



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:01 AM UTC

PDB ID : 2Y1M / pdb_00002y1m
Title : Structure of native c-Cbl
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Deposited on : 2010-12-08
Resolution : 2.67 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

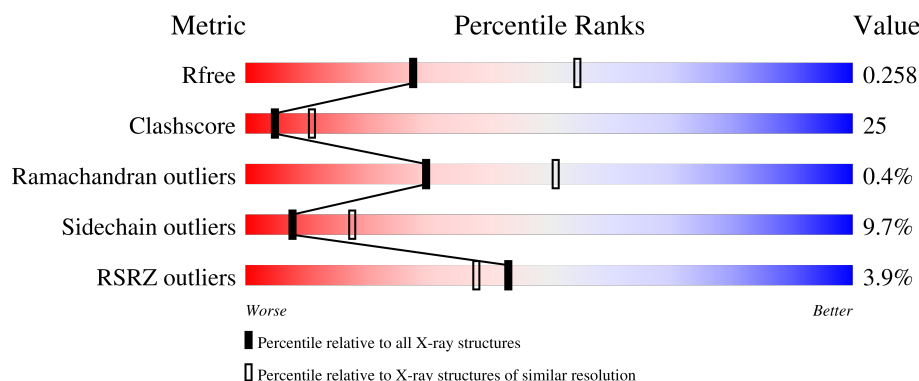
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	389	
1	B	389	
1	C	389	
1	D	389	
1	E	389	

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Mol	Chain	Length	Quality of chain
1	F	389	4% 54% 37% 7% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18832 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 E3 UBIQUITIN-PROTEIN LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			3113	2000	523	565	25			
1	B	385	Total	C	N	O	S	0	0	0
			3121	2006	524	566	25			
1	C	385	Total	C	N	O	S	0	0	0
			3116	2002	524	565	25			
1	D	385	Total	C	N	O	S	0	0	0
			3123	2005	524	569	25			
1	E	383	Total	C	N	O	S	0	0	0
			3106	1996	522	563	25			
1	F	384	Total	C	N	O	S	0	0	0
			3114	2000	523	566	25			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		
2	D	2	Total	Zn	0	0
			2	2		
2	E	2	Total	Zn	0	0
			2	2		
2	F	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

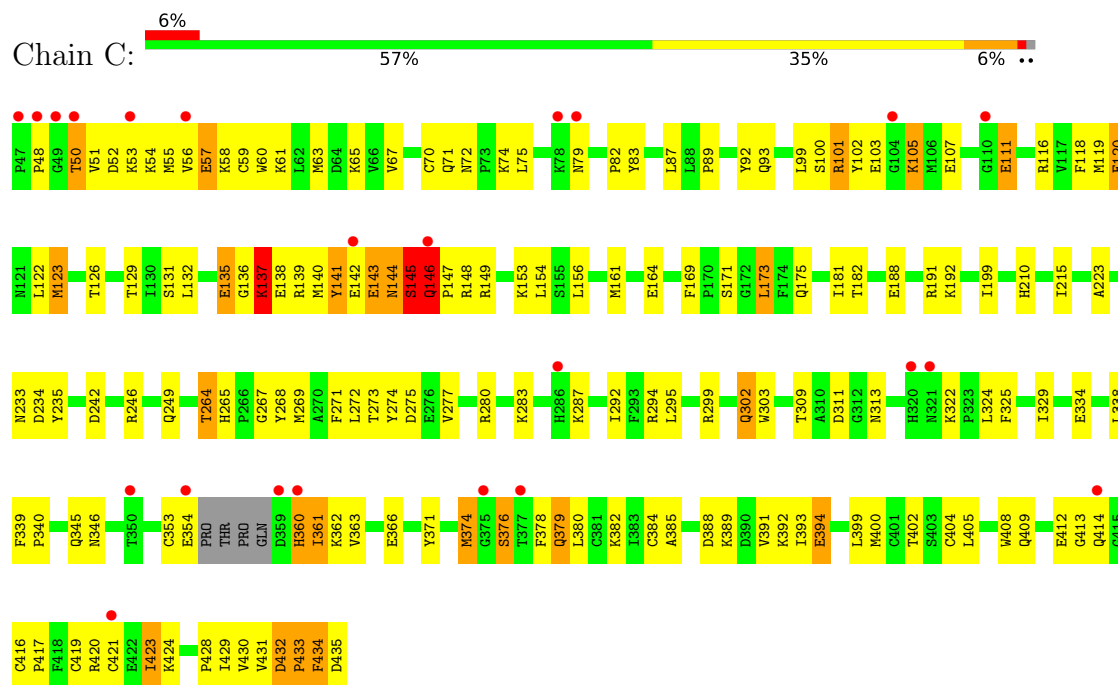
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0

- Molecule 4 is water.

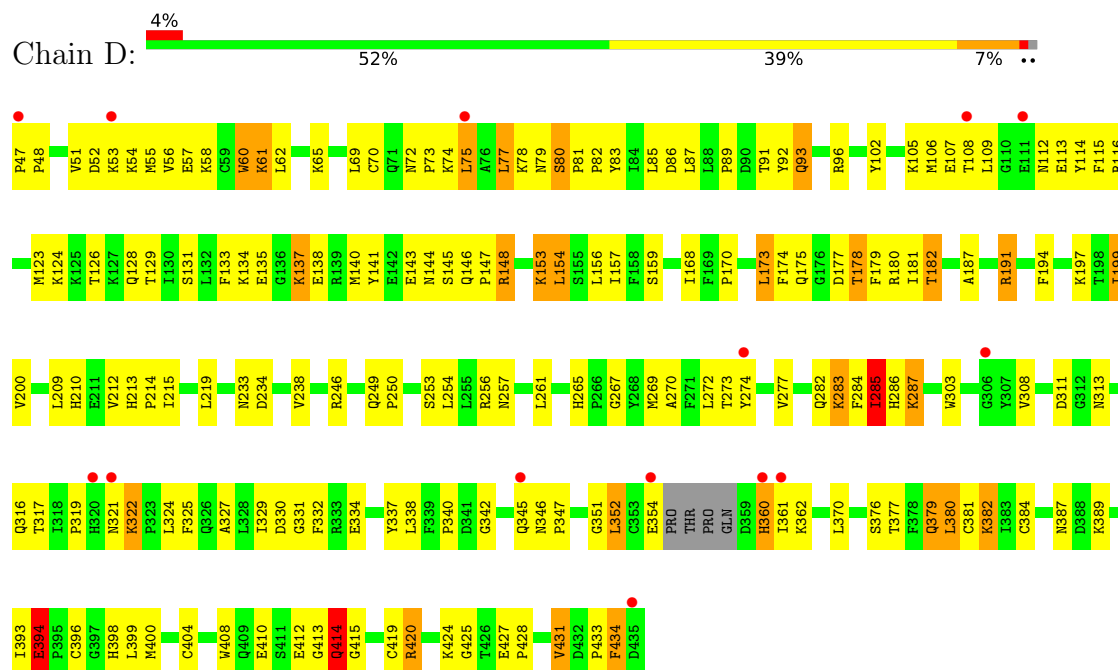
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	32	Total O 32 32	0	0
4	B	23	Total O 23 23	0	0
4	C	27	Total O 27 27	0	0
4	D	17	Total O 17 17	0	0
4	E	12	Total O 12 12	0	0
4	F	10	Total O 10 10	0	0



• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE

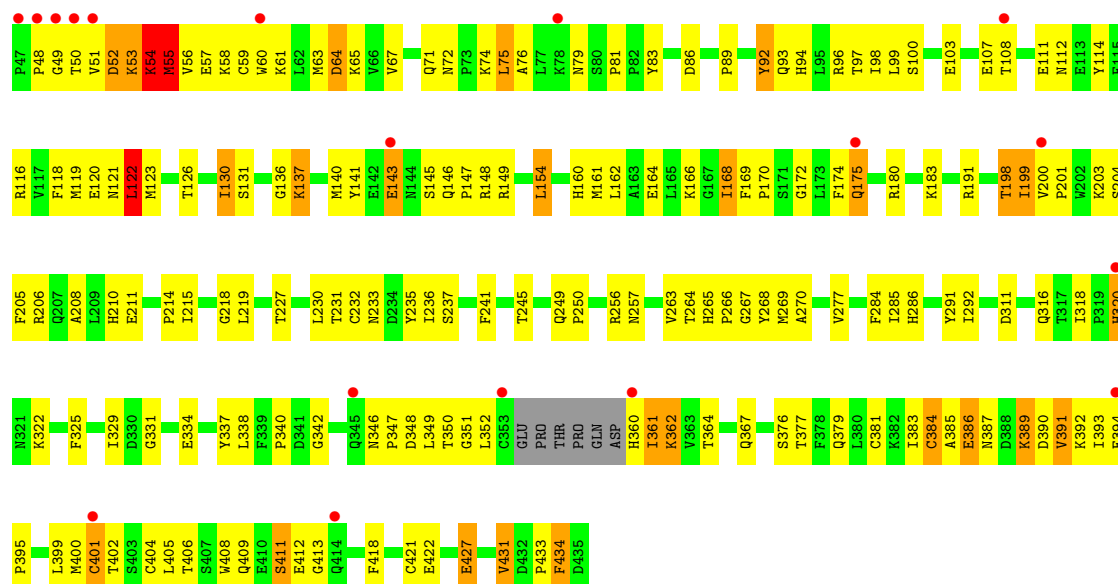


• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE

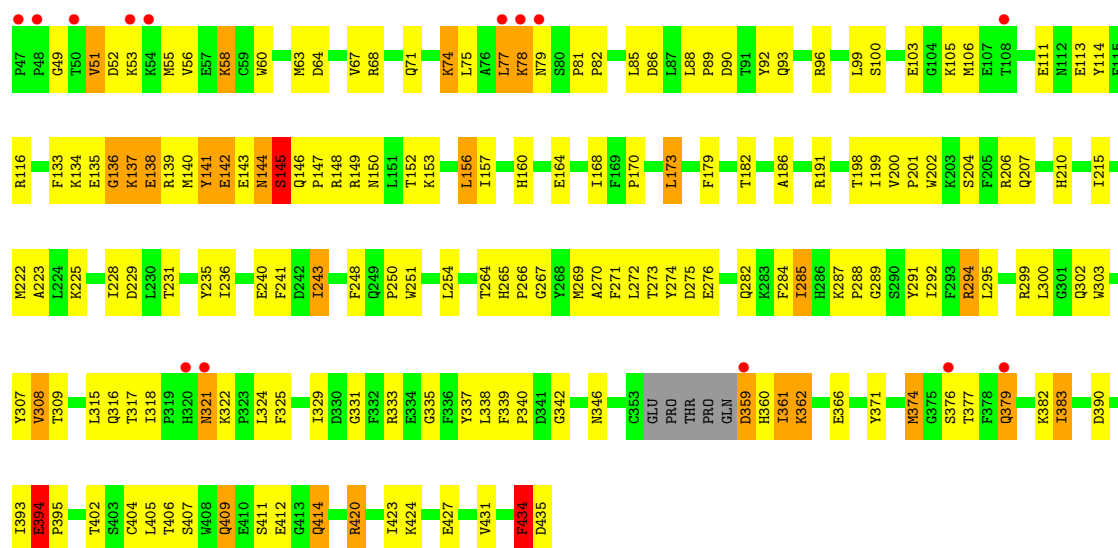


• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE





• Molecule 1: E3 UBIQUITIN-PROTEIN LIGASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	146.80Å 148.56Å 348.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.62 – 2.67 47.62 – 2.67	Depositor EDS
% Data completeness (in resolution range)	94.5 (47.62-2.67) 97.1 (47.62-2.67)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.08 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.218 , 0.263 0.216 , 0.258	Depositor DCC
R_{free} test set	5239 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18832	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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: CA, 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	0.71	0/3192	1.01	10/4310 (0.2%)
1	B	0.70	2/3201 (0.1%)	0.98	9/4323 (0.2%)
1	C	0.65	0/3195	0.97	8/4313 (0.2%)
1	D	0.64	1/3202 (0.0%)	0.97	10/4322 (0.2%)
1	E	0.65	0/3185	1.00	10/4299 (0.2%)
1	F	0.63	0/3193	0.98	8/4310 (0.2%)
All	All	0.66	3/19168 (0.0%)	0.99	55/25877 (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	1
1	C	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	318	ILE	CA-CB	-6.71	1.49	1.54
1	B	385	ALA	CA-CB	-6.29	1.45	1.53
1	D	60	TRP	CA-C	-5.57	1.46	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	145	SER	N-CA-C	-10.12	97.17	110.43
1	A	351	GLY	N-CA-C	-9.33	103.59	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	424	LYS	N-CA-C	-8.74	101.97	114.12
1	B	72	ASN	CA-C-N	8.54	128.24	119.19
1	B	72	ASN	C-N-CA	8.54	128.24	119.19
1	D	352	LEU	N-CA-C	-8.35	102.88	113.23
1	E	54	LYS	N-CA-C	-8.02	103.33	113.43
1	C	141	TYR	N-CA-C	-7.79	103.50	113.16
1	B	375	GLY	N-CA-C	7.49	122.72	114.40
1	C	146	GLN	CA-C-N	-7.44	111.23	118.97
1	C	146	GLN	C-N-CA	-7.44	111.23	118.97
1	D	351	GLY	N-CA-C	-7.18	105.15	114.85
1	D	413	GLY	N-CA-C	-7.11	102.41	112.37
1	F	394	GLU	N-CA-C	-6.80	100.05	110.32
1	D	394	GLU	N-CA-C	-6.73	101.02	110.31
1	F	137	LYS	CB-CA-C	-6.70	108.84	116.54
1	C	137	LYS	CB-CA-C	-6.43	109.17	116.63
1	B	137	LYS	CB-CA-C	-6.42	109.16	116.54
1	B	318	ILE	CB-CA-C	-6.22	104.09	110.13
1	E	55	MET	N-CA-C	-6.20	104.44	111.07
1	A	216	SER	N-CA-C	6.20	120.44	113.01
1	A	273	THR	N-CA-C	-6.18	102.56	110.53
1	A	188	GLU	CB-CA-C	-6.06	101.11	110.81
1	E	137	LYS	CB-CA-C	-6.03	109.61	116.54
1	C	423	ILE	CB-CA-C	-6.02	103.32	111.63
1	D	254	LEU	N-CA-C	5.97	117.58	111.14
1	E	168	ILE	N-CA-C	-5.95	107.01	112.96
1	E	384	CYS	N-CA-C	-5.90	104.79	112.23
1	F	434	PHE	N-CA-C	-5.90	100.58	109.79
1	A	350	THR	N-CA-C	-5.88	102.72	110.43
1	F	136	GLY	N-CA-C	-5.86	107.40	114.66
1	A	434	PHE	N-CA-C	-5.84	99.72	109.24
1	A	81	PRO	O-C-N	5.84	123.89	121.15
1	E	92	TYR	N-CA-C	-5.82	104.57	111.03
1	F	383	ILE	N-CA-C	-5.77	105.46	111.58
1	D	414	GLN	N-CA-C	5.56	117.20	111.03
1	A	228	ILE	CB-CA-C	-5.56	104.94	111.94
1	F	376	SER	N-CA-C	5.55	115.89	108.23
1	D	270	ALA	CB-CA-C	-5.50	110.21	116.54
1	C	143	GLU	N-CA-C	5.42	117.19	111.28
1	B	80	SER	CA-C-N	5.39	125.94	120.38
1	B	80	SER	C-N-CA	5.39	125.94	120.38
1	C	145	SER	N-CA-C	5.35	118.81	112.72
1	D	434	PHE	N-CA-C	-5.32	99.84	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	212	VAL	CB-CA-C	-5.31	105.70	110.91
1	E	391	VAL	N-CA-C	5.23	115.10	107.88
1	B	423	ILE	CB-CA-C	-5.22	103.94	111.19
1	F	58	LYS	N-CA-C	-5.20	105.69	111.36
1	C	302	GLN	N-CA-C	5.17	117.87	109.24
1	E	270	ALA	CB-CA-C	-5.14	110.62	116.54
1	E	218	GLY	N-CA-C	-5.13	107.66	115.66
1	D	287	LYS	CA-C-N	5.12	125.28	119.90
1	D	287	LYS	C-N-CA	5.12	125.28	119.90
1	B	394	GLU	N-CA-C	-5.12	102.27	110.10
1	E	122	LEU	N-CA-C	-5.04	107.52	113.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	321	ASN	Peptide
1	C	144	ASN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3113	0	3082	127	0
1	B	3121	0	3091	136	0
1	C	3116	0	3083	162	0
1	D	3123	0	3088	173	0
1	E	3106	0	3079	206	0
1	F	3114	0	3082	169	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	32	0	0	0	0
4	B	23	0	0	0	0
4	C	27	0	0	0	0
4	D	17	0	0	0	0
4	E	12	0	0	0	0
4	F	10	0	0	0	0
All	All	18832	0	18505	946	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 25.

All (946) 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:F:143:GLU:HG2	1:F:144:ASN:ND2	1.36	1.38
1:E:145:SER:OG	1:E:147:PRO:HD2	1.43	1.17
1:C:361:ILE:O	1:C:361:ILE:HD12	1.45	1.16
1:D:282:GLN:HE22	1:D:285:ILE:HD11	1.08	1.12
1:C:101:ARG:HD3	1:C:173:LEU:HD23	1.31	1.11
1:D:48:PRO:HG2	1:D:116:ARG:HH12	1.10	1.10
1:A:146:GLN:HG3	1:A:379:GLN:NE2	1.68	1.08
1:B:395:PRO:HD3	1:B:424:LYS:HG3	1.35	1.07
1:B:53:LYS:O	1:B:57:GLU:HG2	1.52	1.07
1:C:101:ARG:HD3	1:C:173:LEU:CD2	1.84	1.06
1:C:140:MET:HE2	1:C:147:PRO:HB3	1.35	1.06
1:E:383:ILE:HD11	1:E:404:CYS:HB3	1.34	1.05
1:C:145:SER:O	1:C:147:PRO:HD2	1.58	1.04
1:F:143:GLU:C	1:F:144:ASN:HD22	1.66	1.03
1:D:210:HIS:CD2	1:D:215:ILE:H	1.78	1.00
1:E:53:LYS:C	1:E:53:LYS:HD2	1.84	1.00
1:E:54:LYS:HD3	1:E:55:MET:N	1.77	1.00
1:F:139:ARG:O	1:F:142:GLU:HB2	1.61	1.00
1:C:101:ARG:CD	1:C:173:LEU:HD23	1.92	0.99
1:D:257:ASN:OD1	1:D:352:LEU:HD22	1.60	0.99
1:E:54:LYS:HZ2	1:E:54:LYS:C	1.71	0.99
1:F:143:GLU:HG2	1:F:144:ASN:HD21	1.23	0.98
1:C:361:ILE:HD12	1:C:361:ILE:C	1.88	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:LYS:HD3	1:E:55:MET:H	1.28	0.98
1:C:210:HIS:HD2	1:C:215:ILE:H	1.12	0.98
1:C:132:LEU:HG	1:C:140:MET:HE1	1.43	0.97
1:E:53:LYS:HE3	1:E:57:GLU:OE1	1.64	0.97
1:B:62:LEU:HB3	1:B:126:THR:HG21	1.45	0.96
1:D:282:GLN:NE2	1:D:285:ILE:HD11	1.80	0.96
1:C:376:SER:HB2	1:C:382:LYS:NZ	1.81	0.95
1:A:210:HIS:HD2	1:A:215:ILE:H	1.14	0.95
1:A:265:HIS:CD2	1:A:267:GLY:H	1.85	0.95
1:F:77:LEU:HD12	1:F:77:LEU:H	1.29	0.95
1:E:265:HIS:HD2	1:E:267:GLY:H	1.12	0.94
1:B:431:VAL:O	1:B:433:PRO:HD3	1.67	0.94
1:A:265:HIS:HD2	1:A:267:GLY:H	1.01	0.93
1:C:142:GLU:HB3	1:C:145:SER:HB2	1.50	0.93
1:B:265:HIS:HD2	1:B:267:GLY:H	1.16	0.93
1:D:379:GLN:HG3	1:D:431:VAL:HG13	1.51	0.92
1:D:340:PRO:HD3	1:D:346:ASN:HD22	1.34	0.92
1:C:52:ASP:OD1	1:C:54:LYS:HG2	1.69	0.91
1:F:273:THR:HG22	1:F:275:ASP:H	1.34	0.91
1:F:142:GLU:HB3	1:F:145:SER:OG	1.70	0.91
1:F:143:GLU:CG	1:F:144:ASN:ND2	2.32	0.91
1:B:380:LEU:O	1:B:382:LYS:HE3	1.70	0.91
1:E:121:ASN:OD1	1:E:233:ASN:HB3	1.70	0.90
1:C:432:ASP:HB3	1:C:435:ASP:HB3	1.51	0.90
1:C:265:HIS:HD2	1:C:267:GLY:H	1.18	0.90
1:F:146:GLN:HE21	1:F:377:THR:CG2	1.84	0.90
1:D:210:HIS:HD2	1:D:215:ILE:H	0.93	0.89
1:D:47:PRO:N	1:D:48:PRO:HD2	1.87	0.89
1:E:63:MET:CE	1:E:122:LEU:HD21	2.02	0.89
1:F:143:GLU:HG2	1:F:144:ASN:HD22	1.15	0.89
1:E:256:ARG:HG3	1:E:256:ARG:HH11	1.36	0.89
1:D:52:ASP:OD1	1:D:54:LYS:HB3	1.73	0.88
1:E:331:GLY:HA3	1:E:337:TYR:CD2	2.08	0.88
1:C:142:GLU:HB3	1:C:145:SER:CB	2.04	0.88
1:D:48:PRO:HG2	1:D:116:ARG:NH1	1.87	0.87
1:D:72:ASN:O	1:D:75:LEU:HB2	1.74	0.87
1:A:265:HIS:HD2	1:A:267:GLY:N	1.73	0.87
1:C:142:GLU:O	1:C:145:SER:HB3	1.74	0.87
1:F:282:GLN:HE22	1:F:285:ILE:HD13	1.39	0.87
1:B:412:GLU:O	1:B:412:GLU:HG2	1.74	0.86
1:A:273:THR:HG22	1:A:276:GLU:H	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ASN:HB3	1:D:75:LEU:HD22	1.55	0.86
1:F:100:SER:O	1:F:103:GLU:HG3	1.75	0.86
1:D:210:HIS:HD2	1:D:215:ILE:N	1.73	0.85
1:F:265:HIS:HD2	1:F:267:GLY:H	1.18	0.85
1:A:423:ILE:C	1:A:423:ILE:HD12	2.03	0.84
1:B:354:GLU:OE2	1:B:355:PRO:HD2	1.78	0.83
1:A:210:HIS:CD2	1:A:215:ILE:H	1.97	0.83
1:F:210:HIS:HD2	1:F:215:ILE:H	1.22	0.83
1:E:53:LYS:HE3	1:E:57:GLU:CD	2.04	0.83
1:C:376:SER:HB2	1:C:382:LYS:HZ3	1.40	0.82
1:E:384:CYS:HB2	1:E:386:GLU:HG3	1.62	0.82
1:F:146:GLN:HG3	1:F:379:GLN:OE1	1.79	0.81
1:A:423:ILE:HD12	1:A:423:ILE:O	1.78	0.81
1:F:146:GLN:HE22	1:F:149:ARG:HH11	1.24	0.81
1:E:340:PRO:HD3	1:E:346:ASN:HD22	1.44	0.81
1:D:70:CYS:HA	1:D:75:LEU:HD23	1.61	0.80
1:F:146:GLN:NE2	1:F:149:ARG:HH11	1.78	0.80
1:D:338:LEU:O	1:D:346:ASN:HB2	1.81	0.80
1:E:100:SER:O	1:E:103:GLU:HG2	1.82	0.80
1:E:384:CYS:HB2	1:E:386:GLU:CG	2.12	0.80
1:F:149:ARG:NH1	1:F:377:THR:HG23	1.95	0.79
1:C:131:SER:O	1:C:135:GLU:HG2	1.82	0.79
1:C:140:MET:HE2	1:C:147:PRO:CB	2.11	0.79
1:C:360:HIS:ND1	1:C:360:HIS:N	2.31	0.79
1:B:62:LEU:HB3	1:B:126:THR:CG2	2.13	0.79
1:B:59:CYS:O	1:B:63:MET:HG3	1.82	0.79
1:F:81:PRO:HA	1:F:82:PRO:C	2.07	0.79
1:B:58:LYS:HD3	1:B:123:MET:HE2	1.65	0.78
1:C:139:ARG:O	1:C:142:GLU:HB2	1.84	0.78
1:B:399:LEU:HD22	1:B:429:ILE:HD13	1.65	0.78
1:C:210:HIS:CD2	1:C:215:ILE:H	2.00	0.78
1:C:145:SER:O	1:C:147:PRO:CD	2.32	0.78
1:C:139:ARG:O	1:C:142:GLU:CB	2.31	0.77
1:E:143:GLU:HA	1:E:143:GLU:OE1	1.84	0.77
1:F:141:TYR:CD1	1:F:141:TYR:N	2.48	0.77
1:F:316:GLN:O	1:F:316:GLN:HG3	1.85	0.76
1:F:142:GLU:CB	1:F:145:SER:OG	2.33	0.76
1:C:50:THR:HA	1:C:116:ARG:HD2	1.68	0.76
1:B:210:HIS:HD2	1:B:214:PRO:HA	1.51	0.76
1:F:143:GLU:O	1:F:144:ASN:HB2	1.86	0.76
1:F:321:ASN:C	1:F:321:ASN:HD22	1.94	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:ILE:CG2	1:C:423:ILE:HG13	2.15	0.76
1:E:143:GLU:OE1	1:E:143:GLU:CA	2.33	0.76
1:C:233:ASN:ND2	1:C:235:TYR:HB2	1.99	0.75
1:F:143:GLU:C	1:F:144:ASN:ND2	2.45	0.75
1:D:265:HIS:CD2	1:D:267:GLY:H	2.04	0.75
1:C:101:ARG:CD	1:C:173:LEU:CD2	2.57	0.75
1:F:146:GLN:NE2	1:F:377:THR:HG23	2.02	0.75
1:F:321:ASN:C	1:F:321:ASN:ND2	2.42	0.75
1:D:53:LYS:O	1:D:57:GLU:HG2	1.86	0.74
1:D:233:ASN:O	1:D:234:ASP:HB2	1.87	0.74
1:E:383:ILE:HD11	1:E:404:CYS:CB	2.17	0.74
1:A:261:LEU:HD22	1:A:324:LEU:HD23	1.70	0.74
1:C:182:THR:HB	1:C:246:ARG:HD3	1.69	0.74
1:E:265:HIS:CD2	1:E:267:GLY:H	2.03	0.73
1:A:145:SER:O	1:A:149:ARG:HG2	1.87	0.73
1:D:282:GLN:HE22	1:D:285:ILE:CD1	1.96	0.73
1:C:361:ILE:C	1:C:361:ILE:CD1	2.61	0.73
1:B:235:TYR:O	1:B:236:ILE:HD13	1.89	0.73
1:D:265:HIS:HD2	1:D:267:GLY:H	1.34	0.73
1:E:54:LYS:CD	1:E:55:MET:N	2.50	0.73
1:E:145:SER:OG	1:E:147:PRO:CD	2.31	0.73
1:B:354:GLU:CD	1:B:355:PRO:HD2	2.13	0.72
1:A:434:PHE:CB	1:E:334:GLU:HG2	2.20	0.72
1:D:379:GLN:HG3	1:D:431:VAL:CG1	2.19	0.72
1:D:331:GLY:HA3	1:D:337:TYR:CD2	2.23	0.72
1:B:393:ILE:HG23	1:B:423:ILE:HG23	1.70	0.72
1:C:233:ASN:HD21	1:C:235:TYR:HB2	1.53	0.72
1:E:63:MET:HE1	1:E:122:LEU:HD21	1.71	0.72
1:D:79:ASN:OD1	1:D:79:ASN:C	2.32	0.72
1:F:64:ASP:O	1:F:67:VAL:HG22	1.90	0.72
1:D:47:PRO:N	1:D:48:PRO:CD	2.53	0.71
1:E:219:LEU:HD13	1:E:418:PHE:HB3	1.71	0.71
1:B:58:LYS:HD3	1:B:123:MET:CE	2.20	0.71
1:B:320:HIS:ND1	1:B:320:HIS:N	2.30	0.71
1:D:321:ASN:HB3	1:D:322:LYS:HG2	1.71	0.71
1:B:58:LYS:HD2	1:B:123:MET:HE1	1.71	0.71
1:B:395:PRO:CD	1:B:424:LYS:HG3	2.16	0.71
1:C:361:ILE:O	1:C:361:ILE:CD1	2.34	0.71
1:F:63:MET:O	1:F:67:VAL:HG13	1.91	0.71
1:B:48:PRO:HA	1:B:120:GLU:OE2	1.90	0.70
1:A:75:LEU:O	1:A:148:ARG:NH2	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:CYS:O	1:C:420:ARG:HB2	1.90	0.70
1:F:200:VAL:HG23	1:F:201:PRO:HD2	1.74	0.70
1:B:257:ASN:OD1	1:B:352:LEU:HD13	1.91	0.70
1:F:379:GLN:HA	1:F:431:VAL:HG21	1.74	0.70
1:D:70:CYS:HA	1:D:75:LEU:CD2	2.21	0.70
1:F:282:GLN:NE2	1:F:285:ILE:HD13	2.06	0.70
1:C:59:CYS:O	1:C:63:MET:HG3	1.92	0.69
1:C:431:VAL:O	1:C:433:PRO:HD3	1.92	0.69
1:A:146:GLN:HG3	1:A:379:GLN:HE22	1.56	0.69
1:C:51:VAL:HG12	1:C:52:ASP:N	2.08	0.69
1:D:282:GLN:NE2	1:D:285:ILE:CD1	2.55	0.69
1:C:393:ILE:HG23	1:C:423:ILE:HG13	1.73	0.69
1:E:79:ASN:O	1:E:83:TYR:CE2	2.46	0.69
1:F:340:PRO:HD3	1:F:346:ASN:HD22	1.58	0.69
1:A:299:ARG:HH21	1:A:302:GLN:HE22	1.41	0.69
1:F:143:GLU:O	1:F:144:ASN:CB	2.40	0.69
1:E:112:ASN:O	1:E:116:ARG:HG3	1.92	0.68
1:A:362:LYS:H	1:E:175:GLN:HE22	1.41	0.68
1:A:181:ILE:HD11	1:A:238:VAL:HG23	1.73	0.68
1:E:394:GLU:HB3	1:E:395:PRO:HA	1.75	0.68
1:C:48:PRO:HB3	1:C:120:GLU:HG3	1.74	0.68
1:D:284:PHE:CE1	1:D:342:GLY:HA3	2.28	0.68
1:C:107:GLU:O	1:C:111:GLU:HG2	1.93	0.68
1:B:210:HIS:CD2	1:B:215:ILE:H	2.11	0.68
1:D:51:VAL:HG13	1:D:55:MET:HE3	1.75	0.68
1:E:94:HIS:O	1:E:98:ILE:HG13	1.93	0.68
1:A:334:GLU:HG2	1:F:434:PHE:HB3	1.76	0.68
1:E:360:HIS:CD2	1:E:362:LYS:NZ	2.62	0.68
1:B:210:HIS:CD2	1:B:214:PRO:HA	2.29	0.67
1:B:380:LEU:HD21	1:B:385:ALA:O	1.94	0.67
1:F:146:GLN:HE22	1:F:149:ARG:NH1	1.92	0.67
1:B:174:PHE:CZ	1:B:176:GLY:HA3	2.30	0.67
1:B:399:LEU:HD22	1:B:429:ILE:CD1	2.24	0.66
1:C:132:LEU:HG	1:C:140:MET:CE	2.22	0.66
1:F:393:ILE:HG23	1:F:423:ILE:HG23	1.78	0.66
1:C:122:LEU:HA	1:C:161:MET:HE1	1.78	0.66
1:B:362:LYS:HG2	1:C:171:SER:HB2	1.78	0.65
1:F:78:LYS:HG2	1:F:79:ASN:H	1.61	0.65
1:B:58:LYS:CD	1:B:123:MET:HE1	2.26	0.65
1:C:51:VAL:HG12	1:C:52:ASP:H	1.59	0.65
1:D:361:ILE:HG13	1:D:361:ILE:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:79:ASN:ND2	1:F:79:ASN:O	2.29	0.65
1:F:273:THR:HG22	1:F:275:ASP:N	2.08	0.65
1:A:224:LEU:HG	1:A:228:ILE:HD11	1.78	0.65
1:E:284:PHE:C	1:E:286:HIS:H	2.04	0.65
1:F:317:THR:HG22	1:F:318:ILE:N	2.11	0.65
1:B:265:HIS:CD2	1:B:267:GLY:H	2.07	0.65
1:B:325:PHE:O	1:B:329:ILE:HG13	1.97	0.64
1:F:414:GLN:HB3	1:F:420:ARG:HG3	1.79	0.64
1:F:136:GLY:O	1:F:139:ARG:HB2	1.98	0.64
1:B:406:THR:O	1:B:410:GLU:HG3	1.97	0.64
1:D:265:HIS:HD2	1:D:267:GLY:N	1.94	0.64
1:E:121:ASN:O	1:E:121:ASN:ND2	2.30	0.64
1:A:361:ILE:HD12	1:A:361:ILE:H	1.62	0.64
1:B:340:PRO:HD3	1:B:346:ASN:HD22	1.63	0.64
1:C:265:HIS:CD2	1:C:267:GLY:H	2.07	0.64
1:E:201:PRO:HG2	1:E:204:SER:OG	1.98	0.64
1:A:59:CYS:SG	1:A:122:LEU:HD23	2.38	0.64
1:D:79:ASN:O	1:D:83:TYR:CE2	2.51	0.64
1:F:143:GLU:CG	1:F:144:ASN:HD22	2.00	0.64
1:D:303:TRP:CD2	1:D:324:LEU:HD22	2.33	0.64
1:B:145:SER:HB2	1:B:147:PRO:HD2	1.80	0.63
1:D:73:PRO:C	1:D:75:LEU:H	2.04	0.63
1:D:131:SER:O	1:D:135:GLU:HG2	1.98	0.63
1:F:299:ARG:NH2	1:F:302:GLN:OE1	2.30	0.63
1:D:210:HIS:CD2	1:D:214:PRO:HA	2.34	0.63
1:F:317:THR:HG22	1:F:318:ILE:H	1.60	0.63
1:E:266:PRO:HB2	1:E:340:PRO:HB2	1.80	0.63
1:F:269:MET:HE3	1:F:292:ILE:HG21	1.81	0.63
1:C:153:LYS:NZ	1:C:385:ALA:HB1	2.14	0.63
1:C:265:HIS:HD2	1:C:267:GLY:N	1.93	0.63
1:A:218:GLY:O	1:A:222:MET:HG2	1.97	0.63
1:D:79:ASN:OD1	1:D:80:SER:N	2.32	0.63
1:E:53:LYS:HD2	1:E:53:LYS:O	1.99	0.63
1:E:394:GLU:N	1:E:394:GLU:OE1	2.31	0.63
1:C:54:LYS:CG	1:C:55:MET:N	2.62	0.63
1:E:65:LYS:HB2	1:E:130:ILE:HD11	1.81	0.63
1:F:269:MET:HG3	1:F:292:ILE:HD12	1.80	0.63
1:E:54:LYS:O	1:E:57:GLU:N	2.31	0.62
1:F:85:LEU:O	1:F:89:PRO:HG2	1.99	0.62
1:A:253:SER:O	1:A:257:ASN:ND2	2.32	0.62
1:B:411:SER:O	1:B:412:GLU:CD	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:434:PHE:CD2	1:D:334:GLU:HG3	2.34	0.62
1:D:322:LYS:HE3	1:D:330:ASP:OD2	1.99	0.62
1:E:122:LEU:O	1:E:122:LEU:HG	1.98	0.62
1:F:271:PHE:O	1:F:272:LEU:HD23	1.99	0.62
1:D:134:LYS:O	1:D:137:LYS:HE3	2.00	0.62
1:D:80:SER:OG	1:D:273:THR:HG21	2.00	0.62
1:A:423:ILE:O	1:A:423:ILE:CD1	2.48	0.62
1:C:362:LYS:H	1:D:175:GLN:HE22	1.48	0.62
1:E:364:THR:OG1	1:E:367:GLN:HG3	1.99	0.62
1:E:384:CYS:CB	1:E:386:GLU:HG3	2.28	0.61
1:F:143:GLU:CG	1:F:144:ASN:HD21	2.07	0.61
1:B:62:LEU:CB	1:B:126:THR:HG21	2.26	0.61
1:F:143:GLU:O	1:F:144:ASN:ND2	2.33	0.61
1:D:173:LEU:HD12	1:D:174:PHE:N	2.14	0.61
1:A:393:ILE:HD11	1:A:405:LEU:HD22	1.83	0.61
1:B:264:THR:HG21	1:B:363:VAL:HG22	1.83	0.61
1:D:317:THR:O	1:D:319:PRO:HD3	2.01	0.61
1:A:423:ILE:C	1:A:423:ILE:CD1	2.69	0.61
1:C:132:LEU:O	1:C:140:MET:HE3	2.01	0.61
1:E:75:LEU:HD23	1:E:75:LEU:O	2.00	0.61
1:C:268:TYR:O	1:C:269:MET:HE2	2.00	0.61
1:B:246:ARG:O	1:B:249:GLN:HG2	1.99	0.61
1:C:54:LYS:HG3	1:C:55:MET:N	2.16	0.61
1:E:146:GLN:HB3	1:E:147:PRO:HD3	1.83	0.61
1:E:205:PHE:CE2	1:E:236:ILE:HG21	2.35	0.61
1:F:146:GLN:NE2	1:F:377:THR:CG2	2.57	0.61
1:E:74:LYS:HG2	1:E:141:TYR:CD1	2.35	0.61
1:E:265:HIS:HD2	1:E:267:GLY:N	1.91	0.61
1:F:210:HIS:CD2	1:F:215:ILE:H	2.13	0.60
1:F:287:LYS:HE2	1:F:339:PHE:CD2	2.36	0.60
1:E:433:PRO:HB2	1:E:434:PHE:CD1	2.36	0.60
1:D:72:ASN:CB	1:D:75:LEU:HD22	2.30	0.60
1:A:424:LYS:NZ	1:E:86:ASP:OD2	2.33	0.60
1:F:243:ILE:HD13	1:F:300:LEU:HB3	1.83	0.60
1:A:287:LYS:NZ	1:A:342:GLY:O	2.35	0.60
1:B:58:LYS:CD	1:B:123:MET:CE	2.79	0.60
1:D:384:CYS:HB3	1:D:404:CYS:SG	2.42	0.60
1:C:50:THR:HA	1:C:116:ARG:CD	2.31	0.60
1:F:99:LEU:HD23	1:F:106:MET:HE1	1.84	0.60
1:E:54:LYS:C	1:E:54:LYS:NZ	2.54	0.59
1:E:360:HIS:CD2	1:E:362:LYS:HZ2	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:49:GLY:C	1:F:116:ARG:HD3	2.27	0.59
1:F:53:LYS:HG3	1:F:56:VAL:CG1	2.32	0.59
1:B:266:PRO:HB2	1:B:340:PRO:HB2	1.84	0.59
1:E:60:TRP:CE3	1:E:92:TYR:HE1	2.20	0.59
1:B:82:PRO:HB2	1:B:87:LEU:HD11	1.85	0.59
1:F:149:ARG:HH11	1:F:377:THR:HG23	1.65	0.59
1:D:246:ARG:O	1:D:249:GLN:HG2	2.02	0.59
1:E:54:LYS:NZ	1:E:54:LYS:HB2	2.17	0.59
1:E:61:LYS:O	1:E:64:ASP:HB2	2.03	0.59
1:F:265:HIS:CD2	1:F:267:GLY:H	2.10	0.59
1:D:75:LEU:O	1:D:148:ARG:NH2	2.35	0.58
1:D:253:SER:O	1:D:257:ASN:ND2	2.35	0.58
1:A:299:ARG:HE	1:A:302:GLN:NE2	2.01	0.58
1:E:59:CYS:HB3	1:E:63:MET:HE3	1.84	0.58
1:A:135:GLU:CA	1:A:135:GLU:OE1	2.51	0.58
1:E:56:VAL:HG22	1:E:119:MET:HE2	1.85	0.58
1:C:53:LYS:HA	1:C:56:VAL:HG12	1.84	0.58
1:D:283:LYS:H	1:D:283:LYS:HE2	1.68	0.58
1:D:394:GLU:HG3	1:D:424:LYS:HE2	1.85	0.58
1:D:51:VAL:HG23	1:D:116:ARG:HG2	1.84	0.58
1:F:307:TYR:CE1	1:F:315:LEU:HB2	2.38	0.58
1:D:194:PHE:O	1:D:197:LYS:HG3	2.03	0.58
1:A:417:PRO:O	1:A:420:ARG:NH1	2.37	0.58
1:B:303:TRP:CD2	1:B:324:LEU:HD22	2.39	0.58
1:A:379:GLN:HG3	1:A:431:VAL:HG13	1.85	0.58
1:E:54:LYS:HE3	1:E:55:MET:HA	1.86	0.58
1:E:98:ILE:HD13	1:E:169:PHE:CD2	2.39	0.57
1:C:116:ARG:O	1:C:120:GLU:HB2	2.04	0.57
1:F:92:TYR:CZ	1:F:96:ARG:HD2	2.39	0.57
1:F:146:GLN:HB3	1:F:377:THR:HG21	1.86	0.57
1:A:113:GLU:HG3	1:A:116:ARG:HH21	1.70	0.57
1:E:143:GLU:OE1	1:E:143:GLU:N	2.37	0.57
1:E:205:PHE:CD2	1:E:236:ILE:HG21	2.39	0.57
1:E:256:ARG:HG3	1:E:256:ARG:NH1	2.12	0.57
1:A:380:LEU:O	1:A:382:LYS:CE	2.52	0.57
1:C:105:LYS:C	1:C:107:GLU:H	2.11	0.57
1:F:146:GLN:N	1:F:147:PRO:CD	2.67	0.57
1:B:146:GLN:HA	1:B:149:ARG:HH21	1.69	0.57
1:E:384:CYS:O	1:E:386:GLU:HG2	2.05	0.57
1:E:390:ASP:OD1	1:E:402:THR:HG23	2.04	0.57
1:B:360:HIS:ND1	1:B:360:HIS:N	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:LYS:C	1:E:53:LYS:CD	2.69	0.56
1:E:320:HIS:N	1:E:320:HIS:CD2	2.73	0.56
1:B:92:TYR:OH	1:B:96:ARG:NH1	2.35	0.56
1:C:303:TRP:CD2	1:C:324:LEU:HD22	2.41	0.56
1:F:405:LEU:O	1:F:409:GLN:HG2	2.05	0.56
1:B:146:GLN:OE1	1:B:379:GLN:NE2	2.38	0.56
1:C:137:LYS:HB3	1:C:138:GLU:OE1	2.05	0.56
1:D:257:ASN:OD1	1:D:352:LEU:CD2	2.45	0.56
1:E:121:ASN:CG	1:E:233:ASN:HB3	2.30	0.56
1:F:273:THR:HG22	1:F:274:TYR:N	2.19	0.56
1:F:137:LYS:HB3	1:F:138:GLU:HG3	1.87	0.56
1:D:146:GLN:HB2	1:D:147:PRO:HD3	1.87	0.56
1:E:210:HIS:HD2	1:E:215:ILE:H	1.52	0.56
1:C:242:ASP:O	1:C:246:ARG:HG3	2.06	0.56
1:D:173:LEU:HD12	1:D:174:PHE:H	1.69	0.56
1:E:146:GLN:HG3	1:E:379:GLN:OE1	2.05	0.56
1:F:133:PHE:CE1	1:F:140:MET:HE2	2.41	0.56
1:F:146:GLN:HE21	1:F:377:THR:HG21	1.69	0.56
1:F:329:ILE:O	1:F:333:ARG:HG3	2.05	0.56
1:B:432:ASP:HB3	1:B:435:ASP:HB3	1.88	0.56
1:C:378:PHE:O	1:C:389:LYS:NZ	2.36	0.56
1:E:54:LYS:CE	1:E:55:MET:N	2.69	0.56
1:D:168:ILE:C	1:D:170:PRO:HD3	2.31	0.56
1:F:307:TYR:CZ	1:F:315:LEU:HB2	2.41	0.56
1:E:145:SER:HG	1:E:147:PRO:HD2	1.66	0.56
1:C:295:LEU:HD21	1:C:303:TRP:CZ3	2.41	0.55
1:D:274:TYR:CE1	1:D:316:GLN:HG3	2.41	0.55
1:A:48:PRO:HB3	1:A:120:GLU:OE1	2.06	0.55
1:E:63:MET:HE2	1:E:122:LEU:HD21	1.88	0.55
1:D:60:TRP:O	1:D:61:LYS:C	2.49	0.55
1:F:114:TYR:CD1	1:F:114:TYR:C	2.84	0.55
1:B:360:HIS:N	1:B:360:HIS:HD1	2.02	0.55
1:A:120:GLU:O	1:A:124:LYS:HG3	2.07	0.55
1:D:284:PHE:CZ	1:D:342:GLY:HA3	2.41	0.55
1:B:322:LYS:HB2	1:B:323:PRO:CD	2.37	0.55
1:C:371:TYR:O	1:C:374:MET:HB2	2.07	0.55
1:E:269:MET:HG3	1:E:292:ILE:HD12	1.87	0.55
1:B:121:ASN:HA	1:B:124:LYS:HE3	1.89	0.55
1:C:101:ARG:HD2	1:C:173:LEU:HD23	1.85	0.54
1:C:393:ILE:HG23	1:C:423:ILE:CG1	2.37	0.54
1:F:74:LYS:HB2	1:F:74:LYS:NZ	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:O	1:A:57:GLU:HG2	2.07	0.54
1:A:434:PHE:HB3	1:E:334:GLU:HG2	1.88	0.54
1:B:75:LEU:CD2	1:B:140:MET:O	2.55	0.54
1:B:75:LEU:HD23	1:B:140:MET:O	2.07	0.54
1:D:153:LYS:O	1:D:153:LYS:HE2	2.07	0.54
1:E:54:LYS:HE3	1:E:55:MET:CA	2.37	0.54
1:F:325:PHE:O	1:F:329:ILE:HG13	2.06	0.54
1:C:303:TRP:CE2	1:C:324:LEU:HD22	2.42	0.54
1:D:81:PRO:HA	1:D:82:PRO:C	2.31	0.54
1:A:294:ARG:NH2	1:A:316:GLN:OE1	2.39	0.54
1:B:251:TRP:CD1	1:B:251:TRP:C	2.85	0.54
1:C:139:ARG:O	1:C:142:GLU:HB3	2.06	0.54
1:C:325:PHE:O	1:C:329:ILE:HG13	2.08	0.54
1:C:392:LYS:HB2	1:C:399:LEU:HD23	1.90	0.54
1:E:75:LEU:O	1:E:148:ARG:NH2	2.41	0.54
1:A:331:GLY:HA3	1:A:337:TYR:CD2	2.42	0.54
1:C:434:PHE:N	1:C:434:PHE:CD1	2.74	0.54
1:B:273:THR:HG22	1:B:275:ASP:N	2.22	0.54
1:C:53:LYS:HA	1:C:56:VAL:CG1	2.38	0.54
1:F:90:ASP:O	1:F:93:GLN:HG2	2.07	0.54
1:B:91:THR:O	1:B:95:LEU:HG	2.08	0.53
1:C:105:LYS:C	1:C:107:GLU:N	2.67	0.53
1:E:169:PHE:CE1	1:E:174:PHE:HD1	2.26	0.53
1:E:318:ILE:HG22	1:E:318:ILE:O	2.08	0.53
1:E:384:CYS:C	1:E:386:GLU:HG2	2.33	0.53
1:D:70:CYS:CA	1:D:75:LEU:HD23	2.33	0.53
1:E:55:MET:HE1	1:E:120:GLU:HA	1.89	0.53
1:A:171:SER:HB2	1:F:362:LYS:HG3	1.90	0.53
1:E:146:GLN:N	1:E:147:PRO:CD	2.72	0.53
1:B:383:ILE:HD11	1:B:417:PRO:HB2	1.89	0.53
1:E:383:ILE:HG13	1:E:404:CYS:SG	2.49	0.53
1:E:387:ASN:HB2	1:E:401:CYS:SG	2.47	0.53
1:A:299:ARG:HH21	1:A:302:GLN:NE2	2.05	0.53
1:B:210:HIS:HA	1:B:213:HIS:O	2.08	0.53
1:D:102:TYR:O	1:D:106:MET:HG2	2.09	0.53
1:E:52:ASP:OD1	1:E:52:ASP:N	2.42	0.53
1:C:54:LYS:CG	1:C:55:MET:H	2.22	0.53
1:C:412:GLU:HG2	1:C:412:GLU:O	2.09	0.53
1:D:398:HIS:C	1:D:399:LEU:HD23	2.33	0.53
1:C:111:GLU:HA	1:C:111:GLU:OE1	2.07	0.53
1:F:359:ASP:OD1	1:F:359:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:MET:HA	1:A:126:THR:HG22	1.91	0.53
1:D:267:GLY:O	1:D:269:MET:HG2	2.08	0.53
1:E:107:GLU:HG2	1:E:108:THR:HG23	1.90	0.53
1:E:360:HIS:CD2	1:E:362:LYS:HZ3	2.26	0.53
1:D:123:MET:HA	1:D:126:THR:HG22	1.91	0.53
1:D:269:MET:HB3	1:D:272:LEU:HD11	1.90	0.53
1:A:210:HIS:HD2	1:A:215:ILE:N	1.96	0.53
1:D:284:PHE:O	1:D:285:ILE:C	2.49	0.53
1:A:362:LYS:N	1:E:175:GLN:HE22	2.05	0.52
1:B:392:LYS:HB2	1:B:399:LEU:HD23	1.91	0.52
1:C:277:VAL:HG13	1:C:292:ILE:HD11	1.89	0.52
1:C:405:LEU:O	1:C:409:GLN:HG3	2.09	0.52
1:D:269:MET:HB3	1:D:272:LEU:CD1	2.39	0.52
1:E:405:LEU:O	1:E:409:GLN:HG3	2.10	0.52
1:A:202:TRP:CZ2	1:A:225:LYS:HB2	2.44	0.52
1:E:54:LYS:CE	1:E:55:MET:CA	2.88	0.52
1:E:96:ARG:O	1:E:99:LEU:N	2.41	0.52
1:F:51:VAL:HG13	1:F:55:MET:SD	2.49	0.52
1:C:153:LYS:HZ3	1:C:385:ALA:HB1	1.73	0.52
1:E:52:ASP:O	1:E:54:LYS:N	2.39	0.52
1:F:289:GLY:HA3	1:F:338:LEU:HD12	1.90	0.52
1:F:361:ILE:O	1:F:361:ILE:HG13	2.09	0.52
1:A:49:GLY:O	1:A:116:ARG:HD2	2.10	0.52
1:A:75:LEU:O	1:A:76:ALA:C	2.53	0.52
1:C:142:GLU:HB3	1:C:145:SER:HB3	1.91	0.52
1:E:65:LYS:CB	1:E:130:ILE:HD11	2.39	0.52
1:E:121:ASN:O	1:E:121:ASN:CG	2.51	0.52
1:C:424:LYS:HE3	1:D:86:ASP:OD2	2.09	0.52
1:A:143:GLU:O	1:A:143:GLU:HG2	2.09	0.52
1:D:79:ASN:O	1:D:83:TYR:OH	2.28	0.52
1:D:181:ILE:HB	1:D:187:ALA:HB2	1.91	0.52
1:C:376:SER:HB2	1:C:382:LYS:HZ2	1.71	0.52
1:F:199:ILE:HG12	1:F:235:TYR:HB3	1.91	0.52
1:C:273:THR:HG22	1:C:275:ASP:H	1.75	0.52
1:C:379:GLN:HB2	1:C:431:VAL:HG11	1.92	0.52
1:E:49:GLY:O	1:E:50:THR:C	2.52	0.52
1:E:200:VAL:HG13	1:E:201:PRO:HD2	1.91	0.52
1:E:338:LEU:O	1:E:346:ASN:HB2	2.10	0.52
1:C:72:ASN:HB3	1:C:75:LEU:HG	1.92	0.51
1:D:261:LEU:HD11	1:D:325:PHE:HB3	1.93	0.51
1:E:348:ASP:OD1	1:E:350:THR:OG1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ASP:OD1	1:B:402:THR:HG23	2.09	0.51
1:C:52:ASP:OD1	1:C:54:LYS:CG	2.52	0.51
1:E:55:MET:HE3	1:E:123:MET:HE3	1.92	0.51
1:E:92:TYR:O	1:E:93:GLN:C	2.53	0.51
1:F:86:ASP:C	1:F:89:PRO:HD2	2.35	0.51
1:F:137:LYS:O	1:F:140:MET:HG2	2.11	0.51
1:A:379:GLN:OE1	1:A:379:GLN:N	2.38	0.51
1:F:74:LYS:NZ	1:F:74:LYS:CB	2.73	0.51
1:A:434:PHE:HB2	1:E:334:GLU:HG2	1.92	0.51
1:B:114:TYR:OH	1:B:164:GLU:HG2	2.10	0.51
1:B:210:HIS:HD2	1:B:215:ILE:H	1.58	0.51
1:E:384:CYS:SG	1:E:386:GLU:HG3	2.50	0.51
1:A:173:LEU:HD23	1:A:175:GLN:NE2	2.25	0.51
1:B:146:GLN:OE1	1:B:432:ASP:OD2	2.29	0.51
1:B:377:THR:HB	1:B:379:GLN:HG2	1.93	0.51
1:D:414:GLN:HG2	1:D:415:GLY:N	2.25	0.51
1:F:223:ALA:HB1	1:F:371:TYR:CD2	2.45	0.51
1:F:340:PRO:C	1:F:342:GLY:H	2.17	0.51
1:B:343:ARG:NH2	1:C:181:ILE:O	2.44	0.51
1:E:170:PRO:HD2	1:E:175:GLN:HG3	1.93	0.50
1:E:284:PHE:C	1:E:286:HIS:N	2.68	0.50
1:F:140:MET:O	1:F:148:ARG:CG	2.58	0.50
1:F:331:GLY:HA3	1:F:337:TYR:CD2	2.46	0.50
1:C:169:PHE:HA	1:C:173:LEU:O	2.12	0.50
1:E:54:LYS:CE	1:E:55:MET:HA	2.41	0.50
1:C:271:PHE:O	1:C:272:LEU:HD23	2.11	0.50
1:E:149:ARG:HD2	1:E:377:THR:HG22	1.93	0.50
1:B:434:PHE:O	1:B:435:ASP:OD1	2.29	0.50
1:C:146:GLN:NE2	1:C:149:ARG:HG3	2.27	0.50
1:D:129:THR:OG1	1:D:154:LEU:CD1	2.59	0.50
1:E:362:LYS:N	1:E:362:LYS:CD	2.73	0.50
1:E:434:PHE:CD1	1:E:434:PHE:N	2.76	0.50
1:A:266:PRO:HG3	1:E:180:ARG:HD3	1.94	0.50
1:B:280:ARG:NH1	1:B:341:ASP:OD2	2.45	0.50
1:C:67:VAL:O	1:C:71:GLN:HG3	2.12	0.50
1:D:340:PRO:HD3	1:D:346:ASN:ND2	2.15	0.50
1:D:389:LYS:HE2	1:D:399:LEU:HB2	1.92	0.50
1:A:380:LEU:O	1:A:382:LYS:HE3	2.12	0.50
1:D:177:ASP:OD1	1:D:178:THR:HG23	2.11	0.50
1:A:64:ASP:O	1:A:68:ARG:HG2	2.11	0.50
1:A:75:LEU:HD11	1:A:133:PHE:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:VAL:HG22	1:C:60:TRP:CZ2	2.47	0.50
1:C:70:CYS:HA	1:C:75:LEU:CD1	2.42	0.50
1:E:52:ASP:C	1:E:54:LYS:H	2.20	0.50
1:F:142:GLU:C	1:F:145:SER:OG	2.55	0.50
1:F:272:LEU:HD22	1:F:276:GLU:OE1	2.11	0.50
1:B:139:ARG:NH1	1:B:435:ASP:HB2	2.27	0.50
1:B:269:MET:HG3	1:B:292:ILE:HD12	1.94	0.50
1:B:189:PHE:CG	1:B:251:TRP:CH2	3.00	0.49
1:C:223:ALA:HB1	1:C:371:TYR:CD2	2.47	0.49
1:C:417:PRO:O	1:C:420:ARG:NH1	2.45	0.49
1:D:325:PHE:C	1:D:325:PHE:CD1	2.90	0.49
1:E:79:ASN:C	1:E:79:ASN:OD1	2.54	0.49
1:E:284:PHE:CZ	1:E:342:GLY:HA3	2.47	0.49
1:D:79:ASN:O	1:D:83:TYR:CZ	2.65	0.49
1:D:394:GLU:HG2	1:D:425:GLY:H	1.77	0.49
1:A:135:GLU:OE1	1:A:135:GLU:HA	2.11	0.49
1:A:135:GLU:OE1	1:A:135:GLU:N	2.45	0.49
1:C:379:GLN:HB2	1:C:431:VAL:CG1	2.41	0.49
1:D:274:TYR:HE1	1:D:316:GLN:HG3	1.77	0.49
1:D:394:GLU:HG2	1:D:425:GLY:N	2.27	0.49
1:E:75:LEU:O	1:E:76:ALA:C	2.55	0.49
1:C:423:ILE:O	1:C:423:ILE:HG22	2.12	0.49
1:D:143:GLU:CG	1:D:144:ASN:H	2.26	0.49
1:E:325:PHE:O	1:E:329:ILE:HG13	2.12	0.49
1:E:389:LYS:HE2	1:E:399:LEU:HB2	1.93	0.49
1:E:391:VAL:HG22	1:E:392:LYS:N	2.27	0.49
1:F:200:VAL:CG2	1:F:201:PRO:HD2	2.41	0.49
1:F:316:GLN:O	1:F:316:GLN:CG	2.58	0.49
1:B:380:LEU:CD2	1:B:385:ALA:O	2.60	0.49
1:C:145:SER:O	1:C:145:SER:OG	2.29	0.49
1:D:340:PRO:HG3	1:D:347:PRO:HD3	1.94	0.49
1:E:53:LYS:O	1:E:53:LYS:CD	2.61	0.49
1:A:118:PHE:CD1	1:A:118:PHE:C	2.90	0.49
1:D:419:CYS:O	1:D:420:ARG:HB2	2.11	0.49
1:F:340:PRO:C	1:F:342:GLY:N	2.70	0.49
1:C:299:ARG:NH2	1:C:302:GLN:HE22	2.11	0.49
1:D:112:ASN:HD22	1:D:115:PHE:HB2	1.77	0.49
1:A:224:LEU:HG	1:A:228:ILE:CD1	2.40	0.49
1:F:251:TRP:CZ3	1:F:254:LEU:HD22	2.48	0.49
1:B:126:THR:HG22	1:B:127:LYS:N	2.28	0.49
1:E:433:PRO:HB2	1:E:434:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:LYS:C	1:D:60:TRP:H	2.20	0.48
1:E:392:LYS:HG3	1:E:399:LEU:HD23	1.95	0.48
1:F:270:ALA:O	1:F:294:ARG:HB2	2.12	0.48
1:C:101:ARG:HD3	1:C:173:LEU:HD21	1.85	0.48
1:C:428:PRO:O	1:D:316:GLN:NE2	2.46	0.48
1:E:256:ARG:NH1	1:E:256:ARG:CG	2.74	0.48
1:F:142:GLU:O	1:F:145:SER:OG	2.30	0.48
1:E:408:TRP:CE2	1:E:413:GLY:HA3	2.48	0.48
1:F:405:LEU:O	1:F:409:GLN:CG	2.61	0.48
1:C:100:SER:C	1:C:102:TYR:H	2.21	0.48
1:A:50:THR:HG21	1:A:111:GLU:OE1	2.14	0.48
1:A:81:PRO:HA	1:A:82:PRO:C	2.39	0.48
1:B:99:LEU:HD22	1:B:106:MET:HE1	1.95	0.48
1:C:246:ARG:O	1:C:249:GLN:HG2	2.13	0.48
1:D:361:ILE:O	1:D:362:LYS:HD3	2.14	0.48
1:E:412:GLU:O	1:E:412:GLU:HG2	2.13	0.48
1:B:100:SER:O	1:B:103:GLU:HG3	2.13	0.48
1:B:239:PHE:CZ	1:B:243:ILE:HD11	2.47	0.48
1:B:250:PRO:HD3	1:B:323:PRO:CG	2.44	0.48
1:E:54:LYS:HZ2	1:E:54:LYS:HB2	1.77	0.48
1:E:79:ASN:O	1:E:83:TYR:CZ	2.66	0.48
1:E:168:ILE:HD12	1:E:198:THR:CG2	2.44	0.48
1:E:394:GLU:CB	1:E:395:PRO:HA	2.40	0.48
1:E:331:GLY:HA3	1:E:337:TYR:CE2	2.47	0.48
1:E:362:LYS:HA	1:E:362:LYS:HD2	1.72	0.48
1:E:411:SER:O	1:E:412:GLU:HB3	2.14	0.48
1:A:399:LEU:HD22	1:A:429:ILE:HD13	1.95	0.48
1:B:419:CYS:O	1:B:420:ARG:HB2	2.14	0.48
1:E:250:PRO:HD2	1:E:325:PHE:CE2	2.47	0.48
1:B:233:ASN:O	1:B:234:ASP:HB2	2.12	0.48
1:C:353:CYS:O	1:C:354:GLU:O	2.31	0.48
1:D:393:ILE:HG22	1:D:396:CYS:SG	2.54	0.48
1:F:231:THR:HG23	1:F:240:GLU:OE2	2.14	0.48
1:F:273:THR:CG2	1:F:274:TYR:N	2.76	0.48
1:B:250:PRO:HD3	1:B:323:PRO:HG3	1.96	0.48
1:B:299:ARG:HE	1:B:302:GLN:HE21	1.62	0.47
1:F:377:THR:O	1:F:382:LYS:NZ	2.47	0.47
1:B:263:VAL:HA	1:B:371:TYR:CD1	2.49	0.47
1:B:265:HIS:HD2	1:B:267:GLY:N	1.98	0.47
1:B:273:THR:HG22	1:B:276:GLU:H	1.79	0.47
1:E:54:LYS:HZ2	1:E:54:LYS:CB	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:GLU:OE1	1:E:81:PRO:HD3	2.14	0.47
1:A:88:LEU:HB2	1:A:89:PRO:HD3	1.95	0.47
1:C:164:GLU:O	1:C:164:GLU:HG2	2.14	0.47
1:D:382:LYS:HD3	1:D:382:LYS:HA	1.47	0.47
1:B:72:ASN:OD1	1:B:73:PRO:HD2	2.13	0.47
1:B:146:GLN:HG2	1:B:147:PRO:HD3	1.96	0.47
1:D:380:LEU:O	1:D:382:LYS:HE3	2.14	0.47
1:A:180:ARG:NH2	1:F:264:THR:O	2.48	0.47
1:C:123:MET:O	1:C:126:THR:HG22	2.14	0.47
1:F:138:GLU:HG3	1:F:138:GLU:H	1.35	0.47
1:A:122:LEU:O	1:A:126:THR:HG22	2.14	0.47
1:B:95:LEU:O	1:B:99:LEU:HG	2.14	0.47
1:C:391:VAL:HG22	1:C:392:LYS:N	2.30	0.47
1:D:69:LEU:O	1:D:75:LEU:CD2	2.63	0.47
1:D:128:GLN:HG2	1:D:154:LEU:HD11	1.96	0.47
1:B:431:VAL:C	1:B:433:PRO:HD3	2.38	0.47
1:C:182:THR:CB	1:C:246:ARG:HD3	2.43	0.47
1:D:87:LEU:O	1:D:91:THR:OG1	2.28	0.47
1:D:303:TRP:CE2	1:D:324:LEU:HD22	2.49	0.47
1:E:384:CYS:C	1:E:386:GLU:N	2.73	0.47
1:F:140:MET:O	1:F:148:ARG:HG2	2.14	0.47
1:C:340:PRO:HD3	1:C:346:ASN:HD22	1.80	0.47
1:D:308:VAL:HA	1:D:313:ASN:O	2.15	0.47
1:B:140:MET:O	1:B:148:ARG:HD3	2.15	0.47
1:C:419:CYS:O	1:C:420:ARG:CB	2.57	0.47
1:E:250:PRO:HD2	1:E:325:PHE:HE2	1.80	0.47
1:F:74:LYS:HB2	1:F:74:LYS:HZ2	1.78	0.47
1:F:269:MET:HE3	1:F:292:ILE:CG2	2.44	0.47
1:A:75:LEU:HD11	1:A:133:PHE:HE2	1.80	0.46
1:A:146:GLN:OE1	1:A:146:GLN:HA	2.14	0.46
1:B:75:LEU:HD21	1:B:140:MET:HB3	1.96	0.46
1:C:146:GLN:HA	1:C:149:ARG:HB2	1.97	0.46
1:C:408:TRP:O	1:C:413:GLY:HA3	2.16	0.46
1:D:70:CYS:C	1:D:75:LEU:HD23	2.40	0.46
1:E:203:LYS:HG3	1:E:206:ARG:HH21	1.79	0.46
1:E:54:LYS:HA	1:E:57:GLU:HG2	1.96	0.46
1:E:108:THR:O	1:E:111:GLU:HB2	2.15	0.46
1:E:161:MET:HG3	1:E:231:THR:HG22	1.97	0.46
1:D:287:LYS:HB2	1:F:68:ARG:NH2	2.31	0.46
1:E:54:LYS:NZ	1:E:54:LYS:CB	2.78	0.46
1:A:265:HIS:HD2	1:A:267:GLY:CA	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:PRO:HG3	1:B:156:LEU:HA	1.98	0.46
1:C:59:CYS:HB2	1:C:123:MET:CE	2.44	0.46
1:D:105:LYS:C	1:D:107:GLU:N	2.71	0.46
1:E:146:GLN:N	1:E:147:PRO:HD2	2.30	0.46
1:E:164:GLU:OE2	1:E:237:SER:OG	2.30	0.46
1:E:361:ILE:HA	1:E:361:ILE:HD12	1.66	0.46
1:F:338:LEU:O	1:F:346:ASN:HB2	2.16	0.46
1:F:434:PHE:N	1:F:434:PHE:CD1	2.82	0.46
1:B:56:VAL:HG22	1:B:119:MET:HE2	1.98	0.46
1:B:105:LYS:H	1:B:105:LYS:HG3	1.47	0.46
1:D:73:PRO:C	1:D:75:LEU:N	2.72	0.46
1:E:161:MET:CG	1:E:231:THR:HG22	2.46	0.46
1:E:394:GLU:OE2	1:E:427:GLU:CG	2.64	0.46
1:E:402:THR:O	1:E:405:LEU:N	2.48	0.46
1:F:362:LYS:HD2	1:F:362:LYS:HA	1.46	0.46
1:A:362:LYS:O	1:E:175:GLN:NE2	2.49	0.46
1:E:263:VAL:HG12	1:E:264:THR:HG22	1.96	0.46
1:F:379:GLN:HA	1:F:431:VAL:CG2	2.46	0.46
1:A:50:THR:CG2	1:A:111:GLU:OE1	2.64	0.46
1:C:51:VAL:HG23	1:C:116:ARG:HG2	1.98	0.46
1:C:414:GLN:HB3	1:C:420:ARG:HG3	1.97	0.46
1:D:114:TYR:CD1	1:D:199:ILE:HD12	2.51	0.46
1:D:325:PHE:O	1:D:329:ILE:HG13	2.15	0.46
1:D:256:ARG:HG3	1:D:360:HIS:HB3	1.98	0.46
1:E:257:ASN:OD1	1:E:352:LEU:HD22	2.15	0.46
1:F:144:ASN:C	1:F:145:SER:O	2.52	0.46
1:A:274:TYR:CE2	1:A:278:LYS:HE2	2.51	0.46
1:B:146:GLN:N	1:B:147:PRO:CD	2.78	0.46
1:D:253:SER:O	1:D:257:ASN:CG	2.59	0.46
1:E:57:GLU:O	1:E:61:LYS:HE2	2.15	0.46
1:E:63:MET:HE2	1:E:122:LEU:HD11	1.98	0.46
1:E:154:LEU:HD12	1:E:154:LEU:HA	1.77	0.46
1:F:60:TRP:CD2	1:F:92:TYR:HE1	2.34	0.46
1:A:321:ASN:C	1:A:321:ASN:ND2	2.74	0.46
1:B:86:ASP:C	1:B:89:PRO:HD2	2.41	0.46
1:C:122:LEU:O	1:C:126:THR:HG22	2.16	0.46
1:C:414:GLN:OE1	1:C:414:GLN:HA	2.16	0.46
1:D:92:TYR:OH	1:D:96:ARG:NH1	2.49	0.46
1:D:143:GLU:CG	1:D:144:ASN:N	2.79	0.46
1:D:210:HIS:CD2	1:D:215:ILE:N	2.61	0.46
1:D:265:HIS:HD2	1:D:267:GLY:CA	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:ILE:CG2	1:D:396:CYS:SG	3.03	0.46
1:E:235:TYR:O	1:E:236:ILE:HD13	2.16	0.46
1:F:53:LYS:O	1:F:56:VAL:HG12	2.16	0.46
1:A:378:PHE:HB3	1:E:320:HIS:ND1	2.30	0.45
1:C:379:GLN:HG2	1:C:380:LEU:N	2.32	0.45
1:E:67:VAL:O	1:E:71:GLN:CG	2.64	0.45
1:E:340:PRO:HG3	1:E:347:PRO:HD3	1.98	0.45
1:F:141:TYR:N	1:F:141:TYR:HD1	2.07	0.45
1:F:303:TRP:CD2	1:F:324:LEU:HD22	2.51	0.45
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.61	0.45
1:F:266:PRO:HB2	1:F:340:PRO:HB2	1.98	0.45
1:C:299:ARG:HH21	1:C:302:GLN:HE22	1.64	0.45
1:E:48:PRO:HB3	1:E:116:ARG:HB3	1.97	0.45
1:F:78:LYS:CG	1:F:79:ASN:H	2.29	0.45
1:B:303:TRP:O	1:B:319:PRO:HD2	2.16	0.45
1:C:56:VAL:HG21	1:C:99:LEU:HD11	1.98	0.45
1:C:135:GLU:HG2	1:C:135:GLU:H	1.52	0.45
1:F:250:PRO:HD2	1:F:325:PHE:HE2	1.82	0.45
1:F:299:ARG:HG2	1:F:299:ARG:HH11	1.82	0.45
1:F:411:SER:C	1:F:412:GLU:HG2	2.42	0.45
1:A:250:PRO:HD2	1:A:325:PHE:HE2	1.82	0.45
1:D:143:GLU:HG3	1:D:144:ASN:H	1.81	0.45
1:D:250:PRO:HD2	1:D:325:PHE:HE2	1.82	0.45
1:D:345:GLN:CD	1:D:345:GLN:H	2.23	0.45
1:D:381:CYS:N	1:D:387:ASN:O	2.34	0.45
1:E:140:MET:HE2	1:E:147:PRO:CB	2.46	0.45
1:D:123:MET:O	1:D:126:THR:HG22	2.17	0.45
1:D:410:GLU:C	1:D:412:GLU:H	2.25	0.45
1:E:72:ASN:O	1:E:75:LEU:HB2	2.17	0.45
1:A:122:LEU:HA	1:A:161:MET:HE1	1.97	0.45
1:A:175:GLN:OE1	1:F:362:LYS:N	2.44	0.45
1:B:114:TYR:CD1	1:B:114:TYR:C	2.95	0.45
1:C:264:THR:O	1:D:180:ARG:NH2	2.50	0.45
1:E:54:LYS:NZ	1:E:55:MET:HA	2.32	0.45
1:A:182:THR:HG22	1:A:182:THR:O	2.17	0.45
1:B:77:LEU:O	1:B:78:LYS:C	2.59	0.45
1:C:63:MET:O	1:C:67:VAL:HG23	2.16	0.45
1:C:145:SER:O	1:C:146:GLN:HB2	2.16	0.45
1:C:309:THR:OG1	1:C:313:ASN:HB2	2.16	0.45
1:D:181:ILE:HD11	1:D:238:VAL:HG23	1.98	0.45
1:E:400:MET:HE2	1:E:400:MET:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:PHE:C	1:F:179:PHE:CD1	2.94	0.45
1:F:288:PRO:HA	1:F:308:VAL:HG12	1.98	0.45
1:F:317:THR:CG2	1:F:318:ILE:N	2.80	0.45
1:B:82:PRO:HG2	1:B:155:SER:HB3	1.99	0.45
1:B:77:LEU:HD23	1:B:77:LEU:HA	1.31	0.45
1:C:82:PRO:HG3	1:C:156:LEU:HA	1.98	0.45
1:D:62:LEU:HD13	1:D:126:THR:HG23	1.99	0.45
1:C:277:VAL:HG21	1:C:294:ARG:HD3	2.00	0.44
1:C:384:CYS:HB3	1:C:404:CYS:SG	2.57	0.44
1:D:394:GLU:HG2	1:D:424:LYS:HB3	1.99	0.44
1:E:67:VAL:O	1:E:71:GLN:HG2	2.17	0.44
1:E:384:CYS:C	1:E:386:GLU:H	2.24	0.44
1:F:53:LYS:HG3	1:F:56:VAL:HG11	1.98	0.44
1:D:138:GLU:OE1	1:D:138:GLU:N	2.41	0.44
1:E:94:HIS:O	1:E:94:HIS:CD2	2.71	0.44
1:E:208:ALA:O	1:E:211:GLU:HB2	2.17	0.44
1:F:299:ARG:HG2	1:F:299:ARG:NH1	2.33	0.44
1:A:123:MET:HA	1:A:126:THR:CG2	2.47	0.44
1:A:382:LYS:N	1:A:382:LYS:HD3	2.32	0.44
1:A:423:ILE:O	1:A:423:ILE:CG1	2.64	0.44
1:C:423:ILE:O	1:C:423:ILE:CG2	2.56	0.44
1:E:381:CYS:SG	1:E:383:ILE:HG12	2.57	0.44
1:F:291:TYR:CD1	1:F:337:TYR:HB3	2.53	0.44
1:A:419:CYS:O	1:A:420:ARG:HB2	2.16	0.44
1:B:192:LYS:O	1:B:192:LYS:HG3	2.17	0.44
1:C:287:LYS:HD3	1:C:339:PHE:CD2	2.53	0.44
1:A:233:ASN:O	1:A:234:ASP:HB2	2.17	0.44
1:C:79:ASN:O	1:C:83:TYR:OH	2.32	0.44
1:C:391:VAL:HB	1:C:402:THR:HG23	1.99	0.44
1:D:322:LYS:HE2	1:D:327:ALA:HA	2.00	0.44
1:E:174:PHE:C	1:E:175:GLN:HG2	2.42	0.44
1:B:181:ILE:HD11	1:B:238:VAL:HG23	2.00	0.44
1:C:119:MET:HE3	1:C:119:MET:HB3	1.77	0.44
1:D:394:GLU:OE2	1:D:424:LYS:HE3	2.18	0.44
1:F:67:VAL:HG12	1:F:88:LEU:CD1	2.48	0.44
1:F:160:HIS:CE1	1:F:271:PHE:CE2	3.06	0.44
1:F:229:ASP:OD1	1:F:229:ASP:C	2.60	0.44
1:D:273:THR:O	1:D:277:VAL:HG23	2.18	0.44
1:E:284:PHE:CE1	1:E:342:GLY:HA3	2.53	0.44
1:F:77:LEU:H	1:F:77:LEU:CD1	2.04	0.44
1:F:222:MET:HE3	1:F:222:MET:HB3	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:ILE:O	1:A:316:GLN:HA	2.18	0.44
1:C:345:GLN:OE1	1:D:191:ARG:HG2	2.17	0.44
1:D:58:LYS:C	1:D:60:TRP:N	2.72	0.44
1:D:182:THR:O	1:D:182:THR:HG22	2.17	0.44
1:E:284:PHE:O	1:E:286:HIS:N	2.51	0.44
1:F:114:TYR:OH	1:F:164:GLU:HG2	2.17	0.44
1:F:168:ILE:HD12	1:F:198:THR:CG2	2.48	0.44
1:A:405:LEU:O	1:A:409:GLN:HG3	2.18	0.44
1:B:65:LYS:HD2	1:B:69:LEU:HD11	2.00	0.44
1:B:362:LYS:H	1:C:175:GLN:NE2	2.16	0.44
1:D:145:SER:OG	1:D:148:ARG:HB2	2.17	0.44
1:D:346:ASN:HA	1:D:347:PRO:HD3	1.85	0.44
1:E:268:TYR:O	1:E:269:MET:HE2	2.17	0.44
1:A:210:HIS:CD2	1:A:214:PRO:HA	2.53	0.43
1:B:400:MET:HB3	1:B:400:MET:HE2	1.70	0.43
1:D:53:LYS:HA	1:D:56:VAL:HG12	1.99	0.43
1:D:209:LEU:HD12	1:D:209:LEU:O	2.17	0.43
1:D:332:PHE:CE1	1:D:338:LEU:HD22	2.53	0.43
1:D:376:SER:OG	1:D:377:THR:N	2.50	0.43
1:E:148:ARG:O	1:E:149:ARG:C	2.60	0.43
1:E:210:HIS:CD2	1:E:214:PRO:HA	2.53	0.43
1:F:156:LEU:HA	1:F:156:LEU:HD12	1.44	0.43
1:F:406:THR:O	1:F:407:SER:C	2.61	0.43
1:A:219:LEU:HD12	1:A:219:LEU:HA	1.87	0.43
1:A:321:ASN:C	1:A:321:ASN:HD22	2.26	0.43
1:B:322:LYS:HB2	1:B:323:PRO:HD2	1.99	0.43
1:B:378:PHE:O	1:B:389:LYS:HD2	2.18	0.43
1:C:264:THR:HG21	1:C:363:VAL:HG22	2.00	0.43
1:E:384:CYS:O	1:E:385:ALA:HB3	2.18	0.43
1:F:146:GLN:N	1:F:147:PRO:HD2	2.33	0.43
1:F:228:ILE:HG12	1:F:236:ILE:HD12	2.00	0.43
1:B:139:ARG:C	1:B:141:TYR:H	2.26	0.43
1:B:322:LYS:HD2	1:B:326:GLN:HB3	2.00	0.43
1:D:212:VAL:HG12	1:D:213:HIS:CD2	2.53	0.43
1:A:142:GLU:O	1:A:145:SER:OG	2.35	0.43
1:D:143:GLU:C	1:D:145:SER:H	2.26	0.43
1:D:282:GLN:O	1:D:285:ILE:HG13	2.19	0.43
1:D:370:LEU:HD23	1:D:370:LEU:HA	1.77	0.43
1:E:60:TRP:CD2	1:E:92:TYR:HE1	2.36	0.43
1:A:87:LEU:HD11	1:A:159:SER:HB2	2.00	0.43
1:A:334:GLU:HG2	1:F:434:PHE:CB	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LYS:HB3	1:C:138:GLU:H	1.46	0.43
1:C:273:THR:HG22	1:C:274:TYR:N	2.34	0.43
1:F:75:LEU:HB2	1:F:77:LEU:HD11	2.00	0.43
1:A:59:CYS:O	1:A:63:MET:HG3	2.19	0.43
1:B:392:LYS:HB2	1:B:399:LEU:CD2	2.48	0.43
1:C:100:SER:O	1:C:102:TYR:N	2.51	0.43
1:C:394:GLU:O	1:C:394:GLU:HG2	2.18	0.43
1:D:77:LEU:CD1	1:D:85:LEU:HD12	2.49	0.43
1:D:332:PHE:CD1	1:D:338:LEU:CD2	3.01	0.43
1:E:96:ARG:O	1:E:97:THR:C	2.61	0.43
1:F:186:ALA:HB1	1:F:241:PHE:CE2	2.54	0.43
1:C:55:MET:O	1:C:56:VAL:C	2.60	0.43
1:D:51:VAL:HG13	1:D:55:MET:CE	2.45	0.43
1:D:194:PHE:CD1	1:D:200:VAL:HG11	2.54	0.43
1:A:112:ASN:O	1:A:116:ARG:HG3	2.19	0.43
1:A:146:GLN:N	1:A:147:PRO:CD	2.81	0.43
1:A:183:LYS:HA	1:A:183:LYS:HD3	1.72	0.43
1:B:269:MET:HE3	1:B:292:ILE:CG2	2.48	0.43
1:F:86:ASP:O	1:F:89:PRO:HD2	2.18	0.43
1:F:153:LYS:O	1:F:157:ILE:HG13	2.19	0.43
1:A:84:ILE:HG12	1:A:88:LEU:CD1	2.49	0.43
1:B:219:LEU:HD12	1:B:365:GLN:NE2	2.33	0.43
1:C:416:CYS:HB3	1:C:419:CYS:SG	2.58	0.43
1:D:48:PRO:CG	1:D:116:ARG:NH1	2.71	0.43
1:D:82:PRO:HG3	1:D:156:LEU:HA	2.00	0.43
1:D:146:GLN:HE21	1:D:379:GLN:NE2	2.17	0.43
1:F:105:LYS:O	1:F:106:MET:C	2.62	0.43
1:A:338:LEU:O	1:A:346:ASN:HB2	2.19	0.42
1:B:273:THR:HG22	1:B:275:ASP:H	1.82	0.42
1:C:399:LEU:HD22	1:C:429:ILE:HD13	2.01	0.42
1:D:82:PRO:HB3	1:D:159:SER:HB2	2.01	0.42
1:D:179:PHE:CD1	1:D:179:PHE:C	2.97	0.42
1:E:54:LYS:HD3	1:E:54:LYS:H	1.84	0.42
1:E:263:VAL:HG12	1:E:264:THR:CG2	2.49	0.42
1:E:383:ILE:HG13	1:E:384:CYS:N	2.34	0.42
1:F:294:ARG:HG3	1:F:295:LEU:O	2.19	0.42
1:F:374:MET:HB2	1:F:374:MET:HE2	1.71	0.42
1:B:434:PHE:HB3	1:C:334:GLU:HG2	2.01	0.42
1:C:299:ARG:HH21	1:C:302:GLN:NE2	2.16	0.42
1:D:82:PRO:HB2	1:D:87:LEU:HD11	2.00	0.42
1:E:162:LEU:HD11	1:E:166:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:53:LYS:HA	1:F:56:VAL:HG12	2.00	0.42
1:F:383:ILE:HB	1:F:404:CYS:SG	2.59	0.42
1:F:284:PHE:O	1:F:287:LYS:N	2.37	0.42
1:A:255:LEU:HD23	1:A:255:LEU:HA	1.80	0.42
1:B:299:ARG:HH21	1:B:302:GLN:NE2	2.17	0.42
1:C:82:PRO:HB2	1:C:87:LEU:HD11	2.01	0.42
1:D:79:ASN:O	1:D:83:TYR:HE2	2.02	0.42
1:D:154:LEU:HD23	1:D:154:LEU:HA	1.72	0.42
1:F:88:LEU:N	1:F:89:PRO:CD	2.82	0.42
1:B:88:LEU:HD12	1:B:88:LEU:HA	1.59	0.42
1:B:228:ILE:HG13	1:B:244:PHE:HB2	2.00	0.42
1:B:250:PRO:HD2	1:B:325:PHE:CE2	2.54	0.42
1:D:394:GLU:CG	1:D:424:LYS:HB3	2.49	0.42
1:E:54:LYS:O	1:E:55:MET:C	2.62	0.42
1:E:75:LEU:O	1:E:75:LEU:CD2	2.64	0.42
1:A:191:ARG:NH2	1:A:192:LYS:HA	2.34	0.42
1:A:325:PHE:CD1	1:A:325:PHE:C	2.97	0.42
1:A:349:LEU:O	1:A:350:THR:C	2.62	0.42
1:B:285:ILE:HD12	1:B:285:ILE:HA	1.88	0.42
1:E:48:PRO:HB3	1:E:116:ARG:CB	2.50	0.42
1:E:57:GLU:O	1:E:58:LYS:C	2.63	0.42
1:E:63:MET:HG2	1:E:126:THR:HG21	2.01	0.42
1:E:320:HIS:CD2	1:E:320:HIS:H	2.37	0.42
1:B:251:TRP:O	1:B:251:TRP:CG	2.70	0.42
1:F:99:LEU:CD2	1:F:106:MET:HE1	2.47	0.42
1:F:134:LYS:O	1:F:134:LYS:CG	2.68	0.42
1:A:95:LEU:HD23	1:A:95:LEU:HA	1.87	0.42
1:A:384:CYS:HB3	1:A:404:CYS:SG	2.59	0.42
1:D:400:MET:HE2	1:D:400:MET:HB3	1.84	0.42
1:E:277:VAL:HG13	1:E:292:ILE:HD11	2.01	0.42
1:F:137:LYS:HB3	1:F:138:GLU:H	1.42	0.42
1:B:78:LYS:C	1:B:80:SER:H	2.28	0.42
1:C:136:GLY:O	1:C:139:ARG:HB2	2.20	0.42
1:C:233:ASN:O	1:C:234:ASP:HB2	2.20	0.42
1:D:89:PRO:O	1:D:93:GLN:HG2	2.20	0.42
1:D:362:LYS:HD2	1:D:362:LYS:HA	1.74	0.42
1:E:118:PHE:CD1	1:E:118:PHE:C	2.97	0.42
1:E:160:HIS:HD1	1:E:230:LEU:HB3	1.84	0.42
1:F:291:TYR:OH	1:F:346:ASN:ND2	2.52	0.42
1:B:380:LEU:HD12	1:B:380:LEU:HA	1.92	0.42
1:C:51:VAL:CG1	1:C:52:ASP:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:ALA:HB1	1:C:371:TYR:HD2	1.85	0.42
1:C:379:GLN:HE21	1:C:388:ASP:CG	2.28	0.42
1:D:77:LEU:H	1:D:77:LEU:HG	1.51	0.42
1:D:146:GLN:HG3	1:D:379:GLN:OE1	2.20	0.42
1:E:168:ILE:HD12	1:E:198:THR:HG21	2.01	0.42
1:E:291:TYR:OH	1:E:346:ASN:ND2	2.50	0.42
1:B:123:MET:HE3	1:B:123:MET:HB2	1.87	0.41
1:B:361:ILE:C	1:B:361:ILE:HD12	2.45	0.41
1:C:118:PHE:CD1	1:C:118:PHE:C	2.98	0.41
1:E:89:PRO:O	1:E:92:TYR:HB3	2.19	0.41
1:E:130:ILE:HG22	1:E:131:SER:N	2.34	0.41
1:F:201:PRO:HG2	1:F:204:SER:HB2	2.01	0.41
1:C:56:VAL:HG13	1:C:57:GLU:N	2.34	0.41
1:E:55:MET:O	1:E:56:VAL:C	2.61	0.41
1:E:168:ILE:C	1:E:170:PRO:HD3	2.45	0.41
1:F:79:ASN:O	1:F:79:ASN:CG	2.62	0.41
1:A:224:LEU:CG	1:A:228:ILE:HD11	2.47	0.41
1:A:334:GLU:HG2	1:F:434:PHE:CG	2.54	0.41
1:B:53:LYS:O	1:B:53:LYS:CG	2.68	0.41
1:D:53:LYS:C	1:D:56:VAL:HG12	2.45	0.41
1:D:83:TYR:C	1:D:85:LEU:N	2.78	0.41
1:D:233:ASN:O	1:D:234:ASP:CB	2.61	0.41
1:D:379:GLN:HA	1:D:431:VAL:HG11	2.01	0.41
1:E:183:LYS:HE3	1:E:249:GLN:NE2	2.35	0.41
1:E:241:PHE:CZ	1:E:245:THR:HG21	2.56	0.41
1:B:380:LEU:O	1:B:382:LYS:CE	2.55	0.41
1:D:102:TYR:CD2	1:D:109:LEU:HB2	2.55	0.41
1:E:421:CYS:SG	1:E:422:GLU:N	2.93	0.41
1:F:52:ASP:C	1:F:52:ASP:OD1	2.63	0.41
1:A:80:SER:OG	1:A:81:PRO:HD2	2.21	0.41
1:A:83:TYR:CZ	1:A:85:LEU:HB2	2.55	0.41
1:A:103:GLU:HA	1:A:103:GLU:OE1	2.21	0.41
1:C:129:THR:OG1	1:C:154:LEU:HD13	2.21	0.41
1:D:137:LYS:HB2	1:D:138:GLU:OE1	2.20	0.41
1:E:114:TYR:CD2	1:E:199:ILE:HD12	2.56	0.41
1:B:53:LYS:O	1:B:53:LYS:HG3	2.21	0.41
1:B:273:THR:CG2	1:B:274:TYR:N	2.79	0.41
1:C:280:ARG:O	1:C:283:LYS:HD3	2.21	0.41
1:C:400:MET:HE2	1:C:400:MET:HB3	1.94	0.41
1:E:381:CYS:HB2	1:E:401:CYS:HB3	2.02	0.41
1:F:85:LEU:O	1:F:89:PRO:CG	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:335:GLY:HA2	1:F:338:LEU:HD21	2.02	0.41
1:A:57:GLU:HA	1:A:57:GLU:OE1	2.21	0.41
1:A:123:MET:CA	1:A:126:THR:HG22	2.50	0.41
1:B:74:LYS:HB2	1:B:141:TYR:CD1	2.56	0.41
1:B:382:LYS:HA	1:B:382:LYS:HD3	1.66	0.41
1:C:54:LYS:HG2	1:C:55:MET:H	1.83	0.41
1:D:57:GLU:O	1:D:60:TRP:HB2	2.20	0.41
1:A:114:TYR:CD1	1:A:114:TYR:C	2.99	0.41
1:A:123:MET:O	1:A:126:THR:HG22	2.20	0.41
1:A:368:TYR:O	1:A:369:GLU:C	2.64	0.41
1:C:380:LEU:O	1:C:382:LYS:HE2	2.20	0.41
1:E:136:GLY:O	1:E:137:LYS:C	2.64	0.41
1:A:53:LYS:HG3	1:A:56:VAL:HG12	2.02	0.41
1:A:79:ASN:OD1	1:A:80:SER:N	2.54	0.41
1:B:139:ARG:C	1:B:141:TYR:N	2.75	0.41
1:B:174:PHE:CE1	1:B:176:GLY:HA3	2.56	0.41
1:B:251:TRP:CD1	1:B:251:TRP:O	2.73	0.41
1:C:433:PRO:HB2	1:C:434:PHE:CE1	2.56	0.41
1:D:148:ARG:HA	1:D:148:ARG:HD3	1.87	0.41
1:D:427:GLU:HA	1:D:428:PRO:HD3	1.82	0.41
1:E:379:GLN:HG2	1:E:431:VAL:HG13	2.03	0.41
1:F:182:THR:O	1:F:182:THR:HG22	2.21	0.41
1:F:202:TRP:CH2	1:F:225:LYS:HB2	2.56	0.41
1:F:248:PHE:O	1:F:254:LEU:HD12	2.20	0.41
1:F:411:SER:O	1:F:411:SER:OG	2.34	0.41
1:F:434:PHE:O	1:F:435:ASP:HB2	2.19	0.41
1:B:213:HIS:HE1	1:B:252:SER:O	2.04	0.41
1:B:434:PHE:C	1:B:435:ASP:OD1	2.64	0.41
1:C:299:ARG:HH21	1:C:302:GLN:CD	2.28	0.41
1:C:309:THR:C	1:C:311:ASP:H	2.28	0.41
1:D:74:LYS:HD2	1:D:141:TYR:CD2	2.56	0.41
1:F:390:ASP:OD1	1:F:402:THR:HG22	2.21	0.41
1:A:142:GLU:HG3	1:A:145:SER:OG	2.22	0.40
1:A:280:ARG:O	1:A:280:ARG:HG2	2.20	0.40
1:A:400:MET:HE2	1:A:400:MET:HB3	1.81	0.40
1:B:122:LEU:HA	1:B:161:MET:HE1	2.03	0.40
1:D:219:LEU:HD23	1:D:219:LEU:HA	1.87	0.40
1:E:54:LYS:NZ	1:E:55:MET:N	2.69	0.40
1:A:229:ASP:OD1	1:A:229:ASP:C	2.64	0.40
1:A:325:PHE:O	1:A:329:ILE:HG13	2.21	0.40
1:B:411:SER:O	1:B:412:GLU:CB	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:TYR:CD1	1:C:141:TYR:N	2.87	0.40
1:D:283:LYS:HE2	1:D:283:LYS:N	2.34	0.40
1:D:408:TRP:O	1:D:408:TRP:CG	2.73	0.40
1:E:58:LYS:O	1:E:61:LYS:HB2	2.22	0.40
1:E:349:LEU:C	1:E:351:GLY:H	2.28	0.40
1:C:89:PRO:O	1:C:92:TYR:HB3	2.20	0.40
1:D:133:PHE:CZ	1:D:140:MET:HE2	2.56	0.40
1:E:60:TRP:CD2	1:E:92:TYR:CE1	3.09	0.40
1:E:149:ARG:HH11	1:E:377:THR:HG22	1.85	0.40
1:F:170:PRO:HD2	1:F:173:LEU:O	2.22	0.40
1:F:394:GLU:HA	1:F:395:PRO:HA	1.87	0.40
1:A:71:GLN:O	1:A:72:ASN:C	2.64	0.40
1:A:83:TYR:OH	1:A:85:LEU:HD12	2.21	0.40
1:A:107:GLU:CD	1:A:107:GLU:N	2.78	0.40
1:A:248:PHE:O	1:A:254:LEU:HD12	2.20	0.40
1:B:349:LEU:C	1:B:351:GLY:N	2.78	0.40
1:C:93:GLN:NE2	1:C:93:GLN:HA	2.35	0.40
1:D:284:PHE:O	1:D:286:HIS:N	2.54	0.40
1:E:97:THR:HG22	1:E:172:GLY:HA3	2.03	0.40
1:E:322:LYS:H	1:E:322:LYS:HG2	1.41	0.40
1:A:60:TRP:CZ3	1:A:96:ARG:NH1	2.89	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	380/389 (98%)	356 (94%)	23 (6%)	1 (0%)	36	57
1	B	381/389 (98%)	344 (90%)	37 (10%)	0	100	100
1	C	381/389 (98%)	346 (91%)	32 (8%)	3 (1%)	16	34
1	D	381/389 (98%)	341 (90%)	37 (10%)	3 (1%)	16	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	379/389 (97%)	339 (89%)	39 (10%)	1 (0%)	36	57
1	F	380/389 (98%)	337 (89%)	43 (11%)	0	100	100
All	All	2282/2334 (98%)	2063 (90%)	211 (9%)	8 (0%)	30	51

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	146	GLN
1	C	101	ARG
1	D	182	THR
1	E	285	ILE
1	D	285	ILE
1	D	433	PRO
1	C	433	PRO
1	A	361	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/350 (99%)	321 (93%)	24 (7%)	14	31
1	B	346/350 (99%)	312 (90%)	34 (10%)	7	17
1	C	344/350 (98%)	308 (90%)	36 (10%)	6	15
1	D	346/350 (99%)	313 (90%)	33 (10%)	8	18
1	E	344/350 (98%)	312 (91%)	32 (9%)	8	19
1	F	345/350 (99%)	303 (88%)	42 (12%)	5	10
All	All	2070/2100 (99%)	1869 (90%)	201 (10%)	8	17

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	THR
1	A	59	CYS

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Mol	Chain	Res	Type
1	A	74	LYS
1	A	78	LYS
1	A	100	SER
1	A	103	GLU
1	A	107	GLU
1	A	113	GLU
1	A	135	GLU
1	A	138	GLU
1	A	142	GLU
1	A	145	SER
1	A	148	ARG
1	A	175	GLN
1	A	178	THR
1	A	206	ARG
1	A	216	SER
1	A	273	THR
1	A	285	ILE
1	A	322	LYS
1	A	376	SER
1	A	431	VAL
1	A	432	ASP
1	A	434	PHE
1	B	53	LYS
1	B	59	CYS
1	B	65	LYS
1	B	84	ILE
1	B	88	LEU
1	B	98	ILE
1	B	105	LYS
1	B	124	LYS
1	B	126	THR
1	B	135	GLU
1	B	138	GLU
1	B	146	GLN
1	B	175	GLN
1	B	191	ARG
1	B	197	LYS
1	B	199	ILE
1	B	200	VAL
1	B	206	ARG
1	B	216	SER
1	B	273	THR

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Mol	Chain	Res	Type
1	B	283	LYS
1	B	320	HIS
1	B	349	LEU
1	B	354	GLU
1	B	360	HIS
1	B	362	LYS
1	B	379	GLN
1	B	386	GLU
1	B	391	VAL
1	B	406	THR
1	B	407	SER
1	B	412	GLU
1	B	414	GLN
1	B	424	LYS
1	C	50	THR
1	C	57	GLU
1	C	58	LYS
1	C	61	LYS
1	C	65	LYS
1	C	74	LYS
1	C	103	GLU
1	C	105	LYS
1	C	111	GLU
1	C	120	GLU
1	C	123	MET
1	C	135	GLU
1	C	137	LYS
1	C	143	GLU
1	C	144	ASN
1	C	145	SER
1	C	148	ARG
1	C	173	LEU
1	C	188	GLU
1	C	191	ARG
1	C	192	LYS
1	C	199	ILE
1	C	264	THR
1	C	322	LYS
1	C	338	LEU
1	C	360	HIS
1	C	361	ILE
1	C	366	GLU

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Mol	Chain	Res	Type
1	C	374	MET
1	C	376	SER
1	C	379	GLN
1	C	394	GLU
1	C	421	CYS
1	C	430	VAL
1	C	432	ASP
1	C	434	PHE
1	D	61	LYS
1	D	65	LYS
1	D	75	LEU
1	D	77	LEU
1	D	78	LYS
1	D	80	SER
1	D	93	GLN
1	D	108	THR
1	D	113	GLU
1	D	124	LYS
1	D	137	LYS
1	D	148	ARG
1	D	153	LYS
1	D	154	LEU
1	D	157	ILE
1	D	173	LEU
1	D	178	THR
1	D	191	ARG
1	D	199	ILE
1	D	283	LYS
1	D	285	ILE
1	D	311	ASP
1	D	322	LYS
1	D	354	GLU
1	D	360	HIS
1	D	379	GLN
1	D	380	LEU
1	D	382	LYS
1	D	394	GLU
1	D	414	GLN
1	D	420	ARG
1	D	431	VAL
1	D	434	PHE
1	E	51	VAL

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Mol	Chain	Res	Type
1	E	52	ASP
1	E	53	LYS
1	E	54	LYS
1	E	55	MET
1	E	64	ASP
1	E	75	LEU
1	E	122	LEU
1	E	130	ILE
1	E	143	GLU
1	E	154	LEU
1	E	175	GLN
1	E	191	ARG
1	E	198	THR
1	E	199	ILE
1	E	227	THR
1	E	232	CYS
1	E	311	ASP
1	E	316	GLN
1	E	320	HIS
1	E	361	ILE
1	E	362	LYS
1	E	376	SER
1	E	386	GLU
1	E	389	LYS
1	E	393	ILE
1	E	401	CYS
1	E	406	THR
1	E	411	SER
1	E	427	GLU
1	E	431	VAL
1	E	434	PHE
1	F	51	VAL
1	F	58	LYS
1	F	71	GLN
1	F	74	LYS
1	F	77	LEU
1	F	78	LYS
1	F	111	GLU
1	F	113	GLU
1	F	135	GLU
1	F	138	GLU
1	F	141	TYR

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Mol	Chain	Res	Type
1	F	142	GLU
1	F	144	ASN
1	F	145	SER
1	F	150	ASN
1	F	152	THR
1	F	156	LEU
1	F	173	LEU
1	F	191	ARG
1	F	206	ARG
1	F	207	GLN
1	F	243	ILE
1	F	285	ILE
1	F	294	ARG
1	F	308	VAL
1	F	309	THR
1	F	321	ASN
1	F	322	LYS
1	F	359	ASP
1	F	360	HIS
1	F	361	ILE
1	F	362	LYS
1	F	366	GLU
1	F	374	MET
1	F	379	GLN
1	F	394	GLU
1	F	409	GLN
1	F	414	GLN
1	F	420	ARG
1	F	424	LYS
1	F	427	GLU
1	F	434	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	93	GLN
1	A	150	ASN
1	A	210	HIS
1	A	213	HIS
1	A	257	ASN
1	A	265	HIS

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Mol	Chain	Res	Type
1	A	302	GLN
1	A	320	HIS
1	A	321	ASN
1	A	346	ASN
1	B	71	GLN
1	B	210	HIS
1	B	213	HIS
1	B	233	ASN
1	B	265	HIS
1	B	302	GLN
1	B	321	ASN
1	B	326	GLN
1	B	345	GLN
1	B	346	ASN
1	B	365	GLN
1	B	379	GLN
1	B	387	ASN
1	B	414	GLN
1	C	71	GLN
1	C	93	GLN
1	C	146	GLN
1	C	150	ASN
1	C	160	HIS
1	C	210	HIS
1	C	265	HIS
1	C	346	ASN
1	C	379	GLN
1	D	93	GLN
1	D	112	ASN
1	D	146	GLN
1	D	150	ASN
1	D	175	GLN
1	D	210	HIS
1	D	265	HIS
1	D	282	GLN
1	D	321	ASN
1	D	346	ASN
1	D	387	ASN
1	D	414	GLN
1	E	112	ASN
1	E	146	GLN
1	E	150	ASN

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Mol	Chain	Res	Type
1	E	175	GLN
1	E	210	HIS
1	E	265	HIS
1	E	346	ASN
1	E	360	HIS
1	E	387	ASN
1	F	71	GLN
1	F	79	ASN
1	F	144	ASN
1	F	146	GLN
1	F	160	HIS
1	F	210	HIS
1	F	265	HIS
1	F	282	GLN
1	F	286	HIS
1	F	321	ASN
1	F	346	ASN
1	F	387	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 18 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	384/389 (98%)	0.05	12 (3%)	51	47	31, 46, 79, 109	0
1	B	385/389 (98%)	0.21	8 (2%)	63	60	32, 51, 85, 105	0
1	C	385/389 (98%)	0.37	23 (5%)	27	24	36, 54, 88, 110	0
1	D	385/389 (98%)	0.34	14 (3%)	46	41	36, 56, 89, 112	0
1	E	383/389 (98%)	0.45	18 (4%)	36	32	34, 58, 93, 126	0
1	F	384/389 (98%)	0.41	14 (3%)	46	41	35, 58, 92, 113	0
All	All	2306/2334 (98%)	0.31	89 (3%)	43	38	31, 54, 88, 126	0

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	47	PRO	5.9
1	A	47	PRO	5.5
1	E	47	PRO	5.1
1	C	360	HIS	4.1
1	B	360	HIS	3.9
1	F	47	PRO	3.7
1	B	355	PRO	3.6
1	F	108	THR	3.5
1	E	50	THR	3.4
1	C	47	PRO	3.3
1	B	361	ILE	3.3
1	C	142	GLU	3.3
1	E	48	PRO	3.3
1	A	361	ILE	3.2
1	F	320	HIS	3.2
1	E	49	GLY	3.2
1	C	377	THR	3.2
1	A	435	ASP	3.1
1	F	77	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	310	ALA	3.1
1	F	54	LYS	3.1
1	A	79	ASN	3.0
1	C	359	ASP	3.0
1	F	50	THR	3.0
1	E	394	GLU	3.0
1	A	353	CYS	3.0
1	E	51	VAL	3.0
1	B	376	SER	2.9
1	C	53	LYS	2.9
1	A	376	SER	2.9
1	C	146	GLN	2.9
1	A	188	GLU	2.8
1	A	375	GLY	2.8
1	D	53	LYS	2.8
1	D	361	ILE	2.8
1	E	353	CYS	2.7
1	F	321	ASN	2.7
1	F	379	GLN	2.7
1	C	110	GLY	2.7
1	C	286	HIS	2.7
1	D	320	HIS	2.7
1	F	79	ASN	2.7
1	D	435	ASP	2.7
1	D	274	TYR	2.6
1	E	143	GLU	2.6
1	E	320	HIS	2.5
1	C	354	GLU	2.5
1	C	48	PRO	2.5
1	E	108	THR	2.5
1	F	359	ASP	2.5
1	D	345	GLN	2.5
1	B	146	GLN	2.4
1	E	60	TRP	2.4
1	E	200	VAL	2.4
1	F	48	PRO	2.4
1	C	56	VAL	2.4
1	D	354	GLU	2.3
1	C	421	CYS	2.3
1	C	49	GLY	2.3
1	A	93	GLN	2.3
1	A	414	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	320	HIS	2.3
1	D	360	HIS	2.3
1	F	376	SER	2.3
1	D	321	ASN	2.3
1	B	320	HIS	2.2
1	C	78	LYS	2.2
1	B	321	ASN	2.2
1	A	144	ASN	2.2
1	C	79	ASN	2.2
1	C	375	GLY	2.2
1	E	360	HIS	2.2
1	C	350	THR	2.1
1	E	401	CYS	2.1
1	E	78	LYS	2.1
1	E	414	GLN	2.1
1	D	108	THR	2.1
1	F	53	LYS	2.1
1	C	321	ASN	2.1
1	C	50	THR	2.1
1	D	306	GLY	2.1
1	F	78	LYS	2.1
1	D	75	LEU	2.1
1	A	359	ASP	2.0
1	C	414	GLN	2.0
1	E	345	GLN	2.0
1	D	111	GLU	2.0
1	E	175	GLN	2.0
1	C	104	GLY	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($\text{\AA}^2$)	Q<0.9
3	CA	E	1438	1/1	0.94	0.10	72,72,72,72	0
3	CA	F	1438	1/1	0.94	0.10	77,77,77,77	0
3	CA	A	1438	1/1	0.95	0.07	57,57,57,57	0
3	CA	C	1438	1/1	0.95	0.11	66,66,66,66	0
3	CA	D	1438	1/1	0.96	0.15	63,63,63,63	0
2	ZN	E	1436	1/1	0.97	0.04	70,70,70,70	0
3	CA	B	1438	1/1	0.97	0.09	56,56,56,56	0
2	ZN	A	1436	1/1	0.99	0.02	52,52,52,52	0
2	ZN	E	1437	1/1	0.99	0.03	56,56,56,56	0
2	ZN	C	1436	1/1	0.99	0.02	56,56,56,56	0
2	ZN	C	1437	1/1	0.99	0.02	50,50,50,50	0
2	ZN	F	1437	1/1	1.00	0.02	41,41,41,41	0
2	ZN	B	1436	1/1	1.00	0.02	51,51,51,51	0
2	ZN	D	1436	1/1	1.00	0.04	47,47,47,47	0
2	ZN	D	1437	1/1	1.00	0.04	46,46,46,46	0
2	ZN	B	1437	1/1	1.00	0.03	49,49,49,49	0
2	ZN	A	1437	1/1	1.00	0.02	46,46,46,46	0
2	ZN	F	1436	1/1	1.00	0.03	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.