



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:20 PM UTC

PDB ID : 3DW8 / pdb_00003dw8
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

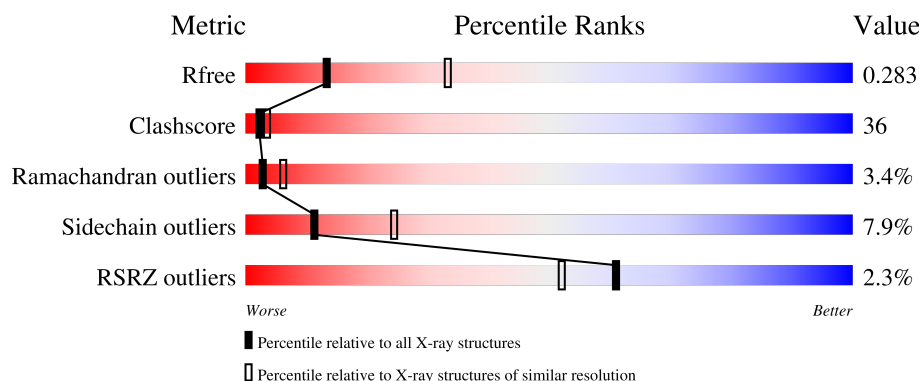
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	582	 3% 35% 54% 10%
1	D	582	 6% 41% 48% 10%
2	B	447	 46% 41% 7% 6%
2	E	447	 52% 35% 6% 6%
3	C	309	 2% 48% 40% 6% 7%

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Mol	Chain	Length	Quality of chain
3	F	309	% 36% 50% 7% 7%
4	G	7	43% 14% 43%
4	H	7	43% 29% 14% 14%

2 Entry composition

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			

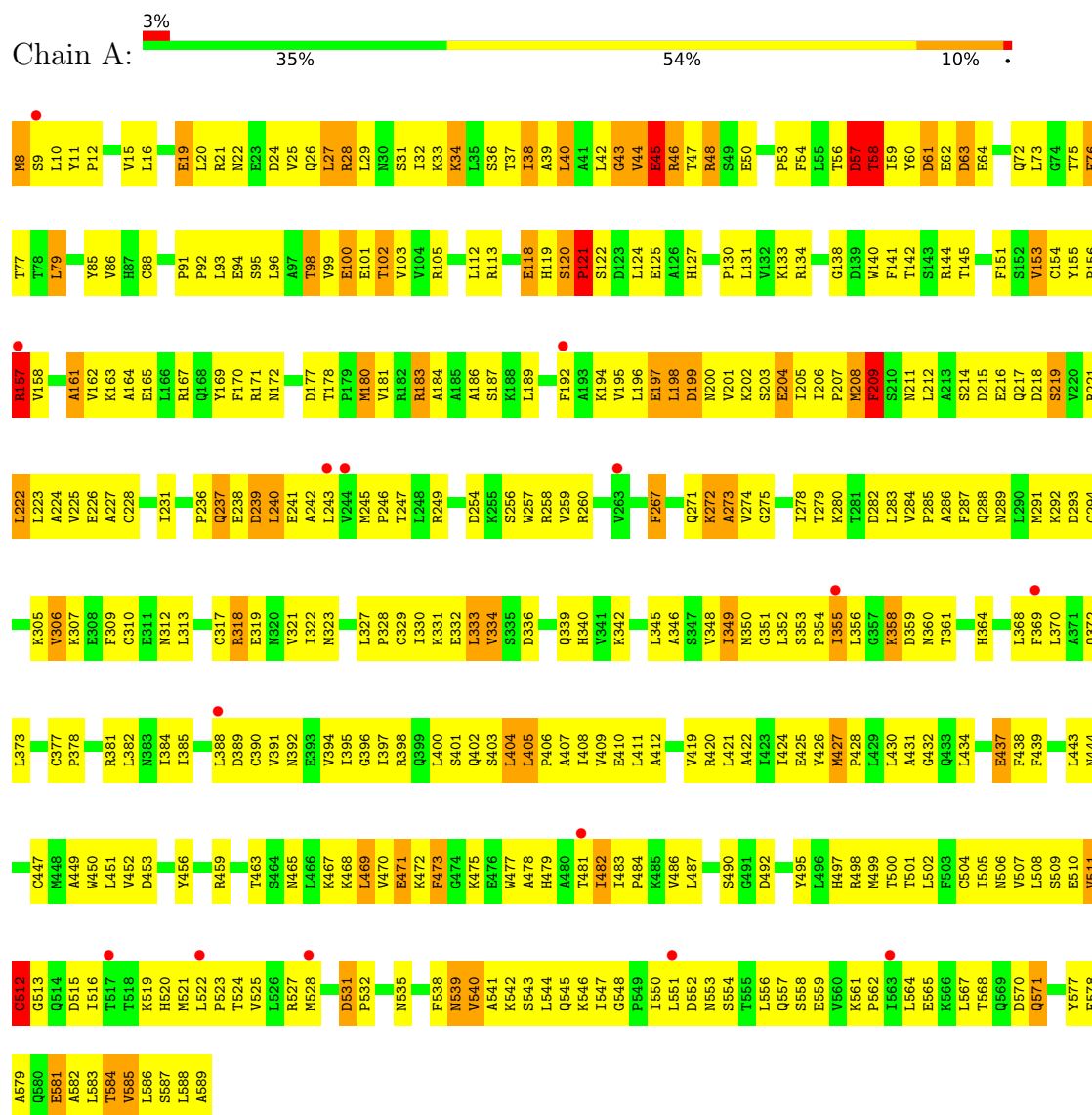
- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

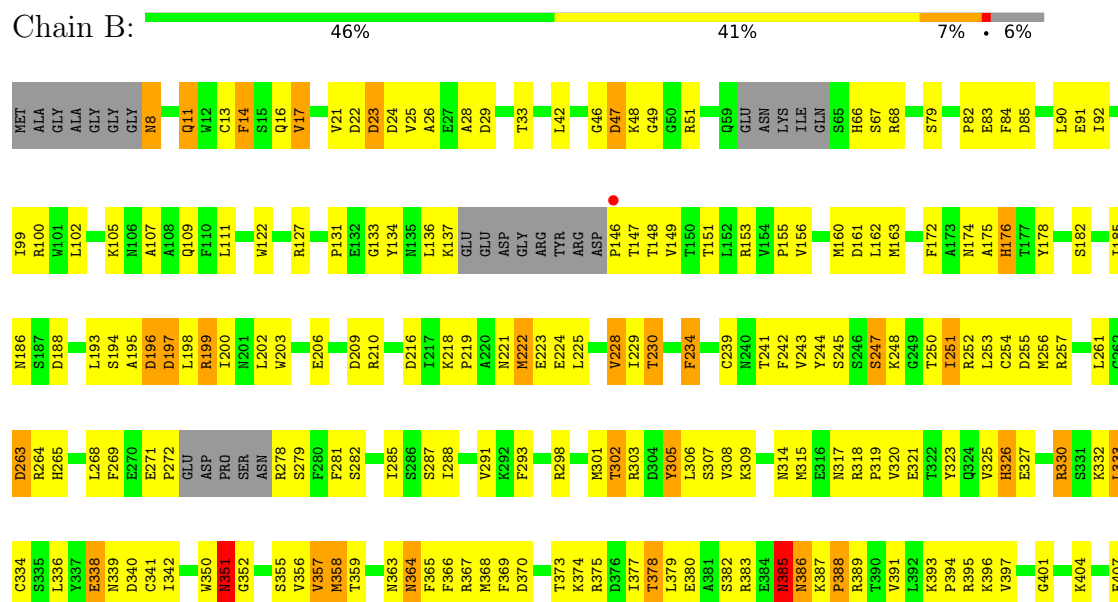
3 Residue-property plots

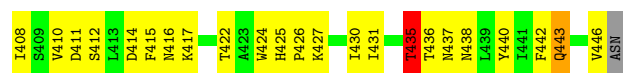
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



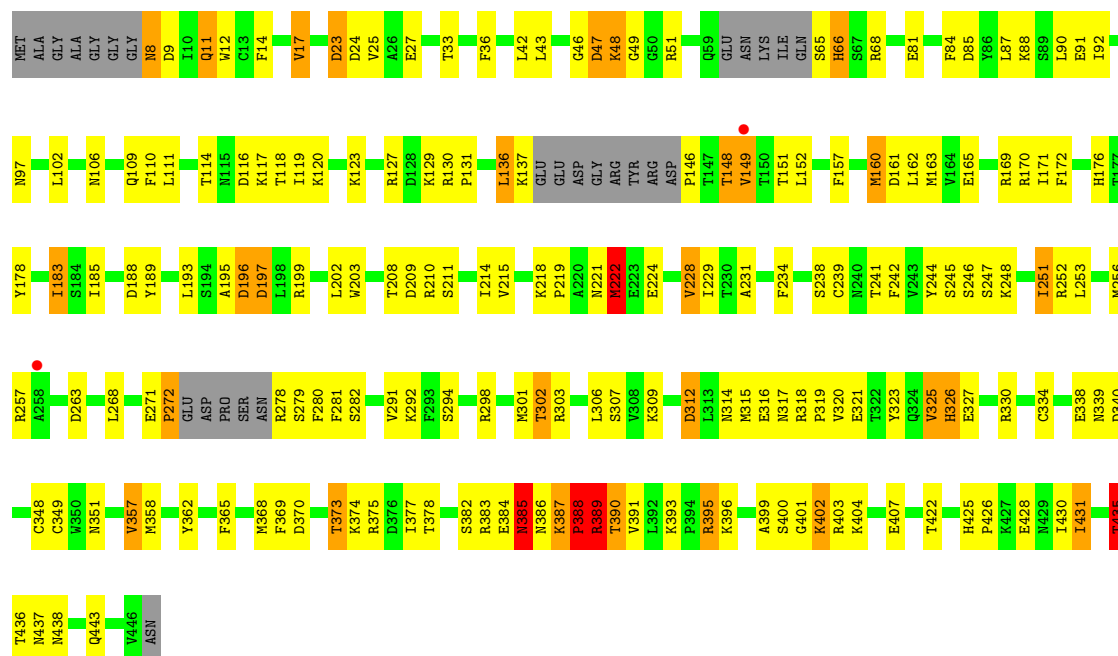
- Molecule 1: Serine/threonine-protein phosphatase 2A 65 kDa regulatory subunit A alpha isoform





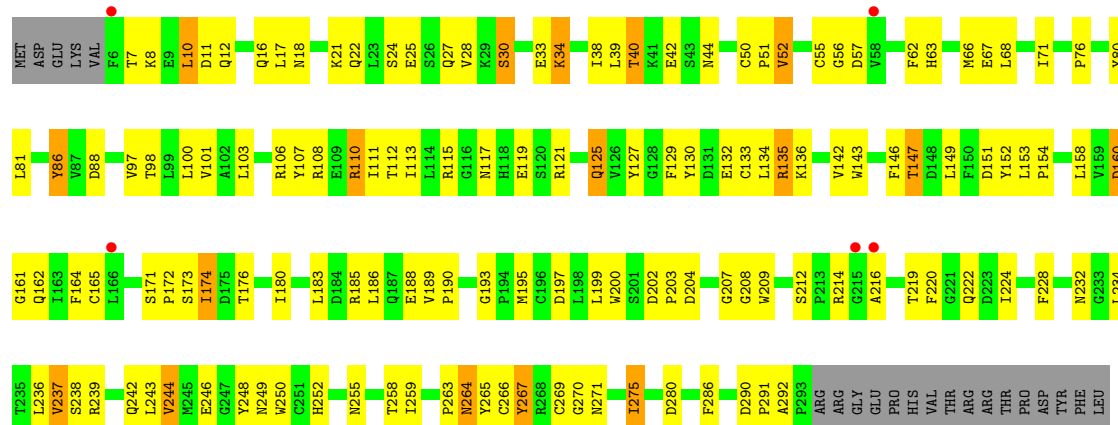
- Molecule 2: Serine/threonine-protein phosphatase 2A 55 kDa regulatory subunit B alpha isoform

Chain E: 52% 35% 6% 6%



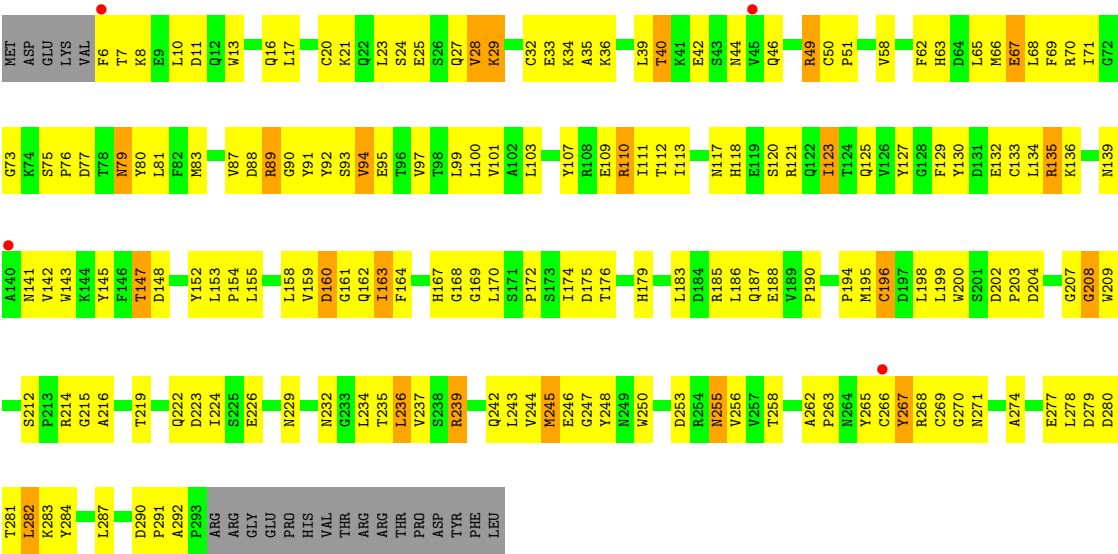
- Molecule 3: Serine/threonine-protein phosphatase 2A catalytic subunit alpha isoform

Chain C: 48% 40% 6% 7%



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

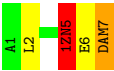
Chain F: 36% 50% 7% 7%



● Molecule 4: microcystin LR



● Molecule 4: microcystin LR



4 Data and refinement statistics

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) 99.2 (49.63-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.91Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.285 0.227 , 0.283	Depositor DCC
R_{free} test set	4180 reflections (4.96%)	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)	0.33 , 74.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for -h-2*1,-k,l	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	1/4609 (0.0%)	1.03	23/6256 (0.4%)
1	D	0.56	1/4609 (0.0%)	1.04	35/6256 (0.6%)
2	B	0.65	0/3501	1.08	22/4730 (0.5%)
2	E	0.69	0/3500	1.11	21/4728 (0.4%)
3	C	0.49	0/2379	0.98	8/3227 (0.2%)
3	F	0.45	0/2379	0.98	9/3227 (0.3%)
4	G	0.44	0/17	0.57	0/19
4	H	0.41	0/17	0.64	0/19
All	All	0.58	2/21011 (0.0%)	1.04	118/28462 (0.4%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	MET	SD-CE	8.85	2.01	1.79
1	D	180	MET	SD-CE	6.35	1.95	1.79

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	48	LYS	N-CA-C	-10.59	99.75	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	48	LYS	N-CA-C	-9.81	100.72	112.89
1	A	47	THR	N-CA-C	-9.75	100.61	111.14
1	D	540	VAL	N-CA-C	-9.30	102.84	111.67
1	D	45	GLU	N-CA-C	-8.06	103.04	113.12
1	A	209	PHE	N-CA-C	-8.04	102.73	112.54
1	A	540	VAL	N-CA-C	-7.95	104.98	111.81
1	A	471	GLU	N-CA-C	-7.64	103.84	113.01
1	D	44	VAL	N-CA-C	-7.48	93.79	109.34
1	D	249	ARG	N-CA-C	-7.27	103.29	111.14
2	E	307	SER	N-CA-C	7.27	119.97	109.14
1	D	471	GLU	N-CA-C	-7.23	104.33	113.01
2	E	47	ASP	N-CA-C	7.19	121.57	110.42
1	A	118	GLU	N-CA-C	-6.99	102.84	113.89
3	C	264	ASN	N-CA-C	-6.93	102.36	111.02
3	F	127	TYR	N-CA-C	6.93	120.62	112.72
3	C	127	TYR	N-CA-C	6.76	120.84	112.59
2	B	176	HIS	N-CA-C	6.71	119.35	108.41
2	E	351	ASN	N-CA-C	-6.65	101.76	110.53
2	E	176	HIS	N-CA-C	6.58	119.13	108.34
1	A	38	ILE	N-CA-C	-6.57	105.34	111.45
1	D	118	GLU	N-CA-C	-6.57	103.51	113.89
1	A	334	VAL	N-CA-C	-6.54	106.60	111.90
1	D	14	ALA	N-CA-C	-6.53	104.25	111.82
2	B	146	PRO	N-CA-CB	6.49	110.13	103.00
1	D	581	GLU	N-CA-C	-6.47	105.39	113.28
2	E	146	PRO	N-CA-CB	6.44	110.08	103.00
2	E	280	PHE	N-CA-C	-6.40	104.23	111.14
3	F	255	ASN	N-CA-C	-6.35	105.69	113.50
2	B	358	MET	N-CA-C	6.32	120.00	109.95
2	B	174	ASN	N-CA-C	6.32	120.30	112.47
2	B	307	SER	N-CA-C	6.27	118.71	109.24
2	B	197	ASP	N-CA-C	-6.25	104.36	112.23
1	A	267	PHE	N-CA-C	6.21	117.74	110.97
1	D	580	GLN	N-CA-C	-6.18	106.28	113.88
2	E	84	PHE	N-CA-C	6.17	119.24	109.50
1	A	531	ASP	CA-C-N	6.11	125.83	119.05
1	A	531	ASP	C-N-CA	6.11	125.83	119.05
1	D	531	ASP	CA-C-N	6.07	125.96	119.28
1	D	531	ASP	C-N-CA	6.07	125.96	119.28
1	D	171	ARG	N-CA-C	-6.06	104.58	111.07
1	D	283	LEU	N-CA-C	6.06	117.88	111.28
2	B	195	ALA	N-CA-C	5.99	119.25	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	334	VAL	N-CA-C	-5.99	106.97	112.96
1	D	490	SER	N-CA-C	-5.96	105.98	113.20
2	E	211	SER	N-CA-C	-5.96	100.01	109.07
2	E	148	THR	N-CA-C	-5.94	104.64	112.72
2	B	305	TYR	N-CA-C	5.93	118.23	111.11
1	A	161	ALA	N-CA-C	-5.93	104.72	111.07
1	A	340	HIS	N-CA-C	-5.93	105.14	112.90
1	A	142	THR	N-CA-C	-5.91	104.47	111.03
2	E	195	ALA	N-CA-C	5.89	119.08	109.24
2	E	238	SER	N-CA-C	5.83	117.95	108.63
1	A	581	GLU	N-CA-C	-5.80	105.97	113.16
2	B	196	ASP	CB-CA-C	-5.79	100.78	114.16
1	D	120	SER	N-CA-C	-5.79	102.29	109.64
1	A	45	GLU	N-CA-C	-5.78	106.58	113.97
3	C	80	TYR	N-CA-C	5.70	118.69	109.40
1	A	27	LEU	N-CA-C	-5.70	104.99	111.14
2	B	85	ASP	N-CA-C	-5.69	95.67	107.67
1	D	331	LYS	N-CA-C	-5.68	105.17	111.36
1	D	42	LEU	N-CA-C	-5.64	103.19	110.19
3	C	52	VAL	CB-CA-C	-5.63	103.13	111.80
2	E	438	ASN	N-CA-C	5.62	118.05	109.95
2	B	263	ASP	N-CA-C	-5.62	107.67	114.75
1	A	183	ARG	N-CA-C	-5.60	105.08	111.07
2	E	294	SER	N-CA-C	-5.59	103.00	110.55
1	A	46	ARG	N-CA-C	-5.58	105.59	112.90
1	D	157	ARG	N-CA-C	5.53	119.51	112.87
1	D	38	ILE	N-CA-C	-5.52	105.47	110.82
1	D	239	ASP	N-CA-C	5.51	119.27	112.54
3	F	80	TYR	N-CA-C	5.51	118.54	109.72
2	E	183	ILE	N-CA-C	-5.51	100.72	108.27
1	D	275	GLY	CA-C-N	5.46	125.29	119.28
1	D	275	GLY	C-N-CA	5.46	125.29	119.28
2	B	351	ASN	N-CA-C	-5.45	101.66	110.32
1	D	116	SER	N-CA-C	-5.45	105.50	111.82
3	F	262	ALA	CA-C-N	5.44	125.61	119.90
3	F	262	ALA	C-N-CA	5.44	125.61	119.90
1	A	120	SER	N-CA-C	-5.41	102.77	109.64
1	D	10	LEU	N-CA-C	5.41	117.18	111.28
2	E	196	ASP	CB-CA-C	-5.40	101.69	114.16
1	D	82	GLY	CA-C-N	5.36	126.54	119.84
1	D	82	GLY	C-N-CA	5.36	126.54	119.84
1	D	579	ALA	N-CA-C	-5.35	107.77	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	326	ILE	N-CA-C	5.34	116.41	111.45
2	B	416	ASN	N-CA-C	-5.33	106.94	113.50
1	A	9	SER	N-CA-C	-5.31	101.87	110.32
1	D	573	VAL	N-CA-C	5.29	115.73	110.23
2	B	254	CYS	N-CA-C	5.28	118.10	109.59
2	E	118	THR	N-CA-C	5.26	118.00	108.69
2	E	435	THR	N-CA-C	-5.25	102.00	110.14
1	D	351	GLY	N-CA-C	-5.24	107.12	115.66
2	E	312	ASP	N-CA-C	-5.22	100.22	108.73
2	B	199	ARG	N-CA-C	5.22	117.31	109.23
2	B	291	VAL	CB-CA-C	-5.21	102.04	110.28
1	A	275	GLY	CA-C-N	5.21	126.36	119.84
1	A	275	GLY	C-N-CA	5.21	126.36	119.84
1	D	399	GLN	N-CA-C	-5.20	106.63	112.87
2	B	397	VAL	N-CA-C	5.20	115.39	108.11
2	B	435	THR	N-CA-C	-5.19	102.78	110.46
3	F	67	GLU	N-CA-C	-5.19	105.62	111.28
1	A	284	VAL	CB-CA-C	-5.18	108.86	114.35
2	E	349	CYS	N-CA-C	5.16	116.83	109.14
2	B	308	VAL	N-CA-C	-5.16	100.95	108.17
1	D	195	VAL	N-CA-C	-5.15	108.11	113.10
3	C	255	ASN	N-CA-C	-5.14	106.86	113.23
3	F	94	VAL	N-CA-C	5.14	115.28	110.30
2	B	438	ASN	N-CA-C	5.11	118.00	110.59
1	D	536	VAL	N-CA-C	-5.10	107.45	113.42
3	C	193	GLY	CA-C-N	5.07	124.24	118.97
3	C	193	GLY	C-N-CA	5.07	124.24	118.97
2	E	197	ASP	N-CA-C	-5.05	105.86	112.23
3	F	163	ILE	N-CA-C	5.05	115.96	108.23
1	D	151	PHE	N-CA-C	5.05	116.63	111.03
3	F	83	MET	N-CA-C	5.04	118.26	112.57
2	B	16	GLN	N-CA-C	5.03	116.83	109.24
3	C	86	TYR	N-CA-C	-5.03	107.32	113.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

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

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	4535	0	4642	436	0
1	D	4535	0	4642	395	0
2	B	3429	0	3323	220	0
2	E	3428	0	3322	190	0
3	C	2322	0	2223	116	0
3	F	2322	0	2223	172	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	1486	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 36.

All (1486) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:323:MET:HE2	1:A:356:LEU:HD13	1.57	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
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:197:GLU:CD	1:A:197:GLU:H	1.88	0.82
1:A:490:SER:HB2	1:A:528:MET:HE3	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:127:ARG:CZ	2:E:163:MET:HE1	2.13	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: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
1:A:571:GLN:CD	1:A:571:GLN:H	1.93	0.77
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
1:A:45:GLU:H	1:A:45:GLU:CD	1.91	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:A:127:HIS:C	1:A:130:PRO:HD2	2.11	0.76
2:B:358:MET:HE3	2:B:366:PHE:CD2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:E:202:LEU:HD22	2:E:256:MET:HE1	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:559:GLU:C	1:A:562:PRO:HD2	2.12	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
2:B:358:MET:HE3	2:B:366:PHE:HD2	1.52	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: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
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:202:LEU:HD22	2:B:256:MET:HE1	1.70	0.72
2:B:373:THR:O	2:B:374:LYS:HB2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:427:MET:HE3	1:A:427:MET:HA	1.71	0.71
2:B:14:PHE:CD1	2:B:14:PHE:C	2.68	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
2:E:222:MET:HA	2:E:222:MET:HE3	1.73	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:D:427:MET:HE3	1:D:427:MET:HA	1.71	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
3:C:243:LEU:HD11	3:C:271:ASN:CG	2.17	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:490:SER:CB	1:D:528:MET:HE2	2.22	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
1:D:127:HIS:C	1:D:130:PRO:HD2	2.20	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:E:127:ARG:HH21	2:E:160:MET:HE1	1.59	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
3:C:266:CYS:C	3:C:267:TYR:HD1	2.03	0.66
1:A:427:MET:N	1:A:428:PRO:HD2	2.11	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:D:490:SER:HB2	1:D:528:MET:HE2	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
1:D:59:ILE:HG22	1:D:59:ILE:O	1.97	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
2:B:336:LEU:HD21	2:B:415:PHE:CE2	2.33	0.63
3:F:95:GLU:CD	3:F:95:GLU:H	2.06	0.63
1:A:391:VAL:HG12	1:A:391:VAL:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:127:ARG:NH2	2:B:163:MET:HE1	2.14	0.63
2:E:163:MET:HE3	2:E:165:GLU:CG	2.28	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: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:A:211:ASN:HA	1:D:8:MET:HE3	1.81	0.62
1:D:57:ASP:HB3	2:E:129:LYS:NZ	2.14	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:483:ILE:O	1:D:487:LEU:HG	2.00	0.61
2:E:163:MET:HE3	2:E:165:GLU:CD	2.24	0.61
2:E:403:ARG:C	2:E:404:LYS:HG3	2.26	0.61
1:A:400:LEU:O	1:A:404:LEU:HD23	2.00	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:127:HIS:O	1:A:130:PRO:HD2	1.99	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
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:131:LEU:HD12	1:D:131:LEU:C	2.25	0.61
1:D:227:ALA:O	1:D:231:ILE:HG13	2.00	0.61
2:E:222:MET:HA	2:E:222:MET:CE	2.30	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
3:F:266:CYS:C	3:F:267:TYR:CD1	2.79	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:D:505:ILE:HG23	1:D:521:MET:HE3	1.84	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:HE3	1:D:588:LEU:O	2.01	0.60
1:D:561:LYS:HB2	1:D:588:LEU:HD13	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:12:TRP:HE1	2:E:368:MET:HE2	1.67	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
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
2:E:85:ASP:CG	2:E:88:LYS:HB2	2.27	0.59
1:A:405:LEU:HB2	1:A:406:PRO:CD	2.31	0.59
1:D:353:SER:C	1:D:355:ILE:H	2.10	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
1:A:208:MET:HB2	1:A:208:MET:HE3	1.84	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
1:A:282:ASP:C	1:A:285:PRO:HD2	2.28	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
3:F:212:SER:C	3:F:214:ARG:H	2.09	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:14:PHE:C	2:B:14:PHE:HD1	2.10	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
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:134:LEU:C	3:F:136:LYS:H	2.11	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:271:GLN:C	1:D:273:ALA:H	2.12	0.58
1:D:490:SER:HB3	1:D:528:MET:HE2	1.85	0.58
2:E:130:ARG:HD3	2:E:160:MET:HE3	1.84	0.58
2:E:291:VAL:C	2:E:292:LYS:HG2	2.28	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
1:A:349:ILE:HG23	1:A:350:MET:HE3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:200:ASN:HA	1:A:203:SER:HG	1.68	0.57
1:A:307:LYS:HD2	1:A:348:VAL:HB	1.85	0.57
1:A:350:MET:HE1	1:A:369:PHE:HB2	1.86	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
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:A:45:GLU:CD	1:A:45:GLU:N	2.63	0.57
2:B:8:ASN:ND2	2:B:375:ARG:HH21	2.03	0.57
1:D:538:PHE:CD1	1:D:538:PHE:C	2.83	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:189:LEU:HD11	1:D:208:MET:HE3	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:332:GLU:C	1:D:334:VAL:H	2.13	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
1:A:57:ASP:O	1:A:58:THR:C	2.48	0.56
3:C:62:PHE:C	3:C:62:PHE:CD1	2.84	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
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
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:A:583:LEU:C	1:A:585:VAL:H	2.14	0.55
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
1:A:505:ILE:HG23	1:A:521:MET:HE3	1.88	0.55
2:B:8:ASN:ND2	2:B:375:ARG:NH2	2.54	0.55
2:B:301:MET:HE1	2:B:357:VAL:HG22	1.88	0.55
2:B:378:THR:O	2:B:379:LEU:HD23	2.07	0.55
1:D:564:LEU:HB3	1:D:583:LEU:HD21	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
1:D:392:ASN:CG	1:D:397:ILE:HG12	2.32	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
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
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
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
1:D:583:LEU:C	1:D:585:VAL:H	2.16	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
1:A:587:SER:C	1:A:589:ALA:H	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:MET:CE	2:B:366:PHE:CD2	2.89	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
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
2:E:358:MET:HE1	2:E:431:ILE:HD13	1.90	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
1:D:398:ARG:HG3	1:D:399:GLN:N	2.22	0.54
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
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
3:C:266:CYS:C	3:C:267:TYR:CD1	2.86	0.54
2:E:170:ARG:HG3	2:E:208:THR:CG2	2.38	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
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:349:ILE:C	1:D:350:MET:HE2	2.34	0.53
1:A:208:MET:CB	1:A:208:MET:HE3	2.39	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:D:524:THR:HG22	1:D:528:MET:HE3	1.91	0.53
3:F:266:CYS:C	3:F:267:TYR:HD1	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:SER:C	1:A:355:ILE:H	2.16	0.53
1:A:397:ILE:HG22	1:A:434:LEU:HD23	1.90	0.53
1:A:472:LYS:HG3	1:A:472:LYS:O	2.07	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
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
1:D:499:MET:HE1	3:F:77:ASP:O	2.08	0.53
2:E:9:ASP:CG	2:E:375:ARG:HH21	2.17	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
2:B:84:PHE:CE1	2:B:91:GLU:HB2	2.44	0.53
3:C:134:LEU:C	3:C:136:LYS:H	2.15	0.53
1:D:473:PHE:HB3	1:D:477:TRP:CE3	2.44	0.53
1:A:28:ARG:HH22	1:A:62:GLU:CD	2.17	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:D:402:GLN:C	1:D:405:LEU:HD11	2.34	0.53
3:F:155:LEU:HD21	3:F:195:MET:HE2	1.90	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
3:F:243:LEU:HD23	3:F:243:LEU:C	2.34	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
1:A:470:VAL:C	1:A:472:LYS:H	2.15	0.52
2:B:377:ILE:HG22	2:B:378:THR:N	2.24	0.52
1:D:57:ASP:O	1:D:58:THR:C	2.50	0.52
1:D:59:ILE:HG12	1:D:96:LEU:CD2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:443:LEU:H	1:D:443:LEU:CD1	2.19	0.52
1:A:470:VAL:C	1:A:472:LYS:N	2.68	0.52
2:E:27:GLU:OE1	2:E:48:LYS:NZ	2.26	0.52
3:F:265:TYR:O	3:F:266:CYS:HB2	2.08	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:E:12:TRP:NE1	2:E:368:MET:HE2	2.24	0.52
1:A:8:MET:SD	1:A:8:MET:C	2.93	0.52
1:D:58:THR:OG1	1:D:59:ILE:N	2.39	0.52
1:D:456:TYR:CD1	1:D:456:TYR:C	2.88	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
1:D:520:HIS:C	1:D:523:PRO:HD2	2.35	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:118:HIS:C	3:F:120:SER:H	2.16	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: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:66:MET:HE2	3:C:66:MET:HA	1.92	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
2:E:435:THR:O	2:E:436:THR:C	2.50	0.52
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:424:TRP:O	2:B:425:HIS:C	2.54	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
1:A:21:ARG:HG3	2:B:131:PRO:CG	2.40	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:D:141:PHE:CD1	1:D:141:PHE:C	2.89	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: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
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:301:MET:HE2	2:B:350:TRP:CE2	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:211:ASN:OD1	1:D:8:MET:HE1	2.09	0.50
1:A:330:ILE:HG23	1:A:345:LEU:HD21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:310:CYS:C	1:D:312:ASN:H	2.19	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
2:E:396:LYS:HD3	2:E:407:GLU:CD	2.37	0.50
3:F:236:LEU:HD12	3:F:250:TRP:CZ3	2.45	0.50
1:A:50:GLU:C	1:A:53:PRO:HD2	2.37	0.50
1:A:124:LEU:HD11	1:A:154:CYS:HB2	1.94	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:141:PHE:C	1:A:141:PHE:CD1	2.89	0.50
1:A:197:GLU:OE2	1:A:200:ASN:ND2	2.38	0.50
1:A:291:MET:HE3	1:A:329:CYS:CB	2.41	0.50
3:F:279:ASP:OD1	3:F:279:ASP:C	2.54	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:406:PRO:O	1:D:407:ALA:C	2.55	0.50
2:B:281:PHE:O	2:B:282:SER:C	2.55	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
2:B:351:ASN:HD22	2:B:351:ASN:C	2.18	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
1:A:349:ILE:HG23	1:A:350:MET:CE	2.42	0.49
1:A:477:TRP:CZ3	1:A:482:ILE:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:B:221:ASN:ND2	2:B:224:GLU:HG3	2.26	0.49
1:D:205:ILE:HA	1:D:208:MET:HE2	1.94	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:A:226:GLU:CD	1:A:227:ALA:N	2.70	0.49
1:D:394:VAL:HG12	1:D:394:VAL:O	2.12	0.49
3:F:6:PHE:O	3:F:7:THR:C	2.54	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
2:B:435:THR:O	2:B:436:THR:C	2.56	0.49
1:D:349:ILE:O	1:D:352:LEU:HD12	2.12	0.49
2:E:193:LEU:HD12	2:E:193:LEU:C	2.37	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:339:GLN:CD	1:A:377:CYS:HB2	2.37	0.49
1:D:352:LEU:C	1:D:354:PRO:HD2	2.37	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:A:197:GLU:CD	1:A:197:GLU:N	2.65	0.49
1:A:495:TYR:CD2	1:A:499:MET:HE2	2.47	0.49
1:D:334:VAL:CG1	1:D:372:GLN:HG2	2.43	0.49
1:D:470:VAL:C	1:D:472:LYS:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:404:LEU:HD23	1:D:404:LEU:H	1.77	0.49
1:D:465:ASN:OD1	1:D:469:LEU:HD12	2.13	0.49
1:A:180:MET:HE3	1:A:183:ARG:HH21	1.78	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:427:MET:HE1	1:D:443:LEU:HD23	1.94	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: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
1:D:448:MET:HE1	1:D:466:LEU:HD21	1.95	0.48
1:D:587:SER:C	1:D:589:ALA:H	2.21	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:271:GLN:C	1:A:273:ALA:H	2.22	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
1:A:133:LYS:HE2	1:A:169:TYR:CE1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:162:LEU:HD23	2:E:162:LEU:C	2.38	0.48
2:E:382:SER:OG	2:E:385:ASN:HB2	2.14	0.48
3:F:134:LEU:C	3:F:136:LYS:N	2.71	0.48
1:A:95:SER:O	1:A:98:THR:HB	2.14	0.48
2:B:410:VAL:C	2:B:412:SER:H	2.22	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:350:MET:C	1:D:352:LEU:H	2.20	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
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
1:A:486:VAL:O	1:A:501:THR:HG23	2.14	0.48
3:C:265:TYR:O	3:C:266:CYS:HB2	2.13	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:398:ARG:C	1:D:400:LEU:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:E:111:LEU:HD12	2:E:111:LEU:C	2.39	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
1:A:227:ALA:O	1:A:228:CYS:C	2.57	0.47
3:C:149:LEU:HD12	3:C:149:LEU:O	2.14	0.47
1:D:60:TYR:O	1:D:61:ASP:CG	2.57	0.47
1:D:303:SER:OG	1:D:333:LEU:HD13	2.15	0.47
3:F:68:LEU:C	3:F:68:LEU:HD23	2.39	0.47
3:F:110:ARG:C	3:F:111:ILE:HG13	2.39	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:368:LEU:C	1:D:370:LEU:N	2.71	0.47
2:E:377:ILE:HG22	2:E:378:THR:H	1.79	0.47
1:A:332:GLU:C	1:A:334:VAL:H	2.22	0.47
2:B:8:ASN:N	2:B:8:ASN:ND2	2.48	0.47
1:D:60:TYR:O	1:D:61:ASP:OD1	2.32	0.47
2:E:231:ALA:HB3	2:E:291:VAL:HG23	1.95	0.47
2:E:253:LEU:C	2:E:253:LEU:HD23	2.39	0.47
1:A:10:LEU:O	1:A:11:TYR:C	2.56	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:204:GLU:C	1:A:207:PRO:HD2	2.40	0.47
1:A:395:ILE:CD1	1:A:400:LEU:HD11	2.45	0.47
2:B:8:ASN:CG	2:B:375:ARG:HH21	2.22	0.47
2:B:176:HIS:ND1	2:B:196:ASP:OD1	2.48	0.47
2:B:368:MET:HE1	2:B:424:TRP:CH2	2.49	0.47
3:C:203:PRO:HB3	3:C:220:PHE:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:212:SER:HA	3:C:219:THR:HG23	1.95	0.47
1:D:58:THR:O	1:D:59:ILE:C	2.57	0.47
1:D:62:GLU:O	1:D:63:ASP:C	2.57	0.47
1:D:129:VAL:N	1:D:130:PRO:CD	2.78	0.47
1:D:282:ASP:C	1:D:285:PRO:HD2	2.40	0.47
1:D:470:VAL:C	1:D:472:LYS:N	2.72	0.47
1:D:486:VAL:O	1:D:501:THR:HG23	2.15	0.47
1:D:505:ILE:C	1:D:507:VAL:H	2.23	0.47
2:E:251:ILE:H	2:E:251:ILE:CD1	2.27	0.47
2:E:281:PHE:O	2:E:282:SER:C	2.56	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
3:C:68:LEU:HD23	3:C:68:LEU:C	2.39	0.47
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:120:SER:C	1:A:122:SER:N	2.70	0.47
1:A:151:PHE:HE2	1:A:170:PHE:HB2	1.80	0.47
1:A:439:PHE:CD1	1:A:439:PHE:C	2.93	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:398:ARG:C	1:D:400:LEU:N	2.72	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
2:B:393:LYS:O	2:B:394:PRO:C	2.58	0.47
3:C:134:LEU:O	3:C:136:LYS:N	2.47	0.47
3:C:212:SER:C	3:C:214:ARG:H	2.23	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:351:ASN:ND2	2:B:351:ASN:C	2.71	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:406:PRO:O	1:A:407:ALA:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:208:GLY:H	3:F:223:ASP:CG	2.23	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
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:189:LEU:CD1	1:D:208:MET:HE3	2.44	0.46
1:D:317:CYS:O	1:D:318:ARG:C	2.58	0.46
1:D:321:VAL:HG23	1:D:322:ILE:N	2.29	0.46
2:E:136:LEU:O	2:E:137:LYS:C	2.58	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
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
2:B:339:ASN:OD1	2:B:341:CYS:SG	2.74	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
3:F:153:LEU:O	3:F:185:ARG:HD2	2.16	0.46
1:A:348:VAL:C	1:A:350:MET:H	2.23	0.46
1:A:348:VAL:C	1:A:350:MET:N	2.72	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: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:310:CYS:C	1:A:312:ASN:H	2.23	0.46
1:A:469:LEU:HD22	1:A:477:TRP:HZ3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:193:LEU:HD12	2:B:193:LEU:C	2.40	0.46
2:B:219:PRO:HD2	2:B:222:MET:HE1	1.98	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
2:B:176:HIS:HD1	2:B:196:ASP:CG	2.23	0.46
1:D:197:GLU:H	1:D:197:GLU:CD	2.24	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
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
1:A:511:VAL:HG23	1:A:511:VAL:O	2.15	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
1:A:354:PRO:C	1:A:355:ILE:HG13	2.41	0.45
1:A:409:VAL:O	1:A:412:ALA:N	2.49	0.45
2:B:332:LYS:O	2:B:333:LEU:C	2.59	0.45
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:O	1:D:452:VAL:HG13	2.14	0.45
1:D:568:THR:HB	1:D:580:GLN:OE1	2.17	0.45
3:F:20:CYS:SG	3:F:92:TYR:CE2	3.10	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
1:A:505:ILE:C	1:A:507:VAL:N	2.74	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:349:ILE:O	1:D:350:MET:HE2	2.16	0.45
1:D:454:HIS:HB3	3:F:287:LEU:HD21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:221:ARG:O	1:A:222:LEU:C	2.59	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:332:GLU:C	1:D:334:VAL:N	2.75	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
3:F:10:LEU:O	3:F:11:ASP:C	2.59	0.45
1:A:39:ALA:HB1	1:A:79:LEU:HD22	1.99	0.45
1:A:120:SER:O	1:A:121:PRO:C	2.59	0.45
1:A:388:LEU:O	1:A:389:ASP:C	2.58	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:A:119:HIS:HB3	1:A:124:LEU:HB2	1.99	0.45
1:A:571:GLN:CD	1:A:571:GLN:N	2.64	0.45
1:D:353:SER:C	1:D:355:ILE:N	2.75	0.45
1:D:522:LEU:N	1:D:523:PRO:HD3	2.32	0.45
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:111:LEU:C	2:B:111:LEU:HD12	2.42	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
1:A:426:TYR:C	1:A:428:PRO:HD2	2.42	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
1:A:16:LEU:HB3	1:A:38:ILE:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:10:LEU:O	3:C:11:ASP:C	2.60	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:58:THR:O	1:A:59:ILE:C	2.59	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
1:D:323:MET:HE2	1:D:356:LEU:HD13	1.98	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:B:22:ASP:CG	2:B:23:ASP:N	2.74	0.44
2:E:120:LYS:HG2	2:E:171:ILE:HG12	1.99	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:520:HIS:C	1:A:523:PRO:HD2	2.43	0.44
1:A:539:ASN:HD22	1:A:539:ASN:HA	1.65	0.44
1:A:561:LYS:HE2	1:A:565:GLU:CD	2.43	0.44
1:D:44:VAL:HG12	1:D:45:GLU:OE2	2.17	0.44
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
1:D:441:GLU:C	1:D:442:LYS:HG2	2.42	0.44
2:E:327:GLU:OE2	2:E:330:ARG:HD2	2.17	0.44
3:F:35:ALA:O	3:F:36:LYS:C	2.60	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:212:LEU:C	1:A:214:SER:H	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:MET:HE3	2:B:160:MET:HB2	1.86	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: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: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:224:ALA:C	1:A:226:GLU:N	2.76	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
2:B:363:ASN:O	2:B:364:ASN:C	2.60	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
3:F:92:TYR:O	3:F:93:SER:C	2.61	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:463:THR:C	1:A:465:ASN:N	2.75	0.44
1:A:483:ILE:HD13	1:A:521:MET:SD	2.57	0.44
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:498:ARG:O	1:D:499:MET:C	2.60	0.44
3:F:158:LEU:HD11	3:F:161:GLY:C	2.42	0.44
1:A:382:LEU:CD1	1:A:411:LEU:HD13	2.47	0.44
1:D:155:TYR:O	1:D:163:LYS:NZ	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:F:198:LEU:C	3:F:199:LEU:HD12	2.42	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:25:GLU:CD	3:F:139:ASN:HD21	2.25	0.43
3:F:40:THR:HG23	3:F:152:TYR:HD2	1.81	0.43
1:A:260:ARG:HH21	1:A:293:ASP:CG	2.25	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
2:B:162:LEU:HD23	2:B:162:LEU:C	2.43	0.43
2:B:198:LEU:C	2:B:199:ARG:HG3	2.43	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
3:F:169:GLY:O	3:F:198:LEU:HA	2.18	0.43
1:A:62:GLU:O	1:A:63:ASP:C	2.61	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
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: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
2:E:370:ASP:CG	2:E:373:THR:HG22	2.43	0.43
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
1:A:209:PHE:CD1	1:A:209:PHE:C	2.96	0.43
1:A:398:ARG:C	1:A:400:LEU:H	2.26	0.43
1:A:456:TYR:CD1	1:A:456:TYR:C	2.95	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:253:LEU:C	2:B:253:LEU:HD23	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:24:ASP:OD1	1:A:24:ASP:C	2.61	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
1:D:352:LEU:O	1:D:353:SER:C	2.60	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
1:A:586:LEU:C	1:A:588:LEU:H	2.26	0.43
2:B:68:ARG:HG2	2:B:68:ARG:NH1	2.33	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
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
1:A:552:ASP:C	1:A:554:SER:N	2.76	0.43
2:B:26:ALA:HB3	2:B:29:ASP:OD2	2.19	0.43
3:C:134:LEU:C	3:C:136:LYS:N	2.73	0.43
1:D:38:ILE:O	1:D:42:LEU:CD2	2.67	0.43
1:D:120:SER:O	1:D:121:PRO:C	2.58	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
2:E:358:MET:HE1	2:E:431:ILE:HG21	2.01	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
2:B:339:ASN:O	2:B:340:ASP:HB2	2.19	0.43
3:C:208:GLY:C	3:C:224:ILE:HD11	2.43	0.43
2:E:14:PHE:CD1	2:E:14:PHE:C	2.97	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
3:C:56:GLY:HA3	3:C:259:ILE:O	2.18	0.43
1:D:321:VAL:CG2	1:D:322:ILE:N	2.81	0.43
2:E:87:LEU:H	2:E:87:LEU:CD1	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:40:THR:C	3:C:42:GLU:H	2.27	0.42
2:E:36:PHE:CE1	2:E:43:LEU:HD13	2.53	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:230:THR:HG22	2:B:245:SER:C	2.44	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:388:LEU:C	1:D:390:CYS:N	2.76	0.42
1:D:437:GLU:HG2	1:D:438:PHE:N	2.34	0.42
2:E:246:SER:C	2:E:248:LYS:H	2.27	0.42
2:E:368:MET:HE3	2:E:368:MET:HB3	1.88	0.42
1:A:286:ALA:C	1:A:288:GLN:N	2.77	0.42
1:A:403:SER:C	1:A:405:LEU:HD12	2.44	0.42
1:A:538:PHE:CD1	1:A:538:PHE:C	2.97	0.42
2:B:14:PHE:HA	2:B:442:PHE:HD1	1.83	0.42
2:B:209:ASP:C	2:B:210:ARG:HG3	2.45	0.42
3:C:121:ARG:HG2	3:C:147:THR:CB	2.49	0.42
1:D:287:PHE:CD1	1:D:291:MET:HE2	2.54	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
2:B:21:VAL:CA	2:B:383:ARG:NH1	2.68	0.42
1:D:505:ILE:C	1:D:507:VAL:N	2.76	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
3:F:253:ASP:O	3:F:253:ASP:CG	2.63	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
1:A:388:LEU:C	1:A:390:CYS:N	2.75	0.42
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:489:MET:HB2	1:D:501:THR:OG1	2.19	0.42
3:F:172:PRO:HG3	3:F:209:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:NH1	2:B:133:GLY:N	2.68	0.42
1:A:239:ASP:O	1:A:240:LEU:C	2.63	0.42
1:A:465:ASN:O	1:A:469:LEU:HB2	2.19	0.42
1:D:180:MET:HE3	1:D:183:ARG:HH21	1.85	0.42
1:D:186:ALA:CA	1:D:212:LEU:HD13	2.49	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: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
2:B:21:VAL:HG22	2:B:21:VAL:O	2.18	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
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:63:ASP:O	1:A:64:GLU:C	2.62	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
1:A:544:LEU:C	1:A:546:LYS:N	2.77	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
2:B:315:MET:HE3	2:B:317:ASN:HD21	1.85	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:301:MET:HE1	2:E:357:VAL:HG22	2.01	0.42
2:E:425:HIS:CG	2:E:426:PRO:HD2	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:42:LEU:HD12	2:B:109:GLN:HG2	2.02	0.41
2:B:222:MET:HE3	2:B:222:MET:HA	2.02	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: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
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:131:LEU:C	1:D:131:LEU:CD1	2.93	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
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
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:323:MET:HE1	1:D:360:ASN:CG	2.45	0.41
1:D:467:LYS:HE2	1:D:471:GLU:OE2	2.19	0.41
1:A:402:GLN:C	1:A:405:LEU:HD11	2.45	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
1:D:57:ASP:HB3	2:E:129:LYS:HZ1	1.86	0.41
1:D:198:LEU:O	1:D:199:ASP:C	2.64	0.41
1:D:332:GLU:O	1:D:334:VAL:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:559:GLU:C	1:D:562:PRO:HD2	2.44	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:305:LYS:O	1:A:306:VAL:C	2.63	0.41
1:A:439:PHE:HE1	1:A:444:ASN:HA	1.86	0.41
1:A:583:LEU:C	1:A:585:VAL:N	2.78	0.41
1:D:58:THR:HA	1:D:60:TYR:HD1	1.85	0.41
1:D:271:GLN:C	1:D:273:ALA:N	2.77	0.41
1:A:170:PHE:HE2	1:A:189:LEU:HD12	1.84	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
1:D:23:GLU:O	1:D:24:ASP:C	2.62	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
1:A:505:ILE:C	1:A:507:VAL:H	2.29	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:291:MET:HB3	1:D:333:LEU:HD11	2.02	0.41
1:D:495:TYR:CD2	1:D:499:MET:HE2	2.54	0.41
1:D:504:CYS:O	1:D:508:LEU:HG	2.20	0.41
1:D:552:ASP:C	1:D:554:SER:H	2.28	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:531:ASP:CG	1:A:532:PRO:HD2	2.46	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
3:C:117:ASN:HB2	3:C:200:TRP:CE2	2.56	0.41
1:D:63:ASP:O	1:D:64:GLU:C	2.64	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:310:CYS:C	1:D:312:ASN:N	2.78	0.41
1:D:423:ILE:HG22	1:D:424:ILE:N	2.36	0.41
1:D:427:MET:HA	1:D:427:MET:CE	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:162:VAL:O	1:A:163:LYS:C	2.63	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:333:LEU:N	2:B:333:LEU:CD2	2.83	0.41
2:B:339:ASN:OD1	2:B:339:ASN:C	2.64	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:246:SER:C	2:E:248:LYS:N	2.79	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
3:F:212:SER:C	3:F:214:ARG:N	2.72	0.41
1:A:256:SER:OG	1:A:259:VAL:HG23	2.21	0.41
1:A:323:MET:HE3	1:A:356:LEU:HD22	2.03	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
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
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
3:F:204:ASP:OD2	3:F:219:THR:HB	2.21	0.40
3:F:239:ARG:HD3	3:F:239:ARG:C	2.46	0.40
2:B:197:ASP:O	2:B:229:ILE:N	2.44	0.40
3:C:16:GLN:HG2	3:C:21:LYS:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:334:VAL:HG13	1:D:372:GLN:CD	2.47	0.40
2:E:222:MET:HE3	2:E:222:MET:CA	2.46	0.40
1:A:183:ARG:O	1:A:184:ALA:C	2.64	0.40
2:B:325:VAL:O	2:B:367:ARG:NE	2.51	0.40
2:B:358:MET:CG	2:B:359:THR:N	2.82	0.40
1:D:284:VAL:HB	1:D:285:PRO:HD3	2.04	0.40
2:E:68:ARG:HB3	2:E:443:GLN:HE22	1.86	0.40
3:F:118:HIS:C	3:F:120:SER:N	2.78	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:398:ARG:C	1:A:400:LEU:N	2.80	0.40
1:A:444:ASN:ND2	1:A:481:THR:HG22	2.37	0.40
2:B:47:ASP:OD2	2:B:51:ARG:NH2	2.54	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:336:ASP:OD2	1:D:341:VAL:HG11	2.22	0.40
1:A:58:THR:C	1:A:60:TYR:N	2.73	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
2:B:351:ASN:O	2:B:352:GLY:C	2.65	0.40
1:D:25:VAL:HA	1:D:28:ARG:NH1	2.36	0.40
1:D:287:PHE:HD1	1:D:291:MET:HE2	1.86	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: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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	580/582 (100%)	441 (76%)	110 (19%)	29 (5%)	1	2
1	D	580/582 (100%)	465 (80%)	88 (15%)	27 (5%)	2	3
2	B	413/447 (92%)	368 (89%)	38 (9%)	7 (2%)	7	16
2	E	413/447 (92%)	364 (88%)	41 (10%)	8 (2%)	6	14
3	C	286/309 (93%)	246 (86%)	35 (12%)	5 (2%)	7	16
3	F	286/309 (93%)	234 (82%)	40 (14%)	12 (4%)	2	3
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	6

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 ⓘ

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%)	470 (92%)	39 (8%)	12	25
1	D	509/509 (100%)	468 (92%)	41 (8%)	11	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	386/408 (95%)	350 (91%)	36 (9%)	8	18
2	E	386/408 (95%)	355 (92%)	31 (8%)	11	24
3	C	254/274 (93%)	235 (92%)	19 (8%)	12	26
3	F	254/274 (93%)	238 (94%)	16 (6%)	16	34
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%)	2120 (92%)	182 (8%)	11	24

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	MET
1	A	19	GLU
1	A	28	ARG
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	76	PHE
1	A	79	LEU
1	A	98	THR
1	A	100	GLU
1	A	102	THR
1	A	103	VAL
1	A	121	PRO
1	A	145	THR
1	A	153	VAL
1	A	157	ARG
1	A	177	ASP
1	A	180	MET
1	A	197	GLU
1	A	199	ASP
1	A	204	GLU
1	A	209	PHE
1	A	219	SER
1	A	222	LEU
1	A	238	GLU

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Mol	Chain	Res	Type
1	A	239	ASP
1	A	404	LEU
1	A	405	LEU
1	A	427	MET
1	A	437	GLU
1	A	447	CYS
1	A	469	LEU
1	A	512	CYS
1	A	539	ASN
1	A	571	GLN
2	B	8	ASN
2	B	11	GLN
2	B	14	PHE
2	B	17	VAL
2	B	23	ASP
2	B	47	ASP
2	B	90	LEU
2	B	100	ARG
2	B	151	THR
2	B	156	VAL
2	B	161	ASP
2	B	200	ILE
2	B	228	VAL
2	B	230	THR
2	B	234	PHE
2	B	247	SER
2	B	248	LYS
2	B	251	ILE
2	B	302	THR
2	B	326	HIS
2	B	330	ARG
2	B	333	LEU
2	B	338	GLU
2	B	351	ASN
2	B	357	VAL
2	B	378	THR
2	B	385	ASN
2	B	386	ASN
2	B	388	PRO
2	B	389	ARG
2	B	408	ILE
2	B	422	THR

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Mol	Chain	Res	Type
2	B	427	LYS
2	B	431	ILE
2	B	435	THR
2	B	443	GLN
3	C	10	LEU
3	C	12	GLN
3	C	18	ASN
3	C	30	SER
3	C	34	LYS
3	C	40	THR
3	C	52	VAL
3	C	57	ASP
3	C	110	ARG
3	C	125	GLN
3	C	147	THR
3	C	160	ASP
3	C	173	SER
3	C	174	ILE
3	C	237	VAL
3	C	239	ARG
3	C	244	VAL
3	C	267	TYR
3	C	275	ILE
1	D	9	SER
1	D	16	LEU
1	D	19	GLU
1	D	23	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	153	VAL
1	D	157	ARG
1	D	180	MET
1	D	196	LEU

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Mol	Chain	Res	Type
1	D	197	GLU
1	D	198	LEU
1	D	204	GLU
1	D	208	MET
1	D	216	GLU
1	D	217	GLN
1	D	222	LEU
1	D	250	GLN
1	D	278	ILE
1	D	306	VAL
1	D	327	LEU
1	D	400	LEU
1	D	405	LEU
1	D	423	ILE
1	D	427	MET
1	D	437	GLU
1	D	443	LEU
1	D	476	GLU
1	D	481	THR
1	D	539	ASN
1	D	559	GLU
1	D	581	GLU
2	E	8	ASN
2	E	11	GLN
2	E	17	VAL
2	E	23	ASP
2	E	81	GLU
2	E	91	GLU
2	E	136	LEU
2	E	160	MET
2	E	169	ARG
2	E	222	MET
2	E	228	VAL
2	E	251	ILE
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

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Mol	Chain	Res	Type
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	58	VAL
3	F	79	ASN
3	F	110	ARG
3	F	123	ILE
3	F	147	THR
3	F	160	ASP
3	F	196	CYS
3	F	235	THR
3	F	236	LEU
3	F	239	ARG
3	F	245	MET
3	F	267	TYR
3	F	282	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	289	ASN
1	A	304	HIS
1	A	339	GLN
1	A	360	ASN
1	A	514	GLN
1	A	539	ASN
1	A	557	GLN
2	B	11	GLN
2	B	109	GLN
2	B	295	HIS

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Mol	Chain	Res	Type
2	B	351	ASN
2	B	438	ASN
3	C	16	GLN
3	C	63	HIS
3	C	122	GLN
3	C	242	GLN
3	C	272	GLN
1	D	230	ASN
1	D	271	GLN
1	D	392	ASN
1	D	444	ASN
1	D	479	HIS
1	D	514	GLN
1	D	539	ASN
1	D	553	ASN
1	D	557	GLN
2	E	104	GLN
2	E	438	ASN
2	E	443	GLN
3	F	16	GLN
3	F	79	ASN
3	F	125	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1ZN	H	5	4	21,23,24	1.46	3 (14%)	25,29,31	1.10	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FGA	G	6	4	6,8,9	2.60	2 (33%)	6,9,11	0.50	0
4	ACB	G	3	4	7,8,9	1.12	0	8,10,12	0.75	0
4	DAM	H	7	3,4	4,5,6	2.50	2 (50%)	3,5,7	3.89	3 (100%)
4	1ZN	G	5	4	21,23,24	1.38	3 (14%)	25,29,31	1.10	2 (8%)
4	FGA	H	6	4	6,8,9	2.57	2 (33%)	6,9,11	0.54	0
4	DAM	G	7	3,4	4,5,6	2.02	1 (25%)	3,5,7	3.85	3 (100%)
4	ACB	H	3	4	7,8,9	1.10	0	8,10,12	1.01	0

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	1ZN	H	5	4	-	5/23/25/27	0/1/1/1
4	FGA	G	6	4	-	4/8/8/9	-
4	ACB	G	3	4	-	2/10/10/12	-
4	DAM	H	7	3,4	-	0/0/4/6	-
4	1ZN	G	5	4	-	5/23/25/27	0/1/1/1
4	FGA	H	6	4	-	4/8/8/9	-
4	DAM	G	7	3,4	-	0/0/4/6	-
4	ACB	H	3	4	-	2/10/10/12	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	6	FGA	O-C	5.35	1.38	1.22
4	G	6	FGA	O-C	5.31	1.37	1.22
4	H	7	DAM	C-CA	4.46	1.52	1.45
4	H	5	1ZN	C3-C2	3.77	1.57	1.52
4	G	7	DAM	C-CA	3.45	1.50	1.45
4	G	5	1ZN	C9-C4	3.03	1.44	1.38
4	G	5	1ZN	C3-C2	2.83	1.56	1.52
4	H	5	1ZN	C9-C4	2.75	1.44	1.38
4	G	6	FGA	OXT-C	-2.66	1.22	1.30
4	H	6	FGA	OXT-C	-2.54	1.22	1.30
4	G	5	1ZN	C6-C5	2.31	1.42	1.38
4	H	5	1ZN	C6-C5	2.22	1.42	1.38
4	H	7	DAM	CM-N	2.05	1.49	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	7	DAM	CM-N-CA	-4.78	116.72	123.98
4	G	7	DAM	CM-N-CA	-4.69	116.86	123.98
4	H	7	DAM	O-C-CA	-4.22	119.84	125.33
4	G	7	DAM	O-C-CA	-4.16	119.92	125.33
4	G	5	1ZN	CA-C18-C	-3.34	106.43	110.67
4	H	5	1ZN	CA-C18-C	-3.14	106.67	110.67
4	G	7	DAM	CB-CA-N	-2.26	120.28	125.84
4	G	5	1ZN	CA-C16-C15	-2.19	120.05	123.62
4	H	7	DAM	CB-CA-N	-2.17	120.49	125.84

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	3	ACB	C4-CB-CG-OD1
4	H	3	ACB	C4-CB-CG-OD1
4	G	5	1ZN	C12-C13-C15-C16
4	H	5	1ZN	C12-C13-C15-C16
4	H	5	1ZN	C14-C13-C15-C16
4	G	6	FGA	OE1-CD-CG-CB
4	H	6	FGA	OE1-CD-CG-CB
4	G	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	3	ACB	CA-CB-CG-OD1
4	H	3	ACB	CA-CB-CG-OD1
4	H	5	1ZN	C2-C3-C4-C9
4	G	5	1ZN	C10-C2-C3-C4
4	H	5	1ZN	C10-C2-C3-C4
4	G	5	1ZN	C2-C3-C4-C9
4	G	5	1ZN	C2-C3-C4-C5
4	G	6	FGA	O-C-CA-N
4	G	6	FGA	OXT-C-CA-N
4	H	6	FGA	OXT-C-CA-N
4	H	6	FGA	O-C-CA-N

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	582/582 (100%)	0.41	15 (2%) 57 48	53, 104, 164, 173	0
1	D	582/582 (100%)	0.42	33 (5%) 29 22	48, 100, 173, 188	0
2	B	421/447 (94%)	-0.08	1 (0%) 91 91	38, 67, 115, 131	0
2	E	421/447 (94%)	-0.21	2 (0%) 87 85	34, 60, 111, 133	0
3	C	288/309 (93%)	0.14	5 (1%) 69 63	60, 88, 119, 154	0
3	F	288/309 (93%)	0.26	4 (1%) 73 67	75, 99, 129, 157	0
4	G	2/7 (28%)	0.79	0 100 100	95, 95, 95, 117	0
4	H	2/7 (28%)	1.10	0 100 100	108, 108, 108, 117	0
All	All	2586/2690 (96%)	0.19	60 (2%) 61 52	34, 88, 161, 188	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	400	LEU	4.3
3	C	6	PHE	3.7
1	D	368	LEU	3.7
2	B	146	PRO	3.4
1	D	404	LEU	3.4
3	F	6	PHE	3.4
1	D	560	VAL	3.2
1	D	528	MET	3.1
1	D	178	THR	3.1
1	D	508	LEU	3.0
1	D	526	LEU	3.0
1	D	352	LEU	2.9
1	D	547	ILE	2.9
1	A	551	LEU	2.8
1	D	382	LEU	2.8
1	D	429	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	369	PHE	2.8
1	A	9	SER	2.8
1	A	388	LEU	2.7
1	D	505	ILE	2.7
1	D	522	LEU	2.7
1	A	355	ILE	2.6
1	D	551	LEU	2.6
1	D	529	ALA	2.6
1	D	384	ILE	2.5
2	E	149	VAL	2.5
3	C	58	VAL	2.4
1	D	520	HIS	2.4
3	F	45	VAL	2.4
1	A	517	THR	2.4
1	D	548	GLY	2.4
1	D	356	LEU	2.4
1	A	563	ILE	2.3
1	D	405	LEU	2.3
1	D	564	LEU	2.3
3	C	166	LEU	2.3
1	A	522	LEU	2.3
1	D	496	LEU	2.2
1	A	481	THR	2.2
3	F	140	ALA	2.2
1	D	348	VAL	2.2
1	A	192	PHE	2.2
1	D	59	ILE	2.2
1	D	397	ILE	2.2
1	A	244	VAL	2.2
3	C	215	GLY	2.2
1	D	544	LEU	2.2
1	A	263	VAL	2.1
1	D	365	LEU	2.1
3	F	266	CYS	2.1
1	D	483	ILE	2.1
1	A	528	MET	2.1
3	C	216	ALA	2.1
1	D	525	VAL	2.1
1	D	225	VAL	2.0
1	D	385	ILE	2.0
2	E	258	ALA	2.0
1	D	540	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	243	LEU	2.0
1	A	157	ARG	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, 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
4	DAL	H	1	5/6	0.81	0.16	108,108,110,112	0
4	FGA	H	6	9/10	0.86	0.17	102,111,118,118	0
4	DAM	G	7	6/7	0.86	0.15	99,101,102,104	0
4	ACB	H	3	9/10	0.87	0.15	108,111,113,113	0
4	FGA	G	6	9/10	0.89	0.18	100,101,106,107	0
4	1ZN	H	5	23/24	0.91	0.21	106,109,113,115	0
4	DAL	G	1	5/6	0.92	0.12	92,94,96,98	0
4	ACB	G	3	9/10	0.93	0.12	93,95,102,104	0
4	1ZN	G	5	23/24	0.94	0.19	99,102,106,107	0
4	DAM	H	7	6/7	0.94	0.11	112,113,116,116	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	C	501	1/1	0.98	0.03	69,69,69,69	0
5	MN	C	502	1/1	0.98	0.03	69,69,69,69	0
5	MN	F	511	1/1	0.98	0.05	82,82,82,82	0
5	MN	F	512	1/1	0.98	0.04	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.