



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:42 AM UTC

PDB ID : 3EIQ / pdb_00003eiq
Title : Crystal structure of Pdcd4-eIF4A
Authors : Loh, P.G.; Cheng, Z.; Song, H.
Deposited on : 2008-09-17
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

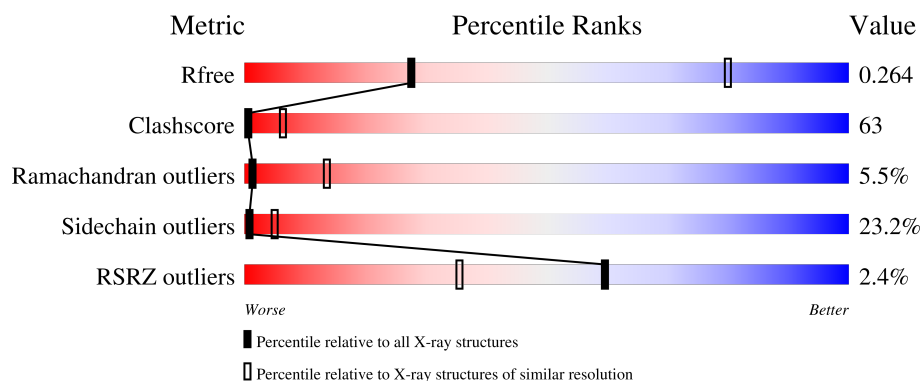
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	414	3% 32% 36% 17% • 12%
1	D	414	% 32% 37% 16% • 10%
2	C	358	% 22% 40% 14% • 22%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8080 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 Eukaryotic initiation factor 4A-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2923	1853	497	554	19			
1	D	371	Total	C	N	O	S	0	0	0
			2979	1887	511	562	19			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP P60842
A	-6	PRO	-	expression tag	UNP P60842
A	-5	LEU	-	expression tag	UNP P60842
A	-4	GLY	-	expression tag	UNP P60842
A	-3	SER	-	expression tag	UNP P60842
A	-2	PRO	-	expression tag	UNP P60842
A	-1	GLU	-	expression tag	UNP P60842
A	0	PHE	-	expression tag	UNP P60842
D	-7	GLY	-	expression tag	UNP P60842
D	-6	PRO	-	expression tag	UNP P60842
D	-5	LEU	-	expression tag	UNP P60842
D	-4	GLY	-	expression tag	UNP P60842
D	-3	SER	-	expression tag	UNP P60842
D	-2	PRO	-	expression tag	UNP P60842
D	-1	GLU	-	expression tag	UNP P60842
D	0	PHE	-	expression tag	UNP P60842

- Molecule 2 is a protein called Programmed cell death protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	278	Total	C	N	O	S	0	0	0
			2178	1380	359	424	15			

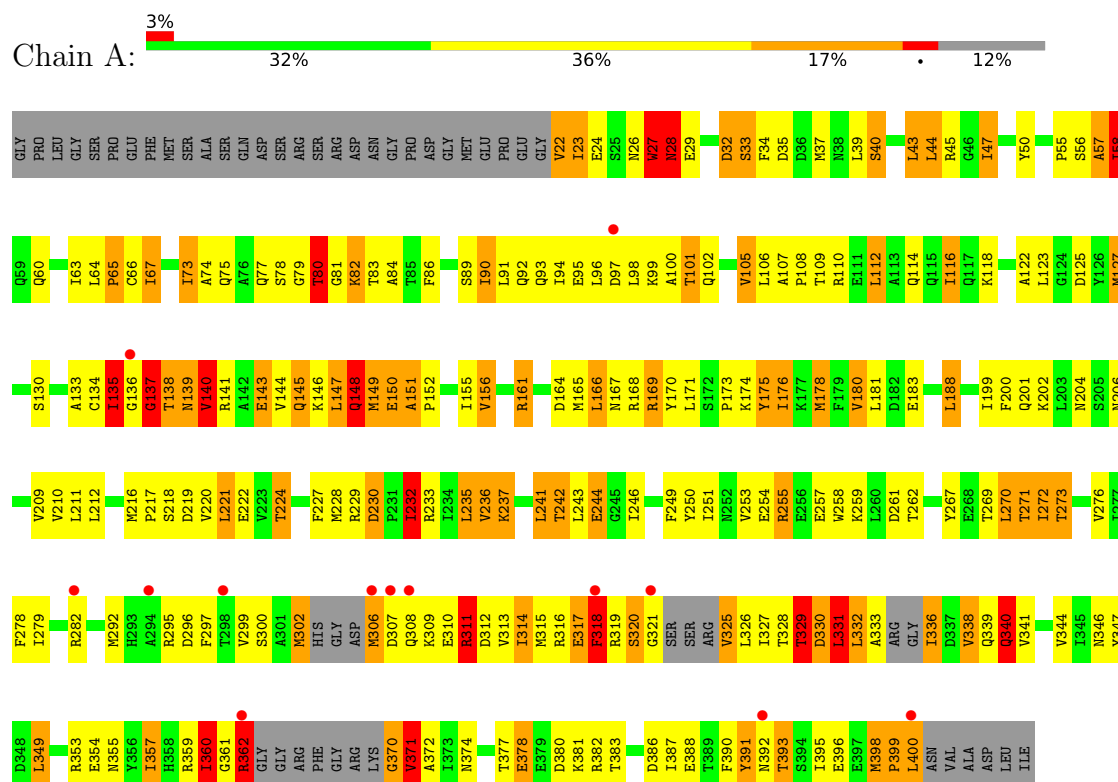
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	112	GLY	-	expression tag	UNP Q61823
C	113	PRO	-	expression tag	UNP Q61823
C	114	LEU	-	expression tag	UNP Q61823
C	115	GLY	-	expression tag	UNP Q61823
C	116	SER	-	expression tag	UNP Q61823
C	117	PRO	-	expression tag	UNP Q61823
C	118	GLU	-	expression tag	UNP Q61823
C	119	PHE	-	expression tag	UNP Q61823

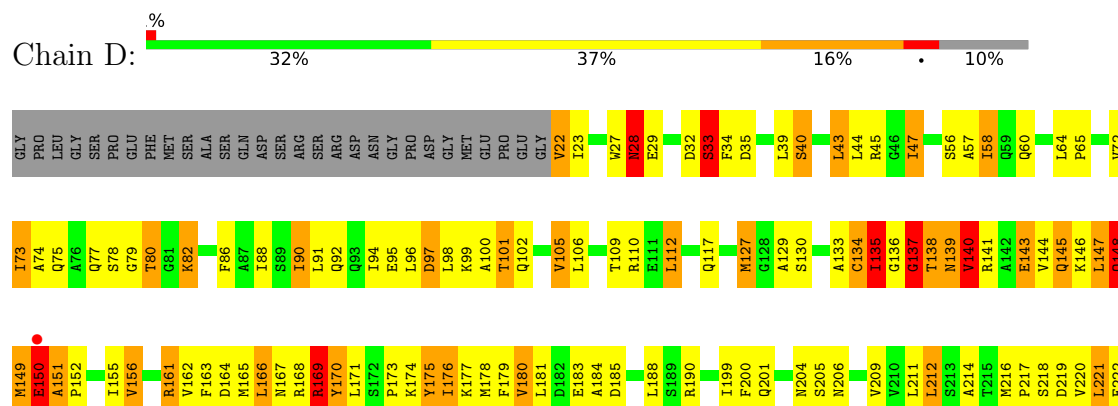
3 Residue-property plots

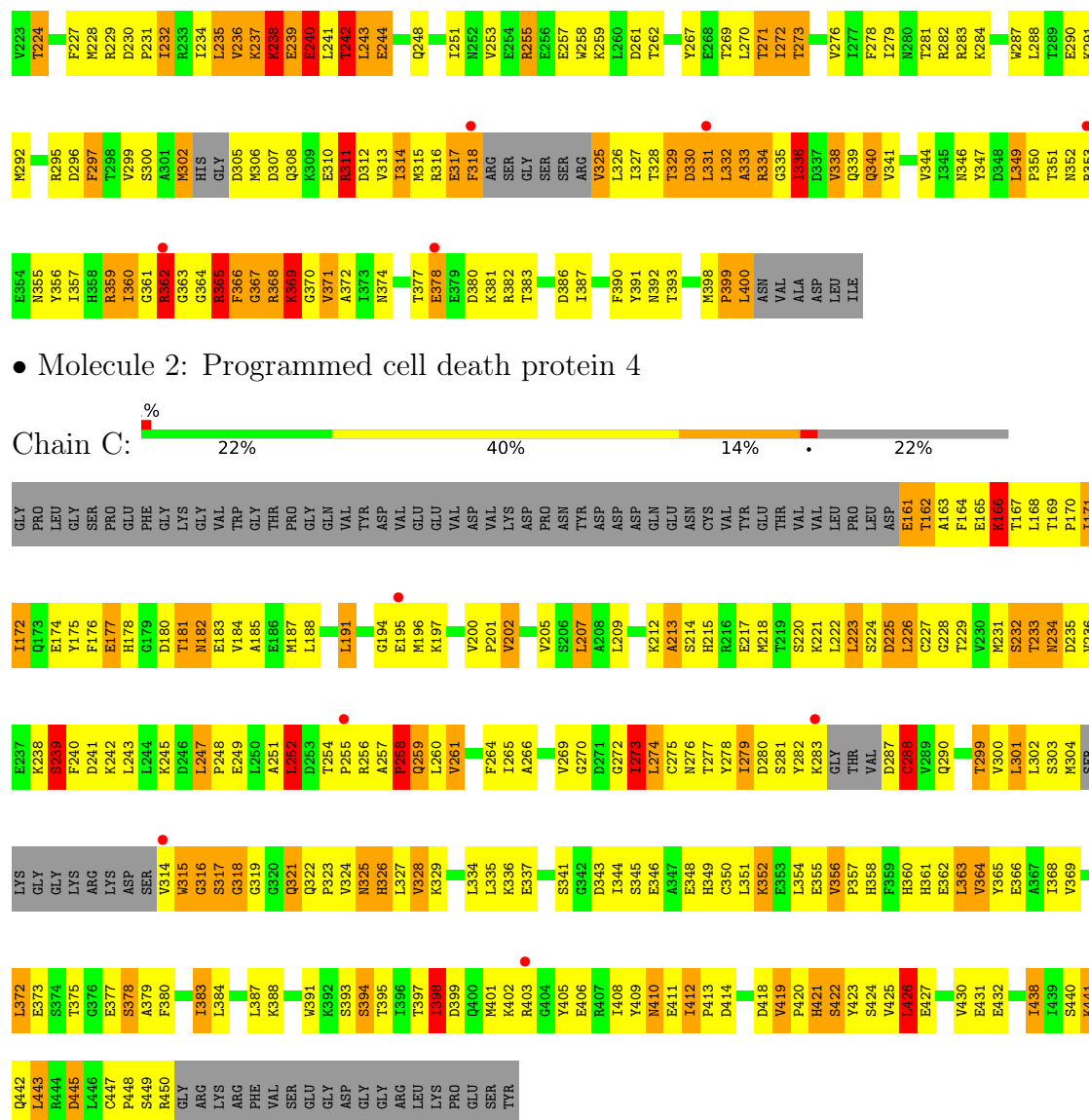
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Eukaryotic initiation factor 4A-I



• Molecule 1: Eukaryotic initiation factor 4A-I





● Molecule 2: Programmed cell death protein 4

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	198.36Å 198.36Å 198.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.91 – 3.50 29.91 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.91-3.50) 99.8 (29.91-3.50)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.44 (at 3.47Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.220 , 0.269 0.217 , 0.264	Depositor DCC
R_{free} test set	1670 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	93.8	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8080	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% 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 i

5.1 Standard geometry i

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	1.16	3/2963 (0.1%)	1.35	34/3998 (0.9%)
1	D	1.22	6/3022 (0.2%)	1.36	21/4077 (0.5%)
2	C	0.89	0/2213	1.26	22/2989 (0.7%)
All	All	1.12	9/8198 (0.1%)	1.33	77/11064 (0.7%)

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	A	0	2
1	D	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	80	THR	CA-CB	7.55	1.67	1.54
1	A	66	CYS	CA-C	-6.04	1.44	1.52
1	D	365	ARG	NE-CZ	-5.85	1.26	1.33
1	D	33	SER	CA-C	-5.56	1.46	1.52
1	D	336	ILE	CA-CB	5.32	1.61	1.54
1	A	67	ILE	CA-CB	-5.23	1.47	1.54
1	D	365	ARG	CD-NE	5.21	1.53	1.46
1	A	148	GLN	CA-C	-5.09	1.48	1.53
1	D	148	GLN	CA-C	-5.02	1.47	1.52

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	365	ARG	N-CA-C	-9.16	97.52	110.35
2	C	351	LEU	N-CA-C	-8.80	101.65	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	171	ILE	CB-CA-C	-8.63	103.47	111.06
1	D	148	GLN	N-CA-C	-8.54	92.63	107.49
1	D	29	GLU	N-CA-C	-8.32	95.83	109.40
1	A	82	LYS	N-CA-C	-8.20	102.42	111.36
1	D	166	LEU	N-CA-C	-8.18	102.45	111.36
2	C	317	SER	N-CA-C	7.89	120.13	108.14
1	D	365	ARG	NE-CZ-NH1	-7.81	113.69	121.50
1	A	137	GLY	N-CA-C	-7.70	90.99	113.30
1	D	365	ARG	NE-CZ-NH2	7.28	125.75	119.20
1	D	340	GLN	N-CA-C	-7.28	103.71	112.59
1	D	362	ARG	CB-CA-C	-7.10	96.30	110.42
1	A	232	ILE	CB-CA-C	-6.98	101.65	111.21
1	A	371	VAL	N-CA-C	6.81	118.74	108.80
1	D	170	TYR	N-CA-C	-6.80	104.98	113.28
1	A	80	THR	N-CA-C	-6.80	96.32	110.80
2	C	316	GLY	N-CA-C	-6.79	101.92	112.85
2	C	172	ILE	N-CA-C	-6.78	103.91	110.42
1	D	82	LYS	N-CA-C	-6.77	103.98	111.36
1	A	29	GLU	N-CA-C	-6.68	99.03	109.72
1	A	327	ILE	CB-CA-C	-6.66	103.26	111.32
1	A	176	ILE	CB-CA-C	-6.58	103.39	111.08
1	A	340	GLN	N-CA-C	-6.53	104.63	112.59
1	A	32	ASP	N-CA-C	6.50	118.03	111.07
1	D	28	ASN	CB-CA-C	6.48	119.46	111.43
1	A	28	ASN	CB-CA-C	6.41	119.81	111.42
1	A	148	GLN	N-CA-C	-6.41	96.31	107.20
1	A	362	ARG	CB-CG-CD	-6.38	96.62	111.30
2	C	412	ILE	CA-C-N	-6.28	113.29	119.64
2	C	412	ILE	C-N-CA	-6.28	113.29	119.64
1	D	43	LEU	N-CA-C	-6.20	104.60	111.36
1	A	371	VAL	CB-CA-C	-6.17	101.70	110.82
1	D	137	GLY	N-CA-C	-6.15	95.47	113.30
1	D	176	ILE	CB-CA-C	-6.14	104.66	111.35
2	C	398	ILE	CB-CA-C	-6.07	102.75	112.16
2	C	273	ILE	N-CA-C	-6.06	105.40	112.98
1	D	80	THR	N-CA-C	-6.03	105.00	112.72
2	C	441	LYS	N-CA-C	-5.89	105.19	112.38
1	A	140	VAL	N-CA-C	-5.86	105.02	110.53
2	C	191	LEU	N-CA-C	-5.76	106.25	113.28
2	C	351	LEU	CA-CB-CG	-5.73	96.23	116.30
1	A	270	LEU	N-CA-C	-5.69	105.99	114.64
1	A	398	MET	CA-C-N	5.67	126.93	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	MET	C-N-CA	5.67	126.93	119.84
2	C	252	LEU	N-CA-C	-5.67	104.72	111.69
1	A	123	LEU	N-CA-C	-5.56	105.22	112.23
2	C	255	PRO	CA-C-N	-5.53	113.64	122.66
2	C	255	PRO	C-N-CA	-5.53	113.64	122.66
1	A	235	LEU	N-CA-C	5.48	119.97	112.68
2	C	162	THR	N-CA-C	-5.48	106.44	113.01
1	D	140	VAL	N-CA-C	-5.47	105.04	111.00
1	D	80	THR	N-CA-CB	5.44	119.90	110.44
1	D	169	ARG	CA-CB-CG	-5.41	103.28	114.10
1	D	205	SER	N-CA-C	-5.28	106.08	113.37
1	D	134	CYS	N-CA-C	5.27	118.15	109.72
1	A	230	ASP	CB-CA-C	-5.26	99.80	110.17
1	A	391	TYR	N-CA-C	-5.25	100.60	108.96
1	A	23	ILE	CB-CA-C	-5.24	103.87	111.68
1	A	188	LEU	N-CA-C	-5.22	105.67	111.36
1	A	125	ASP	CA-C-N	-5.21	112.95	122.38
1	A	125	ASP	C-N-CA	-5.21	112.95	122.38
2	C	181	THR	N-CA-C	-5.20	105.04	111.33
1	A	27	TRP	CA-C-N	-5.18	113.74	121.72
1	A	27	TRP	C-N-CA	-5.18	113.74	121.72
2	C	228	GLY	N-CA-C	-5.18	107.86	114.85
1	A	43	LEU	N-CA-C	-5.15	105.75	111.36
2	C	213	ALA	N-CA-C	-5.14	105.57	111.07
2	C	377	GLU	N-CA-C	5.14	119.56	113.28
2	C	443	LEU	N-CA-C	-5.13	104.66	112.04
1	A	58	ILE	CG1-CB-CG2	-5.12	95.34	110.70
1	A	80	THR	O-C-N	5.11	129.39	122.59
1	A	166	LEU	N-CA-C	-5.11	105.79	111.36
1	A	80	THR	CA-C-N	5.11	131.41	121.41
1	A	80	THR	C-N-CA	5.11	131.41	121.41
2	C	276	ASN	N-CA-C	5.03	116.62	111.03
1	D	32	ASP	N-CA-C	5.03	116.57	111.14

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	THR	Peptide
1	A	370	GLY	Peptide
1	D	150	GLU	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	2923	0	2962	380	1
1	D	2979	0	3020	395	1
2	C	2178	0	2183	281	0
All	All	8080	0	8165	1026	1

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 63.

All (1026) 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:D:367:GLY:HA2	1:D:368:ARG:CG	1.27	1.62
1:A:338:VAL:C	1:A:362:ARG:HH12	1.14	1.55
1:D:338:VAL:CG2	1:D:362:ARG:HH22	1.19	1.54
1:D:135:ILE:CG2	1:D:136:GLY:HA3	1.34	1.54
1:A:135:ILE:CG2	1:A:136:GLY:HA3	1.40	1.51
1:A:338:VAL:CG2	1:A:362:ARG:HH22	1.19	1.51
1:A:150:GLU:CB	1:A:151:ALA:HB2	1.44	1.48
1:D:338:VAL:C	1:D:362:ARG:HH12	1.17	1.48
1:D:135:ILE:HG22	1:D:136:GLY:CA	1.43	1.44
1:D:367:GLY:CA	1:D:368:ARG:HG3	1.46	1.44
1:D:339:GLN:HG2	1:D:362:ARG:CZ	1.51	1.40
1:A:135:ILE:HG22	1:A:136:GLY:CA	1.50	1.39
1:A:150:GLU:HB2	1:A:151:ALA:CB	1.55	1.34
1:D:367:GLY:CA	1:D:368:ARG:CG	1.99	1.34
1:A:339:GLN:OE1	1:A:362:ARG:HD3	1.16	1.33
1:A:338:VAL:HG23	1:A:362:ARG:NH2	0.98	1.29
1:D:338:VAL:HG23	1:D:362:ARG:NH2	0.95	1.28
1:D:338:VAL:C	1:D:362:ARG:NH1	1.89	1.26
1:A:339:GLN:HG2	1:A:362:ARG:NE	1.50	1.25
1:A:339:GLN:HG2	1:A:362:ARG:CZ	1.66	1.24
1:A:339:GLN:CA	1:A:362:ARG:NH1	2.01	1.24
2:C:223:LEU:O	2:C:273:ILE:CD1	1.86	1.24
1:A:339:GLN:N	1:A:362:ARG:NH1	1.86	1.24
1:A:118:LYS:HD3	1:A:307:ASP:OD2	1.34	1.23

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:VAL:C	1:A:362:ARG:NH1	1.94	1.22
1:D:339:GLN:HG2	1:D:362:ARG:NE	1.24	1.22
1:A:339:GLN:CA	1:A:362:ARG:HH11	1.51	1.22
1:D:150:GLU:HB2	1:D:151:ALA:CB	1.69	1.21
2:C:321:GLN:N	2:C:321:GLN:OE1	1.72	1.21
1:A:134:CYS:O	1:A:135:ILE:HG12	1.38	1.20
1:D:235:LEU:HD13	1:D:235:LEU:O	1.41	1.17
2:C:164:PHE:CE1	2:C:168:LEU:HD13	1.79	1.17
1:D:240:GLU:HA	1:D:241:LEU:HB2	1.27	1.16
1:D:147:LEU:CD1	1:D:165:MET:HE1	1.74	1.15
1:A:339:GLN:HA	1:A:362:ARG:NH1	1.57	1.15
1:D:99:LYS:HD3	1:D:150:GLU:OE1	1.45	1.13
1:A:137:GLY:HA2	1:A:140:VAL:HG23	1.29	1.13
1:A:332:LEU:HD12	1:A:332:LEU:N	1.59	1.12
1:D:332:LEU:HD12	1:D:332:LEU:N	1.58	1.12
1:D:367:GLY:HA2	1:D:368:ARG:HG2	1.16	1.12
2:C:317:SER:HB2	2:C:318:GLY:HA3	1.24	1.11
1:D:365:ARG:HA	1:D:367:GLY:N	1.63	1.11
1:A:311:ARG:CG	1:A:311:ARG:HH11	1.63	1.11
1:D:313:VAL:O	1:D:317:GLU:HB2	1.49	1.10
1:D:339:GLN:CG	1:D:362:ARG:NE	2.02	1.10
1:D:150:GLU:HB2	1:D:151:ALA:HB2	1.11	1.09
1:D:339:GLN:N	1:D:362:ARG:NH1	2.00	1.09
1:D:314:ILE:HG22	1:D:336:ILE:HG22	1.32	1.09
1:D:339:GLN:HA	1:D:362:ARG:HH11	1.04	1.08
1:A:339:GLN:CD	1:A:362:ARG:HD3	1.79	1.08
1:A:354:GLU:OE2	2:C:357:PRO:HD2	1.51	1.08
1:D:367:GLY:HA3	1:D:368:ARG:HG3	1.17	1.08
2:C:161:GLU:HG3	2:C:162:THR:N	1.46	1.08
1:D:361:GLY:O	1:D:362:ARG:HG2	1.50	1.07
1:A:110:ARG:HD3	1:A:135:ILE:HG23	1.11	1.07
2:C:317:SER:HB2	2:C:318:GLY:CA	1.82	1.07
1:D:236:VAL:HG22	1:D:236:VAL:O	1.54	1.07
1:D:134:CYS:O	1:D:135:ILE:HG12	1.54	1.07
1:A:311:ARG:HH11	1:A:311:ARG:HG3	0.98	1.07
1:D:241:LEU:O	1:D:242:THR:HG22	1.52	1.07
1:D:338:VAL:CG2	1:D:362:ARG:NH2	1.87	1.07
1:D:314:ILE:CG2	1:D:336:ILE:HG22	1.85	1.06
2:C:287:ASP:O	2:C:288:CYS:HB3	1.52	1.06
1:A:136:GLY:H	1:A:137:GLY:CA	1.68	1.05
1:D:339:GLN:CA	1:D:362:ARG:NH1	2.19	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:GLN:HA	1:D:362:ARG:NH1	1.70	1.05
1:D:136:GLY:H	1:D:137:GLY:CA	1.69	1.05
1:A:22:VAL:CG1	1:A:75:GLN:OE1	2.05	1.05
1:D:110:ARG:CD	1:D:135:ILE:HG23	1.86	1.04
1:D:237:LYS:HG2	1:D:238:LYS:H	1.20	1.04
1:D:101:THR:HB	1:D:152:PRO:O	1.57	1.04
1:D:360:ILE:HG23	1:D:361:GLY:H	1.21	1.04
1:A:147:LEU:CD1	1:A:165:MET:HE1	1.87	1.03
1:D:311:ARG:HG3	1:D:311:ARG:HH11	1.21	1.03
1:A:101:THR:HB	1:A:152:PRO:O	1.55	1.03
1:D:267:TYR:CD2	1:D:297:PHE:CD2	2.47	1.03
1:D:110:ARG:HD3	1:D:135:ILE:HG23	1.07	1.03
1:A:267:TYR:CD2	1:A:297:PHE:HD2	1.75	1.03
1:A:267:TYR:CD2	1:A:297:PHE:CD2	2.45	1.03
1:D:240:GLU:HA	1:D:241:LEU:CB	1.88	1.03
1:A:110:ARG:HD3	1:A:135:ILE:CG2	1.88	1.02
1:A:302:MET:HE1	1:A:310:GLU:HG2	1.40	1.02
1:A:269:THR:O	1:A:270:LEU:HD12	1.58	1.02
1:D:110:ARG:HD3	1:D:135:ILE:CG2	1.88	1.02
1:D:150:GLU:CB	1:D:151:ALA:HB2	1.89	1.02
1:D:314:ILE:O	1:D:318:PHE:HB2	1.57	1.02
1:D:267:TYR:CD2	1:D:297:PHE:HD2	1.77	1.01
1:A:339:GLN:HG2	1:A:362:ARG:CD	1.91	1.01
2:C:426:LEU:O	2:C:430:VAL:HG23	1.60	1.01
1:A:338:VAL:CG2	1:A:362:ARG:NH2	1.95	1.01
1:D:311:ARG:HH11	1:D:311:ARG:CG	1.71	1.01
1:D:368:ARG:O	1:D:369:LYS:HB2	1.58	1.00
1:A:110:ARG:CD	1:A:135:ILE:HG23	1.91	1.00
1:A:339:GLN:OE1	1:A:362:ARG:CD	2.10	0.99
1:D:367:GLY:HA2	1:D:368:ARG:CB	1.87	0.99
1:A:361:GLY:O	1:A:362:ARG:HG2	1.61	0.99
2:C:420:PRO:O	2:C:421:HIS:HB2	1.63	0.99
1:A:302:MET:CE	1:A:310:GLU:HG2	1.93	0.99
1:A:314:ILE:CG2	1:A:336:ILE:HG22	1.92	0.98
1:D:302:MET:HG3	1:D:328:THR:HG22	1.45	0.98
1:D:137:GLY:HA2	1:D:140:VAL:HG23	1.44	0.98
1:D:65:PRO:HB3	1:D:232:ILE:HD11	1.45	0.97
2:C:161:GLU:CG	2:C:162:THR:N	2.25	0.97
1:A:311:ARG:HG3	1:A:311:ARG:NH1	1.65	0.97
1:D:134:CYS:C	1:D:135:ILE:HG12	1.87	0.97
1:D:339:GLN:CG	1:D:362:ARG:CZ	2.40	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:402:LYS:HE2	2:C:406:GLU:OE2	1.66	0.96
1:D:362:ARG:HG3	1:D:369:LYS:HG3	1.46	0.96
2:C:372:LEU:HD21	2:C:426:LEU:HB2	1.48	0.96
1:A:339:GLN:N	1:A:362:ARG:HH12	1.53	0.95
1:A:22:VAL:HG12	1:A:75:GLN:NE2	1.80	0.95
1:D:147:LEU:HD13	1:D:165:MET:HE1	1.44	0.95
1:A:134:CYS:C	1:A:135:ILE:CG1	2.40	0.95
2:C:227:CYS:CB	2:C:273:ILE:HD11	1.97	0.95
1:D:57:ALA:HB1	1:D:236:VAL:HG21	1.48	0.95
1:D:243:LEU:HD12	1:D:243:LEU:H	1.30	0.95
1:A:378:GLU:OE1	1:A:378:GLU:HA	1.67	0.95
2:C:349:HIS:CE1	1:D:283:ARG:HH22	1.85	0.95
1:D:22:VAL:HG12	1:D:75:GLN:NE2	1.79	0.95
2:C:384:LEU:CD2	2:C:432:GLU:HB3	1.97	0.95
1:A:339:GLN:HA	1:A:362:ARG:HH11	0.80	0.94
1:A:23:ILE:HG23	1:A:216:MET:HG3	1.49	0.94
1:A:95:GLU:H	1:A:102:GLN:HE22	1.15	0.94
1:A:302:MET:O	1:A:332:LEU:HD21	1.66	0.94
2:C:402:LYS:O	2:C:406:GLU:HG3	1.67	0.94
1:D:237:LYS:HG2	1:D:238:LYS:N	1.75	0.94
2:C:164:PHE:CD2	2:C:196:MET:CE	2.51	0.94
1:A:79:GLY:HA2	1:A:82:LYS:HB3	1.50	0.93
1:A:22:VAL:HG12	1:A:75:GLN:HE22	1.30	0.93
2:C:442:GLN:HA	2:C:445:ASP:HB2	1.50	0.93
2:C:325:ASN:HA	2:C:328:VAL:HG23	1.49	0.92
2:C:212:LYS:H	2:C:215:HIS:HD2	1.14	0.92
2:C:227:CYS:HB2	2:C:273:ILE:HD11	1.52	0.92
1:A:136:GLY:H	1:A:137:GLY:HA2	1.34	0.92
1:A:314:ILE:O	1:A:318:PHE:HB2	1.69	0.92
1:A:339:GLN:CG	1:A:362:ARG:CD	2.47	0.92
2:C:178:HIS:HD2	2:C:180:ASP:H	1.16	0.91
1:A:360:ILE:HG23	1:A:361:GLY:H	1.35	0.91
1:D:314:ILE:HG21	1:D:335:GLY:O	1.69	0.91
1:D:378:GLU:OE1	1:D:378:GLU:HA	1.70	0.91
1:A:307:ASP:O	1:A:311:ARG:HB2	1.71	0.91
1:D:136:GLY:N	1:D:137:GLY:CA	2.31	0.91
1:A:329:THR:HG21	2:C:174:GLU:OE1	1.71	0.91
1:D:23:ILE:HG23	1:D:216:MET:HG3	1.51	0.90
1:D:235:LEU:O	1:D:235:LEU:CD1	2.20	0.90
2:C:321:GLN:OE1	2:C:321:GLN:CA	2.19	0.90
1:A:134:CYS:C	1:A:135:ILE:HG12	1.96	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:223:LEU:O	2:C:273:ILE:HD11	1.69	0.90
1:D:22:VAL:HG12	1:D:75:GLN:HE22	1.35	0.90
1:D:353:ARG:HG2	1:D:387:ILE:HD13	1.54	0.90
1:D:242:THR:O	1:D:363:GLY:HA2	1.71	0.89
1:D:311:ARG:HG3	1:D:311:ARG:NH1	1.79	0.89
1:D:95:GLU:H	1:D:102:GLN:HE22	1.19	0.89
1:A:236:VAL:HG12	1:A:236:VAL:O	1.72	0.89
1:A:136:GLY:N	1:A:137:GLY:CA	2.30	0.89
1:D:79:GLY:HA2	1:D:82:LYS:HB3	1.54	0.89
1:A:91:LEU:HB3	1:A:127:MET:HE1	1.55	0.89
2:C:384:LEU:HD21	2:C:432:GLU:HB3	1.53	0.89
1:D:367:GLY:CA	1:D:368:ARG:CB	2.42	0.89
1:D:368:ARG:O	1:D:369:LYS:CB	2.21	0.89
1:A:272:ILE:HD12	1:A:273:THR:H	1.36	0.89
1:D:136:GLY:H	1:D:137:GLY:HA2	1.34	0.89
1:D:338:VAL:HG23	1:D:362:ARG:CZ	2.03	0.89
1:A:314:ILE:HG22	1:A:336:ILE:HG22	1.52	0.88
1:D:239:GLU:C	1:D:241:LEU:HG	1.99	0.88
1:A:267:TYR:CE2	1:A:297:PHE:HD2	1.91	0.88
1:A:354:GLU:CD	2:C:357:PRO:HD2	1.99	0.88
1:D:272:ILE:HD12	1:D:273:THR:H	1.35	0.88
1:D:267:TYR:CE2	1:D:297:PHE:HD2	1.92	0.88
1:D:332:LEU:N	1:D:332:LEU:CD1	2.32	0.88
1:D:364:GLY:O	1:D:365:ARG:C	2.17	0.88
1:D:269:THR:O	1:D:270:LEU:HD12	1.73	0.88
1:D:135:ILE:CB	1:D:136:GLY:HA3	1.97	0.87
1:A:380:ASP:O	1:A:383:THR:HG22	1.73	0.87
1:A:147:LEU:HD12	1:A:165:MET:HE1	1.54	0.87
1:A:307:ASP:O	1:A:311:ARG:CB	2.23	0.87
1:A:99:LYS:HD3	1:A:150:GLU:OE1	1.73	0.87
1:D:241:LEU:O	1:D:242:THR:CG2	2.23	0.86
2:C:164:PHE:CD2	2:C:196:MET:HE2	2.11	0.86
2:C:164:PHE:CE1	2:C:168:LEU:CD1	2.59	0.85
1:A:137:GLY:CA	1:A:140:VAL:HG23	2.05	0.85
1:A:241:LEU:N	1:A:241:LEU:HD23	1.90	0.85
1:D:380:ASP:O	1:D:383:THR:HG22	1.76	0.85
1:D:22:VAL:CG1	1:D:75:GLN:OE1	2.24	0.85
1:A:22:VAL:HG12	1:A:75:GLN:CD	2.02	0.85
2:C:248:PRO:HA	2:C:290:GLN:OE1	1.77	0.85
1:D:77:GLN:OE1	1:D:77:GLN:HA	1.76	0.84
2:C:224:SER:HA	2:C:273:ILE:HD12	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:LEU:HB3	1:D:127:MET:HE1	1.60	0.84
1:A:77:GLN:OE1	1:A:77:GLN:HA	1.77	0.84
1:A:302:MET:CE	1:A:310:GLU:CG	2.56	0.84
1:D:241:LEU:C	1:D:242:THR:CG2	2.50	0.84
2:C:247:LEU:HD11	2:C:258:PRO:HA	1.57	0.83
1:A:242:THR:CG2	1:A:242:THR:O	2.26	0.83
1:D:134:CYS:C	1:D:135:ILE:CG1	2.52	0.83
1:A:306:MET:O	1:A:306:MET:HG2	1.77	0.82
2:C:380:PHE:HE1	2:C:432:GLU:HG3	1.42	0.82
1:A:339:GLN:CG	1:A:362:ARG:NE	2.40	0.82
2:C:449:SER:O	2:C:450:ARG:HB3	1.77	0.82
1:D:209:VAL:HG12	1:D:228:MET:HE3	1.60	0.82
2:C:223:LEU:O	2:C:273:ILE:HD12	1.78	0.82
1:D:311:ARG:HH11	1:D:311:ARG:CB	1.91	0.82
1:D:23:ILE:CG2	1:D:216:MET:HG3	2.09	0.82
1:D:147:LEU:HD13	1:D:165:MET:CE	2.10	0.82
1:D:237:LYS:CG	1:D:238:LYS:H	1.91	0.82
2:C:168:LEU:HD22	2:C:200:VAL:HG22	1.58	0.81
1:D:353:ARG:HE	1:D:386:ASP:HB3	1.45	0.81
1:A:332:LEU:HD12	1:A:332:LEU:H	1.41	0.81
1:D:317:GLU:OE2	1:D:317:GLU:HA	1.79	0.81
1:D:105:VAL:HB	1:D:180:VAL:HG13	1.61	0.81
1:D:149:MET:HA	1:D:150:GLU:HB3	1.63	0.81
1:A:151:ALA:H	1:A:152:PRO:CD	1.91	0.81
1:D:338:VAL:HG23	1:D:362:ARG:HH21	1.45	0.81
1:A:135:ILE:CB	1:A:136:GLY:HA3	2.02	0.80
1:D:255:ARG:HG3	1:D:258:TRP:CE3	2.16	0.80
1:D:267:TYR:CE2	1:D:297:PHE:CD2	2.69	0.80
1:A:147:LEU:CD1	1:A:165:MET:CE	2.59	0.80
1:A:242:THR:HG23	1:A:244:GLU:HB2	1.63	0.80
2:C:337:GLU:OE1	1:D:282:ARG:HD3	1.82	0.80
2:C:164:PHE:CE2	2:C:196:MET:HE2	2.17	0.80
1:D:91:LEU:HD22	1:D:127:MET:CE	2.12	0.79
1:D:307:ASP:O	1:D:311:ARG:CB	2.30	0.79
1:D:314:ILE:CG2	1:D:336:ILE:CG2	2.59	0.79
1:D:332:LEU:HD12	1:D:332:LEU:H	1.45	0.79
1:A:22:VAL:HG12	1:A:75:GLN:OE1	1.81	0.79
2:C:164:PHE:CD2	2:C:196:MET:HE1	2.16	0.79
1:D:22:VAL:HG12	1:D:75:GLN:CD	2.06	0.79
1:A:168:ARG:O	1:A:169:ARG:HB2	1.83	0.79
1:A:314:ILE:HG23	1:A:336:ILE:HG22	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ASP:O	1:D:311:ARG:N	2.15	0.79
2:C:164:PHE:CD1	2:C:168:LEU:HD13	2.18	0.79
1:D:332:LEU:O	1:D:335:GLY:N	2.16	0.79
1:A:105:VAL:HB	1:A:180:VAL:HG13	1.63	0.79
1:A:317:GLU:OE2	1:A:321:GLY:O	2.00	0.79
1:A:361:GLY:C	1:A:362:ARG:HG2	2.08	0.78
1:D:360:ILE:HG23	1:D:361:GLY:N	1.98	0.78
1:A:134:CYS:O	1:A:135:ILE:CG1	2.23	0.78
1:A:278:PHE:HE1	1:A:333:ALA:HB2	1.48	0.78
2:C:164:PHE:HE1	2:C:168:LEU:HD13	1.45	0.78
1:D:307:ASP:O	1:D:311:ARG:HB2	1.84	0.78
1:D:302:MET:CA	1:D:305:ASP:OD2	2.32	0.78
2:C:168:LEU:CD2	2:C:200:VAL:HG22	2.14	0.78
1:D:278:PHE:HE1	1:D:333:ALA:HB2	1.47	0.78
1:A:22:VAL:HG11	1:A:75:GLN:OE1	1.82	0.77
2:C:325:ASN:HA	2:C:328:VAL:CG2	2.13	0.77
2:C:380:PHE:CE1	2:C:432:GLU:HG3	2.19	0.77
1:D:149:MET:HA	1:D:150:GLU:CB	2.15	0.77
1:A:360:ILE:HG13	1:A:372:ALA:CB	2.14	0.77
1:A:86:PHE:O	1:A:90:ILE:HG12	1.84	0.77
2:C:349:HIS:CD2	1:D:283:ARG:HH12	2.03	0.77
1:A:204:ASN:C	1:A:206:ASN:H	1.93	0.77
1:A:353:ARG:HG2	1:A:387:ILE:HD13	1.67	0.77
1:D:242:THR:O	1:D:242:THR:OG1	1.99	0.77
1:A:22:VAL:CG1	1:A:75:GLN:CD	2.57	0.76
2:C:349:HIS:CG	1:D:283:ARG:HH12	2.03	0.76
2:C:420:PRO:O	2:C:421:HIS:CB	2.29	0.76
1:A:58:ILE:HG12	1:A:236:VAL:HG21	1.65	0.76
1:D:147:LEU:CD1	1:D:165:MET:CE	2.60	0.76
1:A:295:ARG:O	1:A:296:ASP:HB2	1.85	0.76
1:D:204:ASN:C	1:D:206:ASN:H	1.93	0.76
1:D:82:LYS:HD3	1:D:212:LEU:HD22	1.68	0.76
1:A:92:GLN:O	1:A:92:GLN:HG3	1.85	0.76
1:D:365:ARG:HA	1:D:367:GLY:H	1.50	0.76
2:C:164:PHE:HE1	2:C:168:LEU:CD1	1.97	0.75
1:D:136:GLY:N	1:D:137:GLY:HA2	1.99	0.75
1:A:151:ALA:H	1:A:152:PRO:HD3	1.50	0.75
1:D:339:GLN:HG2	1:D:362:ARG:NH1	2.01	0.75
2:C:414:ASP:OD1	1:D:161:ARG:NH2	2.18	0.75
1:D:338:VAL:O	1:D:362:ARG:NH1	2.09	0.75
1:A:267:TYR:CE2	1:A:297:PHE:CD2	2.71	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PHE:CD1	1:A:227:PHE:CD1	2.75	0.75
2:C:227:CYS:HB3	2:C:273:ILE:HD11	1.67	0.74
1:A:217:PRO:HD2	1:A:220:VAL:HB	1.69	0.74
2:C:212:LYS:H	2:C:215:HIS:CD2	2.04	0.74
1:D:269:THR:C	1:D:270:LEU:HD12	2.12	0.74
1:D:399:PRO:O	1:D:400:LEU:CD1	2.36	0.74
2:C:431:GLU:OE1	2:C:431:GLU:HA	1.87	0.74
2:C:411:GLU:C	2:C:413:PRO:HD2	2.13	0.74
2:C:238:LYS:O	2:C:241:ASP:N	2.21	0.73
1:D:101:THR:CB	1:D:152:PRO:O	2.36	0.73
1:D:150:GLU:HB2	1:D:151:ALA:HB3	1.68	0.73
1:D:332:LEU:CD1	1:D:332:LEU:H	2.00	0.73
1:A:339:GLN:CG	1:A:362:ARG:CZ	2.58	0.73
1:D:135:ILE:HA	1:D:161:ARG:NH1	2.04	0.73
1:D:346:ASN:HD22	1:D:374:ASN:HD21	1.36	0.72
1:D:302:MET:C	1:D:305:ASP:OD2	2.32	0.72
2:C:183:GLU:HG3	2:C:187:MET:HE2	1.71	0.72
1:D:147:LEU:HD12	1:D:165:MET:HE1	1.72	0.72
1:A:361:GLY:O	1:A:362:ARG:CG	2.36	0.72
1:D:353:ARG:O	1:D:391:TYR:OH	2.07	0.72
1:A:23:ILE:CG2	1:A:216:MET:HG3	2.18	0.72
1:D:255:ARG:HD3	1:D:257:GLU:OE1	1.89	0.72
1:A:200:PHE:CE2	1:A:227:PHE:CD2	2.78	0.72
2:C:178:HIS:CD2	2:C:180:ASP:H	2.06	0.72
1:A:134:CYS:C	1:A:135:ILE:HG13	2.14	0.72
2:C:319:GLY:H	2:C:322:GLN:HG3	1.55	0.72
1:D:314:ILE:HG23	1:D:336:ILE:HG22	1.72	0.72
2:C:180:ASP:OD1	2:C:182:ASN:HB3	1.90	0.72
1:A:200:PHE:CE1	1:A:227:PHE:HB3	2.25	0.71
2:C:321:GLN:H	2:C:321:GLN:CD	1.98	0.71
2:C:398:ILE:HG12	2:C:399:ASP:N	1.86	0.71
1:D:253:VAL:HG12	1:D:262:THR:HG21	1.73	0.71
1:D:338:VAL:CB	1:D:362:ARG:HH22	2.02	0.71
1:A:302:MET:HG3	1:A:328:THR:HG22	1.73	0.71
2:C:176:PHE:HB3	2:C:215:HIS:ND1	2.04	0.71
1:D:105:VAL:HG22	1:D:156:VAL:HG13	1.71	0.71
1:D:240:GLU:N	1:D:241:LEU:HG	2.05	0.71
1:A:339:GLN:CG	1:A:362:ARG:HD3	2.18	0.71
1:D:229:ARG:O	1:D:230:ASP:C	2.34	0.71
1:A:267:TYR:HE1	1:A:325:VAL:HG11	1.56	0.71
1:D:241:LEU:C	1:D:242:THR:HG23	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:426:LEU:HD13	2:C:426:LEU:C	2.16	0.71
1:A:200:PHE:CZ	1:A:227:PHE:CG	2.78	0.70
1:D:314:ILE:HG23	1:D:336:ILE:CG2	2.21	0.70
1:D:255:ARG:HG3	1:D:258:TRP:CZ3	2.27	0.70
1:D:365:ARG:NH2	1:D:366:PHE:CZ	2.60	0.70
1:A:317:GLU:OE2	1:A:317:GLU:HA	1.91	0.70
1:A:333:ALA:O	1:A:336:ILE:HD13	1.91	0.70
2:C:258:PRO:O	2:C:259:GLN:C	2.35	0.70
2:C:223:LEU:O	2:C:273:ILE:HD13	1.89	0.70
1:A:319:ARG:O	1:A:320:SER:HB3	1.92	0.70
1:A:338:VAL:HG23	1:A:362:ARG:HH21	1.46	0.70
1:A:255:ARG:HG3	1:A:258:TRP:CE3	2.26	0.70
1:A:333:ALA:HA	1:A:336:ILE:CD1	2.22	0.70
1:A:339:GLN:HG2	1:A:362:ARG:NH1	2.05	0.70
1:D:302:MET:O	1:D:332:LEU:HD21	1.91	0.70
1:A:242:THR:CG2	1:A:244:GLU:HB2	2.21	0.69
1:A:251:ILE:HD13	1:A:398:MET:HB3	1.74	0.69
1:A:269:THR:C	1:A:270:LEU:HD12	2.17	0.69
1:A:272:ILE:HD12	1:A:273:THR:N	2.07	0.69
1:D:365:ARG:NH2	1:D:366:PHE:CE1	2.60	0.69
2:C:384:LEU:HD22	2:C:432:GLU:HB3	1.74	0.69
1:D:217:PRO:HD2	1:D:220:VAL:HB	1.73	0.69
1:D:377:THR:H	1:D:380:ASP:HB2	1.57	0.69
2:C:365:TYR:O	2:C:369:VAL:HG23	1.92	0.69
1:A:56:SER:O	1:A:60:GLN:HG3	1.92	0.69
1:A:161:ARG:NH2	2:C:249:GLU:OE2	2.26	0.69
1:D:168:ARG:O	1:D:169:ARG:HB2	1.91	0.69
1:A:135:ILE:HA	1:A:161:ARG:NH1	2.07	0.69
1:D:221:LEU:O	1:D:224:THR:HB	1.93	0.69
1:A:302:MET:HE2	1:A:310:GLU:CG	2.22	0.69
1:D:311:ARG:O	1:D:315:MET:HB2	1.92	0.69
1:D:272:ILE:HD12	1:D:273:THR:N	2.07	0.69
1:A:23:ILE:H	1:A:75:GLN:HE22	1.40	0.68
1:A:229:ARG:O	1:A:230:ASP:C	2.34	0.68
2:C:161:GLU:O	2:C:164:PHE:CB	2.41	0.68
1:A:360:ILE:HG23	1:A:361:GLY:N	2.07	0.68
2:C:346:GLU:HG2	1:D:281:THR:HG21	1.75	0.68
1:D:136:GLY:H	1:D:137:GLY:HA3	1.58	0.68
1:A:101:THR:CB	1:A:152:PRO:O	2.38	0.68
1:A:105:VAL:HG22	1:A:156:VAL:HG13	1.76	0.68
1:A:339:GLN:OE1	1:A:362:ARG:HB2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:326:HIS:ND1	2:C:326:HIS:C	2.51	0.68
1:A:267:TYR:CD2	1:A:297:PHE:CE2	2.80	0.68
1:A:276:VAL:HG23	1:A:341:VAL:HG11	1.75	0.68
1:A:311:ARG:HH11	1:A:311:ARG:CB	2.07	0.68
2:C:317:SER:CB	2:C:318:GLY:HA3	2.14	0.68
2:C:270:GLY:C	2:C:272:GLY:H	2.01	0.68
2:C:319:GLY:HA3	2:C:354:LEU:O	1.94	0.68
1:D:302:MET:HE1	1:D:310:GLU:HG2	1.76	0.67
1:A:390:PHE:HZ	2:C:356:VAL:HG12	1.59	0.67
1:D:313:VAL:CG1	1:D:326:LEU:HD11	2.24	0.67
2:C:222:LEU:O	2:C:226:LEU:HB2	1.95	0.67
2:C:402:LYS:HE2	2:C:406:GLU:CD	2.20	0.67
1:D:276:VAL:HG23	1:D:341:VAL:HG11	1.77	0.67
1:D:302:MET:CE	1:D:310:GLU:HG2	2.25	0.67
2:C:165:GLU:C	2:C:167:THR:H	2.01	0.67
1:A:333:ALA:HA	1:A:336:ILE:HD11	1.76	0.67
2:C:301:LEU:HA	2:C:304:MET:HE2	1.76	0.67
1:A:311:ARG:O	1:A:315:MET:HB2	1.95	0.66
1:D:236:VAL:O	1:D:236:VAL:CG2	2.29	0.66
1:D:295:ARG:O	1:D:296:ASP:HB2	1.93	0.66
1:A:82:LYS:HD3	1:A:212:LEU:HD22	1.76	0.66
1:A:150:GLU:HB2	1:A:151:ALA:HB2	0.71	0.66
1:A:377:THR:H	1:A:380:ASP:HB2	1.58	0.66
2:C:202:VAL:HG11	2:C:242:LYS:HD3	1.77	0.66
1:D:22:VAL:CG1	1:D:75:GLN:CD	2.68	0.66
2:C:419:VAL:HB	2:C:422:SER:HB3	1.77	0.66
1:D:149:MET:CA	1:D:150:GLU:CB	2.74	0.66
1:A:332:LEU:H	1:A:332:LEU:CD1	2.00	0.66
2:C:364:VAL:O	2:C:368:ILE:HG12	1.96	0.66
1:D:56:SER:O	1:D:60:GLN:HG3	1.94	0.66
1:D:174:LYS:HE3	1:D:175:TYR:CE2	2.31	0.66
2:C:317:SER:CB	2:C:318:GLY:CA	2.57	0.66
1:D:366:PHE:O	1:D:367:GLY:O	2.13	0.66
1:A:338:VAL:O	1:A:362:ARG:NH1	2.27	0.66
1:D:312:ASP:HA	1:D:315:MET:HE2	1.76	0.66
1:A:209:VAL:HG12	1:A:228:MET:CE	2.25	0.65
1:D:365:ARG:HA	1:D:366:PHE:C	2.19	0.65
1:A:151:ALA:N	1:A:152:PRO:CD	2.57	0.65
2:C:161:GLU:CG	2:C:162:THR:H	2.09	0.65
1:A:200:PHE:CG	1:A:227:PHE:CE1	2.85	0.65
1:A:399:PRO:O	1:A:400:LEU:CD1	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:THR:H	1:D:82:LYS:H	1.44	0.65
1:D:267:TYR:CD2	1:D:297:PHE:CE2	2.84	0.65
1:A:242:THR:O	1:A:242:THR:HG22	1.96	0.65
2:C:423:TYR:C	2:C:425:VAL:H	2.04	0.65
1:D:181:LEU:HD12	1:D:181:LEU:N	2.09	0.65
1:D:399:PRO:O	1:D:400:LEU:HD12	1.96	0.65
1:A:118:LYS:CD	1:A:307:ASP:OD2	2.28	0.65
2:C:214:SER:OG	2:C:355:GLU:OE2	2.15	0.64
2:C:222:LEU:HG	2:C:226:LEU:HD22	1.77	0.64
2:C:418:ASP:OD2	1:D:161:ARG:HG3	1.96	0.64
1:A:150:GLU:HB3	1:A:151:ALA:HB2	1.71	0.64
1:A:181:LEU:HD12	1:A:181:LEU:N	2.11	0.64
1:D:137:GLY:CA	1:D:140:VAL:HG23	2.22	0.64
2:C:288:CYS:O	2:C:288:CYS:SG	2.54	0.64
1:D:361:GLY:C	1:D:362:ARG:HG2	2.23	0.64
1:D:23:ILE:H	1:D:75:GLN:HE22	1.43	0.64
1:D:267:TYR:O	1:D:271:THR:HA	1.98	0.64
1:A:255:ARG:HG3	1:A:258:TRP:CZ3	2.32	0.64
1:D:22:VAL:HG12	1:D:75:GLN:OE1	1.96	0.64
1:A:188:LEU:HD13	1:A:219:ASP:HB3	1.80	0.63
1:A:282:ARG:HH12	2:C:171:ILE:HG12	1.63	0.63
1:A:136:GLY:N	1:A:137:GLY:HA2	2.02	0.63
1:A:146:LYS:O	1:A:148:GLN:N	2.32	0.63
1:A:255:ARG:HD3	1:A:257:GLU:OE1	1.99	0.63
1:D:311:ARG:HA	1:D:314:ILE:HG13	1.80	0.63
1:A:137:GLY:HA2	1:A:140:VAL:CG2	2.18	0.63
1:D:302:MET:CB	1:D:305:ASP:OD2	2.47	0.63
1:D:334:ARG:HG2	1:D:334:ARG:HH11	1.64	0.63
1:D:391:TYR:O	1:D:393:THR:N	2.31	0.63
2:C:275:CYS:HB3	2:C:278:TYR:HB2	1.80	0.62
1:A:64:LEU:CB	1:A:65:PRO:CD	2.77	0.62
2:C:218:MET:HE2	2:C:321:GLN:HE21	1.64	0.62
1:D:253:VAL:HG23	1:D:253:VAL:O	1.99	0.62
1:A:311:ARG:HA	1:A:314:ILE:HG13	1.81	0.62
1:A:114:GLN:HG3	1:A:114:GLN:O	1.99	0.62
1:A:174:LYS:HB3	1:A:175:TYR:CD2	2.35	0.62
1:A:331:LEU:C	1:A:331:LEU:HD12	2.25	0.62
2:C:302:LEU:C	2:C:304:MET:H	2.06	0.62
1:D:150:GLU:CB	1:D:151:ALA:CB	2.60	0.62
1:D:188:LEU:HD13	1:D:219:ASP:HB3	1.82	0.62
1:D:360:ILE:HG13	1:D:372:ALA:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:CB	1:A:65:PRO:HD3	2.30	0.62
1:A:200:PHE:CG	1:A:227:PHE:CD1	2.88	0.62
1:A:109:THR:OG1	1:A:112:LEU:HB2	1.99	0.61
1:A:150:GLU:CA	1:A:151:ALA:HB2	2.28	0.61
1:A:136:GLY:H	1:A:137:GLY:HA3	1.60	0.61
1:D:174:LYS:HB3	1:D:175:TYR:CD2	2.36	0.61
2:C:227:CYS:CB	2:C:273:ILE:CD1	2.75	0.61
2:C:393:SER:HG	2:C:395:THR:HG1	1.48	0.61
1:D:110:ARG:CD	1:D:135:ILE:CG2	2.62	0.61
1:A:314:ILE:HG23	1:A:336:ILE:CG2	2.30	0.61
1:A:110:ARG:CD	1:A:135:ILE:CG2	2.65	0.61
2:C:349:HIS:ND1	1:D:283:ARG:NH2	2.47	0.61
2:C:426:LEU:O	2:C:426:LEU:HD22	2.01	0.61
1:A:253:VAL:HG23	1:A:253:VAL:O	2.00	0.61
1:D:74:ALA:O	1:D:212:LEU:HA	2.01	0.61
1:A:314:ILE:CG2	1:A:336:ILE:CG2	2.75	0.61
1:D:267:TYR:HE1	1:D:325:VAL:HG11	1.65	0.61
1:D:146:LYS:O	1:D:148:GLN:N	2.34	0.61
1:A:22:VAL:CG1	1:A:75:GLN:NE2	2.61	0.60
1:A:391:TYR:O	1:A:393:THR:N	2.34	0.60
2:C:409:TYR:CE1	2:C:447:CYS:HA	2.35	0.60
2:C:426:LEU:O	2:C:430:VAL:CG2	2.44	0.60
1:D:175:TYR:CD2	1:D:175:TYR:N	2.69	0.60
1:A:95:GLU:H	1:A:102:GLN:NE2	1.92	0.60
1:A:236:VAL:O	1:A:236:VAL:CG1	2.48	0.60
1:D:302:MET:HA	1:D:305:ASP:OD2	2.01	0.60
1:D:346:ASN:HD22	1:D:374:ASN:ND2	1.99	0.60
1:A:204:ASN:C	1:A:206:ASN:N	2.60	0.60
1:A:242:THR:O	1:A:242:THR:HG23	1.98	0.60
1:A:313:VAL:O	1:A:317:GLU:HB2	2.01	0.60
1:A:353:ARG:HE	1:A:386:ASP:HB3	1.65	0.60
1:A:209:VAL:HG12	1:A:228:MET:HE3	1.82	0.60
1:A:313:VAL:CG1	1:A:326:LEU:HD11	2.32	0.60
1:D:235:LEU:O	1:D:235:LEU:CG	2.49	0.60
1:D:166:LEU:HD21	1:D:171:LEU:HD23	1.82	0.60
1:A:278:PHE:HE1	1:A:333:ALA:CB	2.14	0.59
2:C:401:MET:HE3	2:C:405:TYR:HE1	1.67	0.59
1:A:135:ILE:CG2	1:A:136:GLY:CA	2.37	0.59
2:C:349:HIS:CE1	1:D:283:ARG:NH2	2.65	0.59
1:D:164:ASP:OD2	1:D:168:ARG:NH1	2.34	0.59
1:A:300:SER:HB2	1:A:326:LEU:HD12	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:423:TYR:O	2:C:425:VAL:N	2.36	0.59
1:A:339:GLN:CD	1:A:362:ARG:CD	2.58	0.59
1:D:306:MET:O	1:D:310:GLU:HB2	2.01	0.59
1:D:399:PRO:O	1:D:400:LEU:HD13	2.03	0.59
1:A:112:LEU:O	1:A:116:ILE:HD12	2.03	0.59
1:A:92:GLN:O	1:A:92:GLN:CG	2.47	0.59
1:D:240:GLU:CA	1:D:241:LEU:CB	2.73	0.59
1:A:149:MET:HA	1:A:150:GLU:CB	2.28	0.59
1:A:246:ILE:HA	1:A:370:GLY:HA3	1.84	0.59
2:C:165:GLU:C	2:C:167:THR:N	2.60	0.59
1:D:314:ILE:CG2	1:D:335:GLY:O	2.47	0.59
1:A:80:THR:H	1:A:82:LYS:H	1.51	0.58
1:A:399:PRO:O	1:A:400:LEU:HD12	2.02	0.58
2:C:354:LEU:O	2:C:355:GLU:HB2	2.02	0.58
1:A:346:ASN:HD22	1:A:374:ASN:HD21	1.50	0.58
1:D:251:ILE:HD13	1:D:398:MET:HB3	1.84	0.58
1:A:149:MET:HA	1:A:150:GLU:HB3	1.85	0.58
2:C:238:LYS:O	2:C:239:SER:C	2.47	0.58
1:D:39:LEU:O	1:D:40:SER:C	2.47	0.58
2:C:362:GLU:OE2	2:C:366:GLU:CG	2.51	0.58
2:C:317:SER:HB2	2:C:318:GLY:HA2	1.80	0.58
2:C:409:TYR:OH	2:C:430:VAL:HG11	2.03	0.58
1:D:95:GLU:H	1:D:102:GLN:NE2	1.96	0.58
1:A:339:GLN:OE1	1:A:362:ARG:CB	2.51	0.58
2:C:410:ASN:O	2:C:413:PRO:HD3	2.03	0.58
1:D:378:GLU:O	1:D:381:LYS:HB2	2.03	0.58
1:D:135:ILE:CG2	1:D:136:GLY:CA	2.29	0.58
1:A:147:LEU:HD13	1:A:165:MET:CE	2.34	0.57
2:C:411:GLU:C	2:C:413:PRO:CD	2.77	0.57
1:A:95:GLU:N	1:A:102:GLN:HE22	1.94	0.57
1:A:200:PHE:CE1	1:A:227:PHE:CG	2.92	0.57
2:C:349:HIS:CG	1:D:283:ARG:NH1	2.71	0.57
1:D:300:SER:HB2	1:D:326:LEU:HD12	1.86	0.57
1:A:307:ASP:O	1:A:311:ARG:N	2.33	0.57
1:A:353:ARG:O	1:A:391:TYR:OH	2.14	0.57
2:C:161:GLU:O	2:C:164:PHE:HB2	2.04	0.57
2:C:182:ASN:O	2:C:185:ALA:N	2.37	0.57
1:D:311:ARG:O	1:D:315:MET:N	2.38	0.57
2:C:169:THR:HG23	2:C:207:LEU:HD21	1.85	0.57
2:C:270:GLY:C	2:C:272:GLY:N	2.62	0.57
2:C:165:GLU:O	2:C:167:THR:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:311:ARG:O	1:D:315:MET:CB	2.53	0.57
2:C:423:TYR:O	2:C:427:GLU:HG2	2.04	0.57
1:A:150:GLU:CB	1:A:151:ALA:CB	2.39	0.57
2:C:321:GLN:OE1	2:C:321:GLN:C	2.48	0.57
1:D:133:ALA:HA	1:D:156:VAL:O	2.05	0.57
1:D:302:MET:CE	1:D:310:GLU:CG	2.83	0.57
2:C:384:LEU:HD22	2:C:432:GLU:CB	2.35	0.57
1:A:135:ILE:HG22	1:A:136:GLY:HA3	0.62	0.56
1:A:148:GLN:HE21	1:A:170:TYR:HA	1.70	0.56
1:A:166:LEU:HD21	1:A:171:LEU:HD23	1.87	0.56
1:D:148:GLN:HE21	1:D:170:TYR:HA	1.70	0.56
1:D:204:ASN:C	1:D:206:ASN:N	2.60	0.56
1:D:209:VAL:CG1	1:D:228:MET:HE3	2.32	0.56
1:D:361:GLY:O	1:D:362:ARG:CG	2.41	0.56
2:C:449:SER:O	2:C:450:ARG:CB	2.50	0.56
1:A:360:ILE:HG13	1:A:372:ALA:HB2	1.87	0.56
2:C:393:SER:O	2:C:394:SER:C	2.47	0.56
1:D:57:ALA:HB1	1:D:236:VAL:CG2	2.31	0.56
1:D:155:ILE:O	1:D:155:ILE:HG13	2.05	0.56
1:A:278:PHE:CD1	1:A:359:ARG:HG2	2.41	0.56
2:C:236:VAL:HG11	2:C:273:ILE:HG23	1.88	0.56
1:D:99:LYS:CD	1:D:150:GLU:OE1	2.38	0.56
1:A:200:PHE:CZ	1:A:227:PHE:CB	2.89	0.56
2:C:178:HIS:HD2	2:C:180:ASP:N	1.95	0.56
2:C:423:TYR:C	2:C:425:VAL:N	2.62	0.56
1:D:242:THR:OG1	1:D:244:GLU:HG3	2.06	0.56
1:D:175:TYR:N	1:D:175:TYR:HD2	2.05	0.55
1:D:212:LEU:H	1:D:212:LEU:HD12	1.71	0.55
1:A:302:MET:HE2	1:A:310:GLU:HG3	1.88	0.55
1:A:302:MET:CE	1:A:310:GLU:HG3	2.36	0.55
1:A:319:ARG:O	1:A:320:SER:CB	2.55	0.55
2:C:442:GLN:CA	2:C:445:ASP:HB2	2.31	0.55
2:C:277:THR:O	2:C:280:ASP:HB2	2.05	0.55
1:D:135:ILE:HG22	1:D:136:GLY:HA3	0.59	0.55
2:C:249:GLU:OE1	2:C:249:GLU:HA	2.06	0.55
1:D:352:ASN:HB3	1:D:355:ASN:HB2	1.89	0.55
1:A:329:THR:OG1	1:A:332:LEU:HD11	2.07	0.55
1:A:149:MET:C	1:A:150:GLU:HG3	2.31	0.55
1:A:174:LYS:HB3	1:A:175:TYR:CE2	2.40	0.55
2:C:383:ILE:HG23	2:C:387:LEU:HD12	1.88	0.55
2:C:412:ILE:HD12	2:C:426:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:299:THR:HG22	2:C:300:VAL:N	2.22	0.55
1:A:135:ILE:CB	1:A:136:GLY:CA	2.77	0.54
2:C:317:SER:CB	2:C:318:GLY:HA2	2.37	0.54
1:D:28:ASN:OD1	1:D:28:ASN:O	2.25	0.54
1:D:109:THR:OG1	1:D:112:LEU:HB2	2.06	0.54
1:D:151:ALA:N	1:D:152:PRO:CD	2.71	0.54
1:D:181:LEU:N	1:D:181:LEU:CD1	2.70	0.54
1:A:353:ARG:HG2	1:A:387:ILE:CD1	2.36	0.54
2:C:363:LEU:HD13	2:C:363:LEU:C	2.32	0.54
1:D:339:GLN:CA	1:D:362:ARG:HH11	1.83	0.54
1:A:371:VAL:HG23	1:A:372:ALA:N	2.23	0.54
2:C:227:CYS:SG	2:C:273:ILE:HG12	2.47	0.54
1:D:43:LEU:O	1:D:47:ILE:HG23	2.07	0.54
1:D:243:LEU:HD22	1:D:248:GLN:NE2	2.22	0.54
1:D:278:PHE:CG	1:D:359:ARG:HG2	2.42	0.54
1:D:211:LEU:HD23	1:D:211:LEU:C	2.33	0.54
2:C:423:TYR:HD1	2:C:450:ARG:NH2	2.05	0.54
1:A:43:LEU:O	1:A:47:ILE:HG23	2.08	0.54
1:A:74:ALA:O	1:A:212:LEU:HA	2.08	0.54
1:D:65:PRO:HB3	1:D:232:ILE:CD1	2.27	0.54
1:A:168:ARG:HD3	1:A:170:TYR:CE2	2.43	0.54
1:A:181:LEU:N	1:A:181:LEU:CD1	2.70	0.54
2:C:282:TYR:CD2	2:C:282:TYR:O	2.61	0.54
2:C:426:LEU:HD13	2:C:427:GLU:N	2.23	0.54
1:A:267:TYR:O	1:A:271:THR:HA	2.08	0.54
1:D:253:VAL:CG1	1:D:262:THR:HG21	2.37	0.54
1:A:168:ARG:O	1:A:169:ARG:CB	2.53	0.53
1:A:175:TYR:CD2	1:A:175:TYR:N	2.74	0.53
1:A:242:THR:HG23	1:A:244:GLU:H	1.73	0.53
1:D:179:PHE:CE2	1:D:181:LEU:HD11	2.44	0.53
1:A:382:ARG:HG3	1:A:383:THR:H	1.73	0.53
1:D:212:LEU:HD12	1:D:212:LEU:N	2.23	0.53
1:A:149:MET:CA	1:A:150:GLU:CB	2.86	0.53
2:C:224:SER:C	2:C:226:LEU:H	2.15	0.53
2:C:301:LEU:HA	2:C:304:MET:CE	2.38	0.53
1:D:306:MET:O	1:D:306:MET:HG2	2.09	0.53
1:A:311:ARG:O	1:A:315:MET:N	2.41	0.53
2:C:227:CYS:HB2	2:C:273:ILE:CD1	2.30	0.53
1:D:344:VAL:O	1:D:372:ALA:HA	2.08	0.53
1:A:336:ILE:HG12	1:A:336:ILE:O	2.09	0.53
1:D:99:LYS:HD3	1:D:150:GLU:CD	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ILE:H	1:A:75:GLN:NE2	2.07	0.53
1:A:79:GLY:HA2	1:A:82:LYS:CB	2.32	0.53
2:C:161:GLU:O	2:C:164:PHE:HB3	2.08	0.53
1:D:149:MET:CA	1:D:150:GLU:HB3	2.32	0.53
1:D:336:ILE:HG12	1:D:336:ILE:O	2.08	0.53
2:C:316:GLY:O	2:C:317:SER:HB3	2.08	0.53
1:D:380:ASP:C	1:D:383:THR:HG22	2.34	0.53
1:A:212:LEU:N	1:A:212:LEU:HD12	2.24	0.53
1:A:221:LEU:O	1:A:224:THR:HB	2.09	0.53
1:A:360:ILE:HG13	1:A:372:ALA:HB3	1.91	0.53
1:A:382:ARG:HG3	1:A:383:THR:N	2.23	0.53
1:D:272:ILE:CD1	1:D:273:THR:H	2.17	0.53
2:C:442:GLN:HA	2:C:445:ASP:CB	2.31	0.52
1:D:174:LYS:HB3	1:D:175:TYR:CE2	2.44	0.52
1:A:311:ARG:CG	1:A:311:ARG:NH1	2.35	0.52
1:A:390:PHE:O	2:C:361:HIS:NE2	2.41	0.52
2:C:222:LEU:CD1	2:C:226:LEU:HD22	2.39	0.52
1:D:311:ARG:CG	1:D:311:ARG:NH1	2.40	0.52
1:A:73:ILE:HG12	1:A:73:ILE:O	2.08	0.52
2:C:412:ILE:N	2:C:413:PRO:CD	2.72	0.52
1:A:354:GLU:OE2	2:C:357:PRO:CD	2.42	0.52
2:C:372:LEU:HD21	2:C:426:LEU:CB	2.33	0.52
1:A:391:TYR:HB3	2:C:403:ARG:HH22	1.74	0.52
1:D:91:LEU:HD22	1:D:127:MET:HE3	1.90	0.52
1:D:339:GLN:CB	1:D:362:ARG:HD2	2.35	0.52
1:A:107:ALA:HB1	1:A:108:PRO:HD2	1.92	0.52
1:A:200:PHE:CE1	1:A:227:PHE:CB	2.93	0.52
2:C:175:TYR:C	2:C:177:GLU:H	2.18	0.52
2:C:218:MET:HE2	2:C:321:GLN:NE2	2.24	0.52
1:D:162:VAL:O	1:D:165:MET:HB2	2.10	0.52
1:D:258:TRP:O	1:D:262:THR:HG23	2.10	0.52
2:C:325:ASN:CA	2:C:328:VAL:HG23	2.32	0.51
1:D:365:ARG:CA	1:D:366:PHE:C	2.83	0.51
2:C:223:LEU:C	2:C:273:ILE:HD12	2.35	0.51
2:C:224:SER:O	2:C:226:LEU:N	2.44	0.51
1:A:306:MET:SD	1:A:309:LYS:HD2	2.51	0.51
1:A:330:ASP:OD2	1:A:359:ARG:HD2	2.09	0.51
1:A:360:ILE:CG2	1:A:361:GLY:H	2.16	0.51
2:C:361:HIS:H	2:C:361:HIS:CD2	2.29	0.51
1:D:331:LEU:C	1:D:331:LEU:HD12	2.36	0.51
1:A:311:ARG:O	1:A:315:MET:CB	2.59	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:33:SER:HB3	1:D:35:ASP:H	1.75	0.51
1:D:332:LEU:CD1	1:D:332:LEU:C	2.81	0.51
2:C:247:LEU:CD1	2:C:258:PRO:HG3	2.41	0.51
1:A:155:ILE:HG13	1:A:155:ILE:O	2.11	0.51
2:C:419:VAL:O	2:C:422:SER:HB3	2.11	0.51
1:D:371:VAL:HG23	1:D:372:ALA:N	2.26	0.51
1:A:200:PHE:CE2	1:A:227:PHE:CG	2.98	0.51
2:C:194:GLY:O	2:C:197:LYS:HE2	2.11	0.51
2:C:384:LEU:CD2	2:C:432:GLU:CB	2.81	0.51
1:D:101:THR:HA	1:D:152:PRO:O	2.10	0.51
1:D:135:ILE:CB	1:D:136:GLY:CA	2.73	0.51
1:D:110:ARG:NE	1:D:135:ILE:HG23	2.25	0.51
2:C:343:ASP:CG	2:C:346:GLU:HB2	2.36	0.50
1:D:302:MET:HE2	1:D:310:GLU:CG	2.41	0.50
1:D:149:MET:C	1:D:150:GLU:HG3	2.36	0.50
2:C:383:ILE:CG2	2:C:387:LEU:HD12	2.42	0.50
1:A:91:LEU:HD22	1:A:127:MET:CE	2.42	0.50
1:D:312:ASP:O	1:D:316:ARG:N	2.35	0.50
1:A:110:ARG:NE	1:A:135:ILE:HG23	2.26	0.50
1:A:134:CYS:HA	1:A:143:GLU:OE2	2.11	0.50
1:D:377:THR:N	1:D:380:ASP:HB2	2.26	0.50
2:C:175:TYR:CD2	2:C:222:LEU:HD22	2.46	0.50
1:D:77:GLN:NE2	1:D:239:GLU:OE1	2.43	0.50
1:A:22:VAL:HG11	1:A:75:GLN:CD	2.34	0.50
2:C:227:CYS:HB3	2:C:273:ILE:CD1	2.38	0.50
1:D:92:GLN:O	1:D:92:GLN:HG3	2.08	0.50
1:A:79:GLY:CA	1:A:82:LYS:HB3	2.33	0.50
1:A:138:THR:HG23	1:A:139:ASN:H	1.76	0.50
1:A:349:LEU:HD23	1:A:383:THR:HG23	1.94	0.50
1:A:279:ILE:HD11	1:A:347:TYR:CD1	2.47	0.49
1:A:377:THR:N	1:A:380:ASP:HB2	2.26	0.49
2:C:408:ILE:C	2:C:410:ASN:N	2.69	0.49
1:D:367:GLY:HA3	1:D:368:ARG:CG	1.99	0.49
2:C:231:MET:HG3	2:C:235:ASP:OD2	2.12	0.49
1:D:90:ILE:O	1:D:94:ILE:HG12	2.12	0.49
2:C:304:MET:SD	1:D:290:GLU:HB3	2.52	0.49
2:C:373:GLU:OE2	1:D:110:ARG:NH1	2.45	0.49
1:A:50:TYR:HE1	1:A:311:ARG:NH2	2.10	0.49
1:A:339:GLN:HA	1:A:362:ARG:HD2	1.94	0.49
1:A:361:GLY:C	1:A:362:ARG:CG	2.77	0.49
2:C:175:TYR:CE2	2:C:222:LEU:HD22	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:222:LEU:CG	2:C:226:LEU:HD22	2.43	0.49
1:D:98:LEU:HD23	1:D:98:LEU:O	2.12	0.49
1:D:100:ALA:O	1:D:102:GLN:HG3	2.12	0.49
1:D:243:LEU:HD12	1:D:243:LEU:N	2.12	0.49
1:D:299:VAL:HG21	1:D:327:ILE:HD11	1.93	0.49
1:D:350:PRO:HG3	1:D:359:ARG:NE	2.27	0.49
1:A:133:ALA:HA	1:A:156:VAL:O	2.13	0.49
2:C:247:LEU:N	2:C:248:PRO:HD2	2.28	0.49
1:D:356:TYR:O	1:D:360:ILE:HG22	2.12	0.49
1:D:311:ARG:NH1	1:D:311:ARG:CB	2.69	0.49
1:A:175:TYR:N	1:A:175:TYR:HD2	2.11	0.49
1:A:259:LYS:HB3	1:A:347:TYR:CZ	2.47	0.49
1:A:338:VAL:CB	1:A:362:ARG:HH22	2.11	0.49
2:C:278:TYR:O	2:C:279:ILE:C	2.55	0.49
2:C:304:MET:SD	1:D:290:GLU:CB	3.01	0.49
1:D:353:ARG:HE	1:D:386:ASP:CB	2.21	0.49
1:A:140:VAL:O	1:A:141:ARG:C	2.54	0.49
2:C:224:SER:CA	2:C:273:ILE:HD12	2.38	0.49
2:C:406:GLU:O	2:C:410:ASN:HB2	2.12	0.49
2:C:409:TYR:CD1	2:C:447:CYS:HA	2.48	0.49
2:C:432:GLU:OE2	2:C:432:GLU:HA	2.12	0.49
1:D:239:GLU:OE2	1:D:241:LEU:HD11	2.13	0.49
1:D:314:ILE:HG22	1:D:336:ILE:CG2	2.21	0.49
2:C:181:THR:OG1	2:C:225:ASP:HB2	2.13	0.49
1:D:297:PHE:N	1:D:297:PHE:CD1	2.81	0.49
1:D:364:GLY:O	1:D:365:ARG:O	2.31	0.49
2:C:200:VAL:H	2:C:201:PRO:CD	2.26	0.49
1:D:151:ALA:H	1:D:152:PRO:CD	2.26	0.49
1:A:32:ASP:O	1:A:55:PRO:HD2	2.13	0.48
1:A:64:LEU:HB2	1:A:65:PRO:HD3	1.94	0.48
1:A:253:VAL:HG12	1:A:262:THR:HG21	1.93	0.48
1:D:173:PRO:HA	1:D:176:ILE:HD12	1.94	0.48
1:D:209:VAL:HG12	1:D:228:MET:CE	2.36	0.48
2:C:185:ALA:HB2	2:C:226:LEU:CD1	2.43	0.48
2:C:423:TYR:HD1	2:C:450:ARG:HH21	1.62	0.48
1:D:332:LEU:CD1	1:D:333:ALA:N	2.76	0.48
1:D:364:GLY:C	1:D:365:ARG:O	2.49	0.48
1:A:58:ILE:CG1	1:A:236:VAL:HG21	2.40	0.48
2:C:175:TYR:C	2:C:177:GLU:N	2.70	0.48
1:D:360:ILE:HG12	1:D:361:GLY:N	2.23	0.48
1:A:339:GLN:CG	1:A:362:ARG:NH1	2.73	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:388:LYS:HG2	2:C:438:ILE:HD11	1.94	0.48
2:C:180:ASP:OD1	2:C:182:ASN:CB	2.58	0.48
2:C:362:GLU:OE2	2:C:366:GLU:HG3	2.14	0.48
1:A:302:MET:O	1:A:332:LEU:CD2	2.50	0.48
1:D:328:THR:O	1:D:329:THR:O	2.32	0.48
1:D:353:ARG:NE	1:D:386:ASP:HB3	2.23	0.48
1:A:64:LEU:HB3	1:A:65:PRO:HD3	1.96	0.48
1:A:105:VAL:O	1:A:156:VAL:HA	2.14	0.48
1:D:240:GLU:CA	1:D:241:LEU:HG	2.44	0.48
1:A:299:VAL:HA	1:A:325:VAL:HG23	1.95	0.47
1:D:360:ILE:CG1	1:D:361:GLY:N	2.71	0.47
1:A:100:ALA:O	1:A:102:GLN:HG3	2.14	0.47
1:D:237:LYS:CG	1:D:238:LYS:N	2.52	0.47
1:A:242:THR:HG23	1:A:244:GLU:N	2.28	0.47
1:A:278:PHE:CG	1:A:359:ARG:HG2	2.49	0.47
1:A:297:PHE:N	1:A:297:PHE:CD1	2.83	0.47
1:D:134:CYS:HA	1:D:143:GLU:OE2	2.15	0.47
1:A:101:THR:HA	1:A:152:PRO:O	2.15	0.47
1:A:250:TYR:O	1:A:250:TYR:CG	2.68	0.47
1:A:354:GLU:CD	2:C:357:PRO:CD	2.81	0.47
1:A:34:PHE:HA	1:A:37:MET:HE3	1.97	0.47
1:A:122:ALA:HB2	1:A:311:ARG:HH21	1.79	0.47
1:A:44:LEU:HD12	1:A:44:LEU:HA	1.74	0.47
1:A:95:GLU:O	1:A:96:LEU:C	2.58	0.47
1:A:212:LEU:HD12	1:A:212:LEU:H	1.79	0.47
1:A:332:LEU:CD1	1:A:333:ALA:N	2.78	0.47
1:A:340:GLN:HE21	1:A:340:GLN:HB3	1.54	0.47
2:C:200:VAL:N	2:C:201:PRO:CD	2.77	0.47
2:C:349:HIS:CE1	1:D:283:ARG:HH12	2.33	0.47
2:C:440:SER:C	2:C:442:GLN:N	2.70	0.47
1:D:306:MET:C	1:D:310:GLU:HB2	2.40	0.47
1:D:382:ARG:HG3	1:D:383:THR:H	1.80	0.47
2:C:441:LYS:HG2	2:C:442:GLN:N	2.29	0.47
2:C:166:LYS:O	2:C:166:LYS:HG2	2.15	0.47
2:C:169:THR:HB	2:C:170:PRO:HD3	1.97	0.47
2:C:423:TYR:CD1	2:C:450:ARG:NH2	2.83	0.47
1:D:64:LEU:HD23	1:D:64:LEU:HA	1.68	0.47
1:D:101:THR:CA	1:D:152:PRO:O	2.63	0.47
1:A:328:THR:O	1:A:329:THR:O	2.33	0.46
1:A:346:ASN:HD22	1:A:374:ASN:ND2	2.13	0.46
1:D:353:ARG:HD2	1:D:390:PHE:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:ASP:OD2	1:A:168:ARG:NH1	2.48	0.46
2:C:180:ASP:O	2:C:181:THR:C	2.58	0.46
1:D:272:ILE:CD1	1:D:273:THR:N	2.77	0.46
1:A:332:LEU:HD13	1:A:333:ALA:N	2.31	0.46
2:C:209:LEU:HD23	2:C:209:LEU:HA	1.54	0.46
1:D:79:GLY:CA	1:D:82:LYS:HB3	2.36	0.46
1:D:163:PHE:C	1:D:165:MET:H	2.22	0.46
1:D:368:ARG:O	1:D:369:LYS:CG	2.62	0.46
2:C:247:LEU:HD13	2:C:258:PRO:HG3	1.98	0.46
1:D:144:VAL:O	1:D:145:GLN:C	2.55	0.46
1:D:334:ARG:HB2	1:D:334:ARG:CZ	2.46	0.46
1:A:32:ASP:OD1	1:A:32:ASP:N	2.47	0.46
1:A:199:ILE:O	1:A:200:PHE:C	2.56	0.46
2:C:184:VAL:HG13	2:C:188:LEU:HD11	1.97	0.46
2:C:327:LEU:HD21	2:C:356:VAL:HG11	1.97	0.46
2:C:391:TRP:CB	2:C:438:ILE:HG23	2.45	0.46
1:D:39:LEU:C	1:D:40:SER:O	2.59	0.46
1:D:360:ILE:CG2	1:D:361:GLY:H	2.03	0.46
1:D:365:ARG:HG3	1:D:366:PHE:N	2.26	0.46
2:C:171:ILE:O	2:C:171:ILE:HG22	2.15	0.46
2:C:238:LYS:O	2:C:240:PHE:N	2.49	0.46
2:C:364:VAL:HG22	2:C:387:LEU:HD21	1.98	0.46
1:D:259:LYS:HB3	1:D:347:TYR:CZ	2.51	0.46
1:A:27:TRP:HB2	1:A:232:ILE:CG2	2.46	0.46
1:A:56:SER:O	1:A:57:ALA:C	2.58	0.46
2:C:195:GLU:C	2:C:197:LYS:H	2.23	0.46
1:D:332:LEU:HD12	1:D:333:ALA:H	1.81	0.46
1:D:349:LEU:HD23	1:D:383:THR:HG23	1.98	0.46
1:A:64:LEU:HB2	1:A:65:PRO:CD	2.46	0.46
2:C:169:THR:N	2:C:170:PRO:HD2	2.31	0.46
1:D:369:LYS:HB3	1:D:370:GLY:H	1.66	0.46
1:A:98:LEU:HD21	1:A:100:ALA:HB3	1.98	0.45
2:C:260:LEU:O	2:C:261:VAL:C	2.59	0.45
1:A:272:ILE:CD1	1:A:273:THR:H	2.19	0.45
1:A:330:ASP:OD2	1:A:359:ARG:NH1	2.41	0.45
2:C:319:GLY:N	2:C:322:GLN:HG3	2.28	0.45
2:C:413:PRO:CD	2:C:414:ASP:H	2.29	0.45
1:A:94:ILE:HG22	1:A:95:GLU:N	2.31	0.45
1:A:312:ASP:O	1:A:316:ARG:N	2.39	0.45
2:C:232:SER:C	2:C:234:ASN:N	2.73	0.45
2:C:242:LYS:O	2:C:245:LYS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:PHE:O	1:D:90:ILE:HG12	2.17	0.45
1:D:334:ARG:HH11	1:D:334:ARG:CG	2.27	0.45
1:A:90:ILE:O	1:A:94:ILE:HG12	2.16	0.45
1:A:93:GLN:HB3	1:A:178:MET:HE1	1.98	0.45
2:C:247:LEU:HD11	2:C:258:PRO:CA	2.36	0.45
2:C:251:ALA:HA	2:C:254:THR:O	2.17	0.45
2:C:421:HIS:O	2:C:423:TYR:N	2.49	0.45
1:D:302:MET:HE2	1:D:310:GLU:HG3	1.98	0.45
1:A:332:LEU:CD1	1:A:333:ALA:H	2.29	0.45
2:C:180:ASP:OD1	2:C:182:ASN:N	2.50	0.45
2:C:205:VAL:HG13	2:C:264:PHE:CE1	2.52	0.45
2:C:409:TYR:OH	2:C:430:VAL:CG1	2.63	0.45
1:D:188:LEU:HD23	1:D:188:LEU:HA	1.74	0.45
1:D:279:ILE:HG22	1:D:281:THR:H	1.81	0.45
1:A:278:PHE:CE1	1:A:333:ALA:HB2	2.39	0.45
2:C:441:LYS:O	2:C:445:ASP:HB2	2.16	0.45
1:D:58:ILE:HG13	1:D:236:VAL:CG1	2.47	0.45
1:A:378:GLU:O	1:A:381:LYS:HB2	2.17	0.45
2:C:301:LEU:HD22	2:C:304:MET:HE1	1.99	0.45
1:D:140:VAL:O	1:D:141:ARG:C	2.57	0.45
1:A:200:PHE:C	1:A:202:LYS:H	2.24	0.45
1:A:353:ARG:CZ	2:C:324:VAL:HG23	2.47	0.45
1:A:354:GLU:OE2	2:C:358:HIS:HB2	2.16	0.45
2:C:201:PRO:HD2	2:C:239:SER:OG	2.17	0.45
2:C:364:VAL:HG22	2:C:387:LEU:CD2	2.47	0.45
1:D:102:GLN:NE2	1:D:177:LYS:NZ	2.65	0.45
1:A:332:LEU:O	1:A:333:ALA:C	2.59	0.45
2:C:187:MET:O	2:C:191:LEU:HG	2.17	0.45
1:D:58:ILE:HA	1:D:236:VAL:HG11	1.97	0.45
1:D:211:LEU:HD23	1:D:211:LEU:O	2.17	0.45
1:D:288:LEU:O	1:D:292:MET:HG3	2.17	0.45
2:C:164:PHE:CE2	2:C:196:MET:CE	2.88	0.45
2:C:238:LYS:C	2:C:240:PHE:N	2.74	0.45
1:D:138:THR:HG23	1:D:139:ASN:ND2	2.31	0.45
1:D:229:ARG:O	1:D:231:PRO:N	2.50	0.45
1:D:360:ILE:HG13	1:D:372:ALA:HB3	1.97	0.45
1:A:209:VAL:HG12	1:A:228:MET:HE2	1.97	0.44
2:C:348:GLU:O	2:C:352:LYS:HB2	2.17	0.44
2:C:431:GLU:OE1	2:C:431:GLU:CA	2.57	0.44
1:D:382:ARG:HG3	1:D:383:THR:N	2.32	0.44
1:A:138:THR:HG23	1:A:139:ASN:ND2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:VAL:HG23	1:A:325:VAL:HB	1.99	0.44
1:A:361:GLY:O	1:A:362:ARG:CB	2.65	0.44
2:C:302:LEU:O	2:C:304:MET:N	2.50	0.44
2:C:324:VAL:O	2:C:327:LEU:HB2	2.17	0.44
2:C:412:ILE:HG23	2:C:423:TYR:CZ	2.52	0.44
2:C:418:ASP:OD2	1:D:161:ARG:CG	2.65	0.44
1:D:306:MET:O	1:D:310:GLU:N	2.50	0.44
1:A:388:GLU:OE2	1:A:395:ILE:N	2.32	0.44
2:C:195:GLU:C	2:C:197:LYS:N	2.76	0.44
1:D:73:ILE:O	1:D:73:ILE:HG12	2.16	0.44
1:A:73:ILE:HG21	1:A:73:ILE:HD13	1.52	0.44
1:A:306:MET:O	1:A:306:MET:CG	2.53	0.44
2:C:383:ILE:O	2:C:387:LEU:HD12	2.17	0.44
1:D:311:ARG:CA	1:D:314:ILE:HG13	2.46	0.44
1:A:173:PRO:HA	1:A:176:ILE:HD12	2.00	0.44
2:C:196:MET:HE3	2:C:196:MET:HB2	1.96	0.44
2:C:227:CYS:HB3	2:C:273:ILE:CG1	2.47	0.44
2:C:252:LEU:HD12	2:C:252:LEU:HA	1.82	0.44
1:D:163:PHE:C	1:D:165:MET:N	2.75	0.44
1:D:164:ASP:O	1:D:168:ARG:HG3	2.18	0.44
2:C:274:LEU:HD23	2:C:274:LEU:HA	1.70	0.44
1:A:344:VAL:O	1:A:372:ALA:HA	2.18	0.44
2:C:236:VAL:HG11	2:C:273:ILE:O	2.18	0.44
2:C:349:HIS:ND1	2:C:349:HIS:O	2.49	0.44
2:C:409:TYR:CE1	2:C:447:CYS:CA	3.00	0.44
2:C:443:LEU:HD12	2:C:443:LEU:HA	1.52	0.44
1:D:90:ILE:HD12	1:D:90:ILE:HG21	1.58	0.44
1:A:306:MET:HE2	1:A:306:MET:HB3	1.74	0.44
2:C:287:ASP:O	2:C:288:CYS:CB	2.37	0.44
2:C:224:SER:C	2:C:226:LEU:N	2.76	0.43
2:C:232:SER:O	2:C:233:THR:C	2.61	0.43
2:C:301:LEU:CD2	2:C:304:MET:HE1	2.47	0.43
1:D:302:MET:HB2	1:D:305:ASP:OD2	2.16	0.43
2:C:343:ASP:OD1	2:C:346:GLU:HB2	2.17	0.43
2:C:447:CYS:HA	2:C:448:PRO:HD3	1.80	0.43
1:D:91:LEU:HB3	1:D:127:MET:CE	2.41	0.43
1:D:330:ASP:OD2	1:D:359:ARG:NH1	2.43	0.43
1:A:33:SER:HB3	1:A:35:ASP:H	1.83	0.43
2:C:222:LEU:HG	2:C:226:LEU:CD2	2.46	0.43
1:D:138:THR:HG23	1:D:139:ASN:H	1.82	0.43
1:D:329:THR:OG1	1:D:332:LEU:HD11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:ASN:HB2	1:D:374:ASN:HD22	1.83	0.43
1:A:98:LEU:O	1:A:98:LEU:HD23	2.18	0.43
1:D:47:ILE:HD12	1:D:88:ILE:CD1	2.48	0.43
1:D:94:ILE:HD13	1:D:94:ILE:HA	1.81	0.43
1:A:272:ILE:CD1	1:A:273:THR:N	2.79	0.43
2:C:248:PRO:CA	2:C:290:GLN:OE1	2.58	0.43
1:A:26:ASN:O	1:A:26:ASN:CG	2.61	0.43
1:A:39:LEU:C	1:A:40:SER:O	2.62	0.43
2:C:213:ALA:O	2:C:214:SER:C	2.61	0.43
1:D:110:ARG:NE	1:D:135:ILE:CG2	2.81	0.43
1:D:173:PRO:HA	1:D:176:ILE:CD1	2.49	0.43
1:A:144:VAL:O	1:A:145:GLN:C	2.61	0.43
1:D:64:LEU:CB	1:D:65:PRO:CD	2.96	0.43
1:D:361:GLY:C	1:D:362:ARG:CG	2.87	0.43
1:A:200:PHE:CE1	1:A:227:PHE:CD1	3.06	0.43
1:A:28:ASN:OD1	1:A:28:ASN:O	2.37	0.43
1:A:386:ASP:O	1:A:387:ILE:C	2.60	0.43
1:A:399:PRO:O	1:A:400:LEU:HD13	2.15	0.43
2:C:243:LEU:HA	2:C:243:LEU:HD23	1.71	0.43
2:C:350:CYS:O	2:C:354:LEU:HG	2.19	0.43
2:C:378:SER:O	2:C:379:ALA:C	2.61	0.43
1:D:95:GLU:O	1:D:96:LEU:C	2.61	0.43
1:D:200:PHE:CG	1:D:227:PHE:CD1	3.06	0.43
1:A:173:PRO:HA	1:A:176:ILE:CD1	2.49	0.43
1:A:188:LEU:HD23	1:A:188:LEU:HA	1.68	0.43
1:A:249:PHE:HA	1:A:396:GLU:O	2.19	0.43
1:D:135:ILE:HG22	1:D:136:GLY:C	2.30	0.43
1:A:180:VAL:HA	1:A:210:VAL:O	2.19	0.42
1:D:333:ALA:HA	1:D:336:ILE:CD1	2.49	0.42
1:A:144:VAL:C	1:A:146:LYS:N	2.77	0.42
1:A:209:VAL:CG1	1:A:228:MET:HE3	2.47	0.42
1:D:312:ASP:OD1	1:D:315:MET:CE	2.67	0.42
1:A:232:ILE:HG23	1:A:232:ILE:HD13	1.83	0.42
2:C:164:PHE:HE1	2:C:168:LEU:HD11	1.81	0.42
2:C:227:CYS:CB	2:C:273:ILE:CG1	2.97	0.42
1:D:164:ASP:OD1	1:D:168:ARG:NH1	2.52	0.42
1:D:232:ILE:HG23	1:D:232:ILE:HD13	1.80	0.42
1:D:332:LEU:HD12	1:D:333:ALA:N	2.33	0.42
1:A:58:ILE:HG23	1:A:58:ILE:HD13	1.31	0.42
1:A:220:VAL:O	1:A:221:LEU:C	2.62	0.42
1:A:339:GLN:CG	1:A:362:ARG:HD2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ARG:HD2	1:A:390:PHE:CD2	2.54	0.42
2:C:164:PHE:O	2:C:167:THR:N	2.51	0.42
2:C:265:ILE:O	2:C:266:ALA:C	2.60	0.42
2:C:314:VAL:HB	2:C:315:TRP:O	2.20	0.42
1:D:27:TRP:CE2	1:D:65:PRO:HG3	2.54	0.42
1:D:34:PHE:CD1	1:D:47:ILE:HD11	2.54	0.42
1:D:332:LEU:HD13	1:D:333:ALA:N	2.35	0.42
1:A:24:GLU:O	1:A:233:ARG:HD2	2.18	0.42
1:A:332:LEU:HD12	1:A:333:ALA:H	1.84	0.42
2:C:341:SER:O	1:D:351:THR:HG21	2.18	0.42
2:C:357:PRO:HA	2:C:360:HIS:CE1	2.55	0.42
1:D:164:ASP:CG	1:D:168:ARG:NH1	2.77	0.42
2:C:163:ALA:O	2:C:166:LYS:HD2	2.19	0.42
1:D:82:LYS:HD3	1:D:212:LEU:CD2	2.46	0.42
1:D:284:LYS:O	1:D:287:TRP:HB3	2.19	0.42
1:A:81:GLY:HA2	1:A:84:ALA:HB3	2.00	0.42
1:A:181:LEU:O	1:A:211:LEU:HA	2.19	0.42
2:C:185:ALA:HB2	2:C:226:LEU:HD11	2.01	0.42
2:C:326:HIS:ND1	2:C:326:HIS:O	2.52	0.42
2:C:420:PRO:HG2	1:D:190:ARG:O	2.20	0.42
1:D:102:GLN:NE2	1:D:177:LYS:HZ1	2.18	0.42
1:A:94:ILE:HG23	1:A:94:ILE:HD12	1.70	0.42
2:C:232:SER:N	2:C:235:ASP:OD2	2.49	0.42
1:D:151:ALA:H	1:D:152:PRO:HD2	1.84	0.42
1:A:47:ILE:HD13	1:A:47:ILE:HG21	1.64	0.42
1:A:200:PHE:C	1:A:202:LYS:N	2.78	0.42
2:C:184:VAL:CG1	2:C:188:LEU:HD11	2.50	0.42
2:C:323:PRO:O	2:C:326:HIS:HB3	2.19	0.42
2:C:384:LEU:O	2:C:388:LYS:HG3	2.20	0.42
2:C:413:PRO:HD2	2:C:414:ASP:H	1.85	0.42
1:D:72:VAL:HG22	1:D:232:ILE:HD11	2.01	0.42
1:D:317:GLU:O	1:D:318:PHE:C	2.62	0.42
1:A:312:ASP:HA	1:A:315:MET:HE2	2.02	0.42
1:A:360:ILE:HG12	1:A:361:GLY:N	2.33	0.42
1:D:184:ALA:O	1:D:185:ASP:C	2.62	0.42
1:D:398:MET:HA	1:D:399:PRO:HD3	1.96	0.42
2:C:421:HIS:O	2:C:422:SER:C	2.63	0.41
1:A:200:PHE:CB	1:A:227:PHE:CE1	3.02	0.41
1:A:267:TYR:HD2	1:A:297:PHE:CE2	2.32	0.41
1:A:378:GLU:OE1	1:A:378:GLU:CA	2.51	0.41
2:C:383:ILE:HG23	2:C:387:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:401:MET:HE3	2:C:405:TYR:CE1	2.51	0.41
1:D:64:LEU:CB	1:D:65:PRO:HD3	2.50	0.41
1:A:236:VAL:O	1:A:237:LYS:C	2.63	0.41
2:C:346:GLU:OE2	1:D:283:ARG:HD2	2.21	0.41
1:D:58:ILE:HG21	1:D:58:ILE:HD13	1.55	0.41
1:D:127:MET:C	1:D:129:ALA:H	2.29	0.41
1:D:338:VAL:CA	1:D:362:ARG:HH22	2.32	0.41
1:A:39:LEU:O	1:A:40:SER:C	2.63	0.41
1:D:235:LEU:O	1:D:235:LEU:HD22	2.19	0.41
1:D:271:THR:O	1:D:272:ILE:C	2.64	0.41
1:A:200:PHE:CD2	1:A:227:PHE:CZ	3.09	0.41
1:D:333:ALA:O	1:D:336:ILE:HD13	2.21	0.41
1:A:200:PHE:O	1:A:202:LYS:N	2.54	0.41
2:C:257:ALA:N	2:C:258:PRO:CD	2.84	0.41
2:C:410:ASN:O	2:C:413:PRO:CD	2.68	0.41
1:D:144:VAL:C	1:D:146:LYS:N	2.76	0.41
1:A:27:TRP:CD1	1:A:27:TRP:C	2.99	0.41
1:A:140:VAL:HA	1:A:143:GLU:HB2	2.03	0.41
1:D:148:GLN:HA	1:D:149:MET:HA	1.82	0.41
1:D:199:ILE:O	1:D:200:PHE:C	2.63	0.41
1:A:75:GLN:HB2	1:A:216:MET:HE3	2.02	0.41
1:A:81:GLY:HA2	1:A:84:ALA:CB	2.51	0.41
1:A:83:THR:HA	1:A:86:PHE:CE2	2.56	0.41
1:A:91:LEU:HB3	1:A:127:MET:CE	2.37	0.41
1:A:200:PHE:CD2	1:A:227:PHE:CE2	3.09	0.41
1:A:242:THR:H	1:A:362:ARG:C	2.28	0.41
1:A:267:TYR:CE1	1:A:325:VAL:HG11	2.45	0.41
2:C:426:LEU:HD11	2:C:447:CYS:SG	2.61	0.41
1:D:91:LEU:HD22	1:D:127:MET:HE2	2.00	0.41
1:D:185:ASP:OD2	1:D:214:ALA:HB3	2.21	0.41
1:D:232:ILE:HD12	1:D:232:ILE:HG21	1.74	0.41
1:D:339:GLN:N	1:D:362:ARG:CZ	2.81	0.41
1:A:90:ILE:HG12	1:A:90:ILE:H	1.58	0.41
1:A:307:ASP:O	1:A:311:ARG:HB3	2.14	0.41
2:C:200:VAL:H	2:C:201:PRO:HD2	1.86	0.41
1:D:97:ASP:OD2	1:D:97:ASP:C	2.64	0.41
1:A:331:LEU:C	1:A:331:LEU:CD1	2.93	0.40
2:C:412:ILE:HG21	2:C:423:TYR:CE2	2.55	0.40
2:C:442:GLN:O	2:C:442:GLN:HG2	2.21	0.40
1:D:278:PHE:CE1	1:D:333:ALA:HB2	2.39	0.40
1:D:367:GLY:CA	1:D:368:ARG:HB2	2.43	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ILE:HG13	1:A:89:SER:HB3	2.03	0.40
1:A:148:GLN:HA	1:A:149:MET:HA	1.79	0.40
1:D:380:ASP:CA	1:D:383:THR:HG22	2.52	0.40
1:A:94:ILE:CG2	1:A:95:GLU:N	2.83	0.40
1:A:110:ARG:NE	1:A:135:ILE:CG2	2.82	0.40
1:A:164:ASP:O	1:A:168:ARG:HG3	2.21	0.40
1:A:241:LEU:HB3	1:A:357:ILE:HD11	2.03	0.40
2:C:217:GLU:O	2:C:218:MET:C	2.63	0.40
2:C:335:LEU:HA	2:C:335:LEU:HD23	1.87	0.40
1:A:271:THR:O	1:A:272:ILE:C	2.64	0.40
2:C:161:GLU:HG3	2:C:162:THR:CA	2.42	0.40
2:C:324:VAL:O	2:C:328:VAL:HG23	2.20	0.40
1:D:91:LEU:HD13	1:D:127:MET:HE2	2.02	0.40
1:D:185:ASP:OD1	1:D:185:ASP:N	2.55	0.40
1:D:310:GLU:O	1:D:312:ASP:N	2.54	0.40
1:A:63:ILE:HD13	1:A:63:ILE:HG21	1.80	0.40
1:A:278:PHE:CE1	1:A:333:ALA:CB	3.01	0.40
2:C:426:LEU:C	2:C:426:LEU:CD1	2.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ARG:CD	1:D:99:LYS:CE[12_455]	1.94	0.26

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	354/414 (86%)	297 (84%)	38 (11%)	19 (5%)	1	14
1	D	365/414 (88%)	299 (82%)	45 (12%)	21 (6%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	272/358 (76%)	213 (78%)	44 (16%)	15 (6%)	1	13
All	All	991/1186 (84%)	809 (82%)	127 (13%)	55 (6%)	1	13

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	147	LEU
1	A	151	ALA
1	A	271	THR
1	A	320	SER
1	A	329	THR
1	A	392	ASN
1	D	147	LEU
1	D	151	ALA
1	D	271	THR
1	D	329	THR
1	D	362	ARG
1	D	367	GLY
1	D	368	ARG
1	D	369	LYS
1	D	392	ASN
1	D	399	PRO
1	A	40	SER
1	A	237	LYS
1	A	311	ARG
1	A	330	ASP
1	A	399	PRO
2	C	166	LYS
2	C	225	ASP
2	C	239	SER
2	C	258	PRO
2	C	288	CYS
2	C	303	SER
2	C	394	SER
2	C	422	SER
2	C	426	LEU
1	D	40	SER
1	D	236	VAL
1	D	242	THR
1	D	311	ARG
1	D	330	ASP
1	D	333	ALA

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Mol	Chain	Res	Type
1	A	27	TRP
1	A	57	ALA
1	A	318	PHE
1	A	331	LEU
2	C	233	THR
2	C	318	GLY
1	D	238	LYS
1	D	240	GLU
1	A	135	ILE
1	A	360	ILE
2	C	279	ILE
2	C	182	ASN
2	C	421	HIS
2	C	424	SER
1	D	137	GLY
1	D	366	PHE
1	A	236	VAL
1	D	135	ILE
1	A	137	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	325/363 (90%)	249 (77%)	76 (23%)	1	4
1	D	329/363 (91%)	249 (76%)	80 (24%)	1	4
2	C	245/312 (78%)	192 (78%)	53 (22%)	1	6
All	All	899/1038 (87%)	690 (77%)	209 (23%)	1	5

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	VAL
1	A	28	ASN
1	A	33	SER

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Mol	Chain	Res	Type
1	A	44	LEU
1	A	45	ARG
1	A	47	ILE
1	A	58	ILE
1	A	65	PRO
1	A	73	ILE
1	A	78	SER
1	A	80	THR
1	A	90	ILE
1	A	97	ASP
1	A	101	THR
1	A	105	VAL
1	A	106	LEU
1	A	112	LEU
1	A	116	ILE
1	A	127	MET
1	A	130	SER
1	A	135	ILE
1	A	138	THR
1	A	139	ASN
1	A	140	VAL
1	A	143	GLU
1	A	145	GLN
1	A	148	GLN
1	A	149	MET
1	A	150	GLU
1	A	156	VAL
1	A	161	ARG
1	A	167	ASN
1	A	169	ARG
1	A	175	TYR
1	A	178	MET
1	A	180	VAL
1	A	183	GLU
1	A	201	GLN
1	A	218	SER
1	A	221	LEU
1	A	222	GLU
1	A	224	THR
1	A	232	ILE
1	A	235	LEU
1	A	241	LEU

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Mol	Chain	Res	Type
1	A	242	THR
1	A	243	LEU
1	A	244	GLU
1	A	254	GLU
1	A	255	ARG
1	A	261	ASP
1	A	272	ILE
1	A	273	THR
1	A	292	MET
1	A	302	MET
1	A	306	MET
1	A	308	GLN
1	A	311	ARG
1	A	314	ILE
1	A	317	GLU
1	A	318	PHE
1	A	325	VAL
1	A	331	LEU
1	A	332	LEU
1	A	336	ILE
1	A	338	VAL
1	A	340	GLN
1	A	349	LEU
1	A	355	ASN
1	A	357	ILE
1	A	360	ILE
1	A	362	ARG
1	A	371	VAL
1	A	378	GLU
1	A	393	THR
1	A	400	LEU
2	C	161	GLU
2	C	166	LYS
2	C	172	ILE
2	C	177	GLU
2	C	202	VAL
2	C	207	LEU
2	C	220	SER
2	C	221	LYS
2	C	223	LEU
2	C	226	LEU
2	C	229	THR

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Mol	Chain	Res	Type
2	C	232	SER
2	C	234	ASN
2	C	239	SER
2	C	247	LEU
2	C	252	LEU
2	C	256	ARG
2	C	258	PRO
2	C	259	GLN
2	C	261	VAL
2	C	269	VAL
2	C	273	ILE
2	C	274	LEU
2	C	281	SER
2	C	283	LYS
2	C	288	CYS
2	C	299	THR
2	C	301	LEU
2	C	315	TRP
2	C	321	GLN
2	C	325	ASN
2	C	326	HIS
2	C	328	VAL
2	C	329	LYS
2	C	334	LEU
2	C	336	LYS
2	C	344	ILE
2	C	345	SER
2	C	352	LYS
2	C	356	VAL
2	C	363	LEU
2	C	364	VAL
2	C	372	LEU
2	C	375	THR
2	C	378	SER
2	C	383	ILE
2	C	397	THR
2	C	398	ILE
2	C	410	ASN
2	C	419	VAL
2	C	426	LEU
2	C	438	ILE
2	C	445	ASP

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Mol	Chain	Res	Type
1	D	22	VAL
1	D	28	ASN
1	D	33	SER
1	D	44	LEU
1	D	45	ARG
1	D	47	ILE
1	D	58	ILE
1	D	73	ILE
1	D	78	SER
1	D	90	ILE
1	D	97	ASP
1	D	101	THR
1	D	105	VAL
1	D	106	LEU
1	D	112	LEU
1	D	117	GLN
1	D	127	MET
1	D	130	SER
1	D	135	ILE
1	D	138	THR
1	D	139	ASN
1	D	140	VAL
1	D	143	GLU
1	D	145	GLN
1	D	148	GLN
1	D	149	MET
1	D	150	GLU
1	D	156	VAL
1	D	161	ARG
1	D	167	ASN
1	D	169	ARG
1	D	175	TYR
1	D	178	MET
1	D	180	VAL
1	D	183	GLU
1	D	201	GLN
1	D	212	LEU
1	D	218	SER
1	D	221	LEU
1	D	222	GLU
1	D	224	THR
1	D	232	ILE

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Mol	Chain	Res	Type
1	D	234	ILE
1	D	235	LEU
1	D	237	LYS
1	D	238	LYS
1	D	239	GLU
1	D	240	GLU
1	D	242	THR
1	D	243	LEU
1	D	244	GLU
1	D	255	ARG
1	D	261	ASP
1	D	272	ILE
1	D	273	THR
1	D	291	LYS
1	D	297	PHE
1	D	302	MET
1	D	308	GLN
1	D	311	ARG
1	D	314	ILE
1	D	317	GLU
1	D	318	PHE
1	D	325	VAL
1	D	331	LEU
1	D	332	LEU
1	D	334	ARG
1	D	336	ILE
1	D	338	VAL
1	D	340	GLN
1	D	349	LEU
1	D	357	ILE
1	D	359	ARG
1	D	360	ILE
1	D	362	ARG
1	D	365	ARG
1	D	369	LYS
1	D	371	VAL
1	D	378	GLU
1	D	400	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	38	ASN
1	A	75	GLN
1	A	93	GLN
1	A	102	GLN
1	A	117	GLN
1	A	148	GLN
1	A	206	ASN
1	A	208	GLN
1	A	274	GLN
1	A	280	ASN
1	A	340	GLN
1	A	374	ASN
2	C	173	GLN
2	C	178	HIS
2	C	325	ASN
2	C	358	HIS
2	C	421	HIS
1	D	28	ASN
1	D	38	ASN
1	D	75	GLN
1	D	102	GLN
1	D	139	ASN
1	D	148	GLN
1	D	208	GLN
1	D	248	GLN
1	D	280	ASN
1	D	340	GLN
1	D	374	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	364/414 (87%)	0.15	13 (3%) 46 25	46, 54, 74, 102	0
1	D	371/414 (89%)	-0.03	6 (1%) 70 45	35, 54, 73, 107	0
2	C	278/358 (77%)	-0.09	5 (1%) 67 42	31, 56, 72, 80	4 (1%)
All	All	1013/1186 (85%)	0.02	24 (2%) 59 35	31, 54, 73, 107	4 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	314	VAL	6.4
1	A	321	GLY	5.2
2	C	403	ARG	4.5
1	A	318	PHE	3.9
1	D	362	ARG	3.4
1	A	136	GLY	3.0
1	D	318	PHE	3.0
1	D	378	GLU	2.9
1	A	400	LEU	2.8
1	A	298	THR	2.8
1	A	282	ARG	2.7
1	A	307	ASP	2.6
2	C	283	LYS	2.6
1	D	331	LEU	2.5
1	D	353	ARG	2.5
1	A	97	ASP	2.4
1	A	308	GLN	2.4
1	A	306	MET	2.3
1	A	392	ASN	2.3
1	A	294	ALA	2.2
2	C	195	GLU	2.2
2	C	255	PRO	2.1
1	D	150	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	362	ARG	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.