



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:34 AM UTC

PDB ID : 2PF4 / pdb_00002pf4
Title : Crystal structure of the full-length simian virus 40 small t antigen complexed with the protein phosphatase 2A Aalpha subunit
Authors : Cho, U.; Morrone, S.; Xu, W.
Deposited on : 2007-04-03
Resolution : 3.10 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
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

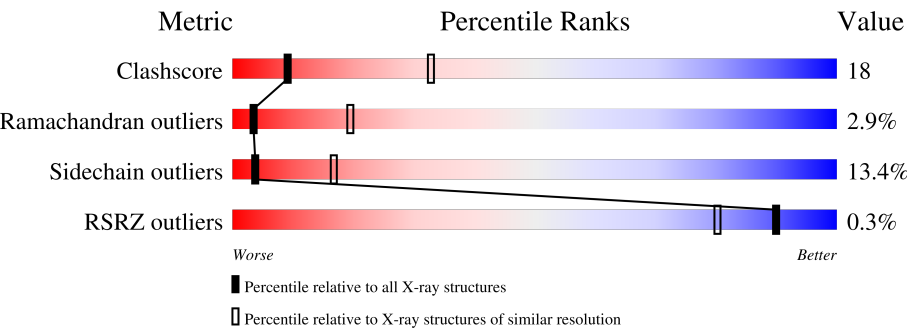
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	589	59%32%6%.
1	B	589	59%34%. .
1	C	589	59%33%6%.
1	D	589	% 58%34%5%. .
2	E	174	46%37%9%. 6%
2	F	174	% 35%36%16%. 13%
2	G	174	% 40%32%8%. 18%

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Mol	Chain	Length	Quality of chain
2	H	174	36% 33% 11% • 18%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22802 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.

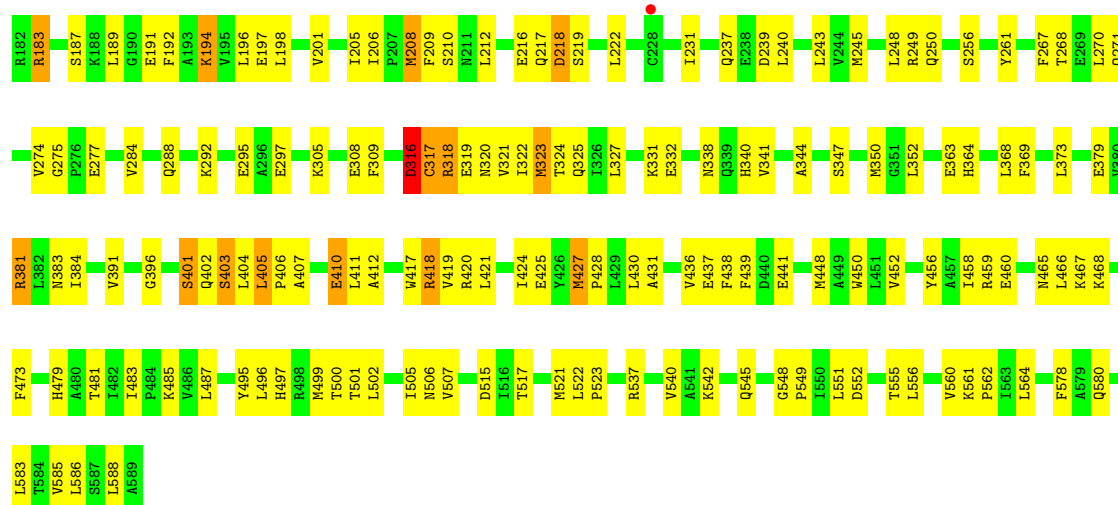
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	0	0
			4472	2840	754	851	27			
1	B	575	Total	C	N	O	S	0	0	0
			4473	2840	754	852	27			
1	C	577	Total	C	N	O	S	0	0	0
			4486	2849	756	854	27			
1	D	577	Total	C	N	O	S	0	0	0
			4492	2852	759	854	27			

- Molecule 2 is a protein called Small T antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	163	Total	C	N	O	S	0	0	0
			1303	836	220	227	20			
2	F	152	Total	C	N	O	S	0	0	0
			1232	790	209	213	20			
2	G	142	Total	C	N	O	S	0	0	0
			1164	748	195	201	20			
2	H	143	Total	C	N	O	S	0	0	0
			1172	751	199	202	20			

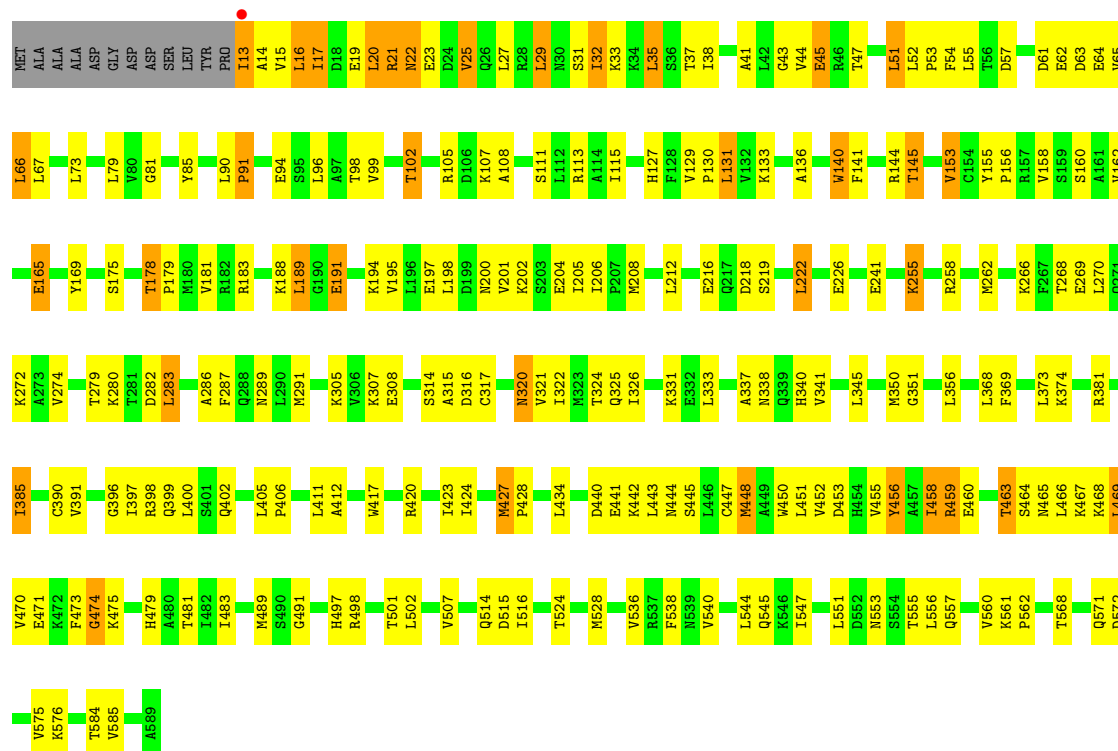
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Zn	0	0
			2	2		
3	F	2	Total	Zn	0	0
			2	2		
3	G	2	Total	Zn	0	0
			2	2		
3	H	2	Total	Zn	0	0
			2	2		



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

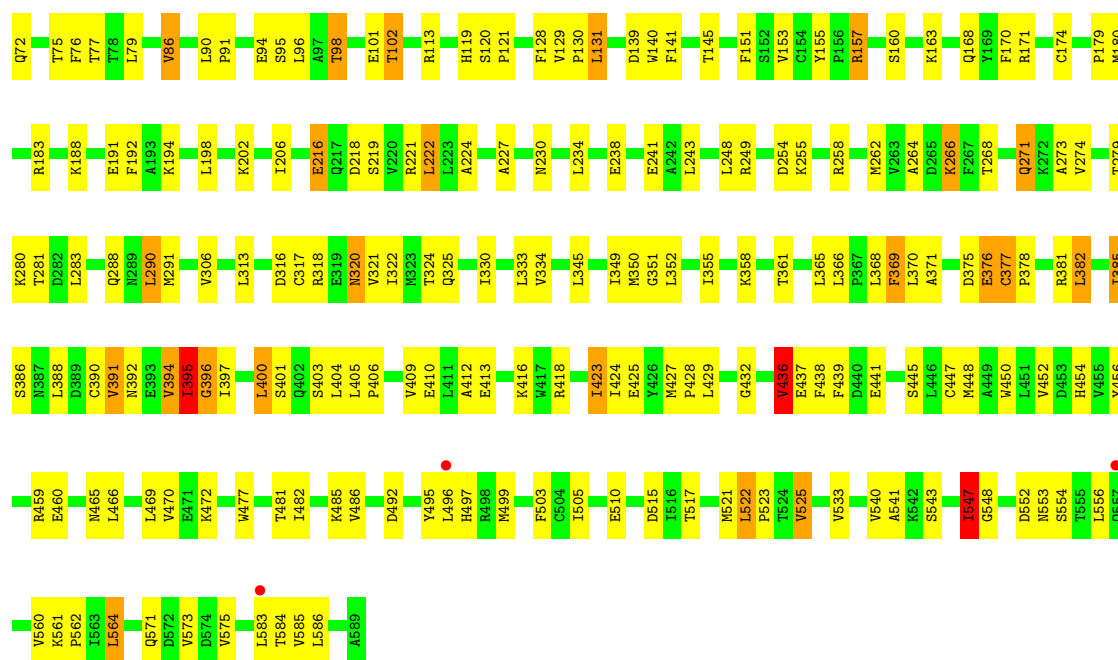
Chain C: 59% 33% 6% .



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

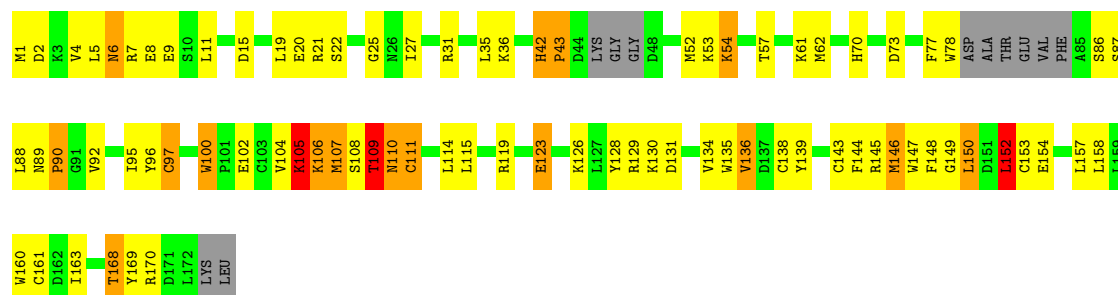
Chain D: 58% 34% 5% ..





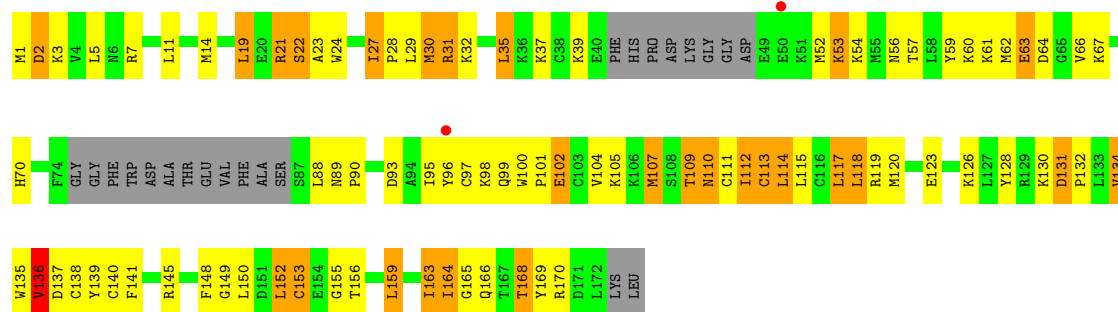
• Molecule 2: Small T antigen

Chain E: 46% 37% 9% 6%



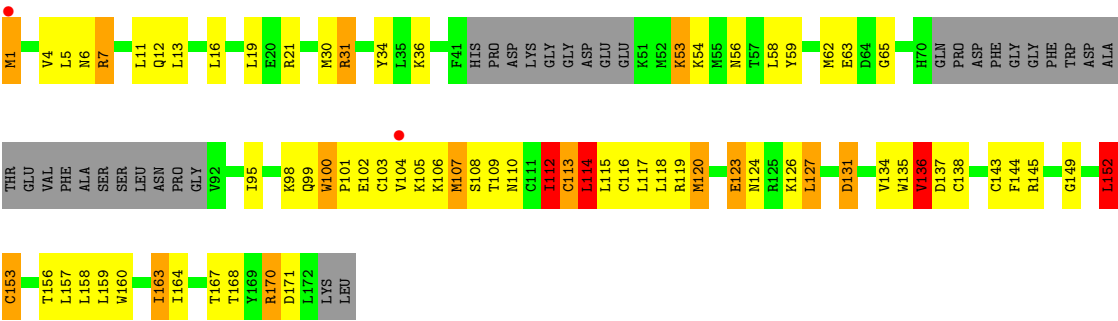
• Molecule 2: Small T antigen

Chain F: 35% 36% 16% 13%

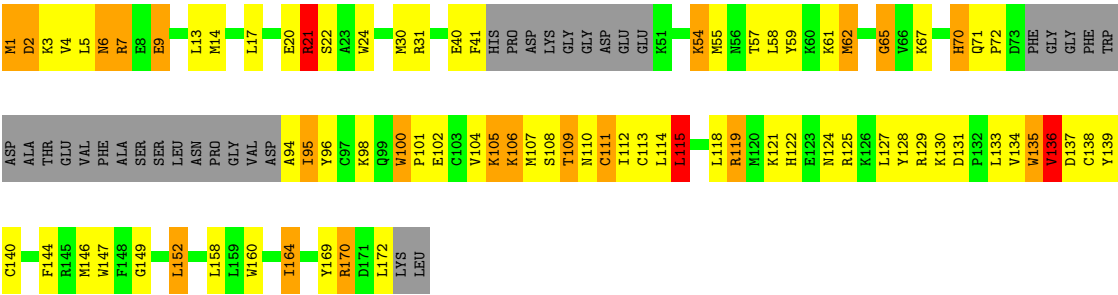


• Molecule 2: Small T antigen

Chain G: 40% 32% 8% 18%



• Molecule 2: Small T antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	94.71Å 105.50Å 111.94Å 115.64° 109.55° 94.11°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.11	Depositor EDS
% Data completeness (in resolution range)	97.4 (20.00-3.10) 87.0 (20.00-3.11)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.244 , 0.304 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	99.6	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 105.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22802	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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:
ZN

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	0.60	0/4544	0.97	6/6170 (0.1%)
1	B	0.62	0/4545	0.98	1/6170 (0.0%)
1	C	0.57	0/4558	0.96	5/6188 (0.1%)
1	D	0.58	0/4564	1.01	15/6195 (0.2%)
2	E	0.68	0/1332	1.03	7/1793 (0.4%)
2	F	0.66	0/1257	1.10	7/1688 (0.4%)
2	G	0.56	0/1186	1.03	3/1590 (0.2%)
2	H	0.63	0/1195	1.10	5/1602 (0.3%)
All	All	0.60	0/23181	1.00	49/31396 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	D	0	2
2	E	0	1
2	H	0	1
All	All	0	6

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	137	ASP	N-CA-C	-11.77	99.62	114.56
1	A	34	LYS	N-CA-C	-11.06	97.54	112.03
1	D	436	VAL	N-CA-C	9.56	122.02	107.78
2	F	23	ALA	N-CA-C	-7.45	104.08	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	23	GLU	N-CA-C	-7.40	98.94	110.42
1	D	394	VAL	N-CA-C	6.95	117.11	111.62
1	D	349	ILE	N-CA-C	6.87	117.02	110.42
1	D	437	GLU	N-CA-C	-6.81	102.88	113.02
2	F	137	ASP	N-CA-C	-6.72	102.29	111.56
2	H	102	GLU	N-CA-C	6.66	120.28	111.75
2	H	71	GLN	CA-C-N	6.57	128.05	119.84
2	H	71	GLN	C-N-CA	6.57	128.05	119.84
1	D	395	ILE	N-CA-C	6.41	117.11	107.75
1	D	64	GLU	N-CA-C	-6.17	105.66	113.43
1	D	59	ILE	N-CA-C	6.15	116.23	106.88
2	E	111	CYS	N-CA-C	6.15	119.23	109.81
1	D	22	ASN	CB-CA-C	-6.03	109.63	116.63
1	A	91	PRO	N-CA-C	5.94	117.95	110.70
1	D	575	VAL	N-CA-C	-5.93	108.07	113.71
2	F	27	ILE	CB-CA-C	-5.92	108.07	113.70
2	H	137	ASP	N-CA-C	-5.92	104.83	111.28
2	G	114	LEU	N-CA-C	-5.81	106.11	113.43
2	E	130	LYS	N-CA-C	-5.77	104.95	112.23
2	E	150	LEU	N-CA-C	5.63	119.00	109.76
2	E	109	THR	N-CA-C	5.62	122.03	113.61
1	A	27	LEU	N-CA-C	-5.53	106.69	113.50
2	F	114	LEU	N-CA-C	5.52	116.97	111.07
2	G	170	ARG	N-CA-C	-5.50	107.14	112.97
1	D	42	LEU	N-CA-C	-5.43	101.62	110.20
2	F	102	GLU	N-CA-C	5.43	119.00	112.38
1	C	456	TYR	N-CA-C	5.38	116.83	111.07
1	A	519	LYS	N-CA-C	5.37	118.17	111.24
1	D	396	GLY	N-CA-C	5.36	120.26	112.55
1	C	22	ASN	N-CA-C	5.35	119.64	113.38
1	C	91	PRO	N-CA-C	5.34	117.22	110.70
1	A	59	ILE	N-CA-C	5.29	115.48	107.75
2	E	100	TRP	CA-C-N	-5.29	113.18	119.05
2	E	100	TRP	C-N-CA	-5.29	113.18	119.05
1	D	377	CYS	CA-C-N	5.23	125.03	119.28
1	D	377	CYS	C-N-CA	5.23	125.03	119.28
2	F	89	ASN	N-CA-C	5.17	117.70	109.64
1	C	102	THR	N-CA-C	5.17	117.65	111.71
1	A	23	GLU	N-CA-C	-5.16	105.98	113.21
1	B	396	GLY	N-CA-C	5.13	119.13	112.25
2	F	109	THR	N-CA-C	5.06	118.01	110.52
1	D	44	VAL	N-CA-C	-5.05	107.78	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	115	LEU	CA-CB-CG	5.05	133.97	116.30
1	C	459	ARG	N-CA-C	-5.04	107.08	113.43
2	E	86	SER	N-CA-C	5.02	116.06	107.28

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	171	ARG	Sidechain
1	B	183	ARG	Sidechain
1	D	22	ASN	Peptide
1	D	436	VAL	Peptide
2	E	108	SER	Peptide
2	H	135	TRP	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	4472	0	4567	150	0
1	B	4473	0	4567	182	0
1	C	4486	0	4583	158	0
1	D	4492	0	4594	146	0
2	E	1303	0	1265	62	0
2	F	1232	0	1222	105	0
2	G	1164	0	1168	47	0
2	H	1172	0	1170	65	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
All	All	22802	0	23136	839	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 18.

All (839) 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)
2:F:31:ARG:NH1	2:F:31:ARG:HB3	1.70	1.07
1:D:24:ASP:HB2	1:D:28:ARG:HH21	1.23	1.03
1:D:24:ASP:HB2	1:D:28:ARG:NH2	1.77	0.99
1:B:405:LEU:HB2	1:B:406:PRO:HD3	1.45	0.99
1:B:456:TYR:HB2	2:H:128:TYR:O	1.64	0.97
1:B:183:ARG:HD3	1:B:219:SER:OG	1.64	0.97
1:B:140:TRP:NE1	2:F:131:ASP:HB3	1.79	0.96
2:H:96:TYR:O	2:H:113:CYS:HB2	1.67	0.95
1:B:421:LEU:HD23	1:D:21:ARG:HH12	1.32	0.92
1:A:16:LEU:O	1:A:19:GLU:HG2	1.71	0.91
1:B:194:LYS:HB3	1:B:194:LYS:HZ2	1.37	0.90
1:A:422:ALA:HB2	1:C:21:ARG:HD3	1.54	0.89
1:A:339:GLN:HB2	2:F:88:LEU:HD13	1.52	0.88
1:D:22:ASN:HB2	1:D:23:GLU:O	1.73	0.87
1:A:338:ASN:HD22	1:A:341:VAL:HG23	1.39	0.87
1:B:194:LYS:HB3	1:B:194:LYS:NZ	1.87	0.87
1:C:255:LYS:HE2	1:C:255:LYS:H	1.41	0.86
1:D:35:LEU:HD21	1:D:55:LEU:HD21	1.59	0.85
2:F:31:ARG:HB3	2:F:31:ARG:HH11	1.37	0.84
1:A:423:ILE:HD13	1:A:423:ILE:H	1.42	0.84
1:C:337:ALA:HB1	2:H:31:ARG:HH21	1.43	0.83
2:F:19:LEU:HD21	2:F:29:LEU:HG	1.59	0.83
1:D:24:ASP:CB	1:D:28:ARG:HH21	1.92	0.83
1:D:492:ASP:OD1	1:D:497:HIS:HB2	1.79	0.83
1:B:133:LYS:HG2	1:B:169:TYR:CE1	2.14	0.81
1:C:321:VAL:HA	1:C:324:THR:HG22	1.62	0.81
1:D:405:LEU:HB3	1:D:406:PRO:HD3	1.61	0.80
1:D:428:PRO:HD3	1:D:465:ASN:ND2	1.97	0.80
1:D:477:TRP:CZ3	1:D:482:ILE:HD11	2.17	0.80
2:F:100:TRP:O	2:F:104:VAL:HG23	1.81	0.80
1:C:13:ILE:HG12	1:C:14:ALA:H	1.45	0.79
2:H:135:TRP:CG	2:H:135:TRP:O	2.33	0.79
1:D:128:PHE:O	1:D:131:LEU:HB3	1.83	0.79
1:B:418:ARG:HG3	1:D:21:ARG:HH11	1.47	0.78
1:B:331:LYS:HG2	1:B:368:LEU:HD21	1.65	0.77
2:G:100:TRP:HB3	2:G:101:PRO:HD3	1.67	0.77
1:C:226:GLU:HB2	1:C:262:MET:HE3	1.67	0.77
2:F:11:LEU:HG	2:F:21:ARG:HD2	1.66	0.77
1:A:24:ASP:CG	1:A:61:ASP:HB3	2.10	0.77
1:C:141:PHE:O	1:C:145:THR:HG23	1.85	0.77
2:H:170:ARG:N	2:H:170:ARG:HD2	1.99	0.76
2:F:1:MET:HE3	2:F:136:VAL:HG11	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:163:ILE:C	2:F:163:ILE:HD13	2.09	0.76
2:G:158:LEU:HB2	2:H:158:LEU:HD21	1.67	0.76
2:H:112:ILE:HG22	2:H:112:ILE:O	1.84	0.76
1:C:411:LEU:HD12	1:C:423:ILE:HD11	1.67	0.76
1:B:456:TYR:CE1	2:H:130:LYS:HD2	2.20	0.76
2:G:106:LYS:HB2	2:G:107:MET:HE2	1.68	0.76
1:B:59:ILE:HG22	1:B:66:LEU:HD21	1.68	0.75
1:A:320:ASN:O	1:A:324:THR:HG22	1.87	0.75
1:C:411:LEU:CD1	1:C:423:ILE:HD11	2.17	0.75
1:C:412:ALA:HB1	1:C:450:TRP:HE1	1.51	0.74
1:A:94:GLU:OE1	1:A:134:ARG:NH2	2.21	0.74
1:D:454:HIS:HD2	2:F:128:TYR:HE1	1.34	0.74
1:A:109:VAL:O	1:A:113:ARG:HG3	1.88	0.74
2:E:15:ASP:OD1	2:E:21:ARG:NH2	2.20	0.73
2:E:104:VAL:HG11	2:E:152:LEU:HD21	1.70	0.73
1:A:52:LEU:HD12	1:A:92:PRO:HG3	1.70	0.73
1:B:140:TRP:HE1	2:F:131:ASP:HB3	1.53	0.73
1:B:405:LEU:HB2	1:B:406:PRO:CD	2.17	0.72
1:C:470:VAL:HG13	1:C:473:PHE:O	1.90	0.72
1:B:171:ARG:HH21	1:B:171:ARG:HB2	1.53	0.72
1:C:314:SER:C	1:C:316:ASP:H	1.96	0.72
1:B:179:PRO:HB2	1:B:183:ARG:HH21	1.54	0.72
1:B:456:TYR:HD2	1:B:459:ARG:HH22	1.36	0.72
2:F:1:MET:HE3	2:F:136:VAL:CG1	2.20	0.72
2:G:98:LYS:O	2:G:103:CYS:SG	2.47	0.72
1:B:402:GLN:HG3	1:B:405:LEU:HD21	1.72	0.71
1:B:320:ASN:O	1:B:324:THR:HG22	1.90	0.71
1:B:134:ARG:HH21	1:B:134:ARG:HG3	1.53	0.71
2:E:96:TYR:CD2	2:E:161:CYS:HB2	2.26	0.71
2:H:2:ASP:CG	2:H:2:ASP:O	2.33	0.71
1:B:22:ASN:C	1:B:24:ASP:H	1.98	0.71
2:E:168:THR:HG23	2:E:170:ARG:HE	1.55	0.71
2:F:100:TRP:HB2	2:F:101:PRO:HD3	1.73	0.71
2:F:163:ILE:HD13	2:F:163:ILE:O	1.91	0.71
1:C:338:ASN:HD22	1:C:341:VAL:HG23	1.56	0.71
1:A:219:SER:HB3	2:E:149:GLY:HA3	1.74	0.70
2:E:95:ILE:HG22	2:E:97:CYS:O	1.91	0.70
1:A:287:PHE:CE1	1:A:291:MET:HE2	2.27	0.69
2:H:1:MET:H1	2:H:136:VAL:HG22	1.57	0.69
1:B:59:ILE:HG22	1:B:66:LEU:CD2	2.23	0.69
1:A:277:GLU:HG2	1:A:280:LYS:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:102:GLU:HB3	2:G:106:LYS:HE2	1.74	0.69
1:B:373:LEU:HD13	1:B:384:ILE:HG21	1.73	0.69
1:D:428:PRO:HD3	1:D:465:ASN:HD21	1.57	0.69
1:A:418:ARG:NH1	1:C:21:ARG:HH21	1.91	0.69
1:B:179:PRO:HB2	1:B:183:ARG:NH2	2.06	0.68
1:D:396:GLY:O	1:D:400:LEU:HB2	1.93	0.68
1:A:388:LEU:O	1:A:392:ASN:HB2	1.93	0.68
1:B:21:ARG:HH21	1:D:418:ARG:HD3	1.58	0.68
1:C:291:MET:HB3	1:C:333:LEU:HD11	1.75	0.68
1:B:517:THR:HA	1:B:521:MET:HE3	1.75	0.68
1:C:197:GLU:HG2	1:C:200:ASN:HD22	1.59	0.68
2:H:121:LYS:O	2:H:125:ARG:HB3	1.94	0.68
1:C:427:MET:N	1:C:428:PRO:HD2	2.08	0.67
1:D:454:HIS:CD2	2:F:128:TYR:HE1	2.12	0.67
1:B:421:LEU:O	1:B:425:GLU:HG3	1.94	0.67
2:H:1:MET:N	2:H:136:VAL:HG22	2.08	0.67
2:F:31:ARG:HB3	2:F:31:ARG:CZ	2.23	0.67
2:G:164:ILE:HA	2:G:167:THR:HG22	1.75	0.67
1:A:24:ASP:OD2	1:A:61:ASP:HB3	1.95	0.67
1:A:373:LEU:HD21	1:A:404:LEU:HD22	1.76	0.67
2:E:1:MET:HB2	2:E:136:VAL:HG22	1.77	0.66
1:A:310:CYS:HA	1:A:313:LEU:HD12	1.77	0.66
2:H:169:TYR:HD1	2:H:172:LEU:HA	1.59	0.66
1:B:338:ASN:HD22	1:B:341:VAL:H	1.41	0.66
1:D:378:PRO:O	1:D:382:LEU:HB2	1.96	0.66
1:B:403:SER:H	1:B:405:LEU:HG	1.61	0.66
2:G:113:CYS:HB2	2:G:116:CYS:HB2	1.79	0.65
1:A:561:LYS:HB3	1:A:562:PRO:HD3	1.79	0.65
1:B:437:GLU:HG2	1:B:438:PHE:H	1.61	0.65
1:D:98:THR:CG2	1:D:140:TRP:HZ3	2.09	0.65
1:D:366:LEU:HD13	1:D:395:ILE:HD12	1.78	0.65
1:C:324:THR:HG23	1:C:325:GLN:HG2	1.77	0.65
1:D:98:THR:HG23	1:D:140:TRP:HZ3	1.61	0.65
1:C:538:PHE:HB3	1:C:575:VAL:HA	1.79	0.65
2:H:14:MET:HE1	2:H:30:MET:HE3	1.78	0.65
1:D:151:PHE:HB3	1:D:192:PHE:CE1	2.32	0.65
2:G:11:LEU:HD22	2:G:21:ARG:HD2	1.77	0.65
1:D:445:SER:HA	1:D:448:MET:HE3	1.78	0.65
1:B:179:PRO:HB3	1:B:217:GLN:NE2	2.12	0.65
1:B:216:GLU:HB2	2:F:22:SER:HB3	1.79	0.64
2:F:24:TRP:CE3	2:F:30:MET:HE1	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:105:LYS:O	2:E:107:MET:N	2.31	0.64
2:H:135:TRP:O	2:H:136:VAL:HG13	1.98	0.64
1:B:98:THR:HG23	1:B:143:SER:OG	1.98	0.64
1:C:545:GLN:HE21	1:C:585:VAL:HG21	1.60	0.64
2:F:110:ASN:HB2	2:G:110:ASN:O	1.97	0.64
1:B:217:GLN:HG2	1:B:219:SER:HB3	1.79	0.64
1:A:216:GLU:H	1:A:216:GLU:CD	2.06	0.63
1:B:427:MET:HB3	1:B:428:PRO:HD3	1.78	0.63
1:C:162:VAL:HA	1:C:165:GLU:OE2	1.98	0.63
2:H:54:LYS:HA	2:H:57:THR:HG22	1.81	0.63
2:G:4:VAL:HG13	2:G:65:GLY:HA3	1.81	0.63
1:A:60:TYR:HA	1:A:66:LEU:HD21	1.80	0.63
1:B:26:GLN:NE2	1:B:30:ASN:HD21	1.97	0.63
1:B:72:GLN:HG3	1:B:76:PHE:HE2	1.64	0.63
2:F:109:THR:HG22	2:F:119:ARG:HH22	1.62	0.63
1:B:427:MET:HE3	1:B:427:MET:HA	1.80	0.62
1:C:412:ALA:HB1	1:C:450:TRP:NE1	2.15	0.62
2:F:159:LEU:O	2:F:163:ILE:HG22	1.98	0.62
2:F:110:ASN:HD21	2:G:112:ILE:HG12	1.63	0.62
1:A:152:SER:HB3	1:A:191:GLU:OE2	2.00	0.62
1:A:217:GLN:HE22	2:E:148:PHE:HA	1.63	0.62
1:D:69:LEU:HD22	1:D:96:LEU:HD11	1.80	0.62
1:D:452:VAL:HG23	1:D:496:LEU:HB3	1.81	0.62
1:D:522:LEU:HB3	1:D:523:PRO:HD3	1.81	0.62
1:C:556:LEU:HD23	1:C:560:VAL:HG21	1.80	0.62
2:F:153:CYS:SG	2:F:155:GLY:N	2.71	0.62
2:F:150:LEU:HD13	2:F:156:THR:HG23	1.81	0.61
1:A:98:THR:CG2	1:A:140:TRP:HE3	2.12	0.61
1:B:218:ASP:N	1:B:218:ASP:OD2	2.34	0.61
2:F:1:MET:HA	2:F:1:MET:HE2	1.82	0.61
1:D:98:THR:HG23	1:D:140:TRP:CZ3	2.36	0.61
1:A:391:VAL:HG12	1:A:395:ILE:HG12	1.82	0.61
1:B:456:TYR:HE1	2:H:130:LYS:HD2	1.63	0.61
2:H:4:VAL:O	2:H:5:LEU:HB2	2.01	0.61
1:D:454:HIS:O	2:F:128:TYR:HD1	1.82	0.61
2:G:131:ASP:OD1	2:G:131:ASP:N	2.30	0.61
1:B:456:TYR:CE1	2:H:130:LYS:HB2	2.36	0.61
2:H:169:TYR:C	2:H:170:ARG:HD2	2.26	0.61
2:F:96:TYR:O	2:F:115:LEU:HG	2.00	0.61
1:C:23:GLU:O	1:C:23:GLU:HG2	1.99	0.61
1:A:178:THR:HG23	2:E:2:ASP:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:LEU:HD11	1:B:270:LEU:HD22	1.82	0.60
1:B:421:LEU:HD23	1:D:21:ARG:NH1	2.10	0.60
2:F:56:ASN:O	2:F:60:LYS:HB2	2.01	0.60
1:B:467:LYS:HB2	1:B:507:VAL:HG12	1.82	0.60
1:B:548:GLY:HA2	1:B:551:LEU:HD12	1.81	0.60
1:A:411:LEU:HB3	1:A:423:ILE:HD12	1.84	0.60
1:B:317:CYS:SG	1:B:317:CYS:O	2.60	0.60
2:E:135:TRP:CZ3	2:E:144:PHE:HB2	2.36	0.60
1:C:424:ILE:HD12	1:C:458:ILE:HG12	1.84	0.60
2:F:96:TYR:OH	2:F:165:GLY:HA2	2.02	0.60
1:B:267:PHE:HA	1:B:270:LEU:HD12	1.83	0.60
1:A:218:ASP:HA	1:A:221:ARG:HB2	1.83	0.60
1:B:405:LEU:CB	1:B:406:PRO:HD3	2.24	0.60
1:A:33:LYS:N	1:A:33:LYS:HD2	2.16	0.59
1:D:227:ALA:HA	1:D:230:ASN:HD22	1.67	0.59
1:B:288:GLN:HE22	1:B:325:GLN:HE21	1.50	0.59
1:A:487:LEU:C	1:A:489:MET:H	2.11	0.59
1:C:572:ASP:HB3	1:C:575:VAL:HB	1.83	0.59
1:D:391:VAL:HG12	1:D:395:ILE:HG13	1.85	0.59
2:E:6:ASN:ND2	2:E:9:GLU:OE1	2.35	0.59
1:B:379:GLU:O	1:B:383:ASN:HB2	2.02	0.59
1:D:556:LEU:HA	1:D:560:VAL:HB	1.84	0.59
2:H:144:PHE:CE1	2:H:160:TRP:HB2	2.37	0.59
1:A:197:GLU:CD	1:A:197:GLU:H	2.10	0.59
1:B:324:THR:HG23	1:B:325:GLN:HG2	1.83	0.59
1:B:288:GLN:HE22	1:B:325:GLN:NE2	2.00	0.59
1:B:483:ILE:O	1:B:487:LEU:HG	2.02	0.59
1:C:268:THR:HG21	1:C:308:GLU:HB2	1.83	0.59
1:B:32:ILE:O	1:B:35:LEU:HB2	2.03	0.59
1:A:553:ASN:O	1:A:557:GLN:HG2	2.03	0.58
2:F:112:ILE:HA	2:F:117:LEU:HD11	1.84	0.58
1:C:468:LYS:C	1:C:470:VAL:H	2.10	0.58
1:A:294:CYS:HB2	2:F:32:LYS:HG3	1.86	0.58
1:D:427:MET:HB3	1:D:465:ASN:HD21	1.68	0.58
2:F:14:MET:HE3	2:F:24:TRP:HB2	1.86	0.58
1:A:500:THR:O	1:A:504:CYS:HB2	2.04	0.58
1:A:350:MET:HB3	1:A:391:VAL:HG21	1.84	0.58
1:B:17:ILE:HG22	1:D:429:LEU:HD13	1.86	0.57
1:C:465:ASN:O	1:C:469:LEU:HB2	2.04	0.57
1:D:180:MET:HG3	2:H:146:MET:HE2	1.85	0.57
1:A:216:GLU:HB3	2:E:22:SER:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:PRO:C	1:A:238:GLU:H	2.13	0.57
1:A:427:MET:HB3	1:A:465:ASN:HD21	1.68	0.57
1:A:90:LEU:HB3	1:A:131:LEU:HD12	1.85	0.57
1:D:279:THR:HA	1:D:283:LEU:HB2	1.84	0.57
1:A:183:ARG:NH1	2:E:146:MET:O	2.36	0.57
2:F:96:TYR:OH	2:F:165:GLY:CA	2.52	0.57
1:A:213:ALA:HB1	1:A:247:THR:HG23	1.86	0.57
1:D:427:MET:CE	1:D:450:TRP:HH2	2.17	0.57
1:C:47:THR:HG23	1:C:51:LEU:HD11	1.86	0.57
1:D:101:GLU:OE1	1:D:102:THR:N	2.37	0.57
2:H:95:ILE:CG2	2:H:113:CYS:HA	2.34	0.57
2:F:136:VAL:CG2	2:F:136:VAL:O	2.52	0.57
2:H:105:LYS:HD3	2:H:152:LEU:HD21	1.85	0.57
1:B:219:SER:HB2	2:F:149:GLY:HA3	1.85	0.57
2:F:21:ARG:O	2:F:22:SER:CB	2.52	0.57
1:B:21:ARG:NH2	1:D:418:ARG:HD3	2.19	0.56
1:B:350:MET:SD	1:B:369:PHE:HB2	2.45	0.56
1:D:183:ARG:HH22	2:H:149:GLY:HA2	1.70	0.56
2:F:96:TYR:HA	2:F:114:LEU:HB2	1.86	0.56
2:H:100:TRP:HB3	2:H:101:PRO:HD3	1.85	0.56
1:C:337:ALA:HB1	2:H:31:ARG:NH2	2.17	0.56
1:C:451:LEU:O	1:C:459:ARG:HG3	2.04	0.56
2:E:15:ASP:CG	2:E:21:ARG:HH21	2.12	0.56
2:F:53:LYS:HD3	2:F:54:LYS:N	2.20	0.56
1:C:155:TYR:O	1:C:158:VAL:HG22	2.05	0.56
1:D:548:GLY:HA3	1:D:586:LEU:HD22	1.87	0.56
1:B:274:VAL:HG23	1:B:275:GLY:H	1.71	0.56
1:A:141:PHE:O	1:A:145:THR:HG23	2.06	0.56
1:B:46:ARG:HA	1:B:49:SER:OG	2.06	0.56
1:B:144:ARG:HG3	1:B:144:ARG:HH11	1.69	0.56
1:B:179:PRO:CB	1:B:217:GLN:NE2	2.67	0.56
2:F:164:ILE:C	2:F:166:GLN:H	2.11	0.56
1:A:349:ILE:HG23	1:A:350:MET:HG2	1.86	0.56
1:C:350:MET:SD	1:C:391:VAL:HG21	2.46	0.56
1:B:373:LEU:HD13	1:B:384:ILE:CG2	2.35	0.56
2:F:88:LEU:O	2:F:168:THR:HA	2.05	0.56
1:D:320:ASN:O	1:D:324:THR:HG22	2.07	0.55
2:G:120:MET:HE2	2:G:120:MET:HA	1.88	0.55
1:D:24:ASP:CB	1:D:28:ARG:NH2	2.58	0.55
1:B:239:ASP:HB3	1:B:243:LEU:HD12	1.88	0.55
2:E:54:LYS:HA	2:E:57:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:SER:HB2	1:D:121:PRO:HD2	1.87	0.55
1:A:77:THR:HG23	1:A:86:VAL:CG1	2.37	0.55
1:A:130:PRO:O	1:A:134:ARG:HG3	2.07	0.55
1:A:131:LEU:C	1:A:131:LEU:HD23	2.32	0.55
1:D:432:GLY:HA2	1:D:472:LYS:HE2	1.88	0.55
1:A:313:LEU:HD13	1:A:321:VAL:CG2	2.36	0.55
2:E:158:LEU:HD21	2:F:100:TRP:CZ3	2.42	0.55
1:A:74:GLY:HA3	1:A:111:SER:OG	2.06	0.55
1:D:517:THR:HA	1:D:521:MET:HB2	1.89	0.55
2:G:107:MET:HB2	2:G:119:ARG:CZ	2.38	0.54
1:B:456:TYR:HD2	1:B:459:ARG:NH2	2.04	0.54
1:B:561:LYS:HB3	1:B:562:PRO:HD3	1.90	0.54
2:F:27:ILE:HB	2:F:28:PRO:HD3	1.88	0.54
2:F:53:LYS:HD3	2:F:54:LYS:H	1.73	0.54
1:A:349:ILE:O	1:A:352:LEU:HD23	2.07	0.54
1:B:237:GLN:HE21	1:B:275:GLY:HA3	1.73	0.54
2:F:168:THR:HG22	2:F:170:ARG:HG3	1.90	0.54
2:H:104:VAL:HG22	2:H:115:LEU:HD21	1.90	0.54
1:A:15:VAL:HG12	1:A:19:GLU:HB3	1.90	0.54
1:D:436:VAL:HG11	1:D:439:PHE:HD1	1.73	0.54
1:D:34:LYS:O	1:D:38:ILE:HG13	2.08	0.54
1:D:448:MET:HE1	1:D:485:LYS:HB2	1.88	0.54
2:H:135:TRP:O	2:H:135:TRP:CD1	2.61	0.54
1:A:418:ARG:HH11	1:C:21:ARG:HH21	1.55	0.54
1:B:495:TYR:O	1:B:499:MET:HB2	2.08	0.54
1:C:568:THR:HA	1:C:576:LYS:HB3	1.90	0.54
1:B:436:VAL:HA	1:B:439:PHE:HB2	1.90	0.54
1:B:556:LEU:HA	1:B:560:VAL:HB	1.90	0.54
1:D:15:VAL:O	1:D:19:GLU:HG2	2.08	0.54
2:E:6:ASN:ND2	2:E:9:GLU:H	2.06	0.54
2:F:141:PHE:CE2	2:F:145:ARG:HD2	2.43	0.54
1:C:561:LYS:HB3	1:C:562:PRO:HD3	1.88	0.53
2:G:120:MET:O	2:G:124:ASN:HB2	2.08	0.53
1:C:156:PRO:HG3	1:C:195:VAL:HB	1.91	0.53
1:D:561:LYS:HA	1:D:564:LEU:HD12	1.89	0.53
1:A:361:THR:HA	1:A:365:LEU:HB2	1.90	0.53
1:B:179:PRO:CB	1:B:217:GLN:HE22	2.21	0.53
1:B:425:GLU:OE1	1:D:54:PHE:CZ	2.62	0.53
1:B:192:PHE:CZ	1:B:196:LEU:HD21	2.43	0.53
1:C:381:ARG:O	1:C:385:ILE:HG12	2.08	0.53
2:G:153:CYS:O	2:G:156:THR:HB	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:LEU:HD23	1:B:438:PHE:HE1	1.74	0.53
1:B:420:ARG:HE	1:B:458:ILE:HD13	1.73	0.53
1:C:468:LYS:O	1:C:470:VAL:N	2.41	0.53
1:D:113:ARG:HG2	1:D:153:VAL:HG11	1.90	0.53
1:D:388:LEU:O	1:D:392:ASN:N	2.39	0.53
2:F:24:TRP:HE3	2:F:30:MET:HE1	1.73	0.53
1:B:183:ARG:NH2	1:B:217:GLN:NE2	2.56	0.53
1:C:470:VAL:HG12	1:C:470:VAL:O	2.08	0.53
1:C:189:LEU:HD13	1:C:212:LEU:HD12	1.91	0.53
1:C:317:CYS:HB2	1:C:320:ASN:HD21	1.74	0.53
2:G:53:LYS:HA	2:G:56:ASN:HD22	1.74	0.53
2:G:135:TRP:CZ2	2:G:163:ILE:HD12	2.44	0.53
1:D:170:PHE:CE2	1:D:174:CYS:SG	3.02	0.53
1:D:350:MET:HE1	1:D:365:LEU:HB3	1.90	0.53
1:D:436:VAL:HG11	1:D:439:PHE:CD1	2.44	0.53
1:C:178:THR:HG22	1:C:181:VAL:H	1.72	0.52
2:F:164:ILE:C	2:F:166:GLN:N	2.67	0.52
2:H:9:GLU:CD	2:H:9:GLU:H	2.17	0.52
1:B:134:ARG:HG3	1:B:134:ARG:NH2	2.23	0.52
1:D:454:HIS:HD2	2:F:128:TYR:CE1	2.21	0.52
1:A:381:ARG:HA	1:A:384:ILE:HG22	1.90	0.52
1:D:56:THR:C	1:D:58:THR:H	2.18	0.52
1:A:313:LEU:HD13	1:A:321:VAL:HG21	1.91	0.52
1:A:409:VAL:HA	1:A:446:LEU:HD11	1.91	0.52
1:B:467:LYS:HB2	1:B:507:VAL:CG1	2.39	0.52
2:E:6:ASN:HD21	2:E:9:GLU:H	1.57	0.52
2:F:31:ARG:HG2	2:F:59:TYR:OH	2.09	0.52
2:H:109:THR:OG1	2:H:111:CYS:HB3	2.09	0.52
1:B:197:GLU:CD	1:B:197:GLU:H	2.18	0.52
1:B:271:GLN:HE22	1:B:309:PHE:HA	1.73	0.52
2:F:56:ASN:O	2:F:60:LYS:HD3	2.09	0.52
1:B:319:GLU:O	1:B:323:MET:HB2	2.09	0.52
1:C:13:ILE:HG12	1:C:14:ALA:N	2.21	0.52
1:A:98:THR:CG2	1:A:140:TRP:CE3	2.92	0.52
1:B:427:MET:HA	1:B:427:MET:CE	2.40	0.52
1:B:274:VAL:HG23	1:B:275:GLY:N	2.25	0.52
1:C:424:ILE:HD12	1:C:458:ILE:CG1	2.39	0.52
2:G:145:ARG:HH21	2:G:152:LEU:N	2.07	0.52
1:B:49:SER:O	1:B:53:PRO:HG2	2.09	0.52
1:D:271:GLN:C	1:D:273:ALA:H	2.18	0.52
1:A:94:GLU:OE1	1:A:131:LEU:HG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:THR:HG23	1:B:305:LYS:HD2	1.92	0.52
1:B:338:ASN:ND2	1:B:341:VAL:H	2.08	0.52
1:C:16:LEU:O	1:C:20:LEU:HB2	2.09	0.52
2:G:135:TRP:HZ2	2:G:163:ILE:HD12	1.75	0.52
1:B:292:LYS:NZ	1:B:332:GLU:OE2	2.43	0.51
1:C:440:ASP:C	1:C:442:LYS:H	2.17	0.51
1:D:218:ASP:OD1	1:D:219:SER:N	2.44	0.51
2:F:54:LYS:HA	2:F:57:THR:HG22	1.92	0.51
1:B:36:SER:O	1:B:40:LEU:HD12	2.11	0.51
1:B:506:ASN:HD22	1:B:506:ASN:N	2.08	0.51
1:D:427:MET:HE2	1:D:450:TRP:HH2	1.75	0.51
2:H:105:LYS:O	2:H:106:LYS:HB3	2.10	0.51
1:A:466:LEU:HB3	1:A:508:LEU:HD21	1.93	0.51
1:A:167:ARG:CZ	1:A:200:ASN:HD22	2.23	0.51
1:B:248:LEU:O	1:B:248:LEU:HD23	2.10	0.51
1:C:201:VAL:O	1:C:206:ILE:HG12	2.10	0.51
1:D:351:GLY:HA2	1:D:390:CYS:SG	2.50	0.51
1:A:427:MET:N	1:A:428:PRO:HD2	2.26	0.51
1:B:401:SER:O	1:B:404:LEU:HB3	2.10	0.51
1:A:178:THR:HG23	2:E:2:ASP:HB2	1.91	0.51
1:A:333:LEU:HB2	1:A:345:LEU:HD11	1.93	0.51
1:B:369:PHE:HE1	1:B:384:ILE:HG23	1.75	0.51
1:C:452:VAL:HG21	1:C:497:HIS:CE1	2.46	0.51
2:E:73:ASP:OD2	2:E:129:ARG:HD2	2.11	0.51
2:E:97:CYS:HB3	2:F:100:TRP:CD1	2.46	0.51
2:G:95:ILE:O	2:G:114:LEU:HB2	2.11	0.51
1:A:105:ARG:NH1	1:A:142:THR:HG22	2.26	0.51
1:D:368:LEU:O	1:D:371:ALA:N	2.44	0.51
1:A:179:PRO:O	1:A:183:ARG:HG3	2.11	0.51
2:G:160:TRP:O	2:G:163:ILE:HG22	2.11	0.51
1:B:552:ASP:HB2	1:B:555:THR:OG1	2.10	0.50
1:D:271:GLN:HA	1:D:274:VAL:HG12	1.92	0.50
2:F:2:ASP:OD2	2:F:3:LYS:HD2	2.11	0.50
1:A:96:LEU:C	1:A:98:THR:H	2.19	0.50
1:A:180:MET:HE1	2:E:147:TRP:HE3	1.76	0.50
1:C:51:LEU:HA	1:C:54:PHE:HB3	1.92	0.50
1:D:25:VAL:HB	1:D:27:LEU:HD23	1.93	0.50
2:H:100:TRP:CB	2:H:101:PRO:HD3	2.40	0.50
1:A:222:LEU:HD23	1:A:222:LEU:C	2.37	0.50
1:B:96:LEU:O	1:B:98:THR:N	2.45	0.50
1:C:61:ASP:CG	1:C:62:GLU:H	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:LEU:HD13	1:C:423:ILE:HD11	1.91	0.50
1:B:381:ARG:NH2	1:B:407:ALA:HA	2.26	0.50
2:G:30:MET:HE2	2:G:62:MET:HE2	1.92	0.50
1:B:497:HIS:O	1:B:500:THR:OG1	2.28	0.50
1:C:553:ASN:O	1:C:557:GLN:HG2	2.11	0.50
1:A:279:THR:HA	1:A:283:LEU:HB2	1.94	0.50
1:D:77:THR:HG23	1:D:86:VAL:CG1	2.42	0.50
1:D:291:MET:HE1	1:D:330:ILE:HD13	1.94	0.50
1:A:471:GLU:HG3	1:A:511:VAL:HG21	1.94	0.49
1:B:96:LEU:C	1:B:98:THR:H	2.20	0.49
1:C:32:ILE:HD13	1:C:35:LEU:HD12	1.93	0.49
1:A:373:LEU:HD23	1:A:403:SER:CB	2.43	0.49
1:C:136:ALA:O	1:C:144:ARG:HG2	2.13	0.49
1:B:178:THR:HG22	2:F:2:ASP:HB3	1.94	0.49
1:C:216:GLU:HG2	2:G:7:ARG:NH1	2.27	0.49
1:C:467:LYS:HE2	1:C:507:VAL:HG21	1.94	0.49
2:E:97:CYS:CB	2:F:100:TRP:CD1	2.95	0.49
2:F:1:MET:HE1	2:F:66:VAL:HG22	1.93	0.49
1:B:268:THR:HG21	1:B:308:GLU:HB3	1.93	0.49
1:D:258:ARG:NH2	2:H:149:GLY:O	2.45	0.49
1:D:410:GLU:HA	1:D:413:GLU:HG2	1.94	0.49
1:A:381:ARG:O	1:A:384:ILE:HG22	2.13	0.49
1:B:72:GLN:CG	1:B:76:PHE:HE2	2.24	0.49
2:F:62:MET:O	2:F:64:ASP:N	2.45	0.49
1:A:24:ASP:OD2	1:A:62:GLU:HG2	2.13	0.49
1:A:236:PRO:O	1:A:238:GLU:N	2.43	0.49
1:A:245:MET:O	1:A:249:ARG:HB2	2.12	0.49
1:C:183:ARG:NH1	1:C:219:SER:OG	2.46	0.49
1:C:498:ARG:O	1:C:501:THR:HB	2.12	0.49
2:E:77:PHE:O	2:E:78:TRP:HB2	2.11	0.49
2:E:104:VAL:HG11	2:E:152:LEU:CD2	2.40	0.49
2:E:114:LEU:HD12	2:E:114:LEU:H	1.78	0.49
1:B:130:PRO:O	1:B:134:ARG:HB2	2.13	0.49
1:B:350:MET:HG3	1:B:391:VAL:HG21	1.94	0.49
1:D:90:LEU:O	1:D:91:PRO:C	2.54	0.49
1:D:206:ILE:HG13	1:D:243:LEU:HD23	1.93	0.49
1:D:268:THR:HA	1:D:271:GLN:HG2	1.95	0.49
1:A:205:ILE:HA	1:A:208:MET:HE3	1.95	0.49
1:A:215:ASP:O	1:A:216:GLU:C	2.55	0.49
1:B:140:TRP:CD1	2:F:131:ASP:HB3	2.45	0.49
1:B:189:LEU:HD21	1:B:205:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:THR:HA	1:C:576:LYS:CB	2.42	0.49
2:E:157:LEU:HD21	2:F:100:TRP:HE1	1.77	0.49
1:A:528:MET:C	1:A:530:GLY:H	2.21	0.49
1:B:344:ALA:O	1:B:347:SER:OG	2.30	0.49
1:B:537:ARG:O	1:B:540:VAL:HB	2.13	0.49
2:E:87:SER:O	2:E:88:LEU:HD22	2.13	0.49
2:H:160:TRP:CZ2	2:H:164:ILE:HD12	2.48	0.49
1:D:241:GLU:OE1	1:D:249:ARG:NH2	2.45	0.49
1:A:178:THR:CG2	2:E:2:ASP:HB3	2.43	0.48
2:E:157:LEU:CD2	2:F:100:TRP:HE1	2.26	0.48
2:G:168:THR:C	2:G:170:ARG:H	2.20	0.48
1:A:317:CYS:O	1:A:321:VAL:HG22	2.13	0.48
1:B:369:PHE:CE1	1:B:384:ILE:HG23	2.48	0.48
1:C:314:SER:C	1:C:316:ASP:N	2.64	0.48
1:C:331:LYS:HG2	1:C:368:LEU:HD21	1.95	0.48
1:D:54:PHE:C	1:D:54:PHE:CD2	2.91	0.48
2:E:97:CYS:HB3	2:F:100:TRP:HD1	1.77	0.48
2:F:136:VAL:O	2:F:136:VAL:HG22	2.12	0.48
2:H:59:TYR:O	2:H:62:MET:HG3	2.13	0.48
1:B:284:VAL:O	1:B:288:GLN:HG3	2.13	0.48
1:C:111:SER:O	1:C:115:ILE:HG12	2.13	0.48
1:C:405:LEU:CD1	1:C:443:LEU:HD13	2.43	0.48
1:C:456:TYR:HD2	1:C:459:ARG:NH2	2.12	0.48
2:G:12:GLN:O	2:G:16:LEU:HG	2.13	0.48
1:C:29:LEU:HD11	1:C:64:GLU:HG2	1.95	0.48
1:C:127:HIS:C	1:C:130:PRO:HD2	2.38	0.48
1:D:179:PRO:O	1:D:180:MET:C	2.57	0.48
1:D:202:LYS:HA	1:D:206:ILE:HG12	1.95	0.48
1:D:499:MET:HE2	1:D:503:PHE:HE1	1.79	0.48
2:E:145:ARG:HG2	2:E:150:LEU:O	2.13	0.48
1:C:113:ARG:NH1	1:C:153:VAL:HG13	2.29	0.48
1:D:375:ASP:OD2	1:D:376:GLU:N	2.47	0.48
2:F:100:TRP:HB2	2:F:101:PRO:CD	2.42	0.48
1:A:316:ASP:OD2	1:A:317:CYS:N	2.47	0.48
1:A:517:THR:HA	1:A:521:MET:HE3	1.95	0.48
1:B:26:GLN:HE21	1:B:30:ASN:HD21	1.61	0.48
1:C:222:LEU:HD12	1:C:222:LEU:C	2.39	0.48
1:D:460:GLU:OE1	2:F:130:LYS:NZ	2.47	0.48
1:A:420:ARG:HA	1:A:423:ILE:HD11	1.95	0.48
1:A:464:SER:O	1:A:468:LYS:HD3	2.14	0.48
1:B:424:ILE:HG12	1:B:450:TRP:CE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:70:HIS:ND1	2:E:170:ARG:HD3	2.29	0.48
2:F:59:TYR:O	2:F:63:GLU:HB2	2.13	0.48
2:F:107:MET:O	2:F:107:MET:HG2	2.12	0.48
1:D:28:ARG:NH1	1:D:61:ASP:OD1	2.47	0.47
2:G:100:TRP:HB3	2:G:101:PRO:CD	2.40	0.47
1:B:412:ALA:HB1	1:B:450:TRP:HZ2	1.79	0.47
2:F:70:HIS:CG	2:F:170:ARG:HD2	2.49	0.47
1:C:37:THR:O	1:C:41:ALA:N	2.34	0.47
2:E:123:GLU:HA	2:E:126:LYS:HG2	1.95	0.47
2:H:95:ILE:HG22	2:H:114:LEU:H	1.78	0.47
1:A:405:LEU:HB3	1:A:406:PRO:HD3	1.96	0.47
1:C:255:LYS:HE2	1:C:255:LYS:N	2.21	0.47
1:D:264:ALA:HB2	1:D:290:LEU:HG	1.96	0.47
1:A:455:VAL:HG13	2:G:127:LEU:HD22	1.96	0.47
1:B:205:ILE:CG2	1:B:231:ILE:HD11	2.44	0.47
1:C:81:GLY:HA3	1:C:85:TYR:HD1	1.80	0.47
1:A:183:ARG:HD3	1:A:219:SER:OG	2.15	0.47
1:A:207:PRO:O	1:A:211:ASN:ND2	2.47	0.47
1:B:381:ARG:HG3	1:B:411:LEU:HD21	1.96	0.47
1:B:548:GLY:HA3	1:B:586:LEU:HD21	1.97	0.47
1:C:279:THR:O	1:C:283:LEU:HB2	2.15	0.47
1:A:176:ASP:OD1	1:A:178:THR:OG1	2.32	0.47
1:A:516:ILE:HG23	1:A:520:HIS:HD2	1.80	0.47
1:C:428:PRO:HD3	1:C:465:ASN:ND2	2.30	0.47
1:D:432:GLY:CA	1:D:472:LYS:HE2	2.44	0.47
2:E:19:LEU:O	2:E:20:GLU:C	2.58	0.47
1:B:30:ASN:O	1:B:33:LYS:HG3	2.15	0.47
1:C:536:VAL:O	1:C:540:VAL:HG23	2.15	0.47
2:F:14:MET:HE1	2:F:30:MET:CE	2.45	0.47
2:F:135:TRP:CH2	2:F:163:ILE:HD12	2.50	0.47
1:A:422:ALA:HB2	1:C:21:ARG:CD	2.38	0.47
1:C:67:LEU:CD2	1:C:107:LYS:HG3	2.45	0.47
1:C:547:ILE:HD12	1:C:551:LEU:HD11	1.97	0.47
1:D:350:MET:HG3	1:D:391:VAL:HG22	1.96	0.47
2:H:112:ILE:O	2:H:112:ILE:CG2	2.56	0.47
1:B:87:HIS:HA	1:B:90:LEU:HD13	1.97	0.46
1:B:144:ARG:HG3	1:B:144:ARG:NH1	2.30	0.46
1:B:174:CYS:SG	1:B:208:MET:HG2	2.55	0.46
1:B:325:GLN:NE2	1:B:325:GLN:HA	2.30	0.46
2:F:21:ARG:O	2:F:22:SER:HB3	2.14	0.46
2:F:163:ILE:O	2:F:163:ILE:CD1	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:O	1:A:206:ILE:HG12	2.14	0.46
1:C:32:ILE:O	1:C:35:LEU:HB2	2.15	0.46
2:E:168:THR:HG23	2:E:170:ARG:NE	2.28	0.46
2:G:1:MET:HG2	2:G:136:VAL:HG21	1.98	0.46
2:H:136:VAL:HG12	2:H:139:TYR:CZ	2.51	0.46
1:D:94:GLU:OE1	1:D:131:LEU:HD22	2.16	0.46
2:F:100:TRP:CB	2:F:101:PRO:HD3	2.44	0.46
1:C:90:LEU:HB2	1:C:91:PRO:HD3	1.96	0.46
1:C:105:ARG:O	1:C:108:ALA:HB3	2.15	0.46
1:D:222:LEU:C	1:D:222:LEU:HD23	2.40	0.46
1:D:436:VAL:HG22	1:D:438:PHE:HB3	1.98	0.46
2:E:144:PHE:CE1	2:E:160:TRP:HB2	2.51	0.46
1:A:498:ARG:O	1:A:501:THR:HB	2.15	0.46
1:A:502:LEU:CD1	1:A:528:MET:SD	3.04	0.46
1:C:258:ARG:NH2	2:G:149:GLY:O	2.49	0.46
2:E:104:VAL:CG1	2:E:152:LEU:HD21	2.44	0.46
1:B:37:THR:HA	1:B:40:LEU:HB2	1.98	0.46
1:C:96:LEU:C	1:C:98:THR:H	2.24	0.46
1:C:183:ARG:HD3	1:C:219:SER:HB2	1.97	0.46
1:C:455:VAL:HB	1:C:458:ILE:HG22	1.97	0.46
2:E:42:HIS:CB	2:E:43:PRO:CD	2.93	0.46
2:G:123:GLU:HA	2:G:126:LYS:HG2	1.97	0.46
1:C:322:ILE:HG21	1:C:356:LEU:HD21	1.97	0.46
1:C:405:LEU:HD12	1:C:443:LEU:HD13	1.97	0.46
1:D:29:LEU:C	1:D:29:LEU:HD13	2.40	0.46
1:D:318:ARG:O	1:D:322:ILE:HG13	2.15	0.46
2:H:122:HIS:C	2:H:122:HIS:CD2	2.93	0.46
1:B:159:SER:OG	1:B:162:VAL:HG23	2.16	0.46
1:B:340:HIS:N	1:B:340:HIS:CD2	2.83	0.46
2:F:114:LEU:HD23	2:F:117:LEU:HD23	1.98	0.46
2:H:94:ALA:C	2:H:95:ILE:HG13	2.41	0.46
1:A:418:ARG:CZ	1:A:418:ARG:HB2	2.44	0.46
1:B:98:THR:HG22	1:B:140:TRP:HE3	1.81	0.46
1:B:128:PHE:O	1:B:131:LEU:HB3	2.16	0.46
1:B:201:VAL:O	1:B:206:ILE:HG12	2.16	0.46
1:C:268:THR:HG23	1:C:305:LYS:HG2	1.97	0.46
1:C:456:TYR:CZ	1:C:460:GLU:HG3	2.51	0.46
1:D:238:GLU:CD	1:D:238:GLU:H	2.23	0.46
1:A:24:ASP:OD1	1:A:61:ASP:HB3	2.16	0.46
1:A:446:LEU:C	1:A:448:MET:H	2.24	0.46
1:B:171:ARG:HB2	1:B:171:ARG:NH2	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:338:ASN:HD21	1:C:340:HIS:HB2	1.80	0.46
1:C:479:HIS:HA	1:C:483:ILE:HB	1.98	0.45
2:E:6:ASN:H	2:E:6:ASN:HD22	1.65	0.45
2:H:144:PHE:CD1	2:H:160:TRP:HB2	2.52	0.45
1:A:52:LEU:HD13	1:A:52:LEU:HA	1.86	0.45
1:C:15:VAL:O	1:C:19:GLU:HG2	2.17	0.45
2:F:2:ASP:OD1	2:F:134:VAL:HG21	2.16	0.45
2:F:98:LYS:O	2:F:99:GLN:HB3	2.16	0.45
2:F:113:CYS:O	2:F:117:LEU:HD22	2.15	0.45
1:C:286:ALA:HA	1:C:289:ASN:HD22	1.81	0.45
1:D:194:LYS:HD3	1:D:234:LEU:HD21	1.99	0.45
1:A:271:GLN:HE22	1:A:309:PHE:HA	1.81	0.45
1:B:545:GLN:HE21	1:B:585:VAL:HG11	1.82	0.45
1:B:561:LYS:HA	1:B:564:LEU:HD12	1.97	0.45
1:D:22:ASN:CB	1:D:23:GLU:O	2.56	0.45
2:E:107:MET:HG3	2:E:119:ARG:NH1	2.31	0.45
2:F:31:ARG:HH22	2:F:35:LEU:CD1	2.30	0.45
2:H:40:GLU:O	2:H:41:PHE:CB	2.64	0.45
1:A:287:PHE:CD1	1:A:291:MET:HE2	2.50	0.45
1:B:556:LEU:HD22	1:B:588:LEU:HD11	1.98	0.45
1:B:580:GLN:HA	1:B:583:LEU:HD12	1.99	0.45
2:H:108:SER:O	2:H:109:THR:HB	2.17	0.45
1:A:537:ARG:O	1:A:540:VAL:HB	2.17	0.45
1:B:406:PRO:O	1:B:410:GLU:HB2	2.17	0.45
1:C:258:ARG:NH1	2:G:149:GLY:O	2.50	0.45
2:F:37:LYS:C	2:F:39:LYS:H	2.25	0.45
2:F:99:GLN:HG2	2:F:102:GLU:HB2	1.99	0.45
1:A:350:MET:HB3	1:A:391:VAL:CG2	2.45	0.45
1:A:524:THR:HG23	1:A:527:ARG:NH2	2.32	0.45
1:D:456:TYR:CZ	2:F:130:LYS:HD2	2.52	0.45
1:A:50:GLU:C	1:A:53:PRO:HD2	2.42	0.45
1:A:138:GLY:O	1:A:144:ARG:NH1	2.50	0.45
1:A:417:TRP:HZ3	1:A:421:LEU:HD12	1.81	0.45
1:A:502:LEU:HD11	1:A:528:MET:SD	2.57	0.45
1:B:59:ILE:CG2	1:B:66:LEU:CD2	2.94	0.45
1:C:456:TYR:CG	2:E:128:TYR:HB3	2.52	0.45
2:E:100:TRP:CZ3	2:E:104:VAL:HG21	2.52	0.45
1:A:452:VAL:HG23	1:A:497:HIS:NE2	2.31	0.45
1:B:318:ARG:O	1:B:322:ILE:HG13	2.17	0.45
1:B:363:GLU:HG2	1:B:364:HIS:CD2	2.51	0.45
1:C:479:HIS:HB2	1:C:483:ILE:HD12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:VAL:HG12	1:D:26:GLN:H	1.81	0.45
2:F:111:CYS:HB3	2:F:113:CYS:HB3	1.98	0.45
2:G:98:LYS:O	2:G:99:GLN:HB3	2.17	0.45
1:B:39:ALA:HB3	1:B:79:LEU:HD23	1.99	0.45
1:C:544:LEU:HD23	1:C:547:ILE:HD11	1.99	0.45
2:G:135:TRP:CD1	2:G:136:VAL:HG23	2.51	0.45
2:H:138:CYS:SG	2:H:140:CYS:HB3	2.57	0.45
1:A:319:GLU:O	1:A:323:MET:HB2	2.17	0.44
1:A:489:MET:C	1:A:491:GLY:H	2.26	0.44
1:B:24:ASP:HB3	1:B:25:VAL:H	1.53	0.44
1:B:46:ARG:O	1:B:50:GLU:N	2.44	0.44
1:B:90:LEU:N	1:B:91:PRO:CD	2.80	0.44
1:C:448:MET:CG	1:C:451:LEU:HD12	2.47	0.44
1:D:505:ILE:HD13	1:D:525:VAL:HG22	2.00	0.44
1:A:200:ASN:OD1	1:A:200:ASN:N	2.50	0.44
1:C:29:LEU:HD13	1:C:65:VAL:HA	2.00	0.44
1:C:466:LEU:HD12	1:C:469:LEU:HD23	2.00	0.44
1:A:67:LEU:HD11	1:A:103:VAL:HG12	2.00	0.44
1:C:22:ASN:O	1:C:23:GLU:HB3	2.18	0.44
1:D:350:MET:HE3	1:D:369:PHE:HB2	1.99	0.44
1:A:417:TRP:CZ3	1:A:421:LEU:HD12	2.52	0.44
1:D:288:GLN:NE2	1:D:325:GLN:HB3	2.32	0.44
2:E:11:LEU:HD22	2:E:21:ARG:HD3	1.99	0.44
2:E:97:CYS:CB	2:F:100:TRP:HD1	2.30	0.44
1:A:28:ARG:O	1:A:32:ILE:HG13	2.18	0.44
1:A:424:ILE:HG12	1:A:450:TRP:CE3	2.52	0.44
1:A:487:LEU:HD22	1:A:524:THR:HG21	2.00	0.44
1:B:77:THR:HG21	1:B:118:GLU:OE1	2.17	0.44
1:B:90:LEU:HD23	1:B:131:LEU:HD13	1.99	0.44
1:B:159:SER:HG	1:B:162:VAL:HG23	1.82	0.44
1:C:498:ARG:HB3	1:C:528:MET:HE1	1.99	0.44
1:D:168:GLN:NE2	1:D:171:ARG:HE	2.15	0.44
2:E:1:MET:SD	2:E:25:GLY:HA2	2.58	0.44
1:A:360:ASN:HA	1:A:363:GLU:HB2	1.99	0.44
1:A:506:ASN:HD21	1:A:543:SER:HA	1.83	0.44
1:B:412:ALA:HB1	1:B:450:TRP:CZ2	2.51	0.44
1:B:545:GLN:NE2	1:B:585:VAL:HG11	2.33	0.44
1:C:497:HIS:N	1:C:497:HIS:CD2	2.86	0.44
1:D:495:TYR:HB3	1:D:533:VAL:HG21	2.00	0.44
2:F:118:LEU:HB3	2:F:140:CYS:HA	2.00	0.44
1:A:171:ARG:HE	1:A:171:ARG:HB2	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLU:HG2	2:F:132:PRO:HB3	2.00	0.44
1:B:402:GLN:O	1:B:403:SER:CB	2.66	0.44
1:D:202:LYS:HA	1:D:206:ILE:CG1	2.47	0.44
2:F:145:ARG:CZ	2:F:152:LEU:HD22	2.47	0.44
1:B:424:ILE:HD11	1:B:458:ILE:HG23	1.98	0.44
1:B:542:LYS:HE2	1:B:578:PHE:CE1	2.53	0.44
1:D:155:TYR:CZ	1:D:163:LYS:HD3	2.52	0.44
1:D:540:VAL:O	1:D:543:SER:HB3	2.18	0.44
2:G:13:LEU:HB2	2:G:58:LEU:HD13	1.99	0.44
2:G:138:CYS:HB3	2:G:143:CYS:SG	2.58	0.44
1:B:173:LEU:O	1:B:176:ASP:HB2	2.18	0.44
1:C:448:MET:HG2	1:C:451:LEU:HD12	1.99	0.44
2:E:154:GLU:HG3	2:F:100:TRP:CH2	2.53	0.44
2:H:54:LYS:HD2	2:H:57:THR:HG21	1.99	0.44
1:A:373:LEU:HD23	1:A:403:SER:HB2	2.00	0.43
1:A:508:LEU:O	1:A:512:CYS:SG	2.75	0.43
1:B:25:VAL:HB	1:B:26:GLN:H	1.60	0.43
1:B:72:GLN:HG3	1:B:76:PHE:CE2	2.50	0.43
1:D:33:LYS:C	1:D:35:LEU:H	2.24	0.43
1:D:224:ALA:O	1:D:227:ALA:N	2.51	0.43
2:E:138:CYS:HB3	2:E:143:CYS:SG	2.58	0.43
1:B:321:VAL:O	1:B:325:GLN:HB2	2.17	0.43
1:B:417:TRP:HB3	1:B:420:ARG:HH11	1.83	0.43
1:C:571:GLN:HG2	1:C:571:GLN:O	2.19	0.43
1:D:61:ASP:OD1	1:D:62:GLU:N	2.46	0.43
1:D:547:ILE:H	1:D:547:ILE:HG13	1.65	0.43
2:F:64:ASP:HA	2:F:67:LYS:HB3	1.99	0.43
2:G:113:CYS:HB3	2:G:116:CYS:H	1.83	0.43
1:A:159:SER:O	1:A:163:LYS:HG3	2.17	0.43
1:C:29:LEU:O	1:C:31:SER:N	2.52	0.43
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.66	0.43
2:E:89:ASN:O	2:E:90:PRO:C	2.62	0.43
2:G:108:SER:H	2:G:119:ARG:NH1	2.16	0.43
1:A:189:LEU:HD11	1:A:205:ILE:HG23	2.01	0.43
1:B:261:TYR:CD1	1:B:261:TYR:C	2.96	0.43
1:C:374:LYS:HA	1:C:381:ARG:HH21	1.83	0.43
1:C:397:ILE:HD11	1:C:434:LEU:HA	2.00	0.43
1:D:262:MET:O	1:D:266:LYS:HG2	2.18	0.43
1:D:412:ALA:HB2	1:D:423:ILE:HG21	2.01	0.43
2:H:125:ARG:NE	2:H:133:LEU:HD11	2.33	0.43
1:A:412:ALA:CB	1:A:450:TRP:HZ2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:PHE:CD1	1:A:538:PHE:C	2.97	0.43
1:B:179:PRO:O	1:B:183:ARG:HG3	2.18	0.43
1:B:316:ASP:HB3	1:B:317:CYS:H	1.61	0.43
1:C:29:LEU:C	1:C:31:SER:N	2.76	0.43
1:D:141:PHE:O	1:D:145:THR:HG23	2.18	0.43
1:D:317:CYS:O	1:D:321:VAL:HG22	2.18	0.43
1:A:256:SER:OG	1:A:259:VAL:HG23	2.18	0.43
1:C:197:GLU:CG	1:C:200:ASN:HD22	2.29	0.43
1:D:95:SER:O	1:D:98:THR:HB	2.19	0.43
1:D:452:VAL:HG22	1:D:452:VAL:O	2.19	0.43
2:E:95:ILE:HD12	2:H:110:ASN:HB3	2.00	0.43
2:F:31:ARG:HH11	2:F:31:ARG:CB	2.17	0.43
2:F:100:TRP:O	2:F:104:VAL:CG2	2.61	0.43
1:A:155:TYR:CZ	1:A:163:LYS:HB3	2.54	0.43
1:B:89:LEU:O	1:B:92:PRO:HD2	2.18	0.43
1:D:254:ASP:OD2	1:D:255:LYS:N	2.52	0.43
1:D:352:LEU:HA	1:D:355:ILE:HD12	2.00	0.43
2:E:97:CYS:HB2	2:F:100:TRP:CD1	2.54	0.43
1:A:197:GLU:CD	1:A:197:GLU:N	2.77	0.43
1:B:145:THR:HG22	1:B:181:VAL:HA	2.00	0.43
1:D:25:VAL:HB	1:D:27:LEU:CD2	2.48	0.43
2:F:145:ARG:O	2:F:148:PHE:O	2.36	0.43
1:B:418:ARG:HG3	1:D:21:ARG:NH1	2.26	0.43
1:B:456:TYR:CZ	2:H:130:LYS:HB2	2.54	0.43
1:B:216:GLU:CG	2:F:22:SER:HB3	2.49	0.42
1:B:437:GLU:HG2	1:B:438:PHE:N	2.31	0.42
1:B:501:THR:O	1:B:505:ILE:HG13	2.19	0.42
1:C:21:ARG:HE	1:C:21:ARG:HA	1.83	0.42
2:F:14:MET:HE1	2:F:24:TRP:HE3	1.83	0.42
2:H:169:TYR:CD1	2:H:172:LEU:HA	2.47	0.42
1:B:288:GLN:NE2	1:B:325:GLN:HE21	2.17	0.42
1:C:67:LEU:HD23	1:C:107:LYS:HG3	2.01	0.42
1:C:369:PHE:CZ	1:C:373:LEU:HD22	2.54	0.42
1:C:428:PRO:HD3	1:C:465:ASN:HD22	1.83	0.42
1:C:445:SER:C	1:C:447:CYS:H	2.27	0.42
1:C:453:ASP:O	1:C:459:ARG:HD3	2.19	0.42
1:D:72:GLN:O	1:D:76:PHE:HD1	2.02	0.42
2:H:4:VAL:HG12	2:H:65:GLY:HA3	2.01	0.42
1:B:58:THR:HG21	1:D:425:GLU:OE2	2.19	0.42
1:B:77:THR:C	1:B:79:LEU:H	2.27	0.42
1:B:402:GLN:HA	1:B:405:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:THR:O	1:C:467:LYS:N	2.40	0.42
1:D:358:LYS:HG3	1:D:394:VAL:HG13	2.00	0.42
1:A:29:LEU:HA	1:A:29:LEU:HD12	1.75	0.42
1:A:413:GLU:O	1:A:413:GLU:HG2	2.19	0.42
1:C:94:GLU:OE1	1:C:131:LEU:HD13	2.19	0.42
1:C:96:LEU:HA	1:C:99:VAL:HG23	2.01	0.42
1:C:98:THR:HG23	1:C:140:TRP:HD1	1.84	0.42
1:C:179:PRO:O	1:C:183:ARG:HG3	2.19	0.42
1:D:183:ARG:NH2	2:H:149:GLY:HA2	2.32	0.42
2:F:62:MET:HE2	2:F:63:GLU:N	2.35	0.42
2:F:152:LEU:HD12	2:F:152:LEU:O	2.19	0.42
2:G:34:TYR:C	2:G:36:LYS:H	2.27	0.42
1:A:353:SER:N	1:A:354:PRO:HD2	2.35	0.42
1:B:338:ASN:HD21	1:B:340:HIS:HB2	1.84	0.42
1:C:16:LEU:HD12	1:C:54:PHE:CE1	2.53	0.42
1:C:280:LYS:HB2	1:C:280:LYS:HE3	1.86	0.42
1:C:427:MET:N	1:C:428:PRO:CD	2.79	0.42
1:D:447:CYS:HA	1:D:450:TRP:CE3	2.54	0.42
2:H:1:MET:HB3	2:H:2:ASP:H	1.46	0.42
1:B:448:MET:HE3	1:B:485:LYS:HD3	2.02	0.42
1:B:452:VAL:HG22	1:B:452:VAL:O	2.19	0.42
1:C:338:ASN:ND2	1:C:341:VAL:HG23	2.30	0.42
1:C:350:MET:HA	1:C:350:MET:HE2	2.00	0.42
1:D:381:ARG:O	1:D:385:ILE:HG12	2.19	0.42
2:E:102:GLU:O	2:E:107:MET:HA	2.20	0.42
1:A:115:ILE:O	1:A:119:HIS:HD2	2.02	0.42
1:A:412:ALA:HB1	1:A:450:TRP:CZ2	2.54	0.42
1:A:547:ILE:HA	1:A:550:ILE:HD12	2.02	0.42
1:C:133:LYS:HE2	1:C:169:TYR:CE2	2.55	0.42
1:C:205:ILE:HA	1:C:208:MET:HE3	2.02	0.42
1:C:489:MET:C	1:C:491:GLY:H	2.27	0.42
1:C:556:LEU:HA	1:C:560:VAL:HB	2.01	0.42
1:D:552:ASP:C	1:D:554:SER:H	2.27	0.42
2:G:99:GLN:HA	2:H:98:LYS:O	2.19	0.42
1:B:140:TRP:CG	2:F:132:PRO:HD2	2.55	0.42
1:B:216:GLU:CB	2:F:22:SER:HB3	2.48	0.42
1:C:29:LEU:O	1:C:32:ILE:N	2.52	0.42
1:C:216:GLU:HG3	2:G:11:LEU:HD21	2.01	0.42
1:C:333:LEU:HB2	1:C:345:LEU:HD22	2.02	0.42
1:C:468:LYS:C	1:C:470:VAL:N	2.77	0.42
2:E:88:LEU:HB3	2:E:89:ASN:H	1.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:LYS:O	2:F:99:GLN:CB	2.67	0.42
2:H:6:ASN:O	2:H:7:ARG:C	2.63	0.42
2:H:106:LYS:C	2:H:108:SER:H	2.28	0.42
1:A:196:LEU:HD13	1:A:200:ASN:HB2	2.02	0.42
1:B:297:GLU:OE2	1:B:297:GLU:N	2.50	0.42
1:C:188:LYS:HD2	1:C:191:GLU:OE2	2.19	0.42
1:C:473:PHE:O	1:C:474:GLY:O	2.37	0.42
1:D:258:ARG:NH1	2:H:149:GLY:O	2.52	0.42
1:D:352:LEU:HD23	1:D:355:ILE:HD12	2.01	0.42
1:A:25:VAL:C	1:A:27:LEU:H	2.27	0.42
1:A:425:GLU:OE1	1:C:17:ILE:HD13	2.20	0.42
1:A:576:LYS:O	1:A:580:GLN:HB2	2.20	0.42
1:B:44:VAL:HG13	1:B:45:GLU:HG3	2.01	0.42
1:D:427:MET:HE3	1:D:450:TRP:HH2	1.84	0.42
1:B:431:ALA:HB1	1:B:473:PHE:CZ	2.55	0.41
1:C:266:LYS:O	1:C:270:LEU:HG	2.19	0.41
1:C:572:ASP:O	1:C:576:LYS:HG2	2.20	0.41
1:D:216:GLU:HB3	2:H:21:ARG:O	2.20	0.41
1:D:436:VAL:HG21	1:D:439:PHE:CD1	2.55	0.41
1:D:456:TYR:HA	1:D:459:ARG:HE	1.83	0.41
2:F:14:MET:CE	2:F:24:TRP:HE3	2.33	0.41
1:A:279:THR:O	1:A:284:VAL:HG23	2.20	0.41
1:B:72:GLN:HE21	1:B:72:GLN:HB2	1.60	0.41
1:B:91:PRO:HB2	1:B:92:PRO:HD3	2.02	0.41
1:D:26:GLN:OE1	1:D:26:GLN:HA	2.19	0.41
1:D:96:LEU:C	1:D:98:THR:H	2.28	0.41
2:G:1:MET:HE3	2:G:4:VAL:HG11	2.01	0.41
1:D:35:LEU:HA	1:D:38:ILE:HD12	2.02	0.41
1:A:448:MET:HE2	1:A:448:MET:HB3	1.80	0.41
1:B:522:LEU:HB3	1:B:523:PRO:HD3	2.01	0.41
1:D:541:ALA:C	1:D:543:SER:H	2.28	0.41
1:D:561:LYS:N	1:D:562:PRO:CD	2.84	0.41
2:F:111:CYS:CB	2:F:113:CYS:H	2.33	0.41
2:G:113:CYS:O	2:G:117:LEU:HD13	2.19	0.41
1:A:128:PHE:O	1:A:131:LEU:HB3	2.20	0.41
1:A:320:ASN:C	1:A:324:THR:HG22	2.43	0.41
1:A:417:TRP:CB	1:A:455:VAL:HG21	2.50	0.41
1:C:61:ASP:H	1:C:66:LEU:HD11	1.85	0.41
1:C:456:TYR:OH	1:C:460:GLU:HG3	2.21	0.41
1:C:514:GLN:C	1:C:516:ILE:H	2.28	0.41
2:E:36:LYS:HE2	2:E:36:LYS:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:138:CYS:SG	2:E:139:TYR:N	2.93	0.41
2:H:13:LEU:O	2:H:17:LEU:HB2	2.21	0.41
2:H:94:ALA:O	2:H:95:ILE:HG13	2.21	0.41
1:B:245:MET:HB3	1:B:249:ARG:NH1	2.36	0.41
1:D:180:MET:HE1	2:H:147:TRP:CE3	2.56	0.41
1:D:221:ARG:HD2	1:D:254:ASP:OD1	2.21	0.41
1:B:134:ARG:NH2	1:B:134:ARG:CG	2.82	0.41
1:C:287:PHE:CE2	1:C:291:MET:SD	3.14	0.41
1:C:396:GLY:H	1:C:399:GLN:NE2	2.18	0.41
1:A:417:TRP:HB3	1:A:455:VAL:HG21	2.03	0.41
1:C:33:LYS:C	1:C:35:LEU:H	2.29	0.41
1:D:29:LEU:HD23	1:D:65:VAL:HA	2.02	0.41
1:D:129:VAL:O	1:D:130:PRO:C	2.62	0.41
1:A:278:ILE:HD12	1:A:278:ILE:H	1.86	0.41
1:A:381:ARG:NH2	1:A:407:ALA:HA	2.35	0.41
1:C:52:LEU:HB2	1:C:53:PRO:HD3	2.03	0.41
1:C:178:THR:HA	1:C:179:PRO:HD3	1.98	0.41
1:C:405:LEU:N	1:C:406:PRO:HD2	2.36	0.41
1:D:198:LEU:O	1:D:202:LYS:HD3	2.21	0.41
1:D:377:CYS:HA	1:D:378:PRO:HD3	1.81	0.41
1:D:452:VAL:CG2	1:D:496:LEU:HB3	2.47	0.41
2:E:109:THR:O	2:E:111:CYS:N	2.54	0.41
2:E:110:ASN:HD21	2:H:95:ILE:HG23	1.86	0.41
2:F:14:MET:HE1	2:F:30:MET:HE1	2.03	0.41
2:F:62:MET:O	2:F:63:GLU:C	2.63	0.41
2:G:100:TRP:O	2:G:104:VAL:HG23	2.21	0.41
2:H:55:MET:O	2:H:55:MET:HG2	2.21	0.41
1:B:151:PHE:CD1	1:B:170:PHE:HD2	2.39	0.41
1:C:29:LEU:C	1:C:31:SER:H	2.29	0.41
1:C:43:GLY:C	1:C:45:GLU:H	2.29	0.41
1:D:188:LYS:HD2	1:D:191:GLU:OE1	2.21	0.41
2:G:144:PHE:CG	2:G:160:TRP:HD1	2.39	0.41
1:A:516:ILE:H	1:A:516:ILE:HG13	1.76	0.40
1:B:240:LEU:HD23	1:B:240:LEU:HA	1.80	0.40
1:C:287:PHE:CD2	1:C:291:MET:HE2	2.57	0.40
1:C:417:TRP:HA	1:C:420:ARG:NH1	2.36	0.40
1:D:424:ILE:HG12	1:D:450:TRP:CE3	2.56	0.40
2:H:20:GLU:C	2:H:22:SER:H	2.28	0.40
1:A:487:LEU:C	1:A:489:MET:N	2.77	0.40
1:C:351:GLY:HA2	1:C:390:CYS:SG	2.61	0.40
1:C:427:MET:HB3	1:C:465:ASN:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1:MET:HA	2:E:4:VAL:HG23	2.02	0.40
2:E:109:THR:C	2:E:111:CYS:H	2.29	0.40
2:G:31:ARG:HG2	2:G:59:TYR:OH	2.22	0.40
1:C:21:ARG:HB3	1:C:22:ASN:H	1.66	0.40
1:D:466:LEU:O	1:D:470:VAL:HG23	2.22	0.40
2:E:27:ILE:H	2:E:27:ILE:HG12	1.74	0.40
2:E:100:TRP:CD1	2:F:95:ILE:HG22	2.57	0.40
2:F:109:THR:HG22	2:F:119:ARG:NH2	2.32	0.40
2:H:119:ARG:HH21	2:H:119:ARG:HG2	1.86	0.40
1:A:33:LYS:N	1:A:33:LYS:CD	2.83	0.40
1:B:86:VAL:HG13	1:B:119:HIS:CE1	2.55	0.40
1:D:556:LEU:HD23	1:D:560:VAL:HG21	2.04	0.40
1:A:42:LEU:O	1:A:46:ARG:HB2	2.22	0.40
1:A:563:ILE:HD13	1:A:563:ILE:HA	1.98	0.40
1:C:131:LEU:HD12	1:C:131:LEU:C	2.46	0.40
1:D:119:HIS:O	1:D:157:ARG:NH1	2.55	0.40
2:F:139:TYR:O	2:F:140:CYS:C	2.63	0.40
2:G:99:GLN:HE21	2:G:102:GLU:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	573/589 (97%)	505 (88%)	53 (9%)	15 (3%)	4	21
1	B	573/589 (97%)	507 (88%)	57 (10%)	9 (2%)	7	30
1	C	575/589 (98%)	502 (87%)	65 (11%)	8 (1%)	9	34
1	D	575/589 (98%)	477 (83%)	85 (15%)	13 (2%)	5	23
2	E	157/174 (90%)	127 (81%)	20 (13%)	10 (6%)	1	6
2	F	146/174 (84%)	112 (77%)	24 (16%)	10 (7%)	1	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	136/174 (78%)	114 (84%)	17 (12%)	5 (4%)	2	15
2	H	137/174 (79%)	106 (77%)	18 (13%)	13 (10%)	0	3
All	All	2872/3052 (94%)	2450 (85%)	339 (12%)	83 (3%)	3	19

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ALA
1	B	97	ALA
1	B	316	ASP
1	B	317	CYS
1	B	401	SER
1	C	25	VAL
1	C	474	GLY
2	E	42	HIS
2	E	106	LYS
2	E	110	ASN
2	F	2	ASP
2	F	63	GLU
2	F	138	CYS
2	G	100	TRP
2	H	3	LYS
2	H	7	ARG
2	H	72	PRO
1	A	237	GLN
1	A	316	ASP
1	A	443	LEU
1	C	315	ALA
1	C	469	LEU
1	D	43	GLY
1	D	160	SER
1	D	369	PHE
1	D	386	SER
1	D	573	VAL
2	E	92	VAL
2	E	105	LYS
2	E	136	VAL
2	E	152	LEU
2	E	169	TYR
2	F	52	MET
2	H	70	HIS

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Mol	Chain	Res	Type
2	H	95	ILE
2	H	100	TRP
2	H	106	LYS
2	H	136	VAL
2	H	152	LEU
1	A	50	GLU
1	A	199	ASP
1	A	320	ASN
1	A	573	VAL
1	B	549	PRO
1	C	441	GLU
1	D	401	SER
1	D	522	LEU
1	D	571	GLN
2	F	5	LEU
2	H	24	TRP
1	A	48	ARG
1	A	349	ILE
1	A	488	ALA
1	B	25	VAL
1	D	564	LEU
2	F	22	SER
2	G	105	LYS
2	H	65	GLY
1	A	97	ALA
1	A	348	VAL
1	A	515	ASP
1	B	403	SER
1	C	44	VAL
1	C	471	GLU
1	C	515	ASP
1	D	57	ASP
1	D	306	VAL
2	F	93	ASP
2	H	21	ARG
2	H	107	MET
1	B	209	PHE
1	B	210	SER
1	D	547	ILE
1	D	553	ASN
2	F	169	TYR
2	G	152	LEU

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Mol	Chain	Res	Type
2	E	90	PRO
2	F	136	VAL
2	G	112	ILE
2	G	136	VAL
1	A	482	ILE
2	E	43	PRO
2	F	90	PRO

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	501/512 (98%)	447 (89%)	54 (11%)	6	25
1	B	501/512 (98%)	446 (89%)	55 (11%)	6	24
1	C	502/512 (98%)	439 (88%)	63 (12%)	4	19
1	D	503/512 (98%)	442 (88%)	61 (12%)	5	20
2	E	138/157 (88%)	113 (82%)	25 (18%)	2	8
2	F	134/157 (85%)	106 (79%)	28 (21%)	1	5
2	G	128/157 (82%)	100 (78%)	28 (22%)	1	4
2	H	128/157 (82%)	103 (80%)	25 (20%)	1	6
All	All	2535/2676 (95%)	2196 (87%)	339 (13%)	4	17

All (339) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	51	LEU
1	A	52	LEU
1	A	55	LEU
1	A	60	TYR
1	A	67	LEU
1	A	72	GLN
1	A	78	THR

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Mol	Chain	Res	Type
1	A	85	TYR
1	A	103	VAL
1	A	107	LYS
1	A	110	GLU
1	A	111	SER
1	A	125	GLU
1	A	152	SER
1	A	159	SER
1	A	175	SER
1	A	178	THR
1	A	187	SER
1	A	194	LYS
1	A	196	LEU
1	A	197	GLU
1	A	200	ASN
1	A	222	LEU
1	A	234	LEU
1	A	235	LEU
1	A	237	GLN
1	A	238	GLU
1	A	241	GLU
1	A	250	GLN
1	A	270	LEU
1	A	271	GLN
1	A	274	VAL
1	A	283	LEU
1	A	323	MET
1	A	327	LEU
1	A	348	VAL
1	A	355	ILE
1	A	363	GLU
1	A	365	LEU
1	A	368	LEU
1	A	370	LEU
1	A	408	ILE
1	A	409	VAL
1	A	413	GLU
1	A	423	ILE
1	A	446	LEU
1	A	466	LEU
1	A	504	CYS
1	A	511	VAL

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Mol	Chain	Res	Type
1	A	516	ILE
1	A	519	LYS
1	A	571	GLN
1	A	576	LYS
1	B	16	LEU
1	B	21	ARG
1	B	23	GLU
1	B	25	VAL
1	B	29	LEU
1	B	34	LYS
1	B	35	LEU
1	B	37	THR
1	B	40	LEU
1	B	44	VAL
1	B	51	LEU
1	B	52	LEU
1	B	64	GLU
1	B	72	GLN
1	B	98	THR
1	B	111	SER
1	B	122	SER
1	B	124	LEU
1	B	125	GLU
1	B	139	ASP
1	B	143	SER
1	B	187	SER
1	B	191	GLU
1	B	194	LYS
1	B	198	LEU
1	B	208	MET
1	B	212	LEU
1	B	218	ASP
1	B	222	LEU
1	B	250	GLN
1	B	256	SER
1	B	277	GLU
1	B	295	GLU
1	B	316	ASP
1	B	318	ARG
1	B	323	MET
1	B	327	LEU
1	B	352	LEU

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Mol	Chain	Res	Type
1	B	381	ARG
1	B	405	LEU
1	B	410	GLU
1	B	418	ARG
1	B	419	VAL
1	B	427	MET
1	B	430	LEU
1	B	441	GLU
1	B	460	GLU
1	B	465	ASN
1	B	466	LEU
1	B	468	LYS
1	B	479	HIS
1	B	481	THR
1	B	496	LEU
1	B	502	LEU
1	B	515	ASP
1	C	13	ILE
1	C	16	LEU
1	C	17	ILE
1	C	20	LEU
1	C	21	ARG
1	C	25	VAL
1	C	27	LEU
1	C	29	LEU
1	C	32	ILE
1	C	35	LEU
1	C	38	ILE
1	C	45	GLU
1	C	51	LEU
1	C	55	LEU
1	C	57	ASP
1	C	63	ASP
1	C	66	LEU
1	C	73	LEU
1	C	79	LEU
1	C	102	THR
1	C	129	VAL
1	C	131	LEU
1	C	140	TRP
1	C	145	THR
1	C	153	VAL

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Mol	Chain	Res	Type
1	C	160	SER
1	C	165	GLU
1	C	175	SER
1	C	178	THR
1	C	189	LEU
1	C	191	GLU
1	C	194	LYS
1	C	198	LEU
1	C	202	LYS
1	C	204	GLU
1	C	218	ASP
1	C	222	LEU
1	C	241	GLU
1	C	255	LYS
1	C	269	GLU
1	C	272	LYS
1	C	274	VAL
1	C	282	ASP
1	C	283	LEU
1	C	307	LYS
1	C	320	ASN
1	C	326	ILE
1	C	385	ILE
1	C	398	ARG
1	C	400	LEU
1	C	402	GLN
1	C	427	MET
1	C	444	ASN
1	C	448	MET
1	C	458	ILE
1	C	463	THR
1	C	464	SER
1	C	475	LYS
1	C	481	THR
1	C	502	LEU
1	C	524	THR
1	C	555	THR
1	C	584	THR
1	D	13	ILE
1	D	16	LEU
1	D	20	LEU
1	D	21	ARG

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Mol	Chain	Res	Type
1	D	25	VAL
1	D	27	LEU
1	D	29	LEU
1	D	32	ILE
1	D	37	THR
1	D	47	THR
1	D	55	LEU
1	D	66	LEU
1	D	67	LEU
1	D	75	THR
1	D	79	LEU
1	D	86	VAL
1	D	98	THR
1	D	102	THR
1	D	131	LEU
1	D	139	ASP
1	D	157	ARG
1	D	216	GLU
1	D	222	LEU
1	D	248	LEU
1	D	266	LYS
1	D	271	GLN
1	D	280	LYS
1	D	281	THR
1	D	290	LEU
1	D	313	LEU
1	D	316	ASP
1	D	320	ASN
1	D	333	LEU
1	D	334	VAL
1	D	345	LEU
1	D	361	THR
1	D	370	LEU
1	D	376	GLU
1	D	382	LEU
1	D	385	ILE
1	D	391	VAL
1	D	395	ILE
1	D	397	ILE
1	D	400	LEU
1	D	403	SER
1	D	404	LEU

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Mol	Chain	Res	Type
1	D	409	VAL
1	D	416	LYS
1	D	423	ILE
1	D	436	VAL
1	D	441	GLU
1	D	469	LEU
1	D	481	THR
1	D	486	VAL
1	D	510	GLU
1	D	515	ASP
1	D	525	VAL
1	D	547	ILE
1	D	583	LEU
1	D	584	THR
1	D	585	VAL
2	E	5	LEU
2	E	6	ASN
2	E	7	ARG
2	E	8	GLU
2	E	31	ARG
2	E	35	LEU
2	E	52	MET
2	E	53	LYS
2	E	54	LYS
2	E	61	LYS
2	E	62	MET
2	E	97	CYS
2	E	105	LYS
2	E	106	LYS
2	E	107	MET
2	E	109	THR
2	E	115	LEU
2	E	123	GLU
2	E	131	ASP
2	E	134	VAL
2	E	146	MET
2	E	152	LEU
2	E	153	CYS
2	E	163	ILE
2	E	168	THR
2	F	7	ARG
2	F	19	LEU

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Mol	Chain	Res	Type
2	F	21	ARG
2	F	30	MET
2	F	31	ARG
2	F	35	LEU
2	F	53	LYS
2	F	61	LYS
2	F	97	CYS
2	F	105	LYS
2	F	107	MET
2	F	110	ASN
2	F	112	ILE
2	F	113	CYS
2	F	117	LEU
2	F	118	LEU
2	F	120	MET
2	F	123	GLU
2	F	126	LYS
2	F	131	ASP
2	F	134	VAL
2	F	136	VAL
2	F	152	LEU
2	F	153	CYS
2	F	159	LEU
2	F	163	ILE
2	F	164	ILE
2	F	168	THR
2	G	1	MET
2	G	5	LEU
2	G	6	ASN
2	G	7	ARG
2	G	19	LEU
2	G	31	ARG
2	G	53	LYS
2	G	54	LYS
2	G	63	GLU
2	G	107	MET
2	G	109	THR
2	G	112	ILE
2	G	113	CYS
2	G	114	LEU
2	G	115	LEU
2	G	118	LEU

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Mol	Chain	Res	Type
2	G	120	MET
2	G	123	GLU
2	G	127	LEU
2	G	131	ASP
2	G	134	VAL
2	G	136	VAL
2	G	152	LEU
2	G	153	CYS
2	G	157	LEU
2	G	159	LEU
2	G	163	ILE
2	G	171	ASP
2	H	1	MET
2	H	2	ASP
2	H	6	ASN
2	H	9	GLU
2	H	21	ARG
2	H	54	LYS
2	H	58	LEU
2	H	61	LYS
2	H	62	MET
2	H	67	LYS
2	H	70	HIS
2	H	105	LYS
2	H	109	THR
2	H	111	CYS
2	H	115	LEU
2	H	118	LEU
2	H	119	ARG
2	H	124	ASN
2	H	127	LEU
2	H	129	ARG
2	H	131	ASP
2	H	134	VAL
2	H	136	VAL
2	H	164	ILE
2	H	170	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN

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Mol	Chain	Res	Type
1	A	117	HIS
1	A	119	HIS
1	A	127	HIS
1	A	217	GLN
1	A	271	GLN
1	A	288	GLN
1	A	338	ASN
1	A	339	GLN
1	A	387	ASN
1	A	465	ASN
1	A	494	ASN
1	A	506	ASN
1	A	571	GLN
1	B	26	GLN
1	B	30	ASN
1	B	72	GLN
1	B	217	GLN
1	B	230	ASN
1	B	237	GLN
1	B	250	GLN
1	B	271	GLN
1	B	289	ASN
1	B	325	GLN
1	B	338	ASN
1	B	340	HIS
1	B	392	ASN
1	B	402	GLN
1	B	465	ASN
1	B	506	ASN
1	B	514	GLN
1	B	520	HIS
1	B	535	ASN
1	B	539	ASN
1	B	545	GLN
1	B	580	GLN
1	C	22	ASN
1	C	119	HIS
1	C	127	HIS
1	C	211	ASN
1	C	230	ASN
1	C	271	GLN
1	C	288	GLN

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Mol	Chain	Res	Type
1	C	289	ASN
1	C	312	ASN
1	C	320	ASN
1	C	325	GLN
1	C	338	ASN
1	C	339	GLN
1	C	399	GLN
1	C	433	GLN
1	C	444	ASN
1	C	465	ASN
1	C	506	ASN
1	C	535	ASN
1	C	539	ASN
1	C	545	GLN
1	C	557	GLN
1	D	119	HIS
1	D	168	GLN
1	D	211	ASN
1	D	230	ASN
1	D	233	GLN
1	D	288	GLN
1	D	289	ASN
1	D	360	ASN
1	D	454	HIS
1	D	465	ASN
1	D	497	HIS
1	D	535	ASN
2	E	6	ASN
2	E	110	ASN
2	E	122	HIS
2	F	110	ASN
2	F	122	HIS
2	G	6	ASN
2	G	12	GLN
2	G	99	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	575/589 (97%)	-0.33	0 100 100	98, 114, 132, 146	0
1	B	575/589 (97%)	-0.36	1 (0%) 91 83	96, 112, 123, 132	0
1	C	577/589 (97%)	-0.29	1 (0%) 91 83	98, 114, 131, 135	0
1	D	577/589 (97%)	-0.19	4 (0%) 84 68	98, 113, 140, 146	0
2	E	163/174 (93%)	-0.39	0 100 100	103, 113, 123, 133	0
2	F	152/174 (87%)	-0.20	2 (1%) 75 56	103, 114, 127, 136	0
2	G	142/174 (81%)	-0.24	2 (1%) 73 53	99, 114, 121, 125	0
2	H	143/174 (82%)	-0.24	0 100 100	96, 112, 121, 127	0
All	All	2904/3052 (95%)	-0.29	10 (0%) 90 80	96, 113, 133, 146	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	23	GLU	3.3
2	G	104	VAL	3.2
1	C	13	ILE	3.1
2	F	96	TYR	2.8
2	G	1	MET	2.5
2	F	50	GLU	2.2
1	B	228	CYS	2.1
1	D	496	LEU	2.1
1	D	557	GLN	2.1
1	D	583	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
3	ZN	E	602	1/1	0.93	0.10	99,99,99,99	0
3	ZN	F	702	1/1	0.95	0.10	100,100,100,100	0
3	ZN	E	601	1/1	0.98	0.09	103,103,103,103	0
3	ZN	G	801	1/1	0.98	0.04	108,108,108,108	0
3	ZN	H	901	1/1	0.98	0.05	101,101,101,101	0
3	ZN	G	802	1/1	0.99	0.04	98,98,98,98	0
3	ZN	F	701	1/1	0.99	0.06	108,108,108,108	0
3	ZN	H	902	1/1	0.99	0.12	98,98,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.