILE:O	1:A:59:ILE:CG2	2.48	0.62
2:E:278:ARG:HG3	2:E:279:SER:H	1.64	0.62
2:E:302:THR:HG22	2:E:309:LYS:HG2	1.82	0.62
2:E:387:LYS:HB3	2:E:388:PRO:HD2	1.80	0.62
3:F:158:LEU:HD21	3:F:161:GLY:HA2	1.80	0.61
1:A:15:VAL:CG2	2:B:136:LEU:HD21	2.28	0.61
1:A:209:PHE:CD2	1:A:231:ILE:HD12	2.35	0.61
1:A:350:MET:HB3	1:A:391:VAL:HG23	1.82	0.61
2:B:278:ARG:HG3	2:B:279:SER:N	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:LYS:HB3	2:B:388:PRO:HD2	1.82	0.61
1:D:287:PHE:CE1	1:D:291:MET:SD	2.93	0.61
1:D:483:ILE:O	1:D:487:LEU:HG	2.00	0.61
1:A:400:LEU:O	1:A:404:LEU:HD23	2.00	0.61
3:C:266:CYS:C	3:C:267:TYR:HD1	2.03	0.61
1:D:467:LYS:HB2	1:D:507:VAL:CG1	2.29	0.61
3:F:199:LEU:N	3:F:199:LEU:HD12	2.15	0.61
3:F:248:TYR:HA	3:F:258:THR:O	2.01	0.61
1:A:200:ASN:HA	1:A:203:SER:OG	2.00	0.61
1:A:385:ILE:CG2	1:A:430:LEU:HD11	2.31	0.61
1:D:536:VAL:O	1:D:540:VAL:HG23	2.00	0.61
2:E:222:MET:CE	2:E:222:MET:HA	2.30	0.61
3:F:281:THR:OG1	3:F:283:LYS:HG2	2.00	0.61
1:A:24:ASP:OD1	1:A:26:GLN:N	2.33	0.61
1:A:120:SER:O	1:A:122:SER:N	2.34	0.61
3:C:248:TYR:HA	3:C:258:THR:O	1.99	0.61
1:A:25:VAL:HA	1:A:28:ARG:NH1	2.15	0.61
1:A:388:LEU:HD11	1:A:430:LEU:HD23	1.83	0.61
1:A:524:THR:HG23	1:A:527:ARG:NH2	2.14	0.61
1:D:227:ALA:O	1:D:231:ILE:HG13	2.00	0.61
1:A:452:VAL:HG23	1:A:497:HIS:ND1	2.15	0.60
2:B:404:LYS:HD2	2:B:407:GLU:OE1	2.00	0.60
1:A:196:LEU:HB2	1:A:201:VAL:CG2	2.31	0.60
1:D:319:GLU:HG3	1:D:356:LEU:CD2	2.32	0.60
2:E:197:ASP:HB3	2:E:228:VAL:HG22	1.83	0.60
3:F:121:ARG:HG3	3:F:188:GLU:OE2	2.01	0.60
1:A:211:ASN:OD1	1:D:8:MET:CE	2.50	0.60
1:A:405:LEU:HB2	1:A:406:PRO:HD3	1.83	0.60
2:B:264:ARG:HG2	2:B:265:HIS:N	2.16	0.60
1:A:94:GLU:HG3	1:A:131:LEU:HD11	1.82	0.60
2:B:330:ARG:CG	2:B:330:ARG:NH1	2.61	0.60
2:B:436:THR:HG23	2:B:437:ASN:H	1.64	0.60
1:D:561:LYS:HB2	1:D:588:LEU:HD13	1.83	0.60
1:D:561:LYS:HE3	1:D:588:LEU:O	2.01	0.60
3:F:121:ARG:HG2	3:F:147:THR:HB	1.83	0.60
1:A:544:LEU:HD12	1:A:564:LEU:HD21	1.82	0.60
2:B:373:THR:HG21	2:B:375:ARG:HB2	1.83	0.60
1:D:392:ASN:HD21	1:D:397:ILE:CG1	2.15	0.60
3:F:195:MET:O	3:F:199:LEU:HD13	2.02	0.60
2:E:358:MET:CE	2:E:431:ILE:HD13	2.32	0.60
3:C:174:ILE:HD13	3:C:180:ILE:HG12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:LYS:HD3	1:D:234:LEU:HD21	1.83	0.60
2:E:317:ASN:O	2:E:318:ARG:HG3	2.02	0.60
3:F:75:SER:OG	3:F:111:ILE:HD11	2.02	0.60
2:B:47:ASP:HB2	2:B:51:ARG:H	1.67	0.60
3:F:164:PHE:HB2	3:F:234:LEU:HD13	1.84	0.60
3:F:239:ARG:O	3:F:258:THR:HA	2.02	0.60
1:D:59:ILE:CD1	1:D:95:SER:HB3	2.26	0.59
1:D:338:ASN:OD1	1:D:340:HIS:N	2.33	0.59
2:E:92:ILE:HD13	2:E:117:LYS:HG3	1.84	0.59
2:E:214:ILE:O	2:E:215:VAL:HG23	2.02	0.59
3:C:135:ARG:HH11	3:C:135:ARG:HG2	1.66	0.59
3:C:243:LEU:HD11	3:C:271:ASN:ND2	2.16	0.59
1:D:578:PHE:O	1:D:582:ALA:HB2	2.03	0.59
1:A:405:LEU:HB2	1:A:406:PRO:CD	2.31	0.59
1:D:421:LEU:O	1:D:425:GLU:HG2	2.02	0.59
1:D:548:GLY:HA3	1:D:586:LEU:CD2	2.32	0.59
2:E:160:MET:HG2	2:E:161:ASP:N	2.16	0.59
3:F:123:ILE:HD11	3:F:200:TRP:CH2	2.36	0.59
2:E:8:ASN:N	2:E:8:ASN:ND2	2.50	0.59
3:F:50:CYS:HB2	3:F:51:PRO:HA	1.83	0.59
3:F:190:PRO:O	3:F:196:CYS:HB2	2.02	0.59
1:A:58:THR:HA	1:A:60:TYR:HD1	1.66	0.59
1:A:373:LEU:HD13	1:A:384:ILE:CG2	2.32	0.59
1:A:492:ASP:O	1:A:498:ARG:HD3	2.02	0.59
1:D:358:LYS:O	1:D:362:ILE:HG13	2.00	0.59
2:B:8:ASN:N	2:B:8:ASN:ND2	2.48	0.59
1:D:267:PHE:CD2	1:D:287:PHE:HD2	2.21	0.59
1:A:208:MET:CE	1:A:208:MET:CG	2.80	0.59
2:B:230:THR:HG21	2:B:288:ILE:O	2.03	0.59
2:B:305:TYR:CE1	2:B:342:ILE:HA	2.37	0.59
3:C:97:VAL:O	3:C:101:VAL:HG23	2.02	0.59
1:D:456:TYR:CG	3:F:73:GLY:HA2	2.38	0.59
2:E:389:ARG:HG3	2:E:389:ARG:HH11	1.67	0.59
2:B:221:ASN:HD21	2:B:224:GLU:HG3	1.66	0.59
1:D:331:LYS:HD3	1:D:368:LEU:HD21	1.84	0.59
1:A:382:LEU:HD12	1:A:411:LEU:HD13	1.84	0.59
1:A:478:ALA:O	1:A:482:ILE:HB	2.03	0.59
2:B:47:ASP:HB3	2:B:49:GLY:H	1.68	0.59
1:D:535:ASN:HA	1:D:538:PHE:CE2	2.38	0.59
1:A:196:LEU:HB2	1:A:201:VAL:HG22	1.85	0.58
2:B:373:THR:CG2	2:B:375:ARG:HB2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:LEU:HD11	3:C:98:THR:HG22	1.84	0.58
1:D:63:ASP:OD1	1:D:101:GLU:HG3	2.03	0.58
3:F:236:LEU:HD12	3:F:250:TRP:HZ3	1.68	0.58
1:D:428:PRO:HD3	1:D:465:ASN:ND2	2.19	0.58
3:F:16:GLN:CG	3:F:21:LYS:HB2	2.32	0.58
1:A:508:LEU:O	1:A:512:CYS:HB2	2.02	0.58
1:A:548:GLY:HA3	1:A:586:LEU:CD2	2.34	0.58
2:B:365:PHE:HA	2:B:379:LEU:O	2.02	0.58
1:A:20:LEU:HD23	1:A:31:SER:HB2	1.85	0.58
1:D:448:MET:HA	1:D:451:LEU:HD12	1.86	0.58
2:E:234:PHE:CD1	2:E:242:PHE:HB3	2.38	0.58
1:A:93:LEU:HB3	1:A:112:LEU:HD21	1.83	0.58
1:A:140:TRP:CH2	2:B:107:ALA:HB2	2.39	0.58
2:B:14:PHE:CZ	2:B:17:VAL:HG22	2.39	0.58
1:D:101:GLU:OE2	2:E:170:ARG:NH2	2.35	0.58
1:D:194:LYS:CD	1:D:234:LEU:HD21	2.34	0.58
3:C:267:TYR:CD1	3:C:267:TYR:N	2.71	0.58
1:A:161:ALA:O	1:A:164:ALA:HB3	2.04	0.58
2:B:333:LEU:HD23	2:B:333:LEU:H	1.69	0.58
3:F:76:PRO:O	3:F:110:ARG:HG2	2.04	0.58
3:F:117:ASN:HB2	3:F:200:TRP:CE2	2.39	0.58
1:A:102:THR:HB	1:A:105:ARG:NH2	2.19	0.57
1:A:346:ALA:HB1	1:A:384:ILE:HD11	1.86	0.57
2:B:306:LEU:O	2:B:325:VAL:HG12	2.03	0.57
2:B:317:ASN:O	2:B:318:ARG:HG3	2.04	0.57
1:D:405:LEU:HD12	1:D:405:LEU:N	2.18	0.57
3:F:95:GLU:CD	3:F:95:GLU:H	2.06	0.57
2:B:251:ILE:HD12	2:B:251:ILE:N	2.14	0.57
1:D:515:ASP:O	1:D:519:LYS:HB2	2.04	0.57
1:A:373:LEU:HD21	1:A:404:LEU:CB	2.25	0.57
3:C:121:ARG:HG2	3:C:147:THR:HB	1.84	0.57
1:D:22:ASN:O	1:D:28:ARG:HD3	2.04	0.57
1:D:353:SER:O	1:D:355:ILE:N	2.37	0.57
1:A:307:LYS:HD2	1:A:348:VAL:HB	1.85	0.57
1:A:323:MET:HE2	1:A:356:LEU:HD13	1.85	0.57
1:D:407:ALA:O	1:D:411:LEU:HG	2.04	0.57
2:E:36:PHE:CD1	2:E:43:LEU:HD13	2.39	0.57
1:A:350:MET:SD	1:A:369:PHE:CD1	2.98	0.57
1:D:494:ASN:HA	3:F:280:ASP:OD1	2.05	0.57
2:E:272:PRO:HG2	2:E:318:ARG:HE	1.69	0.57
1:A:291:MET:O	1:A:333:LEU:HD21	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ARG:HG2	1:A:319:GLU:N	2.19	0.57
1:D:431:ALA:HB1	1:D:473:PHE:CE2	2.36	0.57
1:D:484:PRO:HA	1:D:487:LEU:HD12	1.85	0.57
1:A:19:GLU:HG3	1:A:27:LEU:HB3	1.85	0.57
1:A:157:ARG:HH11	1:A:157:ARG:CB	2.17	0.57
1:D:189:LEU:HD11	1:D:208:MET:HE3	1.87	0.57
2:B:8:ASN:ND2	2:B:375:ARG:HH21	2.03	0.57
2:E:403:ARG:C	2:E:404:LYS:HG3	2.26	0.57
3:F:236:LEU:HG	3:F:237:VAL:N	2.20	0.57
1:A:394:VAL:HG12	1:A:394:VAL:O	2.05	0.56
2:B:11:GLN:HA	2:B:11:GLN:NE2	2.20	0.56
1:A:88:CYS:O	1:A:91:PRO:HD2	2.06	0.56
1:A:294:CYS:SG	2:B:264:ARG:NH1	2.79	0.56
1:A:492:ASP:O	1:A:498:ARG:CD	2.54	0.56
1:A:538:PHE:O	1:A:542:LYS:HG3	2.05	0.56
2:B:268:LEU:HD12	2:B:269:PHE:N	2.21	0.56
1:D:292:LYS:HE2	1:D:329:CYS:SG	2.45	0.56
3:F:67:GLU:HB2	3:F:292:ALA:HB2	1.87	0.56
3:F:81:LEU:HD13	3:F:112:THR:HB	1.86	0.56
1:A:178:THR:CG2	1:A:180:MET:H	2.13	0.56
1:A:286:ALA:O	1:A:289:ASN:N	2.39	0.56
1:A:346:ALA:HB1	1:A:384:ILE:CD1	2.35	0.56
1:A:579:ALA:O	1:A:583:LEU:HG	2.05	0.56
1:D:350:MET:HG3	1:D:369:PHE:CE1	2.41	0.56
1:D:428:PRO:HD3	1:D:465:ASN:HD21	1.69	0.56
1:D:561:LYS:HB2	1:D:588:LEU:HD22	1.88	0.56
2:E:42:LEU:HD12	2:E:109:GLN:HG2	1.86	0.56
1:A:171:ARG:HA	1:A:208:MET:SD	2.46	0.56
2:B:446:VAL:O	2:B:446:VAL:HG13	2.05	0.56
1:D:57:ASP:HB2	2:E:157:PHE:CE2	2.41	0.56
1:D:131:LEU:HD12	1:D:131:LEU:C	2.25	0.56
1:A:381:ARG:O	1:A:385:ILE:HG12	2.06	0.56
1:A:385:ILE:HG23	1:A:430:LEU:HD21	1.87	0.56
1:A:431:ALA:HB1	1:A:473:PHE:CE2	2.39	0.56
2:B:385:ASN:HB3	2:B:386:ASN:OD1	2.06	0.56
2:E:386:ASN:O	2:E:387:LYS:HE2	2.04	0.56
3:F:103:LEU:HB3	3:F:111:ILE:HD13	1.87	0.56
1:A:34:LYS:O	1:A:38:ILE:HD13	2.06	0.56
1:A:186:ALA:CB	1:A:212:LEU:HD13	2.34	0.56
1:A:209:PHE:CZ	1:A:247:THR:HG21	2.41	0.56
1:A:424:ILE:HG12	1:A:450:TRP:CZ3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:544:LEU:HD12	1:D:564:LEU:CD2	2.35	0.56
3:F:123:ILE:HD11	3:F:200:TRP:HH2	1.70	0.56
3:F:266:CYS:C	3:F:267:TYR:CD1	2.79	0.56
1:A:419:VAL:O	1:A:422:ALA:HB3	2.06	0.56
1:D:25:VAL:HG22	1:D:28:ARG:HH12	1.71	0.56
1:D:310:CYS:HB3	1:D:322:ILE:HD11	1.88	0.56
3:F:13:TRP:CZ3	3:F:27:GLN:HB3	2.41	0.56
1:D:438:PHE:O	1:D:442:LYS:HB2	2.05	0.55
1:D:499:MET:HB3	1:D:503:PHE:CE2	2.41	0.55
1:A:29:LEU:HD22	1:A:64:GLU:HG2	1.87	0.55
1:A:313:LEU:HD13	1:A:321:VAL:HG21	1.88	0.55
3:C:195:MET:O	3:C:199:LEU:HD13	2.06	0.55
1:D:502:LEU:HD13	1:D:539:ASN:O	2.06	0.55
1:A:22:ASN:O	1:A:28:ARG:HD3	2.06	0.55
1:A:99:VAL:HG12	1:A:101:GLU:H	1.70	0.55
1:A:151:PHE:CE2	1:A:170:PHE:HB2	2.41	0.55
1:D:331:LYS:HD3	1:D:368:LEU:CD2	2.37	0.55
1:D:442:LYS:HB2	1:D:443:LEU:HD12	1.89	0.55
2:B:8:ASN:ND2	2:B:375:ARG:NH2	2.54	0.55
2:B:378:THR:O	2:B:379:LEU:HD23	2.07	0.55
1:D:398:ARG:HG3	1:D:399:GLN:N	2.22	0.55
1:D:564:LEU:HB3	1:D:583:LEU:HD21	1.88	0.55
2:B:42:LEU:CD1	2:B:109:GLN:HG2	2.37	0.55
2:E:170:ARG:HG3	2:E:208:THR:HG22	1.88	0.55
3:F:29:LYS:O	3:F:33:GLU:HG2	2.05	0.55
1:A:45:GLU:OE1	1:A:46:ARG:N	2.38	0.55
1:A:287:PHE:CZ	1:A:306:VAL:HG22	2.41	0.55
1:D:369:PHE:CE1	1:D:384:ILE:HG23	2.42	0.55
3:F:172:PRO:HA	3:F:209:TRP:CZ2	2.42	0.55
1:A:522:LEU:N	1:A:523:PRO:CD	2.69	0.55
2:B:11:GLN:HE21	2:B:11:GLN:CA	2.20	0.55
2:B:332:LYS:NZ	2:B:410:VAL:HG11	2.22	0.55
1:D:331:LYS:HA	1:D:368:LEU:HD21	1.88	0.55
2:E:136:LEU:CD1	2:E:136:LEU:N	2.69	0.55
2:E:403:ARG:O	2:E:404:LYS:HG3	2.07	0.55
1:A:287:PHE:HZ	1:A:306:VAL:HG22	1.72	0.55
1:A:434:LEU:O	1:A:438:PHE:HB3	2.07	0.55
1:D:334:VAL:HG13	1:D:372:GLN:HG2	1.88	0.55
1:D:522:LEU:N	1:D:523:PRO:CD	2.69	0.55
1:D:548:GLY:HA3	1:D:586:LEU:HD21	1.88	0.55
2:E:85:ASP:CG	2:E:88:LYS:HB2	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:85:ASP:OD2	2:E:88:LYS:HD2	2.07	0.55
2:E:339:ASN:O	2:E:340:ASP:HB2	2.07	0.55
1:A:404:LEU:HD23	1:A:404:LEU:H	1.72	0.55
2:B:358:MET:CE	2:B:366:PHE:CD2	2.89	0.55
1:D:516:ILE:HA	1:D:519:LYS:HB2	1.88	0.55
3:F:176:THR:O	3:F:179:HIS:HB2	2.06	0.55
1:D:353:SER:C	1:D:355:ILE:H	2.10	0.55
1:D:427:MET:HE1	1:D:443:LEU:HD23	1.88	0.55
2:E:136:LEU:N	2:E:136:LEU:HD12	2.22	0.55
1:A:545:GLN:HG3	1:A:585:VAL:HB	1.89	0.54
1:D:375:ASP:O	1:D:381:ARG:NH1	2.40	0.54
2:B:241:THR:HG23	2:B:253:LEU:HD21	1.88	0.54
1:D:288:GLN:NE2	1:D:325:GLN:O	2.38	0.54
3:F:212:SER:C	3:F:214:ARG:H	2.09	0.54
1:A:162:VAL:O	1:A:165:GLU:N	2.40	0.54
1:A:469:LEU:HD22	1:A:477:TRP:CZ3	2.42	0.54
2:E:12:TRP:CZ2	2:E:368:MET:HE1	2.42	0.54
2:E:219:PRO:HD2	2:E:222:MET:HE1	1.88	0.54
3:F:70:ARG:HG3	3:F:70:ARG:HH11	1.70	0.54
1:A:181:VAL:O	1:A:184:ALA:HB3	2.07	0.54
1:A:472:LYS:HG3	1:A:472:LYS:O	2.07	0.54
2:B:134:TYR:HB3	2:B:137:LYS:HA	1.89	0.54
1:D:57:ASP:HB2	2:E:157:PHE:CD2	2.42	0.54
1:D:218:ASP:O	1:D:222:LEU:HD22	2.08	0.54
1:D:307:LYS:HE2	1:D:311:GLU:OE2	2.07	0.54
3:F:65:LEU:HD21	3:F:100:LEU:HD21	1.90	0.54
1:A:388:LEU:HD11	1:A:430:LEU:CD2	2.37	0.54
2:B:377:ILE:HG22	2:B:378:THR:H	1.72	0.54
1:D:248:LEU:HD22	1:D:270:LEU:HD22	1.89	0.54
2:E:370:ASP:HB3	2:E:373:THR:CG2	2.25	0.54
1:A:274:VAL:HG11	1:A:283:LEU:HD11	1.89	0.54
2:B:14:PHE:C	2:B:14:PHE:HD1	2.10	0.54
3:C:171:SER:HB2	3:C:197:ASP:HB2	1.89	0.54
1:D:353:SER:N	1:D:354:PRO:HD2	2.22	0.54
1:D:492:ASP:O	1:D:498:ARG:HD3	2.07	0.54
1:D:545:GLN:HG3	1:D:585:VAL:HB	1.88	0.54
2:E:47:ASP:HB3	2:E:49:GLY:H	1.72	0.54
3:F:121:ARG:HG2	3:F:147:THR:CB	2.38	0.54
1:A:240:LEU:O	1:A:242:ALA:N	2.41	0.54
1:D:48:ARG:HG3	1:D:80:VAL:HG22	1.89	0.54
1:D:392:ASN:OD1	1:D:397:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:222:GLN:HG3	3:C:252:HIS:HB3	1.90	0.54
1:D:391:VAL:O	1:D:391:VAL:HG12	2.08	0.54
3:F:134:LEU:C	3:F:136:LYS:H	2.11	0.54
1:A:483:ILE:HD13	1:A:521:MET:HG3	1.90	0.54
3:C:160:ASP:O	3:C:162:GLN:HG3	2.07	0.54
2:E:170:ARG:HG3	2:E:208:THR:CG2	2.38	0.54
2:E:291:VAL:C	2:E:292:LYS:HG2	2.28	0.54
1:A:32:ILE:O	1:A:72:GLN:NE2	2.40	0.54
1:A:162:VAL:HA	1:A:165:GLU:OE2	2.08	0.54
1:D:38:ILE:O	1:D:42:LEU:HD23	2.07	0.54
2:E:272:PRO:HG2	2:E:318:ARG:HH21	1.73	0.54
3:F:265:TYR:O	3:F:266:CYS:HB2	2.08	0.54
1:A:331:LYS:HG2	1:A:368:LEU:HD21	1.90	0.53
2:B:17:VAL:HG13	2:B:440:TYR:CE2	2.43	0.53
1:D:350:MET:HB3	1:D:391:VAL:HG21	1.89	0.53
1:D:561:LYS:HE2	1:D:565:GLU:OE2	2.08	0.53
1:D:100:GLU:HG3	2:E:106:ASN:ND2	2.09	0.53
1:D:271:GLN:C	1:D:273:ALA:H	2.12	0.53
2:E:209:ASP:O	2:E:210:ARG:HG3	2.08	0.53
2:E:334:CYS:O	2:E:338:GLU:HG2	2.08	0.53
3:F:94:VAL:HG23	3:F:132:GLU:OE2	2.08	0.53
1:A:141:PHE:CE1	1:A:180:MET:SD	2.96	0.53
1:D:46:ARG:HD2	1:D:50:GLU:OE2	2.08	0.53
1:D:392:ASN:HD21	1:D:397:ILE:CD1	2.22	0.53
1:A:397:ILE:HG22	1:A:434:LEU:HD23	1.90	0.53
2:B:285:ILE:HD13	2:B:333:LEU:HD11	1.89	0.53
2:B:435:THR:CG2	2:B:436:THR:N	2.71	0.53
1:A:274:VAL:O	1:A:278:ILE:HD12	2.08	0.53
3:C:164:PHE:HB2	3:C:234:LEU:HD13	1.90	0.53
1:D:405:LEU:CB	1:D:406:PRO:HD3	2.27	0.53
1:A:282:ASP:C	1:A:285:PRO:HD2	2.28	0.53
3:C:30:SER:O	3:C:33:GLU:HB2	2.08	0.53
3:F:93:SER:O	3:F:97:VAL:HG12	2.07	0.53
3:F:159:VAL:HG11	3:F:278:LEU:HD13	1.90	0.53
1:A:58:THR:HG23	1:A:59:ILE:H	1.73	0.53
1:A:323:MET:CE	1:A:356:LEU:HD22	2.39	0.53
2:B:79:SER:HA	2:B:122:TRP:CZ2	2.44	0.53
3:C:174:ILE:HD11	3:C:183:LEU:HD11	1.91	0.53
1:D:498:ARG:HH21	1:D:536:VAL:HG21	1.74	0.53
2:E:65:SER:HA	2:E:428:GLU:OE2	2.08	0.53
3:F:283:LYS:HA	3:F:283:LYS:HE2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:PHE:CE1	2:B:91:GLU:HB2	2.44	0.53
1:D:473:PHE:HB3	1:D:477:TRP:CE3	2.44	0.53
1:A:561:LYS:N	1:A:562:PRO:CD	2.72	0.53
1:D:346:ALA:HA	1:D:349:ILE:CG2	2.39	0.53
1:A:60:TYR:CG	1:A:60:TYR:O	2.61	0.52
2:B:47:ASP:HB3	2:B:49:GLY:N	2.24	0.52
1:D:32:ILE:CA	1:D:35:LEU:HD22	2.39	0.52
1:D:58:THR:HG23	1:D:59:ILE:N	2.19	0.52
1:A:391:VAL:O	1:A:395:ILE:HG12	2.08	0.52
3:C:7:THR:HG22	3:C:11:ASP:OD1	2.10	0.52
1:A:487:LEU:HD22	1:A:524:THR:OG1	2.09	0.52
2:B:68:ARG:HG2	2:B:68:ARG:HH11	1.74	0.52
2:B:377:ILE:HG22	2:B:378:THR:N	2.24	0.52
1:D:59:ILE:HG12	1:D:96:LEU:CD2	2.40	0.52
1:D:443:LEU:H	1:D:443:LEU:CD1	2.19	0.52
2:E:27:GLU:OE1	2:E:48:LYS:NZ	2.26	0.52
1:A:198:LEU:CD2	1:A:202:LYS:HD3	2.39	0.52
1:A:434:LEU:HB3	1:A:438:PHE:HD2	1.75	0.52
3:C:214:ARG:HH21	3:C:242:GLN:HG2	1.73	0.52
2:B:358:MET:HE2	2:B:366:PHE:CD2	2.44	0.52
1:D:58:THR:OG1	1:D:59:ILE:N	2.39	0.52
1:D:538:PHE:CD1	1:D:538:PHE:C	2.83	0.52
1:A:59:ILE:HG13	1:A:96:LEU:HG	1.92	0.52
1:A:198:LEU:HD21	1:A:202:LYS:HD3	1.92	0.52
1:D:61:ASP:HB3	1:D:62:GLU:OE1	2.10	0.52
1:D:330:ILE:O	1:D:334:VAL:HG23	2.10	0.52
3:F:134:LEU:O	3:F:136:LYS:N	2.43	0.52
1:A:46:ARG:O	1:A:50:GLU:N	2.42	0.52
1:A:165:GLU:O	1:A:169:TYR:HD1	1.92	0.52
1:A:567:LEU:O	1:A:570:ASP:HB2	2.10	0.52
3:C:39:LEU:O	3:C:185:ARG:NH2	2.42	0.52
3:C:135:ARG:HG2	3:C:135:ARG:NH1	2.25	0.52
3:F:143:TRP:O	3:F:147:THR:OG1	2.28	0.52
1:A:48:ARG:HD3	1:A:88:CYS:SG	2.50	0.52
1:A:57:ASP:O	1:A:58:THR:C	2.48	0.52
1:A:353:SER:OG	1:A:361:THR:HG21	2.10	0.52
1:A:571:GLN:OE1	1:A:571:GLN:N	2.43	0.52
3:C:290:ASP:HB3	3:C:291:PRO:HD2	1.92	0.52
1:D:331:LYS:CD	1:D:368:LEU:HD21	2.39	0.52
2:E:11:GLN:HG3	2:E:391:VAL:HG11	1.92	0.52
2:E:148:THR:HG22	2:E:148:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:89:ARG:HG3	3:F:265:TYR:OH	2.10	0.52
1:A:8:MET:SD	1:A:8:MET:O	2.68	0.51
1:A:584:THR:HG22	1:A:584:THR:O	2.10	0.51
3:C:103:LEU:HB3	3:C:111:ILE:HD12	1.91	0.51
1:D:332:GLU:C	1:D:334:VAL:H	2.13	0.51
1:A:370:LEU:HG	1:A:403:SER:OG	2.10	0.51
1:A:477:TRP:CE3	1:A:482:ILE:HD11	2.44	0.51
1:D:564:LEU:O	1:D:568:THR:HG23	2.10	0.51
1:D:579:ALA:O	1:D:583:LEU:HG	2.10	0.51
3:F:32:CYS:O	3:F:36:LYS:HG3	2.11	0.51
1:A:61:ASP:HB3	1:A:62:GLU:OE1	2.10	0.51
1:A:94:GLU:HG3	1:A:131:LEU:CD1	2.40	0.51
3:F:290:ASP:HB3	3:F:291:PRO:HD2	1.93	0.51
2:B:102:LEU:HD23	2:B:185:ILE:HG21	1.91	0.51
2:B:333:LEU:HD23	2:B:333:LEU:N	2.25	0.51
1:D:271:GLN:O	1:D:273:ALA:N	2.44	0.51
2:E:12:TRP:CH2	2:E:431:ILE:HD12	2.46	0.51
2:E:358:MET:HE3	2:E:431:ILE:HD13	1.93	0.51
1:A:21:ARG:HG3	2:B:131:PRO:CG	2.40	0.51
3:C:62:PHE:C	3:C:62:PHE:CD1	2.84	0.51
3:C:199:LEU:HD12	3:C:199:LEU:N	2.26	0.51
1:D:100:GLU:HG2	2:E:110:PHE:HZ	1.75	0.51
2:E:325:VAL:HG22	2:E:326:HIS:CD2	2.45	0.51
3:F:99:LEU:HG	3:F:103:LEU:HD11	1.93	0.51
2:B:386:ASN:O	2:B:387:LYS:HE2	2.10	0.51
1:D:256:SER:HB3	1:D:259:VAL:HG23	1.92	0.51
1:D:336:ASP:O	1:D:342:LYS:HD3	2.10	0.51
2:E:221:ASN:ND2	2:E:224:GLU:HG3	2.22	0.51
3:F:200:TRP:CE3	3:F:216:ALA:HB3	2.45	0.51
1:A:29:LEU:O	1:A:33:LYS:HG3	2.10	0.51
1:A:56:THR:O	1:A:59:ILE:HD13	2.10	0.51
1:A:161:ALA:O	1:A:165:GLU:HG3	2.11	0.51
3:C:266:CYS:SG	4:G:2:LEU:CD1	2.99	0.51
1:D:32:ILE:O	1:D:35:LEU:HD22	2.11	0.51
1:A:196:LEU:HD12	1:A:205:ILE:CG1	2.40	0.51
1:A:327:LEU:HB3	1:A:328:PRO:HD3	1.92	0.51
1:A:583:LEU:C	1:A:585:VAL:H	2.14	0.51
1:D:9:SER:O	1:D:12:PRO:HD2	2.10	0.51
1:D:32:ILE:HA	1:D:35:LEU:CD2	2.39	0.51
3:F:100:LEU:CA	3:F:103:LEU:HD12	2.35	0.51
2:B:68:ARG:HD3	2:B:443:GLN:OE1	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ALA:HB1	1:A:578:PHE:O	2.11	0.51
2:B:243:VAL:HG13	2:B:293:PHE:CZ	2.46	0.51
2:B:356:VAL:HG12	2:B:357:VAL:N	2.25	0.51
3:C:152:TYR:HA	3:C:186:LEU:CD2	2.41	0.51
1:D:478:ALA:O	1:D:483:ILE:HG13	2.11	0.51
2:E:425:HIS:HB2	2:E:430:ILE:HB	1.92	0.51
3:F:97:VAL:O	3:F:101:VAL:HG23	2.11	0.51
1:A:330:ILE:HG23	1:A:345:LEU:HD21	1.94	0.50
1:D:267:PHE:O	1:D:270:LEU:HB2	2.10	0.50
1:D:310:CYS:HB3	1:D:322:ILE:CD1	2.40	0.50
1:D:419:VAL:O	1:D:422:ALA:HB3	2.11	0.50
1:A:211:ASN:OD1	1:D:8:MET:SD	2.69	0.50
2:B:351:ASN:O	2:B:351:ASN:ND2	2.41	0.50
2:B:373:THR:HG22	2:B:375:ARG:H	1.76	0.50
1:D:409:VAL:O	1:D:412:ALA:HB3	2.10	0.50
3:F:236:LEU:HD12	3:F:250:TRP:CZ3	2.45	0.50
1:A:124:LEU:HD11	1:A:154:CYS:HB2	1.94	0.50
1:A:291:MET:HE1	1:A:329:CYS:HB2	1.93	0.50
1:A:334:VAL:HG13	1:A:372:GLN:HG2	1.93	0.50
1:A:432:GLY:HA3	1:A:472:LYS:CE	2.35	0.50
2:B:197:ASP:HB3	2:B:228:VAL:CG2	2.40	0.50
3:C:100:LEU:HA	3:C:103:LEU:HD12	1.93	0.50
3:C:263:PRO:HB2	3:C:291:PRO:HD3	1.93	0.50
1:D:291:MET:O	1:D:333:LEU:HD21	2.10	0.50
1:A:197:GLU:OE2	1:A:200:ASN:ND2	2.38	0.50
1:A:62:GLU:OE1	1:A:62:GLU:N	2.45	0.50
1:A:206:ILE:HB	1:A:207:PRO:HD3	1.94	0.50
1:A:443:LEU:HD12	1:A:443:LEU:N	2.26	0.50
1:A:570:ASP:OD1	1:A:571:GLN:OE1	2.30	0.50
3:C:176:THR:HA	3:C:232:ASN:OD1	2.11	0.50
2:E:11:GLN:HG3	2:E:391:VAL:CG1	2.41	0.50
1:A:406:PRO:O	1:A:410:GLU:N	2.41	0.50
2:B:13:CYS:SG	2:B:391:VAL:HA	2.52	0.50
2:B:330:ARG:HG3	2:B:330:ARG:NH1	2.14	0.50
1:D:392:ASN:CG	1:D:397:ILE:HG12	2.32	0.50
1:D:205:ILE:HA	1:D:208:MET:HE2	1.93	0.50
3:F:121:ARG:HG2	3:F:147:THR:HG21	1.94	0.50
1:A:401:SER:OG	1:A:438:PHE:CZ	2.65	0.49
1:D:58:THR:CG2	1:D:59:ILE:H	2.12	0.49
1:D:215:ASP:O	1:D:221:ARG:HD3	2.12	0.49
1:D:427:MET:HG2	1:D:447:CYS:SG	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:ILE:HG23	1:A:350:MET:CE	2.42	0.49
1:A:349:ILE:HG23	1:A:350:MET:HE2	1.94	0.49
1:A:477:TRP:CZ3	1:A:482:ILE:HD11	2.47	0.49
2:B:13:CYS:SG	2:B:391:VAL:HG22	2.51	0.49
3:C:17:LEU:CD1	3:C:98:THR:HG22	2.41	0.49
1:D:448:MET:HE1	1:D:466:LEU:HD21	1.93	0.49
1:D:583:LEU:C	1:D:585:VAL:H	2.16	0.49
3:F:67:GLU:OE1	3:F:70:ARG:NH2	2.45	0.49
1:A:217:GLN:OE1	2:B:239:CYS:CB	2.58	0.49
1:A:587:SER:C	1:A:589:ALA:H	2.15	0.49
2:B:221:ASN:ND2	2:B:224:GLU:HG3	2.26	0.49
2:E:151:THR:HG22	2:E:152:LEU:N	2.27	0.49
2:E:271:GLU:CG	2:E:318:ARG:HG2	2.42	0.49
3:F:199:LEU:N	3:F:199:LEU:CD1	2.76	0.49
1:A:21:ARG:HH12	2:B:133:GLY:N	2.10	0.49
1:D:394:VAL:HG12	1:D:394:VAL:O	2.12	0.49
1:A:198:LEU:HA	1:A:201:VAL:HB	1.95	0.49
1:A:271:GLN:CG	1:A:272:LYS:N	2.75	0.49
1:A:287:PHE:CE1	1:A:291:MET:SD	3.04	0.49
2:B:33:THR:HG21	2:B:99:ILE:HG13	1.93	0.49
2:B:147:THR:O	2:B:147:THR:HG22	2.13	0.49
1:D:349:ILE:O	1:D:352:LEU:HD12	2.12	0.49
3:F:163:ILE:HG23	3:F:236:LEU:CD2	2.41	0.49
3:F:265:TYR:HB3	3:F:269:CYS:HB2	1.95	0.49
1:A:21:ARG:HH12	2:B:133:GLY:H	1.60	0.49
1:A:46:ARG:NH1	2:B:153:ARG:NH1	2.56	0.49
1:A:86:VAL:HG21	1:A:118:GLU:HB2	1.95	0.49
1:A:470:VAL:C	1:A:472:LYS:H	2.15	0.49
3:C:134:LEU:C	3:C:136:LYS:H	2.15	0.49
1:D:552:ASP:OD1	1:D:554:SER:HB3	2.11	0.49
1:A:196:LEU:HD12	1:A:205:ILE:HG12	1.95	0.49
1:D:334:VAL:CG1	1:D:372:GLN:HG2	2.43	0.49
1:A:236:PRO:O	1:A:239:ASP:OD2	2.31	0.49
3:C:25:GLU:HG3	3:C:142:VAL:HG23	1.94	0.49
3:C:71:ILE:HG22	3:C:275:ILE:HD11	1.95	0.49
1:D:313:LEU:HD13	1:D:321:VAL:CG2	2.42	0.49
1:D:527:ARG:HB3	1:D:527:ARG:CZ	2.42	0.49
1:D:564:LEU:HD13	1:D:583:LEU:HD23	1.95	0.49
3:C:264:ASN:ND2	3:C:267:TYR:HA	2.27	0.49
3:C:265:TYR:O	3:C:266:CYS:HB2	2.13	0.49
1:D:404:LEU:HD23	1:D:404:LEU:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:ASN:OD1	1:D:469:LEU:HD12	2.13	0.49
1:A:479:HIS:ND1	1:A:516:ILE:HG23	2.28	0.49
1:A:483:ILE:N	1:A:484:PRO:CD	2.76	0.49
1:D:449:ALA:O	1:D:452:VAL:HG12	2.12	0.49
2:E:114:THR:HG22	2:E:183:ILE:HD13	1.95	0.49
3:F:7:THR:HG22	3:F:11:ASP:OD2	2.13	0.49
3:F:215:GLY:HA3	4:H:5:1ZN:H14	1.95	0.49
1:A:443:LEU:N	1:A:443:LEU:CD1	2.75	0.48
1:A:544:LEU:HD23	1:A:547:ILE:HD11	1.95	0.48
1:D:102:THR:HG22	1:D:105:ARG:NH2	2.26	0.48
1:D:102:THR:CG2	1:D:105:ARG:HH22	2.20	0.48
1:D:411:LEU:HB2	1:D:423:ILE:HG13	1.95	0.48
1:A:187:SER:HB3	1:A:223:LEU:HD22	1.93	0.48
1:A:292:LYS:HE2	1:A:329:CYS:SG	2.53	0.48
3:C:55:CYS:SG	3:C:275:ILE:HG22	2.53	0.48
1:D:58:THR:HA	1:D:60:TYR:CD1	2.47	0.48
1:D:584:THR:HG22	1:D:584:THR:O	2.13	0.48
1:A:267:PHE:CD2	1:A:287:PHE:HD2	2.32	0.48
1:A:353:SER:C	1:A:355:ILE:H	2.16	0.48
1:A:578:PHE:O	1:A:582:ALA:HB2	2.12	0.48
3:C:63:HIS:O	3:C:66:MET:HB2	2.13	0.48
2:E:14:PHE:HZ	2:E:17:VAL:CG2	2.26	0.48
3:F:49:ARG:HG3	3:F:49:ARG:O	2.12	0.48
3:F:76:PRO:HB2	3:F:110:ARG:CG	2.42	0.48
1:A:54:PHE:CE1	2:B:155:PRO:HB2	2.48	0.48
1:A:164:ALA:HA	1:A:167:ARG:NH2	2.29	0.48
1:A:215:ASP:OD1	1:A:216:GLU:N	2.47	0.48
1:A:236:PRO:CG	1:A:239:ASP:OD2	2.59	0.48
1:A:398:ARG:HA	1:A:401:SER:HB3	1.96	0.48
1:A:452:VAL:HG22	1:A:452:VAL:O	2.13	0.48
1:D:62:GLU:OE1	1:D:62:GLU:N	2.45	0.48
1:D:140:TRP:CG	2:E:106:ASN:HA	2.48	0.48
1:D:478:ALA:O	1:D:482:ILE:HB	2.13	0.48
3:F:266:CYS:C	3:F:267:TYR:HD1	2.15	0.48
1:A:133:LYS:HE2	1:A:169:TYR:CE1	2.49	0.48
2:B:358:MET:HE2	2:B:366:PHE:HD2	1.77	0.48
2:B:387:LYS:HB3	2:B:388:PRO:CD	2.43	0.48
1:D:178:THR:HG23	2:E:189:TYR:CE2	2.48	0.48
2:E:228:VAL:HG12	2:E:247:SER:HB3	1.94	0.48
1:A:267:PHE:CE2	1:A:287:PHE:HD2	2.31	0.48
1:A:360:ASN:O	1:A:364:HIS:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:14:PHE:HZ	2:B:17:VAL:HG22	1.79	0.48
2:B:33:THR:HG22	2:B:46:GLY:HA3	1.96	0.48
2:B:387:LYS:HD3	2:B:388:PRO:HD3	1.95	0.48
1:D:267:PHE:O	1:D:270:LEU:N	2.45	0.48
2:E:87:LEU:HD12	2:E:87:LEU:N	2.27	0.48
2:E:382:SER:OG	2:E:385:ASN:HB2	2.14	0.48
1:A:28:ARG:HH22	1:A:62:GLU:CD	2.17	0.48
1:A:95:SER:O	1:A:98:THR:HB	2.14	0.48
1:D:427:MET:HA	1:D:427:MET:CE	2.44	0.48
3:F:170:LEU:HD12	3:F:224:ILE:HG22	1.96	0.48
1:A:157:ARG:HH11	1:A:157:ARG:HB3	1.78	0.48
1:A:291:MET:CE	1:A:329:CYS:HB2	2.43	0.48
1:A:406:PRO:HG2	1:A:407:ALA:H	1.78	0.48
1:A:507:VAL:HA	1:A:510:GLU:OE2	2.13	0.48
1:A:525:VAL:HG13	1:A:540:VAL:HG13	1.96	0.48
1:A:586:LEU:O	1:A:587:SER:HB2	2.13	0.48
1:D:10:LEU:HB2	2:E:149:VAL:HG11	1.96	0.48
1:D:402:GLN:C	1:D:405:LEU:HD11	2.34	0.48
2:E:373:THR:HG23	2:E:375:ARG:CG	2.43	0.48
2:E:373:THR:CG2	2:E:375:ARG:HG3	2.44	0.48
1:A:211:ASN:OD1	1:D:8:MET:HE1	2.12	0.48
1:A:490:SER:HB2	1:A:528:MET:CE	2.44	0.48
2:B:148:THR:HG22	2:B:148:THR:O	2.14	0.48
2:B:230:THR:HG22	2:B:245:SER:OG	2.14	0.48
2:B:373:THR:CG2	2:B:375:ARG:HG3	2.44	0.48
2:B:425:HIS:ND1	2:B:426:PRO:HD2	2.29	0.48
3:C:202:ASP:O	3:C:219:THR:HA	2.13	0.48
1:D:99:VAL:HG12	1:D:101:GLU:H	1.79	0.48
1:D:456:TYR:CD2	3:F:73:GLY:HA2	2.49	0.48
2:E:102:LEU:HD23	2:E:185:ILE:HG21	1.95	0.48
3:F:243:LEU:HD23	3:F:243:LEU:C	2.34	0.48
1:A:470:VAL:C	1:A:472:LYS:N	2.68	0.48
1:A:486:VAL:O	1:A:501:THR:HG23	2.14	0.48
1:D:483:ILE:N	1:D:484:PRO:CD	2.77	0.48
1:D:541:ALA:HB1	1:D:578:PHE:O	2.14	0.48
2:E:404:LYS:HD2	2:E:407:GLU:OE1	2.14	0.48
2:B:414:ASP:OD2	2:B:417:LYS:HE3	2.14	0.47
1:D:59:ILE:HG12	1:D:96:LEU:HD21	1.95	0.47
1:D:219:SER:O	1:D:222:LEU:CD2	2.62	0.47
1:D:495:TYR:CE1	1:D:496:LEU:HG	2.49	0.47
3:F:179:HIS:O	3:F:183:LEU:HG	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:MET:HE2	2:B:350:TRP:CE2	2.49	0.47
1:D:206:ILE:HB	1:D:207:PRO:HD3	1.94	0.47
1:D:424:ILE:HG12	1:D:450:TRP:CZ3	2.48	0.47
3:F:17:LEU:HD21	3:F:23:LEU:HG	1.96	0.47
3:F:25:GLU:OE1	3:F:139:ASN:ND2	2.41	0.47
3:F:185:ARG:O	3:F:187:GLN:N	2.46	0.47
1:A:8:MET:SD	1:A:8:MET:C	2.93	0.47
3:C:244:VAL:HG11	3:C:249:ASN:HB3	1.95	0.47
1:D:19:GLU:HG3	1:D:27:LEU:HB3	1.96	0.47
1:D:57:ASP:O	1:D:58:THR:C	2.50	0.47
3:F:29:LYS:HD2	3:F:145:TYR:CZ	2.48	0.47
3:F:125:GLN:HG2	3:F:130:TYR:CD2	2.50	0.47
3:F:267:TYR:CD1	3:F:267:TYR:N	2.82	0.47
1:A:207:PRO:O	1:A:211:ASN:ND2	2.37	0.47
3:C:149:LEU:HD12	3:C:149:LEU:O	2.14	0.47
1:D:303:SER:OG	1:D:333:LEU:HD13	2.15	0.47
3:F:132:GLU:HG3	3:F:135:ARG:NH2	2.29	0.47
1:A:26:GLN:N	1:A:26:GLN:OE1	2.47	0.47
1:A:93:LEU:CB	1:A:112:LEU:HD21	2.45	0.47
1:A:280:LYS:HD2	1:A:317:CYS:SG	2.54	0.47
1:D:186:ALA:HA	1:D:212:LEU:HD13	1.97	0.47
1:D:456:TYR:CD1	1:D:456:TYR:C	2.88	0.47
2:E:9:ASP:CG	2:E:375:ARG:HH21	2.17	0.47
2:E:377:ILE:HG22	2:E:378:THR:H	1.79	0.47
1:D:60:TYR:O	1:D:61:ASP:OD1	2.32	0.47
1:D:520:HIS:C	1:D:523:PRO:HD2	2.35	0.47
2:E:231:ALA:HB3	2:E:291:VAL:HG23	1.95	0.47
1:A:194:LYS:HG3	1:A:194:LYS:O	2.15	0.47
1:A:202:LYS:HG2	1:A:243:LEU:CD1	2.45	0.47
1:A:395:ILE:CD1	1:A:400:LEU:HD11	2.45	0.47
2:B:176:HIS:ND1	2:B:196:ASP:OD1	2.48	0.47
3:C:203:PRO:HB3	3:C:220:PHE:CE2	2.50	0.47
3:C:212:SER:HA	3:C:219:THR:HG23	1.95	0.47
1:D:129:VAL:N	1:D:130:PRO:CD	2.78	0.47
1:D:486:VAL:O	1:D:501:THR:HG23	2.15	0.47
2:E:251:ILE:H	2:E:251:ILE:CD1	2.27	0.47
2:E:435:THR:O	2:E:436:THR:C	2.50	0.47
3:F:118:HIS:C	3:F:120:SER:H	2.16	0.47
3:F:158:LEU:CD2	3:F:161:GLY:HA2	2.43	0.47
1:A:63:ASP:OD1	1:A:101:GLU:HG3	2.15	0.47
1:A:509:SER:O	1:A:550:ILE:HD13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:VAL:HA	1:D:446:LEU:HD21	1.97	0.47
1:D:434:LEU:O	1:D:438:PHE:HB3	2.15	0.47
3:F:40:THR:HG23	3:F:152:TYR:CD2	2.50	0.47
1:A:45:GLU:CD	1:A:45:GLU:N	2.63	0.47
1:A:151:PHE:HE2	1:A:170:PHE:HB2	1.80	0.47
1:A:451:LEU:O	1:A:500:THR:HG21	2.14	0.47
2:B:387:LYS:HD3	2:B:388:PRO:CD	2.45	0.47
1:D:42:LEU:O	1:D:43:GLY:O	2.33	0.47
1:D:511:VAL:O	1:D:511:VAL:HG23	2.15	0.47
3:F:202:ASP:O	3:F:219:THR:HA	2.14	0.47
3:C:134:LEU:O	3:C:136:LYS:N	2.47	0.47
1:D:280:LYS:HA	1:D:284:VAL:HG23	1.97	0.47
1:D:503:PHE:O	1:D:507:VAL:HG23	2.15	0.47
3:F:274:ALA:HA	3:F:287:LEU:O	2.15	0.47
2:B:82:PRO:O	2:B:83:GLU:HG2	2.14	0.46
2:B:327:GLU:O	2:B:330:ARG:HB2	2.15	0.46
2:B:424:TRP:O	2:B:425:HIS:C	2.54	0.46
3:C:236:LEU:HD12	3:C:237:VAL:H	1.80	0.46
1:D:398:ARG:HH21	1:D:402:GLN:HE22	1.63	0.46
2:E:202:LEU:HB2	2:E:214:ILE:HD13	1.97	0.46
2:E:251:ILE:N	2:E:251:ILE:CD1	2.72	0.46
3:F:174:ILE:HD12	3:F:194:PRO:HB2	1.95	0.46
1:A:504:CYS:O	1:A:508:LEU:HG	2.16	0.46
2:B:244:TYR:CZ	2:B:252:ARG:HD2	2.51	0.46
1:D:427:MET:N	1:D:428:PRO:CD	2.77	0.46
1:A:58:THR:OG1	1:A:59:ILE:N	2.47	0.46
1:A:140:TRP:CZ2	2:B:107:ALA:HB2	2.50	0.46
1:A:490:SER:HB2	1:A:528:MET:HE3	1.96	0.46
2:B:182:SER:O	2:B:194:SER:HA	2.16	0.46
3:C:25:GLU:HG3	3:C:142:VAL:CG2	2.44	0.46
3:C:121:ARG:O	3:C:125:GLN:HG2	2.15	0.46
1:D:24:ASP:OD1	1:D:26:GLN:OE1	2.33	0.46
1:D:57:ASP:O	1:D:58:THR:O	2.33	0.46
1:D:321:VAL:HG23	1:D:322:ILE:N	2.29	0.46
4:G:6:FGA:HG3	4:G:7:DAM:HM1	1.72	0.46
1:A:50:GLU:O	1:A:53:PRO:HD2	2.15	0.46
2:B:221:ASN:O	2:B:223:GLU:N	2.47	0.46
1:D:46:ARG:O	1:D:50:GLU:N	2.49	0.46
1:D:60:TYR:O	1:D:60:TYR:CG	2.68	0.46
1:D:141:PHE:CD1	1:D:141:PHE:C	2.89	0.46
1:D:189:LEU:CD1	1:D:208:MET:HE3	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:68:ARG:HG2	2:E:68:ARG:HH11	1.80	0.46
2:B:172:PHE:HB3	2:B:203:TRP:CZ3	2.51	0.46
1:D:98:THR:HG21	1:D:140:TRP:CE3	2.51	0.46
1:D:330:ILE:O	1:D:330:ILE:HG22	2.14	0.46
1:D:404:LEU:HD12	1:D:408:ILE:HD11	1.97	0.46
2:E:97:ASN:ND2	2:E:116:ASP:OD1	2.46	0.46
2:E:188:ASP:O	2:E:189:TYR:HB2	2.14	0.46
2:E:222:MET:HA	2:E:222:MET:HE2	1.97	0.46
3:F:153:LEU:O	3:F:185:ARG:HD2	2.16	0.46
1:A:439:PHE:CE2	1:A:469:LEU:HD21	2.51	0.46
2:B:243:VAL:HG13	2:B:293:PHE:HZ	1.79	0.46
2:B:380:GLU:OE1	2:B:395:ARG:NH2	2.49	0.46
1:D:310:CYS:C	1:D:312:ASN:H	2.19	0.46
1:D:514:GLN:HA	1:D:517:THR:HB	1.96	0.46
2:E:196:ASP:HB2	2:E:199:ARG:H	1.81	0.46
1:A:178:THR:CG2	1:A:180:MET:HB3	2.45	0.46
1:A:197:GLU:HG2	1:A:199:ASP:OD1	2.15	0.46
2:E:321:GLU:HB3	2:E:323:TYR:CE1	2.50	0.46
1:A:469:LEU:HD22	1:A:477:TRP:HZ3	1.81	0.46
2:B:373:THR:HG22	2:B:375:ARG:HG3	1.97	0.46
3:C:165:CYS:HA	3:C:238:SER:O	2.15	0.46
1:D:200:ASN:HA	1:D:203:SER:OG	2.15	0.46
1:A:427:MET:HE3	1:A:427:MET:HA	1.97	0.46
1:D:331:LYS:HA	1:D:368:LEU:CD2	2.45	0.46
2:E:312:ASP:OD1	2:E:314:ASN:HB2	2.15	0.46
3:F:25:GLU:HG3	3:F:142:VAL:HG23	1.97	0.46
1:A:102:THR:HG23	2:B:206:GLU:OE2	2.15	0.46
1:A:138:GLY:O	1:A:144:ARG:HD3	2.15	0.46
1:A:373:LEU:HD13	1:A:384:ILE:HG21	1.96	0.46
1:A:511:VAL:HG23	1:A:511:VAL:O	2.15	0.46
2:B:251:ILE:H	2:B:251:ILE:CD1	2.18	0.46
3:C:115:ARG:HH21	3:C:189:VAL:HG23	1.81	0.46
1:D:302:ALA:O	1:D:305:LYS:N	2.47	0.46
1:A:224:ALA:O	1:A:226:GLU:N	2.49	0.45
2:B:327:GLU:OE2	2:B:330:ARG:NH1	2.48	0.45
1:D:124:LEU:HD22	1:D:128:PHE:HB3	1.98	0.45
2:E:23:ASP:HB3	2:E:24:ASP:H	1.64	0.45
2:E:65:SER:O	2:E:66:HIS:HB2	2.16	0.45
2:E:358:MET:SD	2:E:422:THR:OG1	2.74	0.45
2:E:396:LYS:HD3	2:E:407:GLU:CD	2.37	0.45
1:A:409:VAL:O	1:A:412:ALA:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:113:ILE:HD12	3:C:153:LEU:HD21	1.98	0.45
1:D:157:ARG:HH11	1:D:157:ARG:CG	2.29	0.45
1:D:427:MET:HB3	1:D:465:ASN:HD21	1.81	0.45
1:D:452:VAL:HG13	1:D:452:VAL:O	2.14	0.45
1:D:568:THR:HB	1:D:580:GLN:OE1	2.17	0.45
3:F:6:PHE:O	3:F:7:THR:C	2.54	0.45
3:F:20:CYS:SG	3:F:92:TYR:CE2	3.10	0.45
3:F:155:LEU:HD21	3:F:195:MET:HE2	1.98	0.45
3:F:279:ASP:OD1	3:F:279:ASP:C	2.54	0.45
1:A:141:PHE:C	1:A:141:PHE:CD1	2.89	0.45
1:A:267:PHE:CZ	1:A:287:PHE:HB2	2.51	0.45
1:A:427:MET:N	1:A:428:PRO:CD	2.79	0.45
3:C:188:GLU:O	3:C:190:PRO:HD3	2.16	0.45
1:D:57:ASP:HB3	2:E:129:LYS:CE	2.46	0.45
1:D:171:ARG:HH12	1:D:204:GLU:HG3	1.82	0.45
1:D:318:ARG:CG	1:D:319:GLU:N	2.64	0.45
1:D:454:HIS:HB3	3:F:287:LEU:HD21	1.97	0.45
2:E:119:ILE:N	2:E:119:ILE:HD12	2.31	0.45
2:E:291:VAL:O	2:E:292:LYS:HG2	2.16	0.45
2:E:389:ARG:HH11	2:E:389:ARG:CG	2.28	0.45
4:H:2:LEU:H	4:H:7:DAM:C	2.30	0.45
1:A:198:LEU:HD11	1:A:236:PRO:HD2	1.98	0.45
1:A:495:TYR:O	1:A:499:MET:HG3	2.16	0.45
1:A:559:GLU:HA	1:A:562:PRO:HG2	1.98	0.45
2:B:47:ASP:HB2	2:B:51:ARG:N	2.31	0.45
2:B:263:ASP:OD1	2:B:263:ASP:N	2.50	0.45
3:C:103:LEU:HB3	3:C:111:ILE:HD13	1.94	0.45
3:C:132:GLU:O	3:C:136:LYS:HG3	2.17	0.45
1:D:57:ASP:HB3	2:E:129:LYS:HE3	1.98	0.45
1:D:267:PHE:CE2	1:D:287:PHE:CD2	3.02	0.45
1:D:561:LYS:N	1:D:562:PRO:CD	2.78	0.45
2:E:130:ARG:HB2	2:E:131:PRO:HD2	1.99	0.45
2:E:172:PHE:HD2	2:E:203:TRP:CE3	2.35	0.45
2:E:396:LYS:HD3	2:E:407:GLU:OE2	2.16	0.45
1:A:39:ALA:HB1	1:A:79:LEU:HD22	1.99	0.45
2:B:382:SER:OG	2:B:385:ASN:HB2	2.17	0.45
3:C:76:PRO:HD3	3:C:107:TYR:CE2	2.51	0.45
1:D:406:PRO:O	1:D:407:ALA:C	2.55	0.45
1:A:119:HIS:HB3	1:A:124:LEU:HB2	1.99	0.45
1:D:352:LEU:C	1:D:354:PRO:HD2	2.37	0.45
1:D:522:LEU:N	1:D:523:PRO:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:539:ASN:HD22	1:D:539:ASN:HA	1.63	0.45
1:A:502:LEU:O	1:A:506:ASN:OD1	2.34	0.45
2:B:281:PHE:O	2:B:282:SER:C	2.55	0.45
2:B:351:ASN:HD22	2:B:351:ASN:C	2.18	0.45
1:D:334:VAL:HG13	1:D:372:GLN:OE1	2.17	0.45
2:E:306:LEU:O	2:E:325:VAL:HG13	2.16	0.45
3:F:76:PRO:HG3	3:F:107:TYR:CE1	2.52	0.45
2:B:92:ILE:N	2:B:92:ILE:HD12	2.31	0.45
2:B:305:TYR:HE1	2:B:341:CYS:O	1.99	0.45
3:C:250:TRP:CZ2	3:C:286:PHE:HE2	2.35	0.45
1:D:516:ILE:CA	1:D:519:LYS:HB2	2.47	0.45
3:F:155:LEU:HD11	3:F:195:MET:HE3	1.99	0.45
1:A:16:LEU:HB3	1:A:38:ILE:HD11	1.99	0.45
1:A:197:GLU:CD	1:A:197:GLU:N	2.65	0.45
1:A:564:LEU:HB3	1:A:583:LEU:HD21	1.99	0.45
2:B:323:TYR:HB3	2:B:369:PHE:CE2	2.52	0.45
3:C:68:LEU:HD23	3:C:68:LEU:O	2.17	0.45
3:C:200:TRP:CE3	3:C:216:ALA:HB3	2.51	0.45
1:A:226:GLU:CD	1:A:227:ALA:N	2.70	0.45
1:A:350:MET:HB3	1:A:391:VAL:HG21	1.95	0.45
1:A:432:GLY:CA	1:A:472:LYS:HE3	2.36	0.45
1:A:522:LEU:HD22	1:A:551:LEU:HD11	1.99	0.45
1:D:350:MET:SD	1:D:369:PHE:CD1	3.10	0.45
1:D:366:LEU:O	1:D:370:LEU:HB2	2.17	0.45
2:B:199:ARG:HG2	2:B:216:ASP:HA	1.99	0.44
2:B:325:VAL:HG13	2:B:326:HIS:CD2	2.52	0.44
2:B:435:THR:O	2:B:436:THR:C	2.56	0.44
3:C:266:CYS:C	3:C:267:TYR:CD1	2.86	0.44
1:D:326:ILE:HD12	1:D:326:ILE:N	2.32	0.44
1:D:334:VAL:HG22	1:D:372:GLN:OE1	2.17	0.44
1:D:440:ASP:HA	1:D:444:ASN:HB2	1.99	0.44
1:D:549:PRO:HD3	1:D:586:LEU:CD2	2.47	0.44
2:E:263:ASP:OD1	2:E:263:ASP:N	2.49	0.44
1:A:254:ASP:O	1:A:260:ARG:HD3	2.17	0.44
2:E:120:LYS:HG2	2:E:171:ILE:HG12	1.99	0.44
2:E:162:LEU:HD23	2:E:162:LEU:C	2.38	0.44
2:E:197:ASP:HB3	2:E:228:VAL:CG2	2.45	0.44
1:A:40:LEU:HD22	1:A:79:LEU:HD21	1.99	0.44
1:A:427:MET:HA	1:A:427:MET:CE	2.47	0.44
1:A:539:ASN:HD22	1:A:539:ASN:HA	1.65	0.44
1:D:44:VAL:HG12	1:D:45:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:LEU:O	1:D:404:LEU:HD23	2.17	0.44
1:D:412:ALA:HA	1:D:450:TRP:HZ2	1.82	0.44
2:E:327:GLU:OE2	2:E:330:ARG:HD2	2.17	0.44
3:F:39:LEU:HD13	3:F:153:LEU:HD23	1.99	0.44
3:F:65:LEU:O	3:F:69:PHE:CD2	2.70	0.44
3:F:79:ASN:HD22	3:F:79:ASN:HA	1.57	0.44
1:A:50:GLU:C	1:A:53:PRO:HD2	2.37	0.44
1:A:257:TRP:CE2	1:A:258:ARG:HG2	2.53	0.44
1:A:502:LEU:HD11	1:A:540:VAL:HG23	1.99	0.44
2:B:28:ALA:HB1	2:B:51:ARG:NH2	2.32	0.44
2:B:47:ASP:OD2	2:B:51:ARG:CZ	2.65	0.44
2:E:193:LEU:HD12	2:E:193:LEU:C	2.37	0.44
2:E:388:PRO:O	2:E:389:ARG:HG2	2.17	0.44
3:F:107:TYR:HB3	3:F:110:ARG:HB2	1.99	0.44
1:A:339:GLN:CD	1:A:377:CYS:HB2	2.37	0.44
1:A:339:GLN:NE2	1:A:377:CYS:HB2	2.32	0.44
1:A:358:LYS:HG2	1:A:359:ASP:N	2.33	0.44
1:A:539:ASN:HD22	1:A:542:LYS:HD2	1.83	0.44
1:D:291:MET:HE1	1:D:329:CYS:HB2	1.99	0.44
1:D:475:LYS:HB2	1:D:512:CYS:HA	1.98	0.44
3:F:139:ASN:OD1	3:F:141:ASN:HB2	2.18	0.44
1:A:245:MET:O	1:A:249:ARG:HB2	2.17	0.44
1:A:502:LEU:HD21	1:A:528:MET:SD	2.58	0.44
2:B:302:THR:HG22	2:B:309:LYS:HG2	1.99	0.44
3:C:129:PHE:HZ	3:C:146:PHE:CD2	2.36	0.44
2:E:47:ASP:HB3	2:E:49:GLY:N	2.33	0.44
1:A:155:TYR:CE2	1:A:196:LEU:HD23	2.52	0.44
1:A:271:GLN:OE1	1:A:309:PHE:CD1	2.71	0.44
1:A:348:VAL:O	1:A:350:MET:N	2.51	0.44
3:C:81:LEU:HD13	3:C:112:THR:CB	2.34	0.44
3:C:158:LEU:HG	3:C:161:GLY:HA2	2.00	0.44
1:D:155:TYR:CE2	1:D:163:LYS:HD3	2.52	0.44
1:D:336:ASP:HB3	1:D:342:LYS:CG	2.47	0.44
1:D:502:LEU:HD11	1:D:540:VAL:CG2	2.48	0.44
1:D:553:ASN:O	1:D:557:GLN:HG2	2.18	0.44
2:E:252:ARG:CZ	2:E:268:LEU:HD13	2.48	0.44
2:E:320:VAL:HG12	2:E:321:GLU:HG3	2.00	0.44
1:A:219:SER:HA	1:A:222:LEU:HD21	2.00	0.44
1:A:287:PHE:HZ	1:A:306:VAL:CG2	2.29	0.44
1:A:483:ILE:HD13	1:A:521:MET:SD	2.57	0.44
2:B:351:ASN:ND2	2:B:351:ASN:C	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:LYS:H	3:C:8:LYS:HG3	1.48	0.44
3:C:76:PRO:HB2	3:C:110:ARG:HG2	1.98	0.44
3:C:188:GLU:HG3	3:C:189:VAL:N	2.33	0.44
1:D:470:VAL:C	1:D:472:LYS:H	2.20	0.44
1:D:587:SER:C	1:D:589:ALA:H	2.21	0.44
1:A:323:MET:CE	1:A:356:LEU:HD13	2.47	0.44
1:A:382:LEU:CD1	1:A:411:LEU:HD13	2.47	0.44
1:D:204:GLU:O	1:D:207:PRO:HD2	2.18	0.44
1:D:267:PHE:CZ	1:D:287:PHE:HB2	2.53	0.44
1:D:483:ILE:HG22	1:D:487:LEU:HD11	1.99	0.44
2:E:127:ARG:CZ	2:E:163:MET:CE	2.96	0.44
2:E:248:LYS:HD3	2:E:248:LYS:HA	1.85	0.44
3:F:91:TYR:CE1	3:F:135:ARG:NH2	2.85	0.44
1:A:19:GLU:OE1	1:A:19:GLU:HA	2.18	0.43
1:A:439:PHE:CZ	1:A:469:LEU:HD11	2.53	0.43
1:A:544:LEU:HA	1:A:547:ILE:HG12	2.00	0.43
2:B:222:MET:CE	2:B:225:LEU:HD13	2.48	0.43
2:B:303:ARG:NH1	2:B:359:THR:OG1	2.47	0.43
1:D:462:ALA:O	1:D:465:ASN:HB3	2.18	0.43
2:E:323:TYR:HB3	2:E:369:PHE:CE2	2.53	0.43
3:F:40:THR:HG23	3:F:152:TYR:HD2	1.81	0.43
2:E:244:TYR:OH	2:E:252:ARG:HD2	2.19	0.43
1:A:133:LYS:HD3	1:A:169:TYR:OH	2.18	0.43
1:A:267:PHE:HE2	1:A:287:PHE:HB2	1.81	0.43
1:A:561:LYS:HD2	1:A:588:LEU:HB3	2.00	0.43
1:D:141:PHE:CE1	1:D:180:MET:CG	3.01	0.43
1:D:155:TYR:CZ	1:D:163:LYS:HD3	2.54	0.43
1:D:165:GLU:O	1:D:169:TYR:HD1	2.00	0.43
1:D:350:MET:C	1:D:352:LEU:H	2.20	0.43
3:F:134:LEU:C	3:F:136:LYS:N	2.71	0.43
3:F:169:GLY:O	3:F:198:LEU:HA	2.18	0.43
1:A:133:LYS:NZ	1:A:165:GLU:OE1	2.46	0.43
1:A:449:ALA:O	1:A:452:VAL:HG12	2.19	0.43
2:B:28:ALA:HB1	2:B:51:ARG:HH21	1.82	0.43
2:B:410:VAL:C	2:B:412:SER:H	2.22	0.43
3:C:180:ILE:O	3:C:183:LEU:HB2	2.19	0.43
3:C:228:PHE:O	3:C:232:ASN:ND2	2.43	0.43
1:D:113:ARG:HG2	1:D:153:VAL:HG11	1.99	0.43
1:D:321:VAL:CG2	1:D:322:ILE:N	2.81	0.43
1:D:519:LYS:HB3	1:D:520:HIS:H	1.67	0.43
2:E:362:TYR:O	2:E:365:PHE:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:399:ALA:HB3	2:E:402:LYS:CE	2.35	0.43
3:F:175:ASP:HB2	3:F:179:HIS:HE1	1.83	0.43
2:B:21:VAL:HG22	2:B:21:VAL:O	2.18	0.43
2:B:241:THR:CG2	2:B:253:LEU:HD21	2.48	0.43
2:B:247:SER:HA	2:B:287:SER:OG	2.18	0.43
2:B:368:MET:HE3	2:B:424:TRP:CZ3	2.53	0.43
2:E:110:PHE:CZ	2:E:123:LYS:HG3	2.52	0.43
3:F:24:SER:OG	3:F:27:GLN:HG3	2.19	0.43
3:F:244:VAL:HG23	3:F:247:GLY:H	1.83	0.43
1:A:332:GLU:C	1:A:334:VAL:H	2.22	0.43
1:A:552:ASP:OD1	1:A:554:SER:HB3	2.18	0.43
2:B:298:ARG:HH21	2:B:314:ASN:ND2	2.12	0.43
3:C:106:ARG:HG3	3:C:106:ARG:HH11	1.83	0.43
1:D:233:GLN:HG3	1:D:273:ALA:HB1	2.01	0.43
2:E:374:LYS:HA	2:E:374:LYS:HD3	1.75	0.43
1:A:329:CYS:O	1:A:333:LEU:HG	2.18	0.43
2:B:68:ARG:HG2	2:B:68:ARG:NH1	2.33	0.43
1:D:368:LEU:C	1:D:370:LEU:N	2.71	0.43
1:D:518:THR:HG22	1:D:518:THR:O	2.19	0.43
2:E:252:ARG:NH2	2:E:268:LEU:HD13	2.34	0.43
3:F:110:ARG:C	3:F:111:ILE:HG13	2.39	0.43
1:A:125:GLU:HG3	1:A:158:VAL:HG12	2.00	0.43
1:A:201:VAL:O	1:A:206:ILE:HG12	2.19	0.43
1:A:535:ASN:HA	1:A:538:PHE:CE2	2.53	0.43
2:B:26:ALA:HB3	2:B:29:ASP:OD2	2.19	0.43
1:D:38:ILE:O	1:D:42:LEU:CD2	2.67	0.43
1:D:127:HIS:O	1:D:130:PRO:HD2	2.19	0.43
1:D:307:LYS:O	1:D:311:GLU:HG3	2.18	0.43
1:D:398:ARG:C	1:D:400:LEU:H	2.22	0.43
3:F:88:ASP:O	3:F:90:GLY:N	2.47	0.43
3:F:118:HIS:HA	3:F:123:ILE:HG21	2.01	0.43
3:F:155:LEU:HD21	3:F:195:MET:CE	2.49	0.43
1:A:348:VAL:C	1:A:350:MET:N	2.72	0.43
2:B:219:PRO:HD2	2:B:222:MET:HE1	2.00	0.43
2:B:339:ASN:O	2:B:340:ASP:HB2	2.19	0.43
2:E:387:LYS:HB3	2:E:388:PRO:CD	2.45	0.43
3:F:209:TRP:CD2	3:F:224:ILE:CD1	3.02	0.43
3:F:263:PRO:HB2	3:F:291:PRO:HD3	2.00	0.43
1:A:28:ARG:NH2	1:A:62:GLU:OE1	2.51	0.43
1:A:46:ARG:NH1	1:A:50:GLU:OE2	2.52	0.43
1:A:201:VAL:O	1:A:201:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLN:C	1:A:273:ALA:H	2.22	0.43
3:C:56:GLY:HA3	3:C:259:ILE:O	2.18	0.43
1:D:60:TYR:O	1:D:61:ASP:CG	2.57	0.43
2:E:87:LEU:H	2:E:87:LEU:CD1	2.28	0.43
2:E:111:LEU:HD12	2:E:111:LEU:C	2.39	0.43
2:E:219:PRO:HG2	2:E:222:MET:HE2	2.01	0.43
1:A:227:ALA:O	1:A:228:CYS:C	2.57	0.42
1:A:439:PHE:CE1	1:A:444:ASN:HA	2.54	0.42
1:A:499:MET:SD	1:A:539:ASN:OD1	2.78	0.42
2:B:134:TYR:CB	2:B:137:LYS:HA	2.48	0.42
3:C:68:LEU:HD23	3:C:68:LEU:C	2.39	0.42
2:E:36:PHE:CE1	2:E:43:LEU:HD13	2.53	0.42
3:F:68:LEU:C	3:F:68:LEU:HD23	2.39	0.42
3:F:130:TYR:O	3:F:133:CYS:HB2	2.19	0.42
1:A:336:ASP:O	1:A:342:LYS:HD3	2.19	0.42
1:A:437:GLU:OE1	1:A:437:GLU:N	2.52	0.42
2:B:28:ALA:CB	2:B:51:ARG:NH2	2.82	0.42
2:B:309:LYS:HD3	2:B:319:PRO:HG3	2.01	0.42
2:B:332:LYS:HA	2:B:332:LYS:HD3	1.88	0.42
3:C:17:LEU:HD11	3:C:98:THR:CG2	2.49	0.42
1:D:322:ILE:O	1:D:322:ILE:HG22	2.19	0.42
1:D:330:ILE:HG23	1:D:345:LEU:HD21	2.00	0.42
1:D:437:GLU:HG2	1:D:438:PHE:N	2.34	0.42
1:A:208:MET:HB2	1:A:208:MET:HE2	1.99	0.42
2:B:14:PHE:HA	2:B:442:PHE:HD1	1.83	0.42
3:C:121:ARG:HG2	3:C:147:THR:CB	2.49	0.42
2:E:253:LEU:C	2:E:253:LEU:HD23	2.39	0.42
3:F:212:SER:C	3:F:214:ARG:N	2.72	0.42
3:F:277:GLU:O	3:F:284:TYR:HA	2.20	0.42
1:A:39:ALA:CB	1:A:79:LEU:HD22	2.49	0.42
1:A:204:GLU:C	1:A:207:PRO:HD2	2.40	0.42
2:B:8:ASN:CG	2:B:375:ARG:HH21	2.22	0.42
2:B:21:VAL:CA	2:B:383:ARG:NH1	2.68	0.42
1:D:58:THR:O	1:D:59:ILE:C	2.57	0.42
1:D:62:GLU:O	1:D:63:ASP:C	2.57	0.42
1:D:505:ILE:C	1:D:507:VAL:H	2.23	0.42
3:F:42:GLU:HB3	3:F:46:GLN:OE1	2.20	0.42
3:F:160:ASP:HB3	3:F:162:GLN:OE1	2.18	0.42
3:F:214:ARG:HH21	3:F:242:GLN:HG2	1.85	0.42
1:A:43:GLY:O	1:A:44:VAL:HG23	2.19	0.42
1:A:75:THR:O	1:A:76:PHE:CD1	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:ARG:HD2	2:B:153:ARG:HA	1.83	0.42
3:C:117:ASN:HB3	3:C:199:LEU:O	2.19	0.42
1:D:470:VAL:C	1:D:472:LYS:N	2.72	0.42
1:D:489:MET:HB2	1:D:501:THR:OG1	2.19	0.42
2:E:281:PHE:O	2:E:282:SER:C	2.56	0.42
3:F:172:PRO:HG3	3:F:209:TRP:CE3	2.55	0.42
1:A:10:LEU:O	1:A:11:TYR:C	2.56	0.42
1:A:21:ARG:NH1	2:B:133:GLY:N	2.68	0.42
1:A:465:ASN:O	1:A:469:LEU:HB2	2.19	0.42
2:B:358:MET:CG	2:B:359:THR:N	2.82	0.42
1:D:186:ALA:CA	1:D:212:LEU:HD13	2.49	0.42
1:D:398:ARG:C	1:D:400:LEU:N	2.72	0.42
1:D:401:SER:HA	1:D:404:LEU:HD21	2.01	0.42
1:D:517:THR:O	1:D:521:MET:HB3	2.20	0.42
1:A:120:SER:C	1:A:122:SER:N	2.70	0.42
1:A:170:PHE:CE2	1:A:189:LEU:HD12	2.54	0.42
1:A:218:ASP:O	1:A:222:LEU:HD22	2.19	0.42
1:A:439:PHE:CD1	1:A:439:PHE:C	2.93	0.42
2:B:178:TYR:HB2	2:B:196:ASP:HB3	2.01	0.42
3:C:88:ASP:OD1	3:C:129:PHE:HB2	2.19	0.42
3:C:165:CYS:SG	3:C:238:SER:HB3	2.60	0.42
1:D:356:LEU:HB3	1:D:360:ASN:HB2	2.00	0.42
1:D:418:ARG:NH2	3:F:70:ARG:NH2	2.67	0.42
2:E:199:ARG:NH2	2:E:218:LYS:HD3	2.34	0.42
2:E:272:PRO:CD	2:E:318:ARG:HE	2.32	0.42
3:F:51:PRO:HA	3:F:278:LEU:O	2.19	0.42
3:F:129:PHE:O	3:F:133:CYS:SG	2.71	0.42
3:F:188:GLU:O	3:F:190:PRO:HD3	2.20	0.42
1:A:553:ASN:OD1	1:A:557:GLN:NE2	2.53	0.42
3:C:212:SER:C	3:C:214:ARG:H	2.23	0.42
1:D:40:LEU:HD23	1:D:79:LEU:HD21	2.01	0.42
2:E:383:ARG:HH11	2:E:383:ARG:HB3	1.85	0.42
2:E:402:LYS:H	2:E:402:LYS:HG3	1.41	0.42
3:F:70:ARG:HG3	3:F:70:ARG:NH1	2.35	0.42
3:F:81:LEU:CD1	3:F:112:THR:HB	2.50	0.42
3:F:91:TYR:HE1	3:F:135:ARG:NH2	2.18	0.42
1:A:178:THR:HG21	1:A:180:MET:HB3	2.01	0.42
1:A:237:GLN:O	1:A:240:LEU:HG	2.19	0.42
1:A:353:SER:O	1:A:355:ILE:N	2.47	0.42
2:B:196:ASP:HB3	2:B:197:ASP:H	1.53	0.42
2:B:255:ASP:OD1	2:B:257:ARG:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:LYS:O	2:B:394:PRO:C	2.58	0.42
3:C:134:LEU:C	3:C:136:LYS:N	2.73	0.42
3:C:172:PRO:HG3	3:C:209:TRP:CD2	2.54	0.42
1:D:524:THR:HG23	1:D:527:ARG:HH22	1.84	0.42
2:E:425:HIS:CG	2:E:426:PRO:HD2	2.55	0.42
1:A:406:PRO:O	1:A:407:ALA:C	2.59	0.42
1:A:468:LYS:HD3	1:A:471:GLU:OE1	2.20	0.42
3:C:133:CYS:SG	3:C:143:TRP:HB2	2.60	0.42
3:C:202:ASP:HB3	3:C:242:GLN:NE2	2.34	0.42
1:D:268:THR:HG21	1:D:308:GLU:OE1	2.19	0.42
1:D:437:GLU:CG	1:D:438:PHE:N	2.82	0.42
1:D:455:VAL:HG13	3:F:71:ILE:HD13	2.01	0.42
2:E:278:ARG:CG	2:E:279:SER:H	2.32	0.42
3:F:117:ASN:H	3:F:167:HIS:CD2	2.38	0.42
3:F:142:VAL:HA	3:F:145:TYR:CD2	2.54	0.42
3:F:208:GLY:H	3:F:223:ASP:CG	2.23	0.42
1:A:400:LEU:HB3	1:A:404:LEU:HD21	2.01	0.41
2:B:17:VAL:HG13	2:B:440:TYR:CD2	2.55	0.41
2:B:22:ASP:CG	2:B:23:ASP:N	2.74	0.41
2:B:42:LEU:HD12	2:B:109:GLN:HG2	2.02	0.41
2:B:332:LYS:HZ2	2:B:410:VAL:HG11	1.84	0.41
1:D:105:ARG:O	1:D:109:VAL:HG23	2.20	0.41
1:D:248:LEU:O	1:D:248:LEU:HD12	2.20	0.41
1:D:317:CYS:O	1:D:318:ARG:C	2.58	0.41
1:D:338:ASN:OD1	1:D:340:HIS:HB3	2.19	0.41
1:D:433:GLN:O	1:D:434:LEU:HG	2.20	0.41
2:E:85:ASP:OD1	2:E:88:LYS:HB2	2.20	0.41
2:E:136:LEU:O	2:E:137:LYS:C	2.58	0.41
3:F:44:ASN:ND2	3:F:183:LEU:O	2.53	0.41
4:G:2:LEU:H	4:G:7:DAM:C	2.33	0.41
1:A:100:GLU:H	1:A:100:GLU:HG3	1.38	0.41
1:A:352:LEU:O	1:A:355:ILE:HB	2.20	0.41
3:C:107:TYR:HB3	3:C:110:ARG:HB2	2.01	0.41
3:C:265:TYR:HB3	3:C:269:CYS:HB2	2.01	0.41
1:D:346:ALA:HB1	1:D:384:ILE:CD1	2.50	0.41
2:E:172:PHE:HB3	2:E:203:TRP:CZ3	2.55	0.41
2:E:272:PRO:HD2	2:E:318:ARG:HE	1.85	0.41
3:F:63:HIS:O	3:F:66:MET:HB2	2.21	0.41
1:A:211:ASN:CA	1:D:8:MET:HE3	2.49	0.41
2:B:230:THR:CG2	2:B:288:ILE:O	2.67	0.41
2:B:370:ASP:HB3	2:B:373:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:LYS:O	2:B:395:ARG:HD3	2.21	0.41
3:C:67:GLU:O	3:C:71:ILE:HG12	2.20	0.41
3:C:86:TYR:CD2	3:C:119:GLU:OE2	2.73	0.41
1:D:35:LEU:HB2	1:D:72:GLN:HG2	2.02	0.41
1:D:467:LYS:HE2	1:D:471:GLU:OE2	2.19	0.41
1:A:348:VAL:C	1:A:350:MET:H	2.23	0.41
2:B:271:GLU:HG3	2:B:318:ARG:HG2	2.03	0.41
2:B:425:HIS:HB2	2:B:430:ILE:HB	2.02	0.41
3:C:66:MET:HE2	3:C:66:MET:HA	2.02	0.41
1:D:332:GLU:O	1:D:334:VAL:N	2.53	0.41
1:D:439:PHE:CE1	1:D:477:TRP:HH2	2.38	0.41
1:D:514:GLN:O	1:D:514:GLN:HG2	2.20	0.41
3:F:176:THR:HA	3:F:232:ASN:OD1	2.19	0.41
3:F:282:LEU:HD23	3:F:282:LEU:HA	1.84	0.41
1:A:36:SER:O	1:A:40:LEU:HB2	2.21	0.41
1:A:121:PRO:O	1:A:125:GLU:HB2	2.20	0.41
1:A:439:PHE:HE1	1:A:444:ASN:HA	1.86	0.41
1:D:58:THR:HA	1:D:60:TYR:HD1	1.85	0.41
1:D:282:ASP:C	1:D:285:PRO:HD2	2.40	0.41
1:A:170:PHE:HE2	1:A:189:LEU:HD12	1.84	0.41
1:A:310:CYS:C	1:A:312:ASN:H	2.23	0.41
2:B:23:ASP:HB3	2:B:24:ASP:H	1.71	0.41
2:B:175:ALA:HB3	2:B:203:TRP:HZ2	1.85	0.41
2:B:193:LEU:HD12	2:B:193:LEU:C	2.40	0.41
2:E:33:THR:HG22	2:E:46:GLY:HA3	2.03	0.41
2:E:388:PRO:CB	2:E:389:ARG:HE	2.33	0.41
2:E:389:ARG:CG	2:E:389:ARG:NH1	2.82	0.41
3:F:245:MET:HA	3:F:271:ASN:HB2	2.03	0.41
1:A:77:THR:HG21	1:A:118:GLU:OE1	2.21	0.41
1:A:420:ARG:O	1:A:424:ILE:HG13	2.21	0.41
2:B:176:HIS:HD1	2:B:196:ASP:CG	2.23	0.41
2:B:339:ASN:OD1	2:B:341:CYS:SG	2.74	0.41
3:C:199:LEU:N	3:C:199:LEU:CD1	2.84	0.41
3:C:222:GLN:HG3	3:C:252:HIS:CB	2.50	0.41
1:D:197:GLU:H	1:D:197:GLU:CD	2.24	0.41
1:D:291:MET:HB3	1:D:333:LEU:HD11	2.02	0.41
1:D:504:CYS:O	1:D:508:LEU:HG	2.20	0.41
2:E:197:ASP:O	2:E:229:ILE:N	2.37	0.41
2:E:388:PRO:HB2	2:E:389:ARG:HE	1.85	0.41
1:A:552:ASP:O	1:A:556:LEU:HG	2.21	0.41
3:C:10:LEU:N	3:C:10:LEU:HD23	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:ASN:HB2	3:C:200:TRP:CE2	2.56	0.41
1:D:256:SER:HB3	1:D:259:VAL:CG2	2.50	0.41
1:D:257:TRP:HD1	2:E:257:ARG:O	2.04	0.41
1:D:423:ILE:HG22	1:D:424:ILE:N	2.36	0.41
2:E:272:PRO:HG2	2:E:318:ARG:NH2	2.35	0.41
3:F:159:VAL:HG11	3:F:278:LEU:CD1	2.51	0.41
3:F:202:ASP:OD2	3:F:214:ARG:HG3	2.21	0.41
3:F:229:ASN:ND2	3:F:255:ASN:HB3	2.35	0.41
1:A:85:TYR:CD1	1:A:85:TYR:N	2.89	0.41
1:A:131:LEU:HA	1:A:134:ARG:NH2	2.35	0.41
1:A:197:GLU:CG	1:A:199:ASP:OD1	2.69	0.41
1:A:322:ILE:CD1	1:A:355:ILE:HG21	2.51	0.41
1:A:391:VAL:O	1:A:391:VAL:CG1	2.67	0.41
2:B:222:MET:HE3	2:B:222:MET:HA	2.02	0.41
2:B:332:LYS:O	2:B:333:LEU:C	2.59	0.41
2:B:333:LEU:N	2:B:333:LEU:CD2	2.83	0.41
3:C:76:PRO:HG3	3:C:107:TYR:CE1	2.56	0.41
3:C:153:LEU:HA	3:C:154:PRO:HD3	1.88	0.41
1:D:32:ILE:O	1:D:35:LEU:CD2	2.69	0.41
1:D:387:ASN:O	1:D:390:CYS:HB3	2.21	0.41
1:D:412:ALA:HB1	1:D:450:TRP:CZ2	2.56	0.41
2:E:149:VAL:O	2:E:149:VAL:HG12	2.20	0.41
2:E:231:ALA:HB3	2:E:245:SER:OG	2.21	0.41
2:E:272:PRO:CG	2:E:318:ARG:HE	2.31	0.41
2:E:301:MET:SD	2:E:357:VAL:CG2	3.09	0.41
2:E:315:MET:CE	2:E:318:ARG:HB2	2.51	0.41
3:F:113:ILE:O	3:F:153:LEU:HD22	2.21	0.41
3:F:154:PRO:HA	3:F:185:ARG:HH11	1.83	0.41
1:A:256:SER:OG	1:A:259:VAL:HG23	2.21	0.41
1:A:354:PRO:C	1:A:355:ILE:HG13	2.41	0.41
1:A:369:PHE:CE1	1:A:384:ILE:HG23	2.56	0.41
2:B:244:TYR:OH	2:B:252:ARG:HD2	2.21	0.41
2:B:250:THR:HB	2:B:268:LEU:CD1	2.41	0.41
2:E:222:MET:HA	2:E:222:MET:HE3	2.00	0.41
1:A:8:MET:CE	1:A:10:LEU:HD23	2.51	0.40
1:A:180:MET:CE	1:A:183:ARG:HH21	2.34	0.40
1:A:221:ARG:O	1:A:222:LEU:C	2.59	0.40
3:C:115:ARG:NH2	3:C:189:VAL:HG23	2.37	0.40
1:D:192:PHE:O	1:D:195:VAL:HG22	2.22	0.40
1:D:586:LEU:O	1:D:587:SER:HB2	2.21	0.40
2:E:301:MET:HG2	2:E:348:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:10:LEU:O	3:F:11:ASP:C	2.59	0.40
3:F:204:ASP:OD2	3:F:219:THR:HB	2.21	0.40
1:A:388:LEU:O	1:A:389:ASP:C	2.58	0.40
2:B:197:ASP:O	2:B:229:ILE:N	2.44	0.40
2:B:309:LYS:HG3	2:B:309:LYS:O	2.20	0.40
3:C:16:GLN:HG2	3:C:21:LYS:HB2	2.03	0.40
1:D:93:LEU:HD23	1:D:93:LEU:HA	1.98	0.40
1:D:248:LEU:CD2	1:D:270:LEU:HD22	2.52	0.40
1:A:120:SER:O	1:A:121:PRO:C	2.59	0.40
1:A:571:GLN:CD	1:A:571:GLN:N	2.64	0.40
2:B:325:VAL:O	2:B:367:ARG:NE	2.51	0.40
1:D:284:VAL:HB	1:D:285:PRO:HD3	2.04	0.40
1:D:353:SER:C	1:D:355:ILE:N	2.75	0.40
2:E:68:ARG:HB3	2:E:443:GLN:HE22	1.86	0.40
3:F:209:TRP:CE2	3:F:224:ILE:HD13	2.56	0.40
3:F:212:SER:HA	3:F:219:THR:CG2	2.51	0.40
1:A:10:LEU:HB2	2:B:149:VAL:HG12	2.03	0.40
1:A:444:ASN:ND2	1:A:481:THR:HG22	2.37	0.40
1:A:505:ILE:C	1:A:507:VAL:N	2.74	0.40
2:B:47:ASP:OD2	2:B:51:ARG:NH2	2.54	0.40
2:B:111:LEU:HD12	2:B:111:LEU:C	2.42	0.40
2:B:221:ASN:HD21	2:B:224:GLU:CG	2.31	0.40
2:B:261:LEU:HB2	2:B:263:ASP:OD1	2.21	0.40
2:B:368:MET:CE	2:B:424:TRP:CZ3	3.05	0.40
3:C:246:GLU:HA	3:C:246:GLU:OE1	2.21	0.40
1:D:332:GLU:C	1:D:334:VAL:N	2.75	0.40
1:D:336:ASP:OD2	1:D:341:VAL:HG11	2.22	0.40
1:A:73:LEU:CD1	1:A:92:PRO:HB2	2.51	0.40
1:A:73:LEU:HD11	1:A:92:PRO:HB2	2.02	0.40
1:A:467:LYS:HB2	1:A:507:VAL:HG12	2.01	0.40
2:B:186:ASN:HB3	2:B:188:ASP:OD1	2.22	0.40
2:B:247:SER:O	2:B:287:SER:HA	2.21	0.40
1:D:25:VAL:HA	1:D:28:ARG:NH1	2.36	0.40
1:D:361:THR:O	1:D:361:THR:HG22	2.22	0.40
1:D:451:LEU:O	1:D:500:THR:HG21	2.22	0.40
1:D:499:MET:HE1	3:F:77:ASP:O	2.21	0.40
1:D:570:ASP:O	1:D:576:LYS:CE	2.65	0.40
3:F:209:TRP:CD2	3:F:224:ILE:HD13	2.57	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	580/582 (100%)	441 (76%)	110 (19%)	29 (5%)	2 6
1	D	580/582 (100%)	465 (80%)	88 (15%)	27 (5%)	2 7
2	B	413/447 (92%)	368 (89%)	38 (9%)	7 (2%)	9 27
2	E	413/447 (92%)	364 (88%)	41 (10%)	8 (2%)	8 24
3	C	286/309 (93%)	246 (86%)	35 (12%)	5 (2%)	9 27
3	F	286/309 (93%)	234 (82%)	40 (14%)	12 (4%)	3 8
4	G	1/7 (14%)	1 (100%)	0	0	100 100
4	H	1/7 (14%)	1 (100%)	0	0	100 100
All	All	2560/2690 (95%)	2120 (83%)	352 (14%)	88 (3%)	3 12

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	58	THR
1	A	157	ARG
1	A	241	GLU
1	A	318	ARG
1	A	558	SER
3	C	207	GLY
1	D	58	THR
1	D	272	LYS
1	D	318	ARG
1	D	558	SER
2	E	66	HIS
2	E	385	ASN
3	F	207	GLY
1	A	44	VAL
1	A	57	ASP
1	A	198	LEU
1	A	237	GLN

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Mol	Chain	Res	Type
1	A	240	LEU
1	A	333	LEU
2	B	66	HIS
2	B	222	MET
2	B	364	ASN
2	B	385	ASN
3	C	135	ARG
3	C	270	GLY
1	D	43	GLY
1	D	44	VAL
1	D	61	ASP
1	D	237	GLN
1	D	333	LEU
2	E	400	SER
3	F	8	LYS
3	F	135	ARG
1	A	61	ASP
1	A	63	ASP
1	A	358	LYS
2	B	67	SER
2	B	411	ASP
1	D	63	ASP
1	D	480	ALA
2	E	389	ARG
3	F	28	VAL
1	A	43	GLY
1	A	121	PRO
1	A	225	VAL
3	C	22	GLN
3	C	280	ASP
1	D	358	LYS
1	D	442	LYS
1	D	473	PHE
1	D	584	THR
2	E	222	MET
3	F	62	PHE
3	F	89	ARG
3	F	186	LEU
1	A	272	LYS
1	A	273	ALA
1	A	473	PHE
1	A	512	CYS

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Mol	Chain	Res	Type
1	D	306	VAL
1	D	401	SER
1	A	355	ILE
1	A	511	VAL
1	A	584	THR
1	D	64	GLU
1	D	233	GLN
1	D	241	GLU
1	D	279	THR
1	D	355	ILE
3	F	29	LYS
3	F	270	GLY
1	D	99	VAL
1	D	482	ILE
3	F	168	GLY
1	A	306	VAL
1	A	349	ILE
1	A	513	GLY
1	D	354	PRO
2	E	149	VAL
2	E	388	PRO
3	F	203	PRO
1	D	511	VAL
1	D	513	GLY
3	F	208	GLY
1	A	482	ILE
1	A	585	VAL
2	B	401	GLY
2	E	401	GLY

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	509/509 (100%)	469 (92%)	40 (8%)	12 31
1	D	509/509 (100%)	475 (93%)	34 (7%)	16 39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	386/408 (95%)	357 (92%)	29 (8%)	13 34
2	E	386/408 (95%)	359 (93%)	27 (7%)	15 37
3	C	254/274 (93%)	239 (94%)	15 (6%)	19 45
3	F	254/274 (93%)	242 (95%)	12 (5%)	26 56
4	G	2/2 (100%)	2 (100%)	0	100 100
4	H	2/2 (100%)	2 (100%)	0	100 100
All	All	2302/2386 (96%)	2145 (93%)	157 (7%)	16 38

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	MET
1	A	19	GLU
1	A	34	LYS
1	A	37	THR
1	A	40	LEU
1	A	45	GLU
1	A	48	ARG
1	A	57	ASP
1	A	58	THR
1	A	63	ASP
1	A	76	PHE
1	A	87	HIS
1	A	100	GLU
1	A	102	THR
1	A	103	VAL
1	A	121	PRO
1	A	141	PHE
1	A	145	THR
1	A	153	VAL
1	A	157	ARG
1	A	177	ASP
1	A	180	MET
1	A	199	ASP
1	A	204	GLU
1	A	209	PHE
1	A	219	SER
1	A	222	LEU
1	A	226	GLU
1	A	238	GLU

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Mol	Chain	Res	Type
1	A	239	ASP
1	A	267	PHE
1	A	404	LEU
1	A	405	LEU
1	A	437	GLU
1	A	439	PHE
1	A	447	CYS
1	A	469	LEU
1	A	495	TYR
1	A	512	CYS
1	A	571	GLN
2	B	8	ASN
2	B	9	ASP
2	B	11	GLN
2	B	14	PHE
2	B	17	VAL
2	B	23	ASP
2	B	47	ASP
2	B	151	THR
2	B	153	ARG
2	B	156	VAL
2	B	161	ASP
2	B	169	ARG
2	B	228	VAL
2	B	230	THR
2	B	234	PHE
2	B	302	THR
2	B	326	HIS
2	B	330	ARG
2	B	333	LEU
2	B	351	ASN
2	B	385	ASN
2	B	386	ASN
2	B	388	PRO
2	B	389	ARG
2	B	403	ARG
2	B	422	THR
2	B	431	ILE
2	B	435	THR
2	B	443	GLN
3	C	12	GLN
3	C	18	ASN

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Mol	Chain	Res	Type
3	C	30	SER
3	C	34	LYS
3	C	40	THR
3	C	49	ARG
3	C	52	VAL
3	C	57	ASP
3	C	110	ARG
3	C	125	GLN
3	C	160	ASP
3	C	173	SER
3	C	239	ARG
3	C	244	VAL
3	C	267	TYR
1	D	9	SER
1	D	16	LEU
1	D	19	GLU
1	D	26	GLN
1	D	28	ARG
1	D	35	LEU
1	D	37	THR
1	D	40	LEU
1	D	58	THR
1	D	76	PHE
1	D	78	THR
1	D	100	GLU
1	D	131	LEU
1	D	141	PHE
1	D	157	ARG
1	D	180	MET
1	D	196	LEU
1	D	204	GLU
1	D	222	LEU
1	D	250	GLN
1	D	267	PHE
1	D	282	ASP
1	D	405	LEU
1	D	423	ILE
1	D	427	MET
1	D	437	GLU
1	D	443	LEU
1	D	444	ASN
1	D	476	GLU

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Mol	Chain	Res	Type
1	D	481	THR
1	D	495	TYR
1	D	539	ASN
1	D	559	GLU
1	D	581	GLU
2	E	8	ASN
2	E	17	VAL
2	E	23	ASP
2	E	81	GLU
2	E	160	MET
2	E	169	ARG
2	E	222	MET
2	E	228	VAL
2	E	272	PRO
2	E	298	ARG
2	E	302	THR
2	E	303	ARG
2	E	316	GLU
2	E	325	VAL
2	E	326	HIS
2	E	357	VAL
2	E	373	THR
2	E	384	GLU
2	E	385	ASN
2	E	387	LYS
2	E	388	PRO
2	E	389	ARG
2	E	390	THR
2	E	395	ARG
2	E	402	LYS
2	E	431	ILE
2	E	435	THR
3	F	34	LYS
3	F	40	THR
3	F	49	ARG
3	F	79	ASN
3	F	110	ARG
3	F	147	THR
3	F	160	ASP
3	F	196	CYS
3	F	236	LEU
3	F	239	ARG

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Mol	Chain	Res	Type
3	F	267	TYR
3	F	282	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	289	ASN
1	A	339	GLN
1	A	514	GLN
1	A	539	ASN
1	A	557	GLN
2	B	11	GLN
2	B	351	ASN
2	B	438	ASN
3	C	16	GLN
3	C	122	GLN
3	C	242	GLN
1	D	230	ASN
1	D	271	GLN
1	D	392	ASN
1	D	402	GLN
1	D	479	HIS
1	D	539	ASN
2	E	11	GLN
2	E	443	GLN
3	F	79	ASN
3	F	125	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	ACB	H	3	4	7,8,9	1.26	0	8,10,12	1.00	0
4	DAM	G	7	4,3	4,5,6	2.09	1 (25%)	3,5,7	3.71	3 (100%)
4	FGA	H	6	4	7,8,9	2.34	2 (28%)	7,9,11	1.87	2 (28%)
4	DAM	H	7	4,3	4,5,6	2.58	2 (50%)	3,5,7	3.75	3 (100%)
4	ACB	G	3	4	7,8,9	1.57	1 (14%)	8,10,12	0.73	0
4	FGA	G	6	4	7,8,9	2.36	2 (28%)	7,9,11	1.80	2 (28%)
4	1ZN	G	5	4	23,23,24	1.29	2 (8%)	24,29,31	1.14	2 (8%)
4	1ZN	H	5	4	23,23,24	1.43	3 (13%)	24,29,31	1.14	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACB	H	3	4	-	1/9/10/12	-
4	DAM	G	7	4,3	-	0/0/4/6	-
4	FGA	H	6	4	-	1/7/8/9	-
4	DAM	H	7	4,3	-	0/0/4/6	-
4	ACB	G	3	4	-	1/9/10/12	-
4	FGA	G	6	4	-	3/7/8/9	-
4	1ZN	G	5	4	-	5/22/25/27	0/1/1/1
4	1ZN	H	5	4	-	5/22/25/27	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	6	FGA	O-C	5.18	1.38	1.22
4	G	6	FGA	O-C	5.14	1.37	1.22
4	H	7	DAM	C-CA	4.65	1.52	1.45
4	H	5	1ZN	C3-C2	3.71	1.57	1.52
4	G	7	DAM	C-CA	3.62	1.50	1.45
4	G	5	1ZN	C9-C4	2.81	1.44	1.38
4	G	3	ACB	CB-CA	2.81	1.57	1.55
4	G	5	1ZN	C3-C2	2.79	1.56	1.52
4	G	6	FGA	OXT-C	-2.56	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	5	1ZN	C9-C4	2.56	1.44	1.38
4	H	6	FGA	OXT-C	-2.44	1.22	1.30
4	H	5	1ZN	C18-CA	-2.13	1.53	1.55
4	H	7	DAM	CM-N	2.05	1.49	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	7	DAM	CM-N-CA	-4.42	116.72	123.45
4	G	7	DAM	CM-N-CA	-4.33	116.86	123.45
4	H	7	DAM	O-C-CA	-4.19	119.84	125.22
4	G	7	DAM	O-C-CA	-4.13	119.92	125.22
4	G	5	1ZN	CA-C18-C	-3.47	106.43	110.72
4	H	6	FGA	OXT-C-CA	3.43	125.06	113.38
4	G	6	FGA	OXT-C-CA	3.29	124.60	113.38
4	H	5	1ZN	CA-C18-C	-3.27	106.67	110.72
4	H	6	FGA	O-C-CA	-3.20	110.84	122.14
4	G	6	FGA	O-C-CA	-3.12	111.14	122.14
4	G	7	DAM	CB-CA-N	-2.32	120.28	125.91
4	G	5	1ZN	CA-C16-C15	-2.31	120.05	123.59
4	H	7	DAM	CB-CA-N	-2.24	120.49	125.91

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	5	1ZN	C12-C13-C15-C16
4	G	5	1ZN	C14-C13-C15-C16
4	H	5	1ZN	C12-C13-C15-C16
4	H	5	1ZN	C14-C13-C15-C16
4	G	6	FGA	CA-CB-CG-CD
4	H	6	FGA	CA-CB-CG-CD
4	H	5	1ZN	C2-C3-C4-C5
4	G	5	1ZN	C2-C3-C4-C5
4	H	5	1ZN	C2-C3-C4-C9
4	G	5	1ZN	C2-C3-C4-C9
4	G	3	ACB	CA-CB-CG-OD1
4	H	3	ACB	CA-CB-CG-OD1
4	G	5	1ZN	C10-C2-C3-C4
4	H	5	1ZN	C10-C2-C3-C4
4	G	6	FGA	O-C-CA-N
4	G	6	FGA	OXT-C-CA-N

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	7	DAM	2	0
4	H	7	DAM	1	0
4	G	6	FGA	1	0
4	H	5	1ZN	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	582/582 (100%)	0.60	77 (13%) 3 2	53, 104, 164, 173	0
1	D	582/582 (100%)	0.80	87 (14%) 2 1	48, 100, 173, 188	0
2	B	421/447 (94%)	0.18	15 (3%) 42 37	38, 67, 115, 131	0
2	E	421/447 (94%)	0.06	8 (1%) 66 64	34, 60, 111, 133	0
3	C	288/309 (93%)	0.18	4 (1%) 75 74	60, 88, 119, 154	0
3	F	288/309 (93%)	0.46	20 (6%) 16 12	75, 99, 129, 157	0
4	G	2/7 (28%)	0.88	0 100 100	95, 95, 95, 117	0
4	H	2/7 (28%)	0.23	0 100 100	108, 108, 108, 117	0
All	All	2586/2690 (96%)	0.43	211 (8%) 11 8	34, 88, 161, 188	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	348	VAL	6.8
1	D	551	LEU	6.8
1	A	511	VAL	6.8
1	D	548	GLY	6.4
1	D	556	LEU	6.2
1	A	589	ALA	6.1
1	A	588	LEU	5.9
1	D	567	LEU	5.3
1	D	549	PRO	5.2
1	D	512	CYS	5.2
1	D	515	ASP	5.1
2	B	446	VAL	5.0
1	A	587	SER	4.8
1	D	547	ILE	4.8
1	A	395	ILE	4.7
1	D	580	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	368	LEU	4.7
1	A	481	THR	4.6
2	E	148	THR	4.6
1	A	388	LEU	4.5
1	D	345	LEU	4.5
1	D	429	LEU	4.4
1	A	512	CYS	4.4
1	D	518	THR	4.4
1	D	560	VAL	4.4
1	D	553	ASN	4.4
1	A	586	LEU	4.4
1	D	526	LEU	4.3
1	A	473	PHE	4.3
3	F	170	LEU	4.3
1	A	352	LEU	4.3
1	D	541	ALA	4.2
1	D	517	THR	4.2
1	A	466	LEU	4.1
1	A	477	TRP	4.0
3	F	39	LEU	4.0
1	D	550	ILE	3.9
1	A	544	LEU	3.9
1	A	349	ILE	3.9
1	D	400	LEU	3.9
1	D	390	CYS	3.9
1	D	525	VAL	3.8
1	D	352	LEU	3.7
1	A	431	ALA	3.7
1	A	508	LEU	3.7
3	F	45	VAL	3.7
1	A	480	ALA	3.6
1	D	505	ILE	3.6
1	D	516	ILE	3.6
1	A	556	LEU	3.6
1	A	564	LEU	3.6
2	B	265	HIS	3.5
1	A	355	ILE	3.5
1	D	344	ALA	3.5
1	D	509	SER	3.5
3	F	152	TYR	3.5
3	F	157	ALA	3.5
1	A	505	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	331	LYS	3.4
1	D	554	SER	3.4
1	D	387	ASN	3.4
3	F	158	LEU	3.4
1	D	562	PRO	3.4
1	A	482	ILE	3.4
1	A	560	VAL	3.4
1	D	347	SER	3.4
3	F	28	VAL	3.4
3	F	238	SER	3.4
1	D	365	LEU	3.3
1	A	469	LEU	3.3
1	D	394	VAL	3.3
1	D	445	SER	3.3
1	D	583	LEU	3.3
1	D	395	ILE	3.3
3	F	180	ILE	3.3
1	D	441	GLU	3.3
1	D	544	LEU	3.3
3	F	146	PHE	3.2
1	D	589	ALA	3.2
1	D	327	LEU	3.2
2	B	264	ARG	3.2
1	D	586	LEU	3.2
1	A	443	LEU	3.1
1	D	349	ILE	3.1
1	D	529	ALA	3.0
1	A	440	ASP	3.0
1	A	479	HIS	3.0
1	A	549	PRO	3.0
2	B	134	TYR	3.0
3	F	225	SER	3.0
1	A	550	ILE	3.0
1	A	369	PHE	3.0
1	D	306	VAL	3.0
1	D	302	ALA	2.9
1	D	399	GLN	2.9
3	C	91	TYR	2.9
2	B	155	PRO	2.8
1	A	551	LEU	2.8
2	B	65	SER	2.8
2	B	131	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	522	LEU	2.8
1	D	568	THR	2.8
1	A	470	VAL	2.8
1	A	516	ILE	2.8
1	D	563	ILE	2.7
2	B	389	ARG	2.7
1	D	304	HIS	2.7
1	D	584	THR	2.7
2	E	149	VAL	2.7
1	A	270	LEU	2.7
1	D	402	GLN	2.7
1	D	511	VAL	2.7
1	A	439	PHE	2.7
1	D	454	HIS	2.7
2	E	65	SER	2.6
1	A	402	GLN	2.6
3	F	229	ASN	2.6
3	F	198	LEU	2.6
1	A	274	VAL	2.6
1	A	520	HIS	2.6
1	A	356	LEU	2.6
3	F	278	LEU	2.6
1	D	528	MET	2.6
1	D	362	ILE	2.6
1	A	401	SER	2.6
1	D	588	LEU	2.5
1	A	561	LYS	2.5
1	D	447	CYS	2.5
1	A	264	ALA	2.5
1	D	557	GLN	2.5
1	A	389	ASP	2.5
1	A	358	LYS	2.5
1	A	444	ASN	2.5
1	A	313	LEU	2.5
1	D	545	GLN	2.5
2	E	150	THR	2.5
1	A	521	MET	2.5
1	A	478	ALA	2.5
1	A	385	ILE	2.5
2	B	386	ASN	2.5
1	D	356	LEU	2.5
1	A	525	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	513	GLY	2.4
1	A	540	VAL	2.4
1	D	540	VAL	2.4
1	A	373	LEU	2.4
2	B	136	LEU	2.4
2	E	151	THR	2.4
1	A	346	ALA	2.4
3	C	216	ALA	2.4
1	A	433	GLN	2.4
1	D	372	GLN	2.4
1	A	547	ILE	2.4
1	D	527	ARG	2.4
1	A	504	CYS	2.4
1	A	438	PHE	2.3
1	D	521	MET	2.3
1	A	396	GLY	2.3
2	E	147	THR	2.3
1	D	404	LEU	2.3
1	D	538	PHE	2.3
1	D	364	HIS	2.3
1	D	431	ALA	2.3
1	D	565	GLU	2.3
3	F	34	LYS	2.3
1	D	569	GLN	2.3
1	A	240	LEU	2.3
1	A	405	LEU	2.3
2	B	267	LYS	2.3
1	D	346	ALA	2.3
1	D	489	MET	2.3
3	F	177	LEU	2.3
1	D	343	SER	2.3
2	B	443	GLN	2.3
1	D	334	VAL	2.3
1	A	447	CYS	2.2
1	D	305	LYS	2.2
1	D	432	GLY	2.2
1	D	350	MET	2.2
1	A	548	GLY	2.2
3	F	140	ALA	2.2
1	D	449	ALA	2.2
1	A	472	LYS	2.2
2	E	265	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	274	VAL	2.2
1	A	559	GLU	2.2
3	F	136	LYS	2.2
1	A	578	PHE	2.2
2	B	127	ARG	2.2
1	D	564	LEU	2.2
1	D	578	PHE	2.2
2	B	59	GLN	2.2
1	A	517	THR	2.1
2	B	149	VAL	2.1
1	A	292	LYS	2.1
1	A	579	ALA	2.1
3	C	58	VAL	2.1
1	A	263	VAL	2.1
1	A	484	PRO	2.1
1	D	444	ASN	2.1
3	F	164	PHE	2.1
1	A	322	ILE	2.0
1	D	388	LEU	2.0
3	C	8	LYS	2.0
1	A	345	LEU	2.0
1	A	487	LEU	2.0
1	A	583	LEU	2.0
3	F	23	LEU	2.0
1	A	268	THR	2.0
1	D	367	PRO	2.0
2	E	258	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FGA	H	6	9/10	0.84	0.23	102,111,118,118	0
4	FGA	G	6	9/10	0.85	0.35	100,101,106,107	0
4	ACB	H	3	9/10	0.89	0.21	108,111,113,113	0
4	1ZN	H	5	23/24	0.90	0.28	106,109,113,115	0
4	1ZN	G	5	23/24	0.92	0.33	99,102,106,107	0
4	DAL	H	1	5/6	0.94	0.17	108,108,110,112	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DAM	H	7	6/7	0.94	0.12	112,113,116,116	0
4	DAM	G	7	6/7	0.95	0.09	99,101,102,104	0
4	ACB	G	3	9/10	0.97	0.23	93,95,102,104	0
4	DAL	G	1	5/6	0.97	0.17	92,94,96,98	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MN	F	511	1/1	0.96	0.19	82,82,82,82	0
5	MN	C	502	1/1	0.98	0.12	69,69,69,69	0
5	MN	F	512	1/1	0.98	0.10	91,91,91,91	0
5	MN	C	501	1/1	0.99	0.19	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.