



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:34 PM UTC

PDB ID : 6JIV / pdb_00006jiv
Title : SspE crystal structure
Authors : Bing, Y.Z.; Yang, H.G.
Deposited on : 2019-02-23
Resolution : 3.31 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

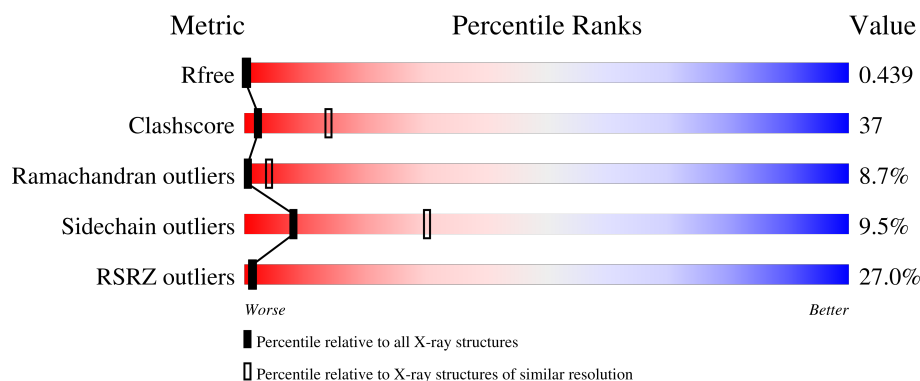
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	771	17% 44% 24% 5% 27%
1	B	771	25% 46% 23% • 27%
1	C	771	17% 39% 26% 7% 28%
1	D	771	18% 43% 24% 5% 27%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15028 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.

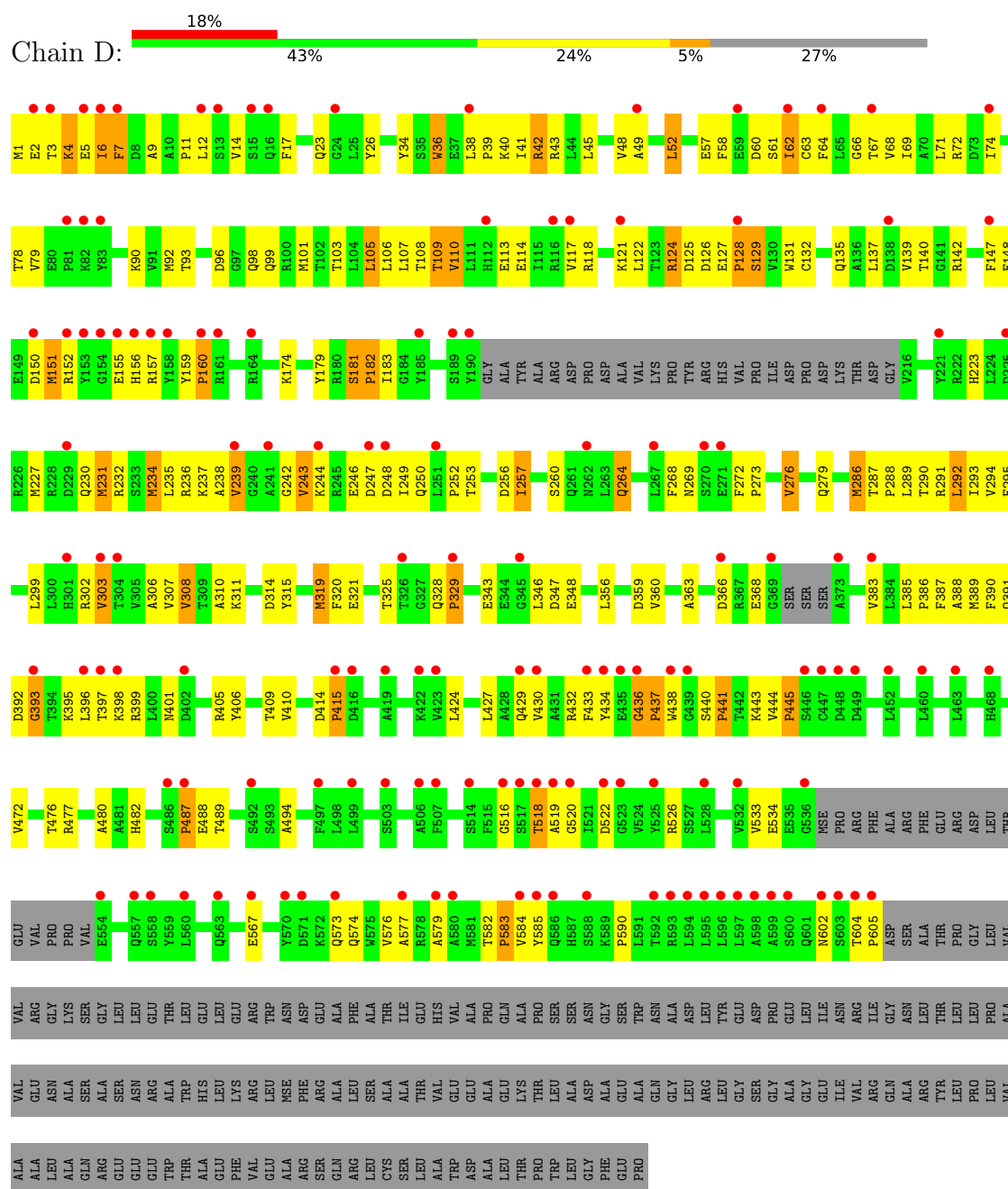
- Molecule 1 is a protein called SspE protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	D	560	Total	C	N	O	S	Se	0	0	0
			3711	2310	674	713	3	11			
1	A	560	Total	C	N	O	S	Se	0	0	0
			3711	2310	674	713	3	11			
1	B	560	Total	C	N	O	S	Se	0	0	0
			3711	2310	674	713	3	11			
1	C	557	Total	C	N	O	S	Se	0	0	0
			3895	2439	697	743	4	12			

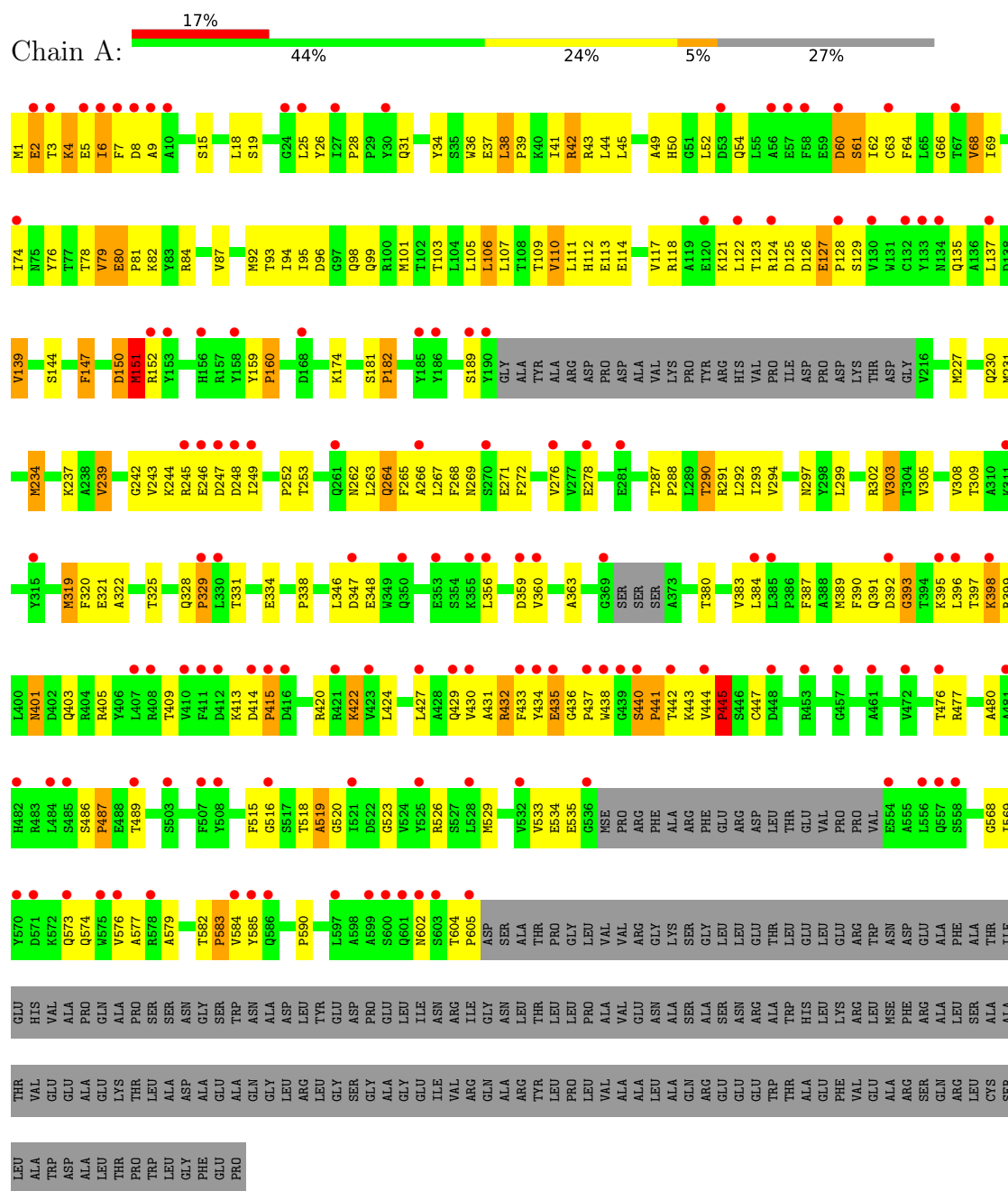
3 Residue-property plots

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.

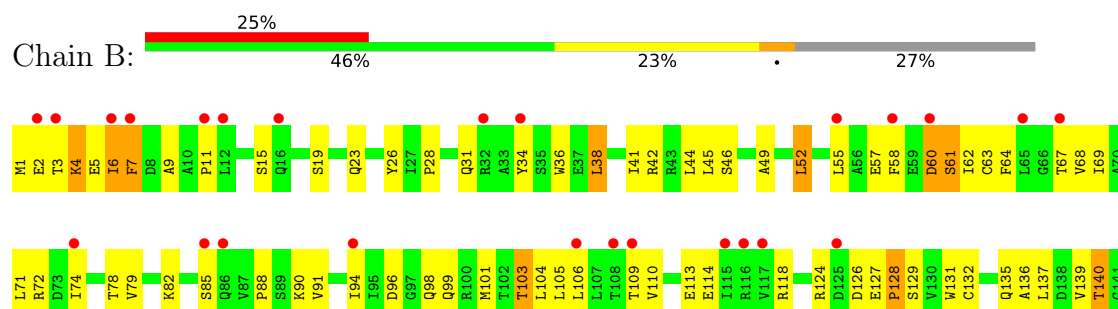
• Molecule 1: SspE protein

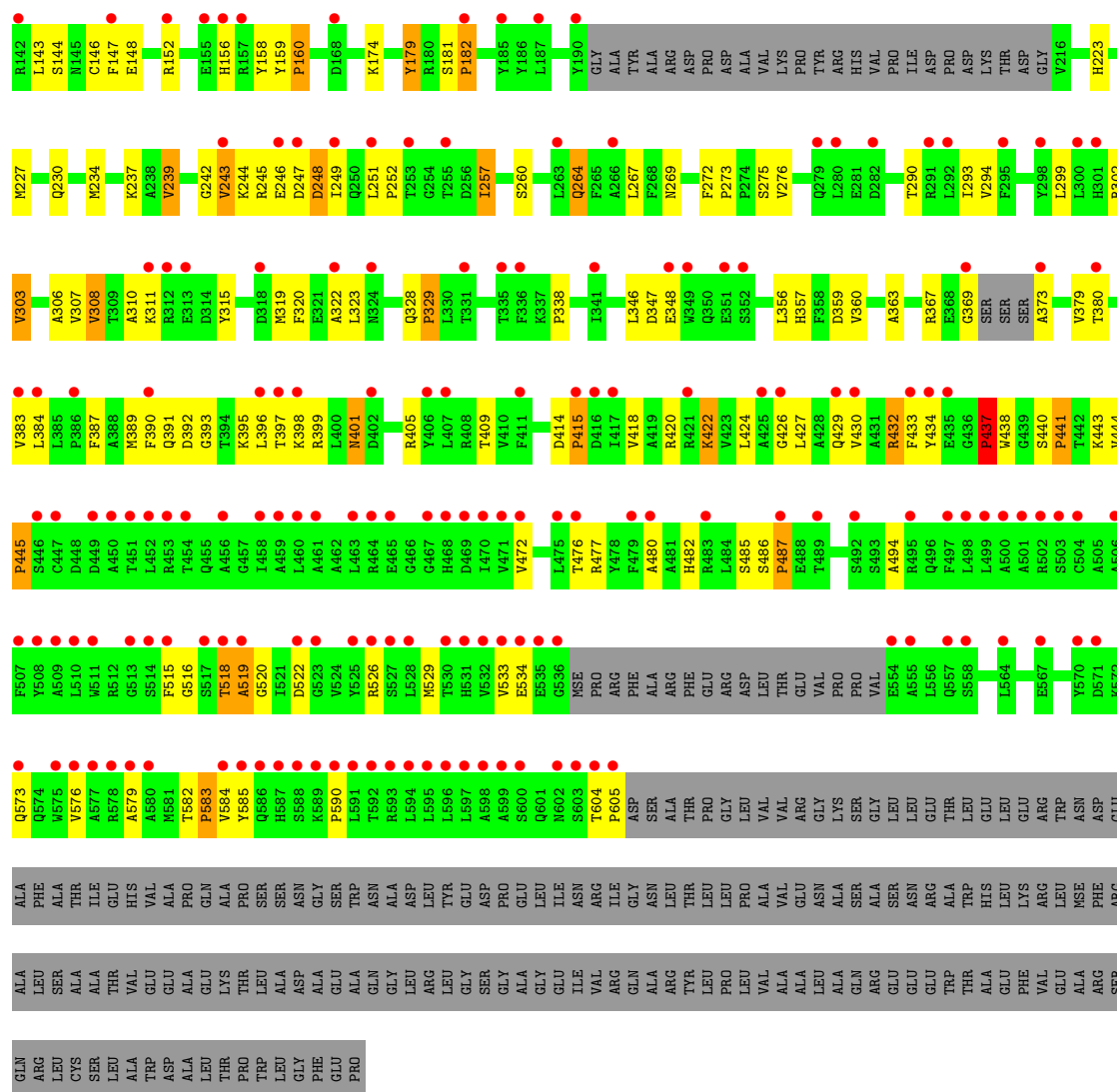


• Molecule 1: SspE protein

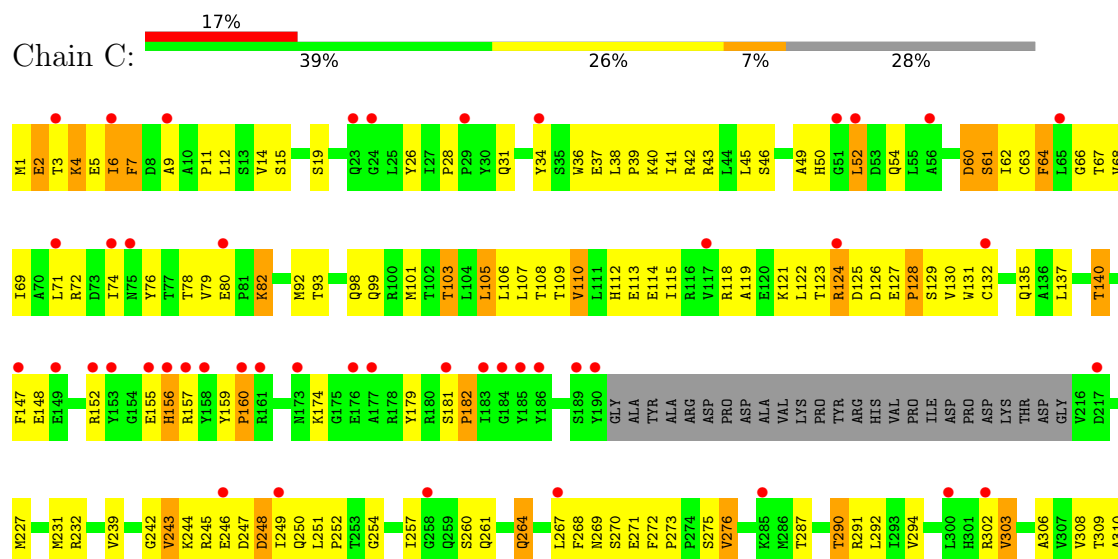


• Molecule 1: SspE protein





• Molecule 1: SspE protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.07Å 138.16Å 293.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.33 – 3.31 125.33 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.5 (125.33-3.31) 99.5 (125.33-3.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.406 , 0.435 0.407 , 0.439	Depositor DCC
R_{free} test set	3357 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	122.6	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 114.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	15028	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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

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	0.62	1/3747 (0.0%)	0.98	14/5100 (0.3%)
1	B	0.52	0/3747	0.90	16/5100 (0.3%)
1	C	0.57	0/3943	0.95	15/5351 (0.3%)
1	D	0.72	0/3747	1.06	14/5100 (0.3%)
All	All	0.61	1/15184 (0.0%)	0.97	59/20651 (0.3%)

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	1
1	C	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	MSE	SE-CE	-6.20	1.76	1.95

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	160	PRO	N-CA-CB	10.75	114.54	103.25
1	A	160	PRO	N-CA-CB	9.27	112.98	103.25
1	A	329	PRO	N-CA-CB	8.99	112.69	103.25
1	B	329	PRO	N-CA-CB	8.66	112.35	103.25
1	C	329	PRO	N-CA-CB	8.54	112.22	103.25
1	D	329	PRO	N-CA-CB	8.46	112.13	103.25
1	B	160	PRO	N-CA-CB	8.37	112.03	103.25
1	C	160	PRO	N-CA-CB	8.34	112.01	103.25
1	A	441	PRO	N-CA-CB	8.27	111.93	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	415	PRO	N-CA-CB	8.19	111.85	103.25
1	C	583	PRO	N-CA-CB	8.15	111.80	103.25
1	B	441	PRO	N-CA-CB	8.13	111.78	103.25
1	B	487	PRO	N-CA-CB	8.04	110.32	103.25
1	B	415	PRO	N-CA-CB	7.97	111.62	103.25
1	C	605	PRO	N-CA-CB	7.88	111.67	103.00
1	D	445	PRO	N-CA-CB	7.74	111.38	103.25
1	D	487	PRO	N-CA-CB	7.72	110.04	103.25
1	B	445	PRO	N-CA-CB	7.69	111.33	103.25
1	A	605	PRO	N-CA-CB	7.69	111.46	103.00
1	C	590	PRO	N-CA-CB	7.66	111.75	103.33
1	A	487	PRO	N-CA-CB	7.64	109.97	103.25
1	C	445	PRO	N-CA-CB	7.59	111.22	103.25
1	A	445	PRO	N-CA-CB	7.40	111.02	103.25
1	A	415	PRO	N-CA-CB	7.34	110.96	103.25
1	D	441	PRO	N-CA-CB	7.33	110.95	103.25
1	C	441	PRO	N-CA-CB	7.20	110.81	103.25
1	A	182	PRO	N-CA-CB	7.19	110.80	103.25
1	A	590	PRO	N-CA-CB	7.14	111.19	103.33
1	A	583	PRO	N-CA-CB	7.13	110.73	103.25
1	B	182	PRO	N-CA-CB	7.08	110.69	103.25
1	B	605	PRO	N-CA-CB	7.03	110.73	103.00
1	D	583	PRO	N-CA-CB	6.85	110.44	103.25
1	C	182	PRO	N-CA-CB	6.81	110.41	103.25
1	D	590	PRO	N-CA-CB	6.62	110.61	103.33
1	D	319	MSE	CB-CG-SE	-6.55	93.05	112.70
1	D	182	PRO	N-CA-CB	6.54	110.12	103.25
1	B	583	PRO	N-CA-CB	6.52	110.09	103.25
1	B	590	PRO	N-CA-CB	6.50	110.48	103.33
1	B	437	PRO	CA-N-CD	-6.39	103.05	112.00
1	D	605	PRO	N-CA-CB	6.37	110.01	103.00
1	B	437	PRO	CB-CA-C	6.33	122.01	111.56
1	C	415	PRO	N-CA-CB	6.32	109.88	103.25
1	C	338	PRO	N-CA-CB	6.24	110.20	103.33
1	A	319	MSE	CB-CG-SE	-6.20	94.09	112.70
1	B	437	PRO	N-CA-CB	-6.10	96.84	103.25
1	C	585	TYR	N-CA-C	-6.03	97.95	110.80
1	A	422	LYS	CB-CA-C	6.01	121.08	110.85
1	B	179	TYR	CA-CB-CG	5.99	124.68	113.90
1	B	319	MSE	CB-CG-SE	-5.97	94.80	112.70
1	D	436	GLY	CA-C-N	5.74	127.02	119.84
1	D	436	GLY	C-N-CA	5.74	127.02	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	PRO	N-CA-CB	5.69	109.59	103.33
1	C	484	LEU	CB-CG-CD1	-5.55	94.03	110.70
1	B	338	PRO	N-CA-CB	5.41	109.42	103.26
1	C	440	SER	CA-C-N	5.28	126.43	119.84
1	C	440	SER	C-N-CA	5.28	126.43	119.84
1	C	250	GLN	N-CA-C	5.19	117.64	108.24
1	D	160	PRO	N-CA-C	-5.16	101.83	112.47
1	A	438	TRP	N-CA-C	-5.05	100.04	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	GLU	Peptide
1	C	477	ARG	Peptide
1	C	584	VAL	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	3711	0	3036	223	0
1	B	3711	0	3038	229	0
1	C	3895	0	3376	335	0
1	D	3711	0	3038	257	0
All	All	15028	0	12488	1009	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 37.

All (1009) 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:C:515:PHE:CZ	1:C:578:ARG:HD3	1.32	1.63
1:D:356:LEU:CA	1:D:427:LEU:HD11	1.17	1.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:LEU:CA	1:A:427:LEU:HD11	1.16	1.59
1:D:356:LEU:HA	1:D:427:LEU:CD1	1.30	1.55
1:D:395:LYS:CE	1:D:526:ARG:HD3	1.37	1.55
1:A:356:LEU:CA	1:A:427:LEU:CD1	1.76	1.55
1:A:356:LEU:HA	1:A:427:LEU:CD1	1.35	1.51
1:D:387:PHE:CA	1:D:429:GLN:NE2	1.71	1.51
1:B:387:PHE:CA	1:B:429:GLN:HE22	1.26	1.48
1:D:356:LEU:CA	1:D:427:LEU:CD1	1.86	1.47
1:D:395:LYS:NZ	1:D:526:ARG:CD	1.75	1.45
1:B:391:GLN:NE2	1:B:422:LYS:HE3	1.14	1.44
1:A:356:LEU:C	1:A:427:LEU:HD11	1.09	1.42
1:B:387:PHE:HA	1:B:429:GLN:NE2	1.18	1.41
1:D:359:ASP:CB	1:D:427:LEU:HD22	1.53	1.38
1:B:387:PHE:HB2	1:B:429:GLN:OE1	1.21	1.37
1:D:356:LEU:C	1:D:427:LEU:HD11	1.09	1.37
1:C:245:ARG:HH12	1:C:523:GLY:N	1.07	1.37
1:C:418:VAL:O	1:C:422:LYS:CE	1.72	1.37
1:D:395:LYS:NZ	1:D:526:ARG:HD2	1.04	1.36
1:C:245:ARG:HH22	1:C:523:GLY:CA	1.38	1.33
1:C:511:TRP:CZ3	1:C:567:GLU:HG3	1.66	1.30
1:B:395:LYS:NZ	1:B:526:ARG:HD2	1.45	1.30
1:C:418:VAL:O	1:C:422:LYS:HE3	1.26	1.30
1:B:395:LYS:CD	1:B:526:ARG:HD3	1.63	1.29
1:D:395:LYS:CE	1:D:526:ARG:CD	2.06	1.28
1:C:432:ARG:HH21	1:C:479:PHE:CB	1.45	1.28
1:D:387:PHE:HA	1:D:429:GLN:NE2	0.96	1.27
1:A:42:ARG:NH2	1:A:247:ASP:OD2	1.68	1.25
1:C:515:PHE:CZ	1:C:578:ARG:CD	2.18	1.25
1:B:391:GLN:NE2	1:B:422:LYS:CE	2.00	1.25
1:A:387:PHE:CB	1:A:429:GLN:OE1	1.80	1.25
1:D:363:ALA:HA	1:D:434:TYR:OH	1.37	1.24
1:D:387:PHE:HB2	1:D:429:GLN:OE1	1.13	1.24
1:D:395:LYS:HD3	1:D:526:ARG:CZ	1.68	1.23
1:B:395:LYS:CE	1:B:526:ARG:HD3	1.69	1.22
1:B:42:ARG:NH2	1:B:247:ASP:OD2	1.74	1.21
1:D:395:LYS:CD	1:D:526:ARG:NH1	2.06	1.19
1:D:432:ARG:HE	1:D:476:THR:CB	1.54	1.19
1:A:433:PHE:CA	1:A:437:PRO:HG2	1.70	1.19
1:C:245:ARG:NH1	1:C:523:GLY:N	1.92	1.18
1:C:356:LEU:CB	1:C:424:LEU:HD23	1.72	1.18
1:C:515:PHE:CE2	1:C:578:ARG:HD3	1.78	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:524:VAL:HG13	1:C:563:GLN:NE2	1.59	1.17
1:B:391:GLN:HE22	1:B:422:LYS:CE	1.55	1.16
1:C:524:VAL:CG1	1:C:563:GLN:OE1	1.93	1.16
1:C:432:ARG:HD3	1:C:476:THR:HA	1.18	1.15
1:C:524:VAL:CG1	1:C:563:GLN:CD	2.19	1.15
1:C:245:ARG:HH22	1:C:523:GLY:HA3	0.98	1.15
1:D:387:PHE:CB	1:D:429:GLN:OE1	1.94	1.14
1:D:429:GLN:O	1:D:433:PHE:CD2	2.01	1.13
1:C:430:VAL:CG1	1:C:434:TYR:HE2	1.61	1.13
1:A:356:LEU:HA	1:A:427:LEU:HD13	1.18	1.12
1:B:356:LEU:CB	1:B:424:LEU:HD23	1.78	1.11
1:D:42:ARG:NH2	1:D:247:ASP:OD2	1.85	1.10
1:B:395:LYS:HD3	1:B:526:ARG:CD	1.82	1.10
1:A:74:ILE:HD11	1:B:1:MSE:SE	2.03	1.09
1:C:528:LEU:CD1	1:C:560:LEU:HD23	1.81	1.09
1:D:395:LYS:HE2	1:D:526:ARG:HD3	1.11	1.09
1:C:568:GLY:O	1:C:578:ARG:NH1	1.86	1.09
1:B:387:PHE:CB	1:B:429:GLN:OE1	2.00	1.08
1:C:555:ALA:O	1:C:559:TYR:HD2	1.35	1.08
1:A:356:LEU:CB	1:A:427:LEU:CD1	2.31	1.08
1:A:433:PHE:HA	1:A:437:PRO:HG2	1.15	1.08
1:A:430:VAL:CG1	1:A:434:TYR:HE2	1.67	1.07
1:C:432:ARG:NH2	1:C:479:PHE:CB	2.17	1.07
1:D:363:ALA:HB2	1:D:430:VAL:HG11	1.37	1.06
1:A:429:GLN:O	1:A:433:PHE:CD2	2.07	1.06
1:C:245:ARG:NH2	1:C:523:GLY:CA	2.18	1.06
1:B:395:LYS:NZ	1:B:526:ARG:CD	2.19	1.06
1:D:432:ARG:HD3	1:D:476:THR:HA	1.36	1.05
1:C:575:TRP:CZ3	1:C:579:ALA:HB2	1.91	1.05
1:D:356:LEU:HA	1:D:427:LEU:HD13	1.38	1.05
1:A:49:ALA:CB	1:A:249:ILE:CG2	2.34	1.04
1:B:395:LYS:CE	1:B:526:ARG:CD	2.35	1.04
1:C:432:ARG:CD	1:C:476:THR:HA	1.77	1.04
1:C:570:TYR:O	1:C:571:ASP:CG	2.00	1.04
1:D:114:GLU:OE1	1:D:118:ARG:NH1	1.91	1.04
1:C:524:VAL:HG13	1:C:563:GLN:CD	1.80	1.04
1:A:430:VAL:HG12	1:A:434:TYR:HE2	1.18	1.03
1:B:395:LYS:HD3	1:B:526:ARG:HD3	1.27	1.03
1:D:432:ARG:NE	1:D:476:THR:CB	2.21	1.03
1:C:359:ASP:CB	1:C:427:LEU:HD22	1.88	1.03
1:C:430:VAL:HG12	1:C:434:TYR:HE2	1.18	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ALA:CB	1:C:249:ILE:CG2	2.37	1.02
1:D:363:ALA:HB2	1:D:430:VAL:CG1	1.90	1.02
1:C:422:LYS:H	1:C:422:LYS:HE2	1.22	1.02
1:A:106:LEU:O	1:A:109:THR:HB	1.58	1.01
1:C:432:ARG:NH2	1:C:477:ARG:HA	1.72	1.01
1:D:74:ILE:HD11	1:C:1:MSE:SE	2.11	1.01
1:A:433:PHE:HA	1:A:437:PRO:CG	1.90	1.01
1:D:395:LYS:HD3	1:D:526:ARG:NH1	1.71	1.00
1:D:74:ILE:CD1	1:C:1:MSE:SE	2.59	1.00
1:D:395:LYS:CD	1:D:526:ARG:HD3	1.90	1.00
1:A:49:ALA:HB2	1:A:249:ILE:HG21	1.37	1.00
1:D:387:PHE:N	1:D:429:GLN:NE2	2.09	0.99
1:C:555:ALA:O	1:C:559:TYR:CD2	2.14	0.99
1:C:515:PHE:CE1	1:C:578:ARG:HD3	1.96	0.99
1:D:42:ARG:CZ	1:D:247:ASP:CG	2.36	0.98
1:D:387:PHE:HA	1:D:429:GLN:CD	1.88	0.98
1:C:245:ARG:NH2	1:C:523:GLY:HA3	1.75	0.97
1:C:432:ARG:CD	1:C:476:THR:CA	2.41	0.97
1:C:418:VAL:O	1:C:422:LYS:HE2	1.62	0.96
1:C:245:ARG:HH22	1:C:523:GLY:HA2	1.30	0.96
1:C:430:VAL:HG12	1:C:434:TYR:CE2	2.01	0.96
1:A:356:LEU:CB	1:A:427:LEU:HD12	1.93	0.96
1:C:245:ARG:HH12	1:C:523:GLY:H	0.98	0.96
1:D:356:LEU:HA	1:D:427:LEU:HD12	1.48	0.96
1:D:387:PHE:CA	1:D:429:GLN:CD	2.39	0.95
1:B:387:PHE:CA	1:B:429:GLN:NE2	2.01	0.95
1:C:422:LYS:HE2	1:C:422:LYS:N	1.80	0.95
1:D:356:LEU:C	1:D:427:LEU:CD1	2.01	0.95
1:A:356:LEU:CB	1:A:427:LEU:HD11	1.92	0.95
1:A:430:VAL:HG12	1:A:434:TYR:CE2	2.01	0.94
1:C:432:ARG:CD	1:C:476:THR:CB	2.46	0.94
1:B:49:ALA:CB	1:B:249:ILE:CG2	2.45	0.93
1:C:429:GLN:O	1:C:433:PHE:CD2	2.22	0.93
1:D:395:LYS:HD2	1:D:526:ARG:NH1	1.81	0.93
1:C:511:TRP:HZ3	1:C:567:GLU:HG3	1.28	0.93
1:C:49:ALA:HB2	1:C:249:ILE:HG21	1.48	0.93
1:C:432:ARG:HD2	1:C:476:THR:CB	1.98	0.93
1:C:515:PHE:HE1	1:C:569:ILE:CD1	1.81	0.93
1:B:49:ALA:HB2	1:B:249:ILE:HG21	1.49	0.93
1:B:432:ARG:NE	1:B:437:PRO:HD2	1.83	0.93
1:C:418:VAL:C	1:C:422:LYS:HE3	1.92	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLU:OE1	1:A:118:ARG:NH1	2.02	0.92
1:C:432:ARG:HD3	1:C:476:THR:CA	2.00	0.92
1:D:395:LYS:NZ	1:D:526:ARG:HH11	1.67	0.92
1:A:433:PHE:C	1:A:437:PRO:HG2	1.94	0.92
1:D:41:ILE:HD12	1:D:227:MSE:HE3	1.51	0.92
1:B:429:GLN:O	1:B:433:PHE:CD2	2.23	0.92
1:B:156:HIS:CE1	1:B:179:TYR:OH	2.23	0.92
1:C:49:ALA:HB2	1:C:249:ILE:CG2	2.00	0.92
1:B:359:ASP:CB	1:B:427:LEU:HD22	2.00	0.91
1:D:395:LYS:CD	1:D:526:ARG:HH11	1.75	0.91
1:C:515:PHE:HE1	1:C:569:ILE:HD11	1.36	0.91
1:B:1:MSE:HB2	1:B:4:LYS:HG3	1.53	0.90
1:B:522:ASP:O	1:B:526:ARG:HG3	1.70	0.90
1:A:356:LEU:CA	1:A:427:LEU:HD12	2.00	0.89
1:B:395:LYS:HZ3	1:B:526:ARG:HD2	1.12	0.89
1:D:395:LYS:HD3	1:D:526:ARG:NE	1.87	0.89
1:A:49:ALA:CB	1:A:249:ILE:HG21	2.02	0.89
1:C:528:LEU:CD1	1:C:560:LEU:CD2	2.50	0.89
1:D:387:PHE:HB2	1:D:429:GLN:CD	1.97	0.88
1:C:524:VAL:HG11	1:C:563:GLN:OE1	1.73	0.88
1:B:49:ALA:CB	1:B:249:ILE:HG21	2.03	0.88
1:A:387:PHE:HB2	1:A:429:GLN:OE1	1.06	0.87
1:C:524:VAL:HG12	1:C:563:GLN:OE1	1.73	0.86
1:C:430:VAL:CG1	1:C:434:TYR:CE2	2.54	0.86
1:D:430:VAL:HA	1:D:433:PHE:HD2	1.40	0.86
1:B:432:ARG:HD2	1:B:437:PRO:HG2	1.55	0.86
1:D:60:ASP:OD1	1:B:315:TYR:OH	1.92	0.86
1:B:395:LYS:HZ3	1:B:526:ARG:CD	1.86	0.86
1:D:363:ALA:CA	1:D:434:TYR:OH	2.21	0.86
1:D:74:ILE:HD13	1:C:1:MSE:SE	2.26	0.86
1:B:395:LYS:HD3	1:B:526:ARG:CZ	2.06	0.85
1:D:356:LEU:CA	1:D:427:LEU:HD12	2.04	0.85
1:D:389:MSE:HE1	1:D:526:ARG:HA	1.57	0.85
1:B:387:PHE:HA	1:B:429:GLN:CD	2.02	0.85
1:B:395:LYS:HZ1	1:B:526:ARG:HD2	1.39	0.85
1:C:511:TRP:CH2	1:C:567:GLU:HG3	2.11	0.85
1:D:363:ALA:CB	1:D:430:VAL:CG1	2.54	0.85
1:D:395:LYS:HZ3	1:D:526:ARG:CD	1.57	0.85
1:D:432:ARG:HD3	1:D:476:THR:CA	2.06	0.85
1:A:429:GLN:O	1:A:433:PHE:HD2	1.55	0.85
1:B:430:VAL:CG1	1:B:434:TYR:HE2	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:VAL:CG1	1:D:434:TYR:HE2	1.89	0.84
1:A:42:ARG:NH2	1:A:247:ASP:CG	2.36	0.84
1:C:515:PHE:HZ	1:C:578:ARG:NH1	1.75	0.84
1:A:363:ALA:CB	1:A:430:VAL:HG13	2.08	0.84
1:C:45:LEU:HD11	1:C:231:MSE:HE3	1.60	0.84
1:A:359:ASP:CB	1:A:427:LEU:HD22	2.08	0.83
1:A:356:LEU:HA	1:A:427:LEU:HD12	1.60	0.83
1:B:395:LYS:HD3	1:B:526:ARG:NE	1.92	0.83
1:C:432:ARG:NH2	1:C:477:ARG:CA	2.36	0.83
1:A:9:ALA:HB3	1:C:9:ALA:HB3	1.61	0.83
1:C:565:ARG:HB3	1:C:565:ARG:CZ	2.06	0.83
1:B:395:LYS:CD	1:B:526:ARG:NH1	2.42	0.82
1:C:568:GLY:O	1:C:578:ARG:CZ	2.26	0.82
1:B:430:VAL:HG12	1:B:434:TYR:HE2	1.42	0.82
1:B:432:ARG:CZ	1:B:437:PRO:CD	2.58	0.82
1:D:264:GLN:HG2	1:D:272:PHE:H	1.43	0.82
1:D:395:LYS:HZ3	1:D:526:ARG:HD2	1.02	0.82
1:A:1:MSE:SE	1:B:74:ILE:HD13	2.30	0.82
1:C:54:GLN:OE1	1:C:405:ARG:NH1	2.13	0.81
1:C:515:PHE:HZ	1:C:578:ARG:HH11	1.27	0.81
1:C:528:LEU:HD11	1:C:560:LEU:HD23	1.61	0.81
1:D:429:GLN:O	1:D:433:PHE:HD2	1.64	0.81
1:D:363:ALA:CB	1:D:430:VAL:HG13	2.10	0.81
1:D:395:LYS:CE	1:D:526:ARG:HH11	1.94	0.81
1:D:395:LYS:HZ1	1:D:526:ARG:CD	1.65	0.81
1:C:565:ARG:HG3	1:C:570:TYR:CD2	2.14	0.81
1:B:391:GLN:HE21	1:B:422:LYS:HE3	1.40	0.81
1:D:522:ASP:O	1:D:526:ARG:HG3	1.79	0.81
1:A:42:ARG:CZ	1:A:247:ASP:OD1	2.29	0.81
1:C:528:LEU:HD12	1:C:560:LEU:CD2	2.09	0.81
1:D:9:ALA:HB3	1:B:9:ALA:HB3	1.63	0.81
1:D:72:ARG:NH2	1:C:1:MSE:HE1	1.96	0.81
1:D:395:LYS:HZ3	1:D:526:ARG:NH1	1.78	0.81
1:D:430:VAL:HA	1:D:433:PHE:CD2	2.17	0.80
1:C:45:LEU:C	1:C:249:ILE:HD13	2.07	0.80
1:A:74:ILE:CD1	1:B:1:MSE:SE	2.80	0.80
1:A:363:ALA:CB	1:A:430:VAL:CG1	2.59	0.80
1:A:389:MSE:HE1	1:A:526:ARG:HA	1.64	0.80
1:C:245:ARG:HH12	1:C:522:ASP:C	1.88	0.79
1:B:156:HIS:HE1	1:B:179:TYR:OH	1.63	0.79
1:A:49:ALA:HB2	1:A:249:ILE:CG2	2.05	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ARG:O	1:A:409:THR:HG23	1.81	0.79
1:C:356:LEU:CB	1:C:424:LEU:CD2	2.59	0.79
1:B:395:LYS:CD	1:B:526:ARG:HH11	1.95	0.79
1:C:42:ARG:CZ	1:C:247:ASP:OD1	2.29	0.79
1:A:363:ALA:HB2	1:A:430:VAL:CG1	2.12	0.79
1:B:422:LYS:HD2	1:B:422:LYS:N	1.96	0.79
1:C:245:ARG:NH1	1:C:523:GLY:H	1.62	0.79
1:A:432:ARG:CB	1:A:432:ARG:HH21	1.95	0.78
1:B:395:LYS:HE2	1:B:526:ARG:HD3	1.64	0.78
1:B:405:ARG:O	1:B:409:THR:HG23	1.82	0.78
1:B:387:PHE:CA	1:B:429:GLN:CD	2.56	0.78
1:B:391:GLN:HE22	1:B:422:LYS:HE3	0.96	0.78
1:B:106:LEU:O	1:B:109:THR:HB	1.83	0.78
1:B:346:LEU:O	1:B:348:GLU:N	2.16	0.78
1:A:42:ARG:CZ	1:A:247:ASP:CG	2.56	0.78
1:B:387:PHE:N	1:B:429:GLN:HE22	1.82	0.78
1:C:156:HIS:HE1	1:C:179:TYR:OH	1.66	0.77
1:A:45:LEU:HB3	1:A:249:ILE:CD1	2.14	0.77
1:A:1:MSE:SE	1:B:74:ILE:CD1	2.82	0.77
1:C:524:VAL:CG1	1:C:563:GLN:NE2	2.40	0.77
1:B:387:PHE:HB2	1:B:429:GLN:CD	2.09	0.77
1:D:346:LEU:O	1:D:348:GLU:N	2.17	0.77
1:A:413:LYS:CB	1:A:422:LYS:NZ	2.47	0.77
1:D:260:SER:O	1:D:264:GLN:NE2	2.18	0.77
1:A:431:ALA:O	1:A:435:GLU:HG2	1.83	0.77
1:A:49:ALA:HB1	1:A:249:ILE:CG2	2.15	0.77
1:C:389:MSE:HE1	1:C:526:ARG:HA	1.67	0.76
1:C:405:ARG:O	1:C:409:THR:HG23	1.84	0.76
1:D:356:LEU:CB	1:D:427:LEU:CD1	2.62	0.76
1:A:245:ARG:NH1	1:A:519:ALA:HB1	2.01	0.76
1:B:356:LEU:CB	1:B:424:LEU:CD2	2.63	0.76
1:C:5:GLU:O	1:C:7:PHE:N	2.19	0.76
1:A:346:LEU:O	1:A:348:GLU:N	2.19	0.76
1:C:565:ARG:HA	1:C:570:TYR:HB3	1.68	0.76
1:D:49:ALA:CB	1:D:249:ILE:CG2	2.63	0.75
1:C:484:LEU:HD13	1:C:490:VAL:HA	1.68	0.75
1:D:42:ARG:CZ	1:D:247:ASP:OD2	2.34	0.75
1:A:432:ARG:HA	1:A:432:ARG:NH2	2.02	0.75
1:A:430:VAL:CG1	1:A:434:TYR:CE2	2.60	0.75
1:B:360:VAL:H	1:B:427:LEU:CD2	1.99	0.74
1:B:395:LYS:CD	1:B:526:ARG:CD	2.43	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:ARG:CZ	1:D:472:VAL:O	2.35	0.74
1:D:1:MSE:HB2	1:D:4:LYS:HG3	1.70	0.74
1:C:245:ARG:NH2	1:C:523:GLY:HA2	1.94	0.74
1:D:395:LYS:CD	1:D:526:ARG:CD	2.57	0.74
1:A:432:ARG:O	1:A:437:PRO:HD3	1.87	0.74
1:C:42:ARG:NE	1:C:247:ASP:CG	2.41	0.74
1:C:1:MSE:HB2	1:C:4:LYS:HG3	1.70	0.74
1:D:99:GLN:O	1:D:103:THR:HG23	1.88	0.74
1:D:232:ARG:O	1:D:236:ARG:CB	2.36	0.73
1:B:15:SER:O	1:B:19:SER:OG	2.07	0.73
1:B:395:LYS:HD3	1:B:526:ARG:NH1	2.02	0.73
1:C:251:LEU:HD23	1:C:291:ARG:HB3	1.71	0.73
1:D:363:ALA:CB	1:D:430:VAL:HG11	2.16	0.73
1:B:432:ARG:CZ	1:B:437:PRO:CG	2.66	0.73
1:C:511:TRP:CD1	1:C:521:ILE:HG13	2.24	0.73
1:B:430:VAL:HG12	1:B:434:TYR:CE2	2.23	0.73
1:B:390:PHE:HB2	1:B:429:GLN:NE2	2.03	0.73
1:B:432:ARG:CD	1:B:437:PRO:HG2	2.18	0.72
1:C:46:SER:N	1:C:249:ILE:HD13	2.04	0.72
1:C:452:LEU:HA	1:C:502:ARG:NH2	2.04	0.72
1:D:430:VAL:HG12	1:D:434:TYR:HE2	1.53	0.72
1:B:5:GLU:O	1:B:7:PHE:N	2.23	0.72
1:D:387:PHE:CB	1:D:429:GLN:CD	2.56	0.72
1:B:244:LYS:HD2	1:B:248:ASP:CB	2.20	0.72
1:D:237:LYS:O	1:D:239:VAL:N	2.21	0.72
1:B:1:MSE:O	1:B:3:THR:N	2.22	0.72
1:C:510:LEU:O	1:C:514:SER:N	2.23	0.72
1:A:64:PHE:HZ	1:C:7:PHE:HE1	1.37	0.71
1:A:68:VAL:HG11	1:A:101:MSE:HE3	1.72	0.71
1:C:430:VAL:HG13	1:C:434:TYR:HE2	1.53	0.71
1:D:395:LYS:HD3	1:D:526:ARG:CD	2.20	0.71
1:A:433:PHE:CA	1:A:437:PRO:CG	2.58	0.71
1:B:45:LEU:C	1:B:249:ILE:HD13	2.15	0.71
1:B:430:VAL:HA	1:B:433:PHE:HD2	1.56	0.71
1:C:156:HIS:CE1	1:C:179:TYR:OH	2.43	0.71
1:B:389:MSE:HE1	1:B:526:ARG:HA	1.72	0.71
1:D:41:ILE:HG23	1:D:231:MSE:HE3	1.71	0.71
1:C:114:GLU:OE1	1:C:118:ARG:NH1	2.20	0.71
1:C:484:LEU:HD11	1:C:493:SER:OG	1.91	0.71
1:B:260:SER:O	1:B:264:GLN:NE2	2.24	0.70
1:D:49:ALA:HB2	1:D:249:ILE:HG21	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:CYS:HB3	1:A:303:VAL:HB	1.72	0.70
1:D:1:MSE:O	1:D:3:THR:N	2.25	0.70
1:D:106:LEU:O	1:D:109:THR:HB	1.91	0.70
1:B:391:GLN:HE22	1:B:422:LYS:NZ	1.88	0.70
1:B:49:ALA:HB2	1:B:249:ILE:CG2	2.17	0.70
1:B:432:ARG:CZ	1:B:437:PRO:HD2	2.20	0.70
1:D:405:ARG:O	1:D:409:THR:HG23	1.92	0.70
1:D:430:VAL:CA	1:D:433:PHE:HD2	2.05	0.70
1:D:518:THR:O	1:D:520:GLY:N	2.25	0.70
1:A:432:ARG:HH21	1:A:432:ARG:CG	2.05	0.70
1:C:49:ALA:CB	1:C:249:ILE:HG23	2.22	0.70
1:C:260:SER:O	1:C:264:GLN:NE2	2.25	0.70
1:B:432:ARG:NE	1:B:437:PRO:CD	2.55	0.70
1:A:391:GLN:NE2	1:A:422:LYS:HG2	2.07	0.69
1:B:390:PHE:HB2	1:B:429:GLN:HE21	1.57	0.69
1:C:49:ALA:CB	1:C:249:ILE:HG21	2.14	0.69
1:C:524:VAL:HG13	1:C:563:GLN:HE22	1.57	0.69
1:C:524:VAL:HG11	1:C:563:GLN:CD	2.10	0.69
1:A:264:GLN:HG2	1:A:272:PHE:H	1.57	0.69
1:C:515:PHE:CE1	1:C:569:ILE:HD11	2.25	0.69
1:D:74:ILE:HD13	1:C:1:MSE:CE	2.23	0.69
1:D:26:TYR:CE2	1:D:79:VAL:HA	2.27	0.69
1:A:49:ALA:CB	1:A:249:ILE:HG23	2.20	0.69
1:C:429:GLN:O	1:C:433:PHE:HD2	1.75	0.69
1:C:528:LEU:HD12	1:C:560:LEU:HD23	1.62	0.69
1:D:356:LEU:CB	1:D:427:LEU:HD12	2.22	0.69
1:D:359:ASP:CB	1:D:427:LEU:CD2	2.50	0.69
1:D:363:ALA:HA	1:D:434:TYR:HH	1.56	0.68
1:D:356:LEU:CB	1:D:424:LEU:HD23	2.23	0.68
1:A:1:MSE:HB2	1:A:4:LYS:HG3	1.76	0.68
1:A:265:PHE:CE1	1:A:271:GLU:HB2	2.27	0.68
1:D:34:TYR:OH	1:D:103:THR:HG22	1.92	0.68
1:D:42:ARG:NH2	1:D:247:ASP:CG	2.47	0.68
1:A:389:MSE:SE	1:A:526:ARG:HG2	2.43	0.68
1:C:515:PHE:CE2	1:C:578:ARG:CD	2.65	0.68
1:C:563:GLN:O	1:C:566:SER:OG	2.07	0.68
1:D:395:LYS:HZ3	1:D:526:ARG:CZ	2.07	0.67
1:D:430:VAL:HG12	1:D:434:TYR:CE2	2.29	0.67
1:B:395:LYS:HZ3	1:B:526:ARG:HH11	1.42	0.67
1:C:26:TYR:CE2	1:C:79:VAL:HA	2.28	0.67
1:A:391:GLN:NE2	1:A:422:LYS:CG	2.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ILE:HA	1:C:308:VAL:HG23	1.75	0.67
1:D:429:GLN:O	1:D:433:PHE:CE2	2.47	0.67
1:C:360:VAL:H	1:C:427:LEU:CD2	2.08	0.67
1:D:5:GLU:O	1:D:7:PHE:N	2.27	0.67
1:D:135:GLN:O	1:D:139:VAL:HG23	1.95	0.67
1:B:429:GLN:O	1:B:433:PHE:HD2	1.77	0.67
1:C:515:PHE:CE1	1:C:578:ARG:CD	2.69	0.67
1:C:390:PHE:HB2	1:C:429:GLN:HE21	1.60	0.67
1:B:395:LYS:HD2	1:B:526:ARG:NH1	2.10	0.67
1:A:432:ARG:N	1:A:432:ARG:HD2	2.09	0.67
1:D:395:LYS:HE2	1:D:526:ARG:CD	1.95	0.67
1:B:45:LEU:HB3	1:B:249:ILE:CD1	2.25	0.67
1:C:245:ARG:HH12	1:C:523:GLY:CA	2.06	0.66
1:D:52:LEU:HD13	1:D:252:PRO:HD2	1.77	0.66
1:D:105:LEU:O	1:D:108:THR:OG1	2.13	0.66
1:D:395:LYS:HZ3	1:D:526:ARG:HH11	1.31	0.66
1:D:264:GLN:HG3	1:D:272:PHE:CD1	2.30	0.66
1:D:397:THR:O	1:D:399:ARG:N	2.28	0.66
1:B:418:VAL:O	1:B:422:LYS:HD3	1.96	0.66
1:D:395:LYS:HZ3	1:D:526:ARG:NE	1.94	0.66
1:A:432:ARG:O	1:A:437:PRO:CD	2.44	0.66
1:D:360:VAL:H	1:D:427:LEU:CD2	2.09	0.66
1:D:395:LYS:HZ1	1:D:526:ARG:HD2	0.84	0.66
1:D:66:GLY:HA2	1:B:322:ALA:HB1	1.77	0.65
1:D:476:THR:O	1:D:480:ALA:HB2	1.95	0.65
1:A:69:ILE:HA	1:A:308:VAL:HG23	1.78	0.65
1:B:156:HIS:CE1	1:B:179:TYR:CZ	2.84	0.65
1:C:46:SER:N	1:C:249:ILE:CD1	2.59	0.65
1:A:9:ALA:HB2	1:A:308:VAL:HG12	1.76	0.65
1:B:387:PHE:HA	1:B:429:GLN:HE22	0.52	0.65
1:A:245:ARG:HH11	1:A:519:ALA:HB1	1.61	0.65
1:D:429:GLN:C	1:D:433:PHE:CD2	2.75	0.65
1:C:515:PHE:CE1	1:C:569:ILE:CD1	2.72	0.65
1:C:15:SER:O	1:C:19:SER:OG	2.09	0.65
1:C:486:SER:O	1:C:488:GLU:N	2.28	0.65
1:C:564:LEU:O	1:C:569:ILE:HG22	1.96	0.65
1:C:61:SER:HB2	1:C:405:ARG:HH12	1.62	0.65
1:D:386:PRO:C	1:D:429:GLN:NE2	2.54	0.65
1:A:45:LEU:HD11	1:A:231:MSE:HE3	1.77	0.65
1:B:357:HIS:HA	1:B:427:LEU:HD21	1.79	0.65
1:B:387:PHE:N	1:B:429:GLN:NE2	2.42	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ILE:HD12	1:B:227:MSE:HE3	1.79	0.64
1:B:26:TYR:CE2	1:B:79:VAL:HA	2.32	0.64
1:D:286:MSE:O	1:D:290:THR:OG1	2.15	0.64
1:A:1:MSE:O	1:A:3:THR:N	2.30	0.64
1:C:26:TYR:OH	1:C:80:GLU:HB2	1.97	0.64
1:D:139:VAL:HG21	1:D:293:ILE:HG23	1.78	0.64
1:A:69:ILE:HD13	1:A:319:MSE:HE3	1.80	0.64
1:C:397:THR:O	1:C:399:ARG:N	2.30	0.64
1:C:515:PHE:CZ	1:C:578:ARG:NH1	2.64	0.64
1:C:507:PHE:CD1	1:C:564:LEU:HD21	2.33	0.64
1:B:114:GLU:OE1	1:B:118:ARG:NH1	2.31	0.63
1:C:34:TYR:OH	1:C:103:THR:HG22	1.99	0.63
1:C:432:ARG:O	1:C:437:PRO:HD2	1.98	0.63
1:D:49:ALA:CB	1:D:249:ILE:HG21	2.29	0.63
1:C:257:ILE:HD13	1:C:294:VAL:HG21	1.81	0.63
1:C:147:PHE:HB2	1:C:148:GLU:HG2	1.81	0.62
1:A:253:THR:HA	1:A:291:ARG:HD2	1.81	0.62
1:B:42:ARG:CZ	1:B:247:ASP:CG	2.72	0.62
1:A:227:MSE:O	1:A:231:MSE:HG3	1.99	0.62
1:A:476:THR:O	1:A:480:ALA:HB2	1.98	0.62
1:C:486:SER:HA	1:C:490:VAL:HG23	1.81	0.62
1:D:68:VAL:HG11	1:D:101:MSE:HE2	1.80	0.62
1:D:273:PRO:HB2	1:D:276:VAL:HB	1.82	0.62
1:D:363:ALA:HB1	1:D:430:VAL:HG13	1.80	0.62
1:A:356:LEU:CB	1:A:424:LEU:HD23	2.30	0.62
1:C:395:LYS:HD3	1:C:526:ARG:NH2	2.15	0.61
1:C:486:SER:HB3	1:C:487:PRO:HD2	1.81	0.61
1:D:90:LYS:HE2	1:D:92:MSE:HE2	1.80	0.61
1:A:41:ILE:HD12	1:A:227:MSE:HE3	1.82	0.61
1:A:433:PHE:O	1:A:437:PRO:HG2	2.01	0.61
1:C:570:TYR:O	1:C:571:ASP:OD1	2.18	0.61
1:A:391:GLN:CD	1:A:422:LYS:HG2	2.25	0.61
1:A:432:ARG:O	1:A:437:PRO:CG	2.48	0.61
1:D:42:ARG:CZ	1:D:247:ASP:OD1	2.49	0.61
1:A:237:LYS:O	1:A:239:VAL:N	2.34	0.61
1:A:436:GLY:N	1:A:437:PRO:HD3	2.15	0.61
1:B:36:TRP:CE3	1:B:103:THR:HG21	2.36	0.61
1:C:45:LEU:HB3	1:C:249:ILE:CD1	2.31	0.61
1:C:76:TYR:HB2	1:C:82:LYS:HE3	1.83	0.61
1:B:42:ARG:NH2	1:B:247:ASP:CG	2.56	0.61
1:B:387:PHE:CA	1:B:429:GLN:OE1	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:VAL:CG1	1:D:434:TYR:CE2	2.79	0.61
1:B:383:VAL:HA	1:B:433:PHE:CZ	2.36	0.61
1:C:42:ARG:NH1	1:C:247:ASP:OD1	2.33	0.61
1:C:112:HIS:CE1	1:C:140:THR:HG22	2.36	0.61
1:B:42:ARG:CZ	1:B:247:ASP:OD2	2.48	0.60
1:C:36:TRP:CE3	1:C:103:THR:HG21	2.36	0.60
1:C:435:GLU:OE1	1:C:482:HIS:CE1	2.54	0.60
1:A:34:TYR:OH	1:A:103:THR:HG22	2.01	0.60
1:C:107:LEU:HD13	1:C:231:MSE:HE2	1.83	0.60
1:A:356:LEU:C	1:A:427:LEU:CD1	1.97	0.60
1:B:363:ALA:CB	1:B:430:VAL:CG1	2.80	0.60
1:A:36:TRP:O	1:A:227:MSE:HE2	2.01	0.60
1:C:565:ARG:HA	1:C:570:TYR:CB	2.30	0.60
1:C:569:ILE:O	1:C:569:ILE:HG23	2.01	0.60
1:D:17:PHE:CE2	1:D:101:MSE:HE3	2.37	0.60
1:D:287:THR:N	1:D:288:PRO:HD2	2.17	0.60
1:B:69:ILE:HA	1:B:308:VAL:HG23	1.83	0.60
1:D:360:VAL:N	1:D:427:LEU:CD2	2.65	0.59
1:A:123:THR:O	1:A:125:ASP:N	2.34	0.59
1:B:245:ARG:NH1	1:B:519:ALA:O	2.32	0.59
1:D:389:MSE:HA	1:D:393:GLY:HA2	1.83	0.59
1:A:118:ARG:O	1:A:121:LYS:HG2	2.02	0.59
1:B:34:TYR:OH	1:B:103:THR:HG22	2.02	0.59
1:C:28:PRO:HG2	1:C:31:GLN:HG2	1.84	0.59
1:A:39:PRO:O	1:A:43:ARG:HG3	2.02	0.59
1:B:267:LEU:HD12	1:B:294:VAL:HG13	1.84	0.59
1:C:1:MSE:O	1:C:3:THR:N	2.34	0.59
1:A:5:GLU:O	1:A:7:PHE:N	2.36	0.59
1:D:249:ILE:HG22	1:D:250:GLN:N	2.18	0.59
1:C:514:SER:HB3	1:C:575:TRP:CE3	2.36	0.59
1:D:128:PRO:O	1:D:276:VAL:HG23	2.02	0.59
1:D:432:ARG:CD	1:D:476:THR:CA	2.78	0.59
1:C:245:ARG:CZ	1:C:523:GLY:CA	2.79	0.59
1:A:440:SER:O	1:A:442:THR:N	2.34	0.59
1:D:359:ASP:CA	1:D:427:LEU:HD22	2.30	0.59
1:A:60:ASP:OD1	1:A:61:SER:N	2.34	0.59
1:A:397:THR:O	1:A:399:ARG:N	2.36	0.59
1:B:430:VAL:HA	1:B:433:PHE:CD2	2.37	0.59
1:A:126:ASP:OD1	1:A:127:GLU:N	2.36	0.58
1:C:106:LEU:O	1:C:109:THR:HB	2.03	0.58
1:A:26:TYR:CE2	1:A:79:VAL:HA	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLN:O	1:A:103:THR:HG23	2.02	0.58
1:B:367:ARG:O	1:B:379:VAL:HG21	2.03	0.58
1:B:432:ARG:NH2	1:B:437:PRO:HG3	2.18	0.58
1:A:38:LEU:N	1:A:227:MSE:HE1	2.17	0.58
1:A:413:LYS:CB	1:A:422:LYS:HZ1	2.16	0.58
1:B:363:ALA:CB	1:B:430:VAL:HG13	2.34	0.58
1:C:570:TYR:O	1:C:571:ASP:CB	2.51	0.58
1:A:1:MSE:SE	1:B:74:ILE:HD11	2.52	0.58
1:C:528:LEU:HD12	1:C:560:LEU:HD21	1.84	0.58
1:A:42:ARG:NE	1:A:247:ASP:CG	2.61	0.58
1:C:52:LEU:HD13	1:C:252:PRO:HD2	1.85	0.58
1:D:1:MSE:SE	1:C:74:ILE:HD13	2.54	0.58
1:A:267:LEU:HD12	1:A:294:VAL:HG13	1.86	0.58
1:C:50:HIS:HB2	1:C:399:ARG:NH1	2.19	0.58
1:D:5:GLU:OE2	1:D:311:LYS:HE2	2.04	0.58
1:A:383:VAL:HA	1:A:433:PHE:CZ	2.38	0.58
1:A:42:ARG:HG3	1:A:234:MSE:SE	2.54	0.57
1:C:92:MSE:HE1	1:C:309:THR:OG1	2.04	0.57
1:B:357:HIS:CA	1:B:427:LEU:HD21	2.35	0.57
1:C:575:TRP:CE3	1:C:579:ALA:HB2	2.38	0.57
1:B:237:LYS:O	1:B:239:VAL:N	2.37	0.57
1:C:41:ILE:HD12	1:C:227:MSE:HE3	1.86	0.57
1:C:430:VAL:HG13	1:C:434:TYR:CE2	2.34	0.57
1:B:34:TYR:CE1	1:B:36:TRP:HB2	2.38	0.57
1:C:418:VAL:O	1:C:422:LYS:CD	2.52	0.57
1:C:430:VAL:HA	1:C:433:PHE:HD2	1.69	0.57
1:D:126:ASP:OD1	1:D:127:GLU:N	2.38	0.57
1:A:41:ILE:CD1	1:A:227:MSE:HE3	2.34	0.57
1:A:390:PHE:HB2	1:A:429:GLN:HE21	1.68	0.57
1:C:395:LYS:HB2	1:C:526:ARG:HH21	1.70	0.57
1:C:518:THR:O	1:C:520:GLY:N	2.37	0.57
1:B:397:THR:O	1:B:399:ARG:N	2.37	0.57
1:D:36:TRP:CE3	1:D:103:THR:HG21	2.40	0.57
1:B:42:ARG:CZ	1:B:247:ASP:OD1	2.53	0.57
1:C:245:ARG:NH1	1:C:523:GLY:CA	2.66	0.56
1:D:96:ASP:HB2	1:D:320:PHE:CD2	2.40	0.56
1:B:395:LYS:NZ	1:B:526:ARG:HH11	2.01	0.56
1:C:11:PRO:O	1:C:12:LEU:HD23	2.05	0.56
1:C:118:ARG:O	1:C:121:LYS:HG2	2.05	0.56
1:B:38:LEU:HA	1:B:227:MSE:HE1	1.87	0.56
1:B:62:ILE:HG23	1:B:302:ARG:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:GLU:OE1	1:C:482:HIS:HE1	1.88	0.56
1:C:565:ARG:HB3	1:C:565:ARG:NH2	2.20	0.56
1:A:244:LYS:O	1:A:246:GLU:N	2.37	0.56
1:D:321:GLU:O	1:D:325:THR:HG22	2.05	0.56
1:B:264:GLN:HG2	1:B:272:PHE:H	1.70	0.56
1:D:38:LEU:N	1:D:227:MSE:HE1	2.20	0.56
1:B:391:GLN:NE2	1:B:422:LYS:NZ	2.49	0.56
1:D:432:ARG:NH2	1:D:472:VAL:O	2.39	0.56
1:B:223:HIS:O	1:B:227:MSE:HG2	2.05	0.56
1:C:568:GLY:O	1:C:578:ARG:NH2	2.39	0.56
1:C:132:CYS:SG	1:C:290:THR:HG23	2.46	0.56
1:D:249:ILE:CG2	1:D:250:GLN:N	2.69	0.56
1:A:109:THR:O	1:A:174:LYS:NZ	2.34	0.56
1:D:49:ALA:HB2	1:D:249:ILE:CG2	2.33	0.55
1:D:429:GLN:C	1:D:433:PHE:CE2	2.85	0.55
1:A:42:ARG:NE	1:A:247:ASP:OD1	2.39	0.55
1:B:113:GLU:HG3	1:B:114:GLU:N	2.21	0.55
1:C:511:TRP:CH2	1:C:567:GLU:CG	2.86	0.55
1:B:136:ALA:O	1:B:140:THR:OG1	2.23	0.55
1:C:411:PHE:CE1	1:C:419:ALA:HB1	2.41	0.55
1:C:515:PHE:CD1	1:C:578:ARG:HB3	2.41	0.55
1:B:360:VAL:N	1:B:427:LEU:CD2	2.67	0.55
1:A:45:LEU:HB3	1:A:249:ILE:HD11	1.88	0.55
1:C:105:LEU:O	1:C:108:THR:OG1	2.24	0.55
1:C:515:PHE:HE1	1:C:569:ILE:HD12	1.70	0.55
1:B:46:SER:N	1:B:249:ILE:HD13	2.21	0.55
1:C:490:VAL:O	1:C:493:SER:OG	2.22	0.55
1:D:287:THR:H	1:D:288:PRO:HD2	1.71	0.55
1:A:389:MSE:HA	1:A:393:GLY:HA2	1.89	0.55
1:B:363:ALA:HB2	1:B:430:VAL:CG1	2.36	0.55
1:C:511:TRP:CZ3	1:C:567:GLU:CG	2.62	0.55
1:B:128:PRO:HG2	1:B:275:SER:CB	2.37	0.54
1:B:432:ARG:HE	1:B:437:PRO:HD2	1.70	0.54
1:A:331:THR:O	1:A:334:GLU:N	2.39	0.54
1:B:126:ASP:OD1	1:B:127:GLU:N	2.39	0.54
1:C:123:THR:O	1:C:125:ASP:N	2.41	0.54
1:C:243:VAL:O	1:C:244:LYS:HG3	2.06	0.54
1:A:126:ASP:OD1	1:A:129:SER:OG	2.19	0.54
1:A:64:PHE:CZ	1:C:7:PHE:HE1	2.21	0.54
1:A:518:THR:O	1:A:520:GLY:N	2.40	0.54
1:C:155:GLU:O	1:C:157:ARG:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLU:O	1:A:129:SER:N	2.41	0.54
1:C:424:LEU:C	1:C:483:ARG:HH22	2.16	0.54
1:A:432:ARG:HH21	1:A:432:ARG:CA	2.20	0.54
1:B:246:GLU:O	1:B:247:ASP:OD1	2.26	0.54
1:D:42:ARG:NH1	1:D:247:ASP:OD1	2.41	0.54
1:A:430:VAL:HG13	1:A:434:TYR:HE2	1.63	0.54
1:B:432:ARG:NH2	1:B:437:PRO:CG	2.71	0.54
1:C:71:LEU:HD22	1:C:313:GLU:HB3	1.90	0.54
1:C:410:VAL:HG12	1:C:422:LYS:HG2	1.89	0.54
1:C:515:PHE:CD1	1:C:515:PHE:N	2.76	0.53
1:D:72:ARG:HH21	1:C:1:MSE:HE1	1.71	0.53
1:D:432:ARG:CD	1:D:476:THR:CB	2.86	0.53
1:A:436:GLY:N	1:A:437:PRO:CD	2.72	0.53
1:C:475:LEU:C	1:C:477:ARG:H	2.16	0.53
1:C:49:ALA:HB3	1:C:249:ILE:CG2	2.36	0.53
1:C:156:HIS:HE1	1:C:179:TYR:CZ	2.27	0.53
1:C:385:LEU:HD22	1:C:396:LEU:HB3	1.89	0.53
1:D:132:CYS:SG	1:D:289:LEU:HD23	2.48	0.53
1:B:45:LEU:HB3	1:B:249:ILE:HD12	1.90	0.53
1:B:5:GLU:O	1:B:6:ILE:C	2.52	0.53
1:B:518:THR:O	1:B:520:GLY:N	2.40	0.53
1:C:515:PHE:CE1	1:C:569:ILE:HD12	2.42	0.53
1:A:299:LEU:HA	1:A:303:VAL:CG1	2.38	0.53
1:B:264:GLN:HG3	1:B:272:PHE:CD1	2.44	0.53
1:B:299:LEU:HA	1:B:303:VAL:HG13	1.89	0.53
1:D:148:GLU:OE2	1:D:179:TYR:CE1	2.62	0.53
1:A:432:ARG:HA	1:A:432:ARG:CZ	2.38	0.53
1:B:244:LYS:O	1:B:246:GLU:N	2.42	0.52
1:D:14:VAL:HG23	1:D:303:VAL:HG22	1.92	0.52
1:C:124:ARG:O	1:C:124:ARG:NH1	2.43	0.52
1:D:5:GLU:OE1	1:D:311:LYS:HB2	2.08	0.52
1:B:63:CYS:HB3	1:B:303:VAL:HB	1.90	0.52
1:C:5:GLU:OE2	1:C:311:LYS:HE2	2.09	0.52
1:C:113:GLU:HG3	1:C:114:GLU:N	2.25	0.52
1:B:44:LEU:HD23	1:B:45:LEU:HD12	1.92	0.52
1:D:52:LEU:HD12	1:D:295:PHE:HD1	1.74	0.52
1:B:420:ARG:O	1:B:424:LEU:HG	2.10	0.52
1:C:127:GLU:O	1:C:129:SER:N	2.42	0.52
1:D:57:GLU:HG3	1:D:58:PHE:HD1	1.72	0.52
1:A:430:VAL:O	1:A:434:TYR:CD2	2.62	0.52
1:C:565:ARG:NH2	1:C:565:ARG:CB	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:TRP:O	1:B:135:GLN:HG2	2.10	0.52
1:C:515:PHE:N	1:C:515:PHE:HD1	2.07	0.52
1:D:7:PHE:HE1	1:B:64:PHE:HZ	1.57	0.52
1:D:387:PHE:CA	1:D:429:GLN:OE1	2.46	0.52
1:A:69:ILE:HG12	1:A:308:VAL:CG2	2.39	0.52
1:C:452:LEU:HA	1:C:502:ARG:HH22	1.74	0.52
1:B:430:VAL:CG1	1:B:434:TYR:CE2	2.81	0.51
1:C:314:ASP:OD1	1:C:315:TYR:N	2.43	0.51
1:A:28:PRO:HG2	1:A:31:GLN:HG2	1.92	0.51
1:A:49:ALA:HB1	1:A:249:ILE:HG22	1.90	0.51
1:B:476:THR:O	1:B:480:ALA:HB2	2.10	0.51
1:C:5:GLU:OE1	1:C:311:LYS:HB2	2.10	0.51
1:C:360:VAL:N	1:C:427:LEU:CD2	2.73	0.51
1:D:52:LEU:HD22	1:D:252:PRO:HG3	1.93	0.51
1:B:147:PHE:HB2	1:B:148:GLU:HG2	1.93	0.51
1:C:49:ALA:HB3	1:C:249:ILE:HG23	1.89	0.51
1:C:565:ARG:CZ	1:C:565:ARG:CB	2.85	0.51
1:C:54:GLN:NE2	1:C:405:ARG:HD2	2.25	0.51
1:D:181:SER:O	1:D:183:ILE:N	2.44	0.51
1:A:432:ARG:HG3	1:A:476:THR:HA	1.91	0.51
1:C:52:LEU:HD21	1:C:294:VAL:HG12	1.91	0.51
1:D:432:ARG:HH22	1:D:472:VAL:CB	2.24	0.51
1:A:5:GLU:O	1:A:6:ILE:C	2.54	0.51
1:A:64:PHE:HZ	1:C:7:PHE:CE1	2.23	0.51
1:B:9:ALA:HB2	1:B:308:VAL:HG12	1.92	0.51
1:C:68:VAL:HG11	1:C:101:MSE:HE2	1.92	0.51
1:C:528:LEU:HG	1:C:563:GLN:NE2	2.25	0.51
1:C:49:ALA:CB	1:C:249:ILE:HG22	2.37	0.51
1:B:156:HIS:HE1	1:B:179:TYR:CZ	2.27	0.50
1:C:45:LEU:HD11	1:C:231:MSE:CE	2.39	0.50
1:A:7:PHE:CZ	1:C:306:ALA:HB2	2.46	0.50
1:C:430:VAL:O	1:C:434:TYR:CD2	2.64	0.50
1:D:107:LEU:HA	1:D:110:VAL:CG1	2.41	0.50
1:B:576:VAL:O	1:B:579:ALA:HB3	2.10	0.50
1:D:124:ARG:HG3	1:D:125:ASP:OD1	2.11	0.50
1:B:23:GLN:HG3	1:B:90:LYS:HD3	1.93	0.50
1:C:46:SER:CA	1:C:249:ILE:HD13	2.41	0.50
1:C:267:LEU:HD12	1:C:294:VAL:HG13	1.92	0.50
1:D:244:LYS:O	1:D:246:GLU:N	2.45	0.50
1:D:260:SER:C	1:D:264:GLN:NE2	2.69	0.50
1:D:1:MSE:SE	1:C:74:ILE:CD1	3.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:5:GLU:O	1:D:6:ILE:C	2.55	0.50
1:D:576:VAL:O	1:D:579:ALA:HB3	2.11	0.50
1:B:49:ALA:CB	1:B:249:ILE:HG22	2.40	0.50
1:B:432:ARG:O	1:B:432:ARG:HD3	2.12	0.50
1:C:510:LEU:O	1:C:514:SER:OG	2.27	0.50
1:D:42:ARG:HG3	1:D:234:MSE:SE	2.62	0.50
1:D:78:THR:HG21	1:D:93:THR:HG21	1.93	0.50
1:A:429:GLN:O	1:A:433:PHE:CE2	2.64	0.50
1:B:49:ALA:HB3	1:B:249:ILE:CG2	2.38	0.50
1:A:395:LYS:NZ	1:A:523:GLY:HA2	2.26	0.49
1:C:45:LEU:HB3	1:C:249:ILE:HD12	1.94	0.49
1:C:46:SER:CB	1:C:249:ILE:HG12	2.42	0.49
1:C:507:PHE:HD1	1:C:564:LEU:HD21	1.75	0.49
1:A:321:GLU:O	1:A:325:THR:HG22	2.12	0.49
1:A:363:ALA:HB3	1:A:430:VAL:CG1	2.41	0.49
1:C:389:MSE:HA	1:C:393:GLY:HA2	1.93	0.49
1:D:63:CYS:SG	1:D:64:PHE:N	2.84	0.49
1:D:118:ARG:O	1:D:121:LYS:HG2	2.12	0.49
1:A:391:GLN:NE2	1:A:422:LYS:HG3	2.28	0.49
1:B:38:LEU:N	1:B:227:MSE:HE1	2.26	0.49
1:B:99:GLN:O	1:B:103:THR:HG23	2.13	0.49
1:C:424:LEU:HB3	1:C:483:ARG:NH2	2.28	0.49
1:B:109:THR:HG23	1:B:174:LYS:HG3	1.95	0.49
1:B:128:PRO:HG2	1:B:275:SER:HB3	1.95	0.49
1:B:430:VAL:CA	1:B:433:PHE:HD2	2.24	0.49
1:D:17:PHE:O	1:D:23:GLN:NE2	2.45	0.49
1:C:245:ARG:NH1	1:C:519:ALA:O	2.46	0.49
1:B:46:SER:N	1:B:249:ILE:CD1	2.76	0.49
1:C:128:PRO:HG2	1:C:275:SER:CB	2.42	0.49
1:C:562:GLU:HG3	1:C:565:ARG:HH22	1.78	0.49
1:A:390:PHE:HB2	1:A:429:GLN:NE2	2.28	0.49
1:A:432:ARG:HH21	1:A:432:ARG:HA	1.75	0.49
1:C:62:ILE:HG23	1:C:302:ARG:O	2.13	0.49
1:C:379:VAL:O	1:C:382:SER:OG	2.08	0.49
1:C:455:GLN:CB	1:C:502:ARG:HH21	2.24	0.49
1:C:315:TYR:O	1:C:319:MSE:HB2	2.12	0.49
1:D:249:ILE:CG2	1:D:250:GLN:H	2.26	0.48
1:A:44:LEU:HD23	1:A:45:LEU:HD12	1.95	0.48
1:A:363:ALA:CB	1:A:430:VAL:HG11	2.40	0.48
1:C:243:VAL:O	1:C:244:LYS:CG	2.61	0.48
1:C:396:LEU:HD21	1:C:406:TYR:CB	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:511:TRP:CG	1:C:521:ILE:HG13	2.48	0.48
1:D:150:ASP:C	1:D:151:MSE:HG2	2.38	0.48
1:B:245:ARG:NH1	1:B:519:ALA:HA	2.28	0.48
1:C:559:TYR:O	1:C:562:GLU:HB3	2.13	0.48
1:D:109:THR:HG22	1:D:110:VAL:N	2.27	0.48
1:D:230:GLN:O	1:D:234:MSE:HG3	2.13	0.48
1:D:257:ILE:HD13	1:D:294:VAL:HG21	1.95	0.48
1:D:306:ALA:HB2	1:B:7:PHE:CE1	2.48	0.48
1:A:62:ILE:HG22	1:A:63:CYS:O	2.13	0.48
1:A:230:GLN:O	1:A:234:MSE:HG3	2.12	0.48
1:B:432:ARG:HD3	1:B:432:ARG:C	2.39	0.48
1:C:72:ARG:HB2	1:C:309:THR:CG2	2.43	0.48
1:C:515:PHE:CG	1:C:578:ARG:HB3	2.48	0.48
1:D:360:VAL:HA	1:D:430:VAL:HG21	1.94	0.48
1:B:401:ASN:N	1:B:401:ASN:OD1	2.46	0.48
1:C:131:TRP:O	1:C:135:GLN:HG2	2.13	0.48
1:B:395:LYS:HZ3	1:B:526:ARG:NH1	2.08	0.48
1:B:432:ARG:HH22	1:B:472:VAL:HA	1.79	0.48
1:C:46:SER:HB3	1:C:249:ILE:HG12	1.96	0.48
1:C:418:VAL:CA	1:C:422:LYS:HE3	2.43	0.48
1:B:104:LEU:HD11	1:B:299:LEU:HD11	1.96	0.48
1:C:430:VAL:O	1:C:434:TYR:HD2	1.97	0.48
1:C:527:SER:C	1:C:529:MSE:H	2.21	0.48
1:D:7:PHE:HB2	1:B:11:PRO:HG3	1.96	0.48
1:D:279:GLN:HB3	1:D:286:MSE:HE2	1.95	0.48
1:A:63:CYS:SG	1:A:64:PHE:N	2.87	0.48
1:B:69:ILE:HG12	1:B:308:VAL:CG2	2.44	0.48
1:C:264:GLN:HG3	1:C:272:PHE:CG	2.49	0.48
1:C:480:ALA:O	1:C:484:LEU:HG	2.14	0.48
1:A:432:ARG:HH21	1:A:432:ARG:HG3	1.79	0.47
1:C:37:GLU:N	1:C:37:GLU:OE1	2.46	0.47
1:D:430:VAL:O	1:D:433:PHE:HB2	2.12	0.47
1:A:576:VAL:O	1:A:579:ALA:HB3	2.15	0.47
1:B:387:PHE:CB	1:B:429:GLN:CD	2.71	0.47
1:D:268:PHE:HD2	1:D:272:PHE:HE1	1.61	0.47
1:A:109:THR:HG23	1:A:174:LYS:HG3	1.97	0.47
1:A:363:ALA:HB2	1:A:430:VAL:HG11	1.93	0.47
1:B:46:SER:HA	1:B:249:ILE:HD13	1.95	0.47
1:C:395:LYS:HD3	1:C:526:ARG:HH22	1.79	0.47
1:D:430:VAL:HG13	1:D:434:TYR:HE2	1.73	0.47
1:A:45:LEU:HB3	1:A:249:ILE:HD13	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:ALA:HB1	1:C:66:GLY:HA2	1.97	0.47
1:C:388:ALA:HB1	1:C:394:THR:O	2.14	0.47
1:D:69:ILE:HA	1:D:308:VAL:HG23	1.96	0.47
1:C:60:ASP:OD1	1:C:61:SER:N	2.48	0.47
1:D:45:LEU:HB3	1:D:249:ILE:CD1	2.45	0.47
1:D:48:VAL:HG23	1:D:303:VAL:HG11	1.96	0.47
1:D:62:ILE:HG23	1:D:302:ARG:O	2.14	0.47
1:D:68:VAL:CG1	1:D:101:MSE:HE2	2.44	0.47
1:D:253:THR:HG22	1:D:256:ASP:OD1	2.14	0.47
1:A:430:VAL:HG13	1:A:434:TYR:CE2	2.44	0.47
1:B:273:PRO:O	1:B:276:VAL:HG12	2.15	0.47
1:D:129:SER:O	1:D:132:CYS:HB3	2.15	0.47
1:A:78:THR:HG21	1:A:93:THR:OG1	2.14	0.47
1:A:430:VAL:HA	1:A:433:PHE:HD2	1.79	0.47
1:B:127:GLU:O	1:B:129:SER:N	2.47	0.47
1:A:60:ASP:CG	1:A:61:SER:H	2.19	0.47
1:B:380:THR:O	1:B:384:LEU:HG	2.14	0.47
1:B:432:ARG:NE	1:B:437:PRO:CG	2.77	0.47
1:C:41:ILE:CD1	1:C:227:MSE:HE3	2.45	0.47
1:C:429:GLN:O	1:C:433:PHE:CE2	2.68	0.47
1:C:486:SER:HA	1:C:490:VAL:CG2	2.45	0.47
1:D:129:SER:H	1:D:131:TRP:H	1.62	0.46
1:D:234:MSE:HE2	1:D:234:MSE:HB3	1.88	0.46
1:D:360:VAL:N	1:D:427:LEU:HD23	2.30	0.46
1:A:80:GLU:HB3	1:A:81:PRO:HD3	1.97	0.46
1:C:128:PRO:HG2	1:C:275:SER:HB2	1.97	0.46
1:C:528:LEU:HG	1:C:563:GLN:HE22	1.80	0.46
1:D:299:LEU:HA	1:D:303:VAL:HG13	1.96	0.46
1:B:129:SER:O	1:B:132:CYS:HB3	2.14	0.46
1:D:243:VAL:O	1:D:244:LYS:HG3	2.15	0.46
1:D:476:THR:O	1:D:480:ALA:CB	2.62	0.46
1:A:76:TYR:CB	1:A:82:LYS:HE3	2.46	0.46
1:A:389:MSE:HE3	1:A:529:MSE:HG3	1.98	0.46
1:D:234:MSE:O	1:D:235:LEU:C	2.57	0.46
1:D:390:PHE:HB2	1:D:429:GLN:HE21	1.81	0.46
1:A:25:LEU:HD13	1:A:94:ILE:HD11	1.97	0.46
1:A:401:ASN:OD1	1:A:401:ASN:N	2.49	0.46
1:C:34:TYR:OH	1:C:41:ILE:HD11	2.15	0.46
1:C:514:SER:HB2	1:C:515:PHE:HD1	1.80	0.46
1:D:7:PHE:CE1	1:B:306:ALA:HB2	2.51	0.46
1:A:113:GLU:HG3	1:A:114:GLU:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:HIS:CE1	1:C:179:TYR:CZ	3.02	0.46
1:D:109:THR:HG23	1:D:174:LYS:HG3	1.97	0.46
1:D:150:ASP:O	1:D:151:MSE:HG2	2.16	0.46
1:D:387:PHE:N	1:D:429:GLN:CD	2.68	0.46
1:A:1:MSE:HB2	1:A:4:LYS:CG	2.44	0.46
1:A:389:MSE:HE3	1:A:389:MSE:HB3	1.91	0.46
1:C:273:PRO:HB2	1:C:276:VAL:HB	1.98	0.46
1:C:432:ARG:HH21	1:C:477:ARG:HA	1.74	0.46
1:A:18:LEU:HD13	1:A:105:LEU:HD13	1.98	0.46
1:B:390:PHE:CE2	1:B:477:ARG:HA	2.51	0.46
1:A:262:ASN:O	1:A:266:ALA:CB	2.64	0.46
1:A:430:VAL:O	1:A:434:TYR:HD2	1.99	0.46
1:C:71:LEU:HD12	1:C:310:ALA:O	2.16	0.46
1:C:110:VAL:HB	1:C:232:ARG:HA	1.97	0.46
1:D:96:ASP:HB2	1:D:320:PHE:HD2	1.79	0.46
1:D:385:LEU:HD22	1:D:396:LEU:HB3	1.97	0.46
1:B:38:LEU:CA	1:B:227:MSE:HE1	2.46	0.46
1:B:57:GLU:HG3	1:B:58:PHE:N	2.31	0.46
1:C:510:LEU:C	1:C:514:SER:HG	2.24	0.46
1:D:155:GLU:O	1:D:157:ARG:N	2.49	0.46
1:A:363:ALA:HB3	1:A:430:VAL:HG13	1.93	0.46
1:C:349:TRP:O	1:C:351:GLU:N	2.49	0.46
1:C:430:VAL:HA	1:C:433:PHE:CD2	2.50	0.46
1:C:477:ARG:C	1:C:479:PHE:N	2.72	0.46
1:B:45:LEU:C	1:B:249:ILE:CD1	2.87	0.45
1:C:367:ARG:O	1:C:379:VAL:HG21	2.16	0.45
1:C:599:ALA:O	1:C:601:GLN:N	2.50	0.45
1:A:74:ILE:HD13	1:B:1:MSE:CE	2.46	0.45
1:A:398:LYS:O	1:A:403:GLN:NE2	2.49	0.45
1:A:476:THR:O	1:A:480:ALA:CB	2.63	0.45
1:A:574:GLN:O	1:A:577:ALA:HB3	2.17	0.45
1:B:7:PHE:HZ	1:B:323:LEU:HD11	1.80	0.45
1:C:49:ALA:HB1	1:C:249:ILE:CG2	2.38	0.45
1:C:245:ARG:HH11	1:C:522:ASP:HB2	1.81	0.45
1:B:85:SER:HA	1:C:270:SER:CB	2.46	0.45
1:B:88:PRO:HG2	1:B:91:VAL:CG2	2.45	0.45
1:B:395:LYS:HD2	1:B:526:ARG:HH11	1.72	0.45
1:C:363:ALA:HB2	1:C:430:VAL:CG1	2.47	0.45
1:C:601:GLN:C	1:C:603:SER:H	2.24	0.45
1:D:264:GLN:HG3	1:D:272:PHE:CE1	2.52	0.45
1:A:265:PHE:HE1	1:A:271:GLU:HB2	1.77	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:SER:O	1:B:487:PRO:N	2.50	0.45
1:D:388:ALA:O	1:D:393:GLY:HA2	2.17	0.45
1:A:112:HIS:HB3	1:A:174:LYS:NZ	2.31	0.45
1:B:391:GLN:HE21	1:B:422:LYS:CE	2.07	0.45
1:C:36:TRP:O	1:C:227:MSE:HE2	2.17	0.45
1:C:264:GLN:H	1:C:264:GLN:HE21	1.64	0.45
1:D:1:MSE:HG2	1:D:4:LYS:HZ1	1.81	0.45
1:D:7:PHE:HB2	1:B:11:PRO:CG	2.47	0.45
1:D:268:PHE:HD2	1:D:272:PHE:CE1	2.35	0.45
1:A:135:GLN:O	1:A:139:VAL:HG23	2.17	0.45
1:B:68:VAL:HG11	1:B:101:MSE:HE3	1.98	0.45
1:C:63:CYS:SG	1:C:64:PHE:N	2.89	0.45
1:A:84:ARG:HD2	1:A:87:VAL:CG1	2.47	0.45
1:A:420:ARG:O	1:A:424:LEU:HG	2.15	0.45
1:D:148:GLU:OE2	1:D:179:TYR:HE1	1.99	0.45
1:A:50:HIS:HB2	1:A:399:ARG:CZ	2.47	0.45
1:A:139:VAL:HG21	1:A:293:ILE:HG23	1.98	0.45
1:C:46:SER:CA	1:C:249:ILE:CD1	2.95	0.45
1:C:383:VAL:HG22	1:C:433:PHE:CE2	2.51	0.45
1:D:9:ALA:HB2	1:D:308:VAL:HG12	1.98	0.45
1:D:26:TYR:CZ	1:D:79:VAL:HA	2.51	0.45
1:D:45:LEU:C	1:D:249:ILE:HD13	2.42	0.45
1:D:390:PHE:CE2	1:D:477:ARG:HA	2.52	0.45
1:A:432:ARG:HH21	1:A:432:ARG:HB3	1.80	0.45
1:B:42:ARG:NE	1:B:247:ASP:CG	2.75	0.45
1:B:68:VAL:HG11	1:B:101:MSE:CE	2.46	0.45
1:B:257:ILE:HD13	1:B:294:VAL:HG21	1.99	0.45
1:C:321:GLU:O	1:C:325:THR:HG22	2.17	0.45
1:C:486:SER:CB	1:C:487:PRO:HD2	2.47	0.45
1:D:292:LEU:HD12	1:D:292:LEU:HA	1.76	0.44
1:A:92:MSE:HE1	1:A:309:THR:OG1	2.16	0.44
1:D:38:LEU:HA	1:D:227:MSE:HE1	1.99	0.44
1:A:396:LEU:HD23	1:A:396:LEU:HA	1.67	0.44
1:B:422:LYS:N	1:B:422:LYS:CD	2.73	0.44
1:C:389:MSE:HE3	1:C:389:MSE:HB3	1.83	0.44
1:A:113:GLU:O	1:A:117:VAL:HG22	2.16	0.44
1:B:245:ARG:HH11	1:B:519:ALA:HA	1.82	0.44
1:C:432:ARG:CZ	1:C:479:PHE:CB	2.90	0.44
1:C:515:PHE:CZ	1:C:578:ARG:NE	2.82	0.44
1:D:574:GLN:O	1:D:577:ALA:HB3	2.18	0.44
1:C:243:VAL:C	1:C:244:LYS:HG3	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:514:SER:HB2	1:C:515:PHE:CD1	2.52	0.44
1:D:1:MSE:HB2	1:D:4:LYS:CG	2.43	0.44
1:D:57:GLU:HG3	1:D:58:PHE:N	2.32	0.44
1:A:62:ILE:HG12	1:C:315:TYR:OH	2.17	0.44
1:A:487:PRO:O	1:A:489:THR:N	2.50	0.44
1:D:7:PHE:HB2	1:B:11:PRO:HD3	1.98	0.44
1:B:72:ARG:CZ	1:B:90:LYS:HG3	2.48	0.44
1:A:436:GLY:H	1:A:437:PRO:HD3	1.79	0.44
1:B:49:ALA:HB1	1:B:249:ILE:CG2	2.40	0.44
1:C:36:TRP:CD1	1:C:99:GLN:HB3	2.52	0.44
1:C:69:ILE:HG23	1:C:319:MSE:CE	2.46	0.44
1:C:126:ASP:OD1	1:C:129:SER:OG	2.21	0.44
1:C:570:TYR:C	1:C:571:ASP:CG	2.83	0.44
1:D:406:TYR:CE2	1:D:410:VAL:HG21	2.52	0.44
1:A:2:GLU:HG2	1:A:3:THR:H	1.82	0.44
1:A:62:ILE:HD13	1:A:62:ILE:HA	1.75	0.44
1:A:109:THR:HG22	1:A:110:VAL:N	2.33	0.44
1:A:360:VAL:H	1:A:427:LEU:CD2	2.31	0.44
1:C:76:TYR:O	1:C:79:VAL:HG12	2.17	0.44
1:C:244:LYS:HB2	1:C:248:ASP:CB	2.48	0.44
1:C:528:LEU:CD1	1:C:560:LEU:HD21	2.43	0.44
1:C:575:TRP:CZ3	1:C:579:ALA:CB	2.81	0.44
1:D:38:LEU:N	1:D:39:PRO:HD2	2.33	0.44
1:A:1:MSE:HB2	1:A:4:LYS:CD	2.48	0.44
1:A:2:GLU:C	1:A:4:LYS:H	2.26	0.44
1:A:445:PRO:O	1:A:447:CYS:N	2.44	0.44
1:A:49:ALA:HB3	1:A:249:ILE:HG23	1.97	0.43
1:A:319:MSE:HB3	1:A:319:MSE:HE2	1.43	0.43
1:B:128:PRO:HG2	1:B:275:SER:HB2	1.99	0.43
1:C:475:LEU:O	1:C:477:ARG:N	2.49	0.43
1:D:11:PRO:O	1:D:12:LEU:HD23	2.17	0.43
1:D:90:LYS:CE	1:D:92:MSE:HE2	2.48	0.43
1:D:487:PRO:O	1:D:489:THR:N	2.44	0.43
1:A:391:GLN:HE22	1:A:422:LYS:HG3	1.82	0.43
1:A:429:GLN:C	1:A:433:PHE:CD2	2.90	0.43
1:B:46:SER:CA	1:B:249:ILE:HD13	2.48	0.43
1:C:63:CYS:HB3	1:C:303:VAL:HB	1.99	0.43
1:C:125:ASP:HA	1:C:130:VAL:CG1	2.49	0.43
1:D:113:GLU:O	1:D:117:VAL:HG22	2.18	0.43
1:B:60:ASP:OD1	1:B:61:SER:N	2.51	0.43
1:C:2:GLU:C	1:C:4:LYS:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:GLU:O	1:C:6:ILE:HD13	2.18	0.43
1:C:383:VAL:HA	1:C:433:PHE:CZ	2.53	0.43
1:D:36:TRP:CE2	1:D:40:LYS:HD3	2.53	0.43
1:D:62:ILE:HD13	1:D:62:ILE:HA	1.83	0.43
1:D:72:ARG:HB3	1:D:311:LYS:HG2	2.00	0.43
1:A:96:ASP:HB2	1:A:320:PHE:CD2	2.53	0.43
1:B:28:PRO:HG2	1:B:31:GLN:HG2	1.99	0.43
1:B:243:VAL:C	1:B:244:LYS:HG3	2.44	0.43
1:C:155:GLU:C	1:C:157:ARG:H	2.27	0.43
1:C:395:LYS:HG3	1:C:395:LYS:O	2.18	0.43
1:D:482:HIS:HA	1:D:494:ALA:HB1	2.00	0.43
1:B:369:GLY:O	1:B:373:ALA:N	2.51	0.43
1:C:112:HIS:NE2	1:C:140:THR:HG22	2.33	0.43
1:A:234:MSE:HB3	1:A:234:MSE:HE2	1.68	0.43
1:A:252:PRO:O	1:A:291:ARG:HG2	2.17	0.43
1:B:96:ASP:HB2	1:B:320:PHE:CD1	2.53	0.43
1:C:427:LEU:O	1:C:430:VAL:HB	2.18	0.43
1:A:38:LEU:N	1:A:39:PRO:HD2	2.34	0.43
1:B:429:GLN:C	1:B:433:PHE:CD2	2.92	0.43
1:C:115:ILE:HG12	1:C:292:LEU:HB3	2.01	0.43
1:C:122:LEU:HD23	1:C:122:LEU:HA	1.80	0.43
1:D:64:PHE:CE1	1:B:7:PHE:HE1	2.37	0.43
1:D:363:ALA:CB	1:D:434:TYR:OH	2.66	0.43
1:D:366:ASP:C	1:D:368:GLU:H	2.27	0.43
1:D:429:GLN:C	1:D:433:PHE:HD2	2.22	0.43
1:A:54:GLN:OE1	1:A:405:ARG:NH1	2.51	0.43
1:B:34:TYR:C	1:B:34:TYR:CD1	2.95	0.43
1:C:401:ASN:OD1	1:C:401:ASN:N	2.47	0.43
1:C:515:PHE:CZ	1:C:578:ARG:CZ	3.02	0.43
1:D:383:VAL:HA	1:D:433:PHE:CZ	2.54	0.43
1:A:62:ILE:HG23	1:A:302:ARG:O	2.19	0.43
1:A:262:ASN:O	1:A:266:ALA:HB2	2.19	0.43
1:D:223:HIS:O	1:D:227:MSE:HG2	2.19	0.42
1:D:252:PRO:O	1:D:291:ARG:HG2	2.19	0.42
1:D:432:ARG:NH2	1:D:472:VAL:C	2.77	0.42
1:A:107:LEU:HD13	1:A:231:MSE:HE2	2.00	0.42
1:A:380:THR:O	1:A:384:LEU:HG	2.19	0.42
1:A:432:ARG:NH2	1:A:432:ARG:CG	2.72	0.42
1:B:395:LYS:CE	1:B:526:ARG:HH11	2.31	0.42
1:D:71:LEU:HA	1:D:310:ALA:O	2.19	0.42
1:D:122:LEU:C	1:D:124:ARG:H	2.26	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:SER:C	1:D:132:CYS:H	2.26	0.42
1:A:15:SER:O	1:A:19:SER:OG	2.33	0.42
1:B:267:LEU:CD1	1:B:294:VAL:HG13	2.46	0.42
1:C:46:SER:HA	1:C:249:ILE:HD13	2.01	0.42
1:C:113:GLU:HB3	1:C:174:LYS:NZ	2.34	0.42
1:D:290:THR:O	1:D:294:VAL:HG23	2.19	0.42
1:A:76:TYR:HB2	1:A:82:LYS:HE3	2.00	0.42
1:A:139:VAL:HG21	1:A:297:ASN:HD21	1.85	0.42
1:B:71:LEU:HA	1:B:310:ALA:O	2.20	0.42
1:B:94:ILE:CD1	1:B:101:MSE:HG3	2.49	0.42
1:D:156:HIS:CE1	1:D:179:TYR:CE2	3.08	0.42
1:B:128:PRO:O	1:B:276:VAL:HG23	2.19	0.42
1:B:482:HIS:HA	1:B:494:ALA:HB1	2.02	0.42
1:C:14:VAL:HG23	1:C:303:VAL:HG22	2.01	0.42
1:C:46:SER:N	1:C:249:ILE:HD11	2.33	0.42
1:C:61:SER:O	1:C:62:ILE:HD13	2.20	0.42
1:C:396:LEU:HD23	1:C:396:LEU:HA	1.75	0.42
1:A:34:TYR:C	1:A:34:TYR:CD1	2.98	0.42
1:B:251:LEU:HA	1:B:252:PRO:HD2	1.87	0.42
1:C:363:ALA:CB	1:C:430:VAL:HG13	2.50	0.42
1:C:429:GLN:C	1:C:433:PHE:CD2	2.96	0.42
1:C:510:LEU:C	1:C:514:SER:OG	2.62	0.42
1:D:7:PHE:CE1	1:D:319:MSE:SE	3.23	0.42
1:A:37:GLU:C	1:A:227:MSE:HE1	2.44	0.42
1:D:246:GLU:O	1:D:247:ASP:OD1	2.38	0.42
1:C:268:PHE:HD2	1:C:272:PHE:HE1	1.67	0.42
1:D:396:LEU:HD21	1:D:406:TYR:HB2	2.01	0.42
1:B:396:LEU:HD23	1:B:396:LEU:HA	1.61	0.42
1:C:1:MSE:HB2	1:C:4:LYS:CG	2.45	0.42
1:C:42:ARG:NE	1:C:247:ASP:OD1	2.51	0.42
1:C:418:VAL:CB	1:C:422:LYS:HE3	2.50	0.42
1:A:84:ARG:HD2	1:A:87:VAL:HG11	2.01	0.42
1:B:139:VAL:HG21	1:B:293:ILE:HG23	2.02	0.42
1:B:143:LEU:O	1:B:146:CYS:HB2	2.20	0.42
1:C:261:GLN:HG3	1:C:271:GLU:OE2	2.20	0.42
1:A:263:LEU:HD21	1:A:294:VAL:HG11	2.01	0.41
1:A:290:THR:O	1:A:294:VAL:HG23	2.19	0.41
1:C:108:THR:O	1:C:112:HIS:N	2.46	0.41
1:C:113:GLU:HB3	1:C:174:LYS:HZ1	1.85	0.41
1:C:245:ARG:NH1	1:C:522:ASP:CB	2.83	0.41
1:C:338:PRO:O	1:C:342:LYS:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:GLY:O	1:C:521:ILE:C	2.62	0.41
1:D:64:PHE:CZ	1:B:7:PHE:HE1	2.38	0.41
1:A:432:ARG:NH2	1:A:432:ARG:HG3	2.35	0.41
1:B:42:ARG:NE	1:B:247:ASP:OD1	2.52	0.41
1:C:109:THR:HG23	1:C:174:LYS:HG3	2.02	0.41
1:C:254:GLY:HA3	1:C:287:THR:HG23	2.02	0.41
1:A:66:GLY:O	1:A:305:VAL:HG23	2.20	0.41
1:A:432:ARG:NH2	1:A:432:ARG:CA	2.73	0.41
1:C:5:GLU:O	1:C:6:ILE:C	2.63	0.41
1:C:119:ALA:O	1:C:122:LEU:HB2	2.20	0.41
1:C:432:ARG:HD3	1:C:476:THR:CB	2.39	0.41
1:A:268:PHE:CD2	1:A:272:PHE:HE1	2.38	0.41
1:B:88:PRO:HG2	1:B:91:VAL:HG22	2.01	0.41
1:B:103:THR:HG23	1:B:103:THR:H	1.57	0.41
1:B:346:LEU:C	1:B:348:GLU:N	2.79	0.41
1:B:430:VAL:O	1:B:434:TYR:HD2	2.03	0.41
1:B:432:ARG:NH1	1:B:437:PRO:CD	2.82	0.41
1:C:105:LEU:HA	1:C:105:LEU:HD13	1.76	0.41
1:C:78:THR:HG21	1:C:93:THR:OG1	2.20	0.41
1:C:396:LEU:HD21	1:C:406:TYR:HB2	2.02	0.41
1:C:509:ALA:O	1:C:513:GLY:HA3	2.20	0.41
1:D:3:THR:O	1:D:4:LYS:O	2.38	0.41
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.80	0.41
1:C:39:PRO:O	1:C:43:ARG:HG3	2.20	0.41
1:C:264:GLN:HG3	1:C:272:PHE:CD1	2.55	0.41
1:D:319:MSE:HB3	1:D:319:MSE:HE2	1.65	0.41
1:A:122:LEU:HD23	1:A:122:LEU:HA	1.82	0.41
1:A:390:PHE:CE2	1:A:477:ARG:HA	2.55	0.41
1:B:230:GLN:O	1:B:234:MSE:HG3	2.20	0.41
1:B:430:VAL:O	1:B:434:TYR:CD2	2.73	0.41
1:D:113:GLU:HB3	1:D:174:LYS:NZ	2.35	0.41
1:D:253:THR:O	1:D:257:ILE:N	2.52	0.41
1:D:363:ALA:CA	1:D:434:TYR:HH	2.23	0.41
1:A:429:GLN:HB3	1:A:433:PHE:HE2	1.86	0.41
1:B:5:GLU:HB3	1:B:311:LYS:HD3	2.02	0.41
1:B:49:ALA:HB1	1:B:249:ILE:HG22	2.01	0.41
1:B:52:LEU:O	1:B:55:LEU:HB3	2.21	0.41
1:B:426:GLY:O	1:B:430:VAL:HG23	2.21	0.41
1:C:2:GLU:C	1:C:4:LYS:N	2.78	0.41
1:D:39:PRO:O	1:D:43:ARG:HG3	2.21	0.41
1:D:122:LEU:HD23	1:D:122:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:PHE:CD1	1:D:320:PHE:C	2.99	0.40
1:A:1:MSE:HE1	1:B:72:ARG:NH2	2.36	0.40
1:B:245:ARG:NH1	1:B:519:ALA:C	2.79	0.40
1:D:260:SER:C	1:D:264:GLN:HE22	2.29	0.40
1:A:144:SER:HA	1:A:147:PHE:CE2	2.57	0.40
1:B:432:ARG:NE	1:B:437:PRO:HG2	2.35	0.40
1:C:244:LYS:O	1:C:246:GLU:N	2.53	0.40
1:D:314:ASP:OD1	1:D:315:TYR:N	2.54	0.40
1:A:36:TRP:CE3	1:A:103:THR:HG21	2.57	0.40
1:A:287:THR:N	1:A:288:PRO:HD2	2.36	0.40
1:A:389:MSE:CE	1:A:529:MSE:HG3	2.51	0.40
1:C:518:THR:OG1	1:C:519:ALA:N	2.54	0.40
1:D:60:ASP:OD1	1:B:315:TYR:CZ	2.71	0.40
1:D:287:THR:N	1:D:288:PRO:CD	2.83	0.40
1:A:150:ASP:HB3	1:A:151:MSE:H	1.71	0.40
1:C:107:LEU:HB2	1:C:231:MSE:HE1	2.03	0.40
1:D:4:LYS:O	1:D:5:GLU:C	2.64	0.40
1:D:276:VAL:HG22	1:D:286:MSE:HE1	2.04	0.40
1:A:109:THR:HG23	1:A:174:LYS:HE3	2.03	0.40
1:B:360:VAL:HA	1:B:430:VAL:HG21	2.02	0.40
1:C:37:GLU:O	1:C:40:LYS:N	2.51	0.40
1:C:103:THR:H	1:C:103:THR:HG23	1.59	0.40
1:C:572:LYS:O	1:C:573:GLN:C	2.64	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	552/771 (72%)	429 (78%)	73 (13%)	50 (9%)	0 3
1	B	552/771 (72%)	437 (79%)	70 (13%)	45 (8%)	0 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	549/771 (71%)	423 (77%)	80 (15%)	46 (8%)	0	4
1	D	552/771 (72%)	427 (77%)	75 (14%)	50 (9%)	0	3
All	All	2205/3084 (72%)	1716 (78%)	298 (14%)	191 (9%)	0	4

All (191) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	2	GLU
1	D	4	LYS
1	D	6	ILE
1	D	61	SER
1	D	129	SER
1	D	159	TYR
1	D	160	PRO
1	D	182	PRO
1	D	238	ALA
1	D	243	VAL
1	D	248	ASP
1	D	328	GLN
1	D	329	PRO
1	D	398	LYS
1	D	414	ASP
1	D	415	PRO
1	D	437	PRO
1	D	441	PRO
1	D	443	LYS
1	D	444	VAL
1	D	445	PRO
1	D	518	THR
1	D	519	ALA
1	D	582	THR
1	D	583	PRO
1	D	585	TYR
1	A	2	GLU
1	A	4	LYS
1	A	6	ILE
1	A	159	TYR
1	A	160	PRO
1	A	181	SER
1	A	182	PRO
1	A	243	VAL

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Mol	Chain	Res	Type
1	A	328	GLN
1	A	329	PRO
1	A	347	ASP
1	A	398	LYS
1	A	414	ASP
1	A	415	PRO
1	A	441	PRO
1	A	443	LYS
1	A	444	VAL
1	A	445	PRO
1	A	573	GLN
1	A	582	THR
1	A	583	PRO
1	A	585	TYR
1	B	2	GLU
1	B	4	LYS
1	B	6	ILE
1	B	61	SER
1	B	152	ARG
1	B	159	TYR
1	B	160	PRO
1	B	181	SER
1	B	182	PRO
1	B	243	VAL
1	B	328	GLN
1	B	329	PRO
1	B	347	ASP
1	B	393	GLY
1	B	398	LYS
1	B	414	ASP
1	B	415	PRO
1	B	437	PRO
1	B	441	PRO
1	B	443	LYS
1	B	444	VAL
1	B	445	PRO
1	B	486	SER
1	B	573	GLN
1	B	582	THR
1	B	583	PRO
1	B	585	TYR
1	C	2	GLU

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Mol	Chain	Res	Type
1	C	4	LYS
1	C	6	ILE
1	C	152	ARG
1	C	159	TYR
1	C	160	PRO
1	C	181	SER
1	C	182	PRO
1	C	243	VAL
1	C	328	GLN
1	C	329	PRO
1	C	393	GLY
1	C	398	LYS
1	C	414	ASP
1	C	415	PRO
1	C	441	PRO
1	C	443	LYS
1	C	444	VAL
1	C	445	PRO
1	C	487	PRO
1	C	515	PHE
1	C	571	ASP
1	C	582	THR
1	C	583	PRO
1	C	585	TYR
1	D	234	MSE
1	D	239	VAL
1	D	347	ASP
1	D	534	GLU
1	D	567	GLU
1	D	573	GLN
1	A	124	ARG
1	A	128	PRO
1	A	152	ARG
1	A	189	SER
1	A	393	GLY
1	A	515	PHE
1	A	534	GLU
1	A	535	GLU
1	B	128	PRO
1	B	518	THR
1	C	60	ASP
1	C	61	SER

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Mol	Chain	Res	Type
1	C	128	PRO
1	C	437	PRO
1	C	573	GLN
1	D	516	GLY
1	D	533	VAL
1	A	60	ASP
1	A	61	SER
1	A	80	GLU
1	A	239	VAL
1	A	248	ASP
1	A	486	SER
1	A	516	GLY
1	A	568	GLY
1	B	60	ASP
1	B	248	ASP
1	B	515	PHE
1	B	516	GLY
1	C	242	GLY
1	C	248	ASP
1	C	476	THR
1	C	510	LEU
1	C	519	ALA
1	D	124	ARG
1	D	128	PRO
1	D	152	ARG
1	D	438	TRP
1	D	488	GLU
1	A	151	MSE
1	A	435	GLU
1	A	519	ALA
1	A	602	ASN
1	B	158	TYR
1	B	239	VAL
1	B	519	ALA
1	B	533	VAL
1	C	124	ARG
1	C	347	ASP
1	C	602	ASN
1	D	151	MSE
1	D	181	SER
1	D	393	GLY
1	D	602	ASN

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Mol	Chain	Res	Type
1	D	604	THR
1	A	8	ASP
1	A	242	GLY
1	A	440	SER
1	A	604	THR
1	B	124	ARG
1	B	438	TRP
1	B	440	SER
1	B	534	GLU
1	C	239	VAL
1	C	438	TRP
1	C	440	SER
1	C	584	VAL
1	D	343	GLU
1	D	391	GLN
1	A	95	ILE
1	A	584	VAL
1	B	82	LYS
1	B	584	VAL
1	B	604	THR
1	C	82	LYS
1	C	156	HIS
1	C	572	LYS
1	C	604	THR
1	D	584	VAL
1	B	242	GLY
1	D	436	GLY
1	D	440	SER
1	A	533	VAL
1	D	242	GLY
1	A	569	ILE

5.3.2 Protein sidechains [i](#)

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

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	268/637 (42%)	244 (91%)	24 (9%)	9 32
1	B	268/637 (42%)	243 (91%)	25 (9%)	8 31
1	C	322/637 (50%)	291 (90%)	31 (10%)	8 29
1	D	268/637 (42%)	241 (90%)	27 (10%)	7 27
All	All	1126/2548 (44%)	1019 (90%)	107 (10%)	8 30

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	7	PHE
1	D	36	TRP
1	D	42	ARG
1	D	52	LEU
1	D	62	ILE
1	D	67	THR
1	D	98	GLN
1	D	105	LEU
1	D	109	THR
1	D	110	VAL
1	D	137	LEU
1	D	140	THR
1	D	142	ARG
1	D	147	PHE
1	D	231	MSE
1	D	257	ILE
1	D	264	GLN
1	D	269	ASN
1	D	276	VAL
1	D	286	MSE
1	D	292	LEU
1	D	303	VAL
1	D	307	VAL
1	D	308	VAL
1	D	392	ASP
1	D	401	ASN
1	D	437	PRO
1	A	38	LEU
1	A	42	ARG
1	A	52	LEU

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Mol	Chain	Res	Type
1	A	68	VAL
1	A	79	VAL
1	A	98	GLN
1	A	106	LEU
1	A	110	VAL
1	A	137	LEU
1	A	139	VAL
1	A	147	PHE
1	A	150	ASP
1	A	151	MSE
1	A	234	MSE
1	A	264	GLN
1	A	269	ASN
1	A	276	VAL
1	A	278	GLU
1	A	290	THR
1	A	292	LEU
1	A	303	VAL
1	A	392	ASP
1	A	401	ASN
1	A	432	ARG
1	B	7	PHE
1	B	38	LEU
1	B	52	LEU
1	B	67	THR
1	B	78	THR
1	B	98	GLN
1	B	103	THR
1	B	105	LEU
1	B	110	VAL
1	B	137	LEU
1	B	140	THR
1	B	144	SER
1	B	257	ILE
1	B	264	GLN
1	B	269	ASN
1	B	290	THR
1	B	303	VAL
1	B	307	VAL
1	B	308	VAL
1	B	392	ASP
1	B	401	ASN

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Mol	Chain	Res	Type
1	B	422	LYS
1	B	432	ARG
1	B	437	PRO
1	B	529	MSE
1	C	7	PHE
1	C	38	LEU
1	C	52	LEU
1	C	64	PHE
1	C	67	THR
1	C	98	GLN
1	C	103	THR
1	C	105	LEU
1	C	110	VAL
1	C	137	LEU
1	C	140	THR
1	C	264	GLN
1	C	269	ASN
1	C	276	VAL
1	C	290	THR
1	C	303	VAL
1	C	392	ASP
1	C	395	LYS
1	C	401	ASN
1	C	422	LYS
1	C	486	SER
1	C	490	VAL
1	C	503	SER
1	C	515	PHE
1	C	518	THR
1	C	521	ILE
1	C	526	ARG
1	C	565	ARG
1	C	567	GLU
1	C	569	ILE
1	C	575	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	31	GLN
1	D	50	HIS
1	D	112	HIS

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Mol	Chain	Res	Type
1	D	156	HIS
1	D	264	GLN
1	D	324	ASN
1	A	98	GLN
1	A	112	HIS
1	A	156	HIS
1	A	269	ASN
1	A	391	GLN
1	B	156	HIS
1	B	264	GLN
1	B	391	GLN
1	B	429	GLN
1	C	156	HIS
1	C	324	ASN
1	C	391	GLN
1	C	482	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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	548/771 (71%)	1.29	129 (23%) 2 2	53, 109, 176, 219	0
1	B	548/771 (71%)	1.78	193 (35%) 1 1	62, 120, 274, 329	0
1	C	545/771 (70%)	1.38	130 (23%) 2 1	30, 104, 136, 171	0
1	D	548/771 (71%)	1.31	139 (25%) 1 1	37, 91, 169, 223	0
All	All	2189/3084 (70%)	1.44	591 (26%) 1 1	30, 106, 216, 329	0

All (591) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	514	SER	8.9
1	B	591	LEU	7.7
1	C	325	THR	7.1
1	D	3	THR	7.0
1	B	593	ARG	7.0
1	D	596	LEU	6.5
1	B	168	ASP	6.4
1	B	579	ALA	6.4
1	C	382	SER	6.3
1	B	301	HIS	6.2
1	C	156	HIS	6.2
1	A	481	ALA	6.2
1	B	533	VAL	6.1
1	B	398	LYS	6.1
1	B	502	ARG	6.0
1	B	251	LEU	5.9
1	B	554	GLU	5.9
1	C	353	GLU	5.9
1	D	602	ASN	5.8
1	A	600	SER	5.8
1	B	501	ALA	5.7

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Mol	Chain	Res	Type	RSRZ
1	C	430	VAL	5.6
1	D	397	THR	5.6
1	D	579	ALA	5.5
1	B	108	THR	5.2
1	D	156	HIS	5.2
1	D	595	LEU	5.1
1	A	439	GLY	5.1
1	D	554	GLU	5.1
1	B	511	TRP	5.0
1	A	153	TYR	5.0
1	B	513	GLY	5.0
1	C	571	ASP	5.0
1	C	357	HIS	5.0
1	A	246	GLU	5.0
1	D	430	VAL	4.9
1	B	471	VAL	4.9
1	B	597	LEU	4.9
1	B	185	TYR	4.9
1	C	427	LEU	4.8
1	C	532	VAL	4.8
1	B	584	VAL	4.7
1	A	369	GLY	4.7
1	B	253	THR	4.7
1	B	470	ILE	4.7
1	A	185	TYR	4.7
1	D	448	ASP	4.7
1	D	446	SER	4.7
1	C	360	VAL	4.7
1	A	281	GLU	4.7
1	B	497	PHE	4.6
1	D	438	TRP	4.6
1	D	598	ALA	4.5
1	D	536	GLY	4.5
1	B	507	PHE	4.5
1	A	416	ASP	4.5
1	D	600	SER	4.4
1	B	255	THR	4.4
1	B	65	LEU	4.4
1	B	11	PRO	4.4
1	C	356	LEU	4.4
1	B	522	ASP	4.4
1	B	2	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	500	ALA	4.4
1	C	157	ARG	4.4
1	A	571	ASP	4.4
1	A	602	ASN	4.3
1	B	246	GLU	4.3
1	B	369	GLY	4.3
1	D	605	PRO	4.3
1	C	435	GLU	4.3
1	B	557	GLN	4.3
1	A	415	PRO	4.3
1	A	605	PRO	4.3
1	C	497	PHE	4.3
1	C	347	ASP	4.3
1	D	429	GLN	4.2
1	B	373	ALA	4.2
1	C	419	ALA	4.2
1	C	448	ASP	4.2
1	B	7	PHE	4.2
1	C	74	ILE	4.2
1	B	433	PHE	4.1
1	D	267	LEU	4.1
1	D	247	ASP	4.1
1	D	262	ASN	4.1
1	B	352	SER	4.1
1	D	436	GLY	4.1
1	B	594	LEU	4.1
1	A	435	GLU	4.1
1	B	458	ILE	4.1
1	B	460	LEU	4.0
1	D	301	HIS	4.0
1	B	576	VAL	4.0
1	C	155	GLU	4.0
1	A	122	LEU	4.0
1	D	7	PHE	4.0
1	B	411	PHE	4.0
1	B	416	ASP	4.0
1	A	484	LEU	4.0
1	A	63	CYS	3.9
1	A	557	GLN	3.9
1	C	56	ALA	3.9
1	B	463	LEU	3.9
1	B	475	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	121	LYS	3.9
1	B	519	ALA	3.9
1	B	530	THR	3.9
1	D	398	LYS	3.9
1	D	153	TYR	3.9
1	D	189	SER	3.9
1	D	5	GLU	3.8
1	B	508	TYR	3.8
1	C	559	TYR	3.8
1	A	249	ILE	3.8
1	B	397	THR	3.8
1	B	266	ALA	3.8
1	A	407	LEU	3.8
1	A	427	LEU	3.8
1	C	433	PHE	3.8
1	D	423	VAL	3.8
1	B	469	ASP	3.8
1	B	74	ILE	3.8
1	B	577	ALA	3.7
1	D	592	THR	3.7
1	C	518	THR	3.7
1	B	349	TRP	3.7
1	B	510	LEU	3.7
1	B	526	ARG	3.7
1	A	189	SER	3.7
1	D	532	VAL	3.6
1	B	592	THR	3.6
1	A	156	HIS	3.6
1	B	155	GLU	3.6
1	B	588	SER	3.6
1	B	476	THR	3.6
1	B	263	LEU	3.6
1	C	479	PHE	3.6
1	A	603	SER	3.6
1	D	248	ASP	3.6
1	D	528	LEU	3.6
1	A	6	ILE	3.6
1	A	30	TYR	3.6
1	C	434	TYR	3.6
1	D	588	SER	3.6
1	B	249	ILE	3.6
1	A	168	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	597	LEU	3.6
1	A	437	PRO	3.5
1	C	190	TYR	3.5
1	A	278	GLU	3.5
1	C	562	GLU	3.5
1	A	124	ARG	3.5
1	D	522	ASP	3.5
1	A	137	LEU	3.5
1	C	153	TYR	3.5
1	A	433	PHE	3.5
1	B	468	HIS	3.5
1	B	295	PHE	3.4
1	B	503	SER	3.4
1	B	282	ASP	3.4
1	B	465	GLU	3.4
1	C	29	PRO	3.4
1	B	407	LEU	3.4
1	B	487	PRO	3.4
1	A	430	VAL	3.4
1	C	161	ARG	3.4
1	C	483	ARG	3.4
1	C	429	GLN	3.4
1	C	354	SER	3.4
1	A	528	LEU	3.4
1	B	571	ASP	3.4
1	B	109	THR	3.4
1	B	479	PHE	3.3
1	C	349	TRP	3.3
1	A	120	GLU	3.3
1	C	246	GLU	3.3
1	B	523	GLY	3.3
1	C	24	GLY	3.3
1	B	156	HIS	3.3
1	D	117	VAL	3.3
1	D	492	SER	3.3
1	B	504	CYS	3.3
1	B	157	ARG	3.3
1	B	532	VAL	3.3
1	C	258	GLY	3.3
1	D	185	TYR	3.3
1	B	125	ASP	3.3
1	A	396	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	558	SER	3.2
1	A	482	HIS	3.2
1	B	573	GLN	3.2
1	C	3	THR	3.2
1	C	363	ALA	3.2
1	D	435	GLU	3.2
1	B	348	GLU	3.2
1	D	422	LYS	3.2
1	B	292	LEU	3.2
1	B	595	LEU	3.2
1	D	433	PHE	3.2
1	D	241	ALA	3.2
1	A	507	PHE	3.2
1	C	181	SER	3.2
1	A	601	GLN	3.2
1	B	417	ILE	3.2
1	C	160	PRO	3.2
1	C	23	GLN	3.2
1	A	60	ASP	3.2
1	C	502	ARG	3.2
1	D	82	LYS	3.2
1	D	584	VAL	3.2
1	B	243	VAL	3.2
1	C	569	ILE	3.2
1	D	580	ALA	3.1
1	B	558	SER	3.1
1	B	598	ALA	3.1
1	C	575	TRP	3.1
1	B	570	TYR	3.1
1	D	599	ALA	3.1
1	A	261	GLN	3.1
1	A	442	THR	3.1
1	B	3	THR	3.1
1	B	472	VAL	3.1
1	B	152	ARG	3.1
1	C	361	VAL	3.1
1	B	590	PRO	3.1
1	A	521	ILE	3.1
1	C	553	VAL	3.1
1	C	567	GLU	3.1
1	A	599	ALA	3.0
1	B	459	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	476	THR	3.0
1	B	386	PRO	3.0
1	A	347	ASP	3.0
1	C	498	LEU	3.0
1	A	24	GLY	3.0
1	B	489	THR	3.0
1	C	249	ILE	3.0
1	D	449	ASP	3.0
1	A	134	ASN	3.0
1	B	58	PHE	3.0
1	A	74	ILE	3.0
1	D	221	TYR	3.0
1	B	312	ARG	3.0
1	C	369	GLY	3.0
1	C	524	VAL	3.0
1	B	390	PHE	3.0
1	D	519	ALA	3.0
1	A	8	ASP	3.0
1	B	247	ASP	3.0
1	B	602	ASN	3.0
1	D	12	LEU	2.9
1	B	300	LEU	2.9
1	A	270	SER	2.9
1	D	271	GLU	2.9
1	A	190	TYR	2.9
1	B	429	GLN	2.9
1	A	584	VAL	2.9
1	B	600	SER	2.9
1	D	74	ILE	2.9
1	B	564	LEU	2.9
1	B	596	LEU	2.9
1	A	414	ASP	2.9
1	A	56	ALA	2.9
1	B	509	ALA	2.9
1	C	579	ALA	2.9
1	A	5	GLU	2.9
1	D	507	PHE	2.9
1	B	86	GLN	2.8
1	C	418	VAL	2.8
1	B	291	ARG	2.8
1	B	447	CYS	2.8
1	D	6	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	508	TYR	2.8
1	B	106	LEU	2.8
1	D	557	GLN	2.8
1	A	440	SER	2.8
1	D	419	ALA	2.8
1	C	425	ALA	2.8
1	D	415	PRO	2.8
1	A	423	VAL	2.8
1	A	472	VAL	2.8
1	D	244	LYS	2.8
1	B	396	LEU	2.8
1	C	460	LEU	2.8
1	A	570	TYR	2.8
1	B	421	ARG	2.8
1	A	53	ASP	2.8
1	C	521	ILE	2.8
1	D	570	TYR	2.8
1	B	500	ALA	2.8
1	C	437	PRO	2.8
1	D	452	LEU	2.8
1	A	385	LEU	2.8
1	B	451	THR	2.8
1	C	438	TRP	2.8
1	B	426	GLY	2.8
1	C	577	ALA	2.8
1	D	603	SER	2.8
1	A	2	GLU	2.8
1	D	147	PHE	2.7
1	B	147	PHE	2.7
1	B	335	THR	2.8
1	C	476	THR	2.8
1	B	467	GLY	2.7
1	C	563	GLN	2.7
1	A	356	LEU	2.7
1	D	59	GLU	2.7
1	A	554	GLU	2.7
1	D	138	ASP	2.7
1	A	573	GLN	2.7
1	D	38	LEU	2.7
1	A	434	TYR	2.7
1	B	12	LEU	2.7
1	B	415	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	586	GLN	2.7
1	D	2	GLU	2.7
1	A	536	GLY	2.7
1	A	311	LYS	2.7
1	D	586	GLN	2.7
1	A	329	PRO	2.7
1	B	527	SER	2.7
1	A	9	ALA	2.7
1	D	396	LEU	2.7
1	A	444	VAL	2.7
1	B	406	TYR	2.7
1	D	366	ASP	2.7
1	B	535	GLU	2.6
1	B	384	LEU	2.6
1	C	6	ILE	2.6
1	C	574	GLN	2.6
1	C	51	GLY	2.6
1	B	518	THR	2.6
1	A	438	TRP	2.6
1	B	430	VAL	2.6
1	B	492	SER	2.6
1	C	578	ARG	2.6
1	B	142	ARG	2.6
1	A	27	ILE	2.6
1	C	352	SER	2.6
1	B	279	GLN	2.6
1	C	573	GLN	2.6
1	B	536	GLY	2.6
1	C	80	GLU	2.6
1	C	176	GLU	2.6
1	C	383	VAL	2.6
1	B	446	SER	2.6
1	C	601	GLN	2.6
1	D	520	GLY	2.6
1	D	523	GLY	2.6
1	B	449	ASP	2.6
1	C	217	ASP	2.6
1	A	130	VAL	2.6
1	B	483	ARG	2.6
1	D	329	PRO	2.5
1	A	132	CYS	2.5
1	C	508	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	383	VAL	2.5
1	A	248	ASP	2.5
1	A	392	ASP	2.5
1	D	49	ALA	2.5
1	D	497	PHE	2.5
1	D	487	PRO	2.5
1	A	186	TYR	2.5
1	D	15	SER	2.5
1	D	439	GLY	2.5
1	B	85	SER	2.5
1	C	568	GLY	2.5
1	B	480	ALA	2.5
1	B	575	TRP	2.5
1	C	528	LEU	2.5
1	C	486	SER	2.5
1	D	571	ASP	2.5
1	A	152	ARG	2.5
1	B	34	TYR	2.5
1	C	267	LEU	2.5
1	C	499	LEU	2.5
1	B	435	GLU	2.5
1	A	411	PHE	2.5
1	A	25	LEU	2.5
1	D	303	VAL	2.5
1	A	429	GLN	2.5
1	C	183	ILE	2.4
1	A	575	TRP	2.4
1	B	60	ASP	2.4
1	B	324	ASN	2.4
1	B	454	THR	2.4
1	B	528	LEU	2.4
1	D	112	HIS	2.4
1	D	577	ALA	2.4
1	B	16	GLN	2.4
1	C	350	GLN	2.4
1	D	447	CYS	2.4
1	A	485	SER	2.4
1	A	597	LEU	2.4
1	B	187	LEU	2.4
1	B	67	THR	2.4
1	C	326	THR	2.4
1	B	298	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	158	TYR	2.4
1	C	184	GLY	2.4
1	D	16	GLN	2.4
1	B	311	LYS	2.4
1	B	313	GLU	2.4
1	B	515	PHE	2.4
1	C	302	ARG	2.4
1	D	304	THR	2.4
1	A	489	THR	2.4
1	D	225	ASP	2.4
1	D	416	ASP	2.4
1	D	369	GLY	2.4
1	B	434	TYR	2.4
1	C	185	TYR	2.4
1	B	461	ALA	2.4
1	A	355	LYS	2.4
1	A	395	LYS	2.4
1	C	515	PHE	2.4
1	C	344	GLU	2.4
1	D	128	PRO	2.4
1	A	3	THR	2.4
1	A	461	ALA	2.4
1	A	585	TYR	2.4
1	B	402	ASP	2.4
1	B	555	ALA	2.4
1	C	147	PHE	2.4
1	A	330	LEU	2.4
1	B	452	LEU	2.4
1	A	57	GLU	2.4
1	C	527	SER	2.4
1	A	398	LYS	2.3
1	B	587	HIS	2.3
1	D	190	TYR	2.3
1	D	593	ARG	2.3
1	C	124	ARG	2.3
1	B	534	GLU	2.3
1	D	13	SER	2.3
1	B	517	SER	2.3
1	B	603	SER	2.3
1	C	189	SER	2.3
1	D	24	GLY	2.3
1	D	83	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	585	TYR	2.3
1	D	251	LEU	2.3
1	D	594	LEU	2.3
1	B	499	LEU	2.3
1	D	573	GLN	2.3
1	B	567	GLU	2.3
1	D	239	VAL	2.3
1	A	532	VAL	2.3
1	D	116	ARG	2.3
1	D	160	PRO	2.3
1	B	182	PRO	2.3
1	C	393	GLY	2.3
1	C	467	GLY	2.3
1	B	425	ALA	2.3
1	C	9	ALA	2.3
1	C	34	TYR	2.3
1	D	499	LEU	2.3
1	C	300	LEU	2.3
1	B	318	ASP	2.3
1	C	313	GLU	2.3
1	B	383	VAL	2.3
1	C	432	ARG	2.3
1	C	445	PRO	2.3
1	C	493	SER	2.3
1	D	463	LEU	2.3
1	B	55	LEU	2.3
1	A	133	TYR	2.3
1	C	173	ASN	2.3
1	A	421	ARG	2.3
1	B	605	PRO	2.3
1	C	470	ILE	2.3
1	D	506	ALA	2.3
1	D	460	LEU	2.3
1	A	556	LEU	2.3
1	B	280	LEU	2.3
1	B	498	LEU	2.3
1	B	531	HIS	2.3
1	B	604	THR	2.3
1	C	335	THR	2.3
1	A	503	SER	2.3
1	C	446	SER	2.3
1	A	578	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	578	ARG	2.3
1	B	117	VAL	2.3
1	D	567	GLU	2.2
1	B	351	GLU	2.2
1	C	149	GLU	2.2
1	D	67	THR	2.2
1	D	326	THR	2.2
1	D	518	THR	2.2
1	B	525	TYR	2.2
1	C	600	SER	2.2
1	D	157	ARG	2.2
1	B	32	ARG	2.2
1	A	350	GLN	2.2
1	A	586	GLN	2.2
1	A	448	ASP	2.2
1	B	341	ILE	2.2
1	D	81	PRO	2.2
1	D	373	ALA	2.2
1	A	10	ALA	2.2
1	A	128	PRO	2.2
1	A	516	GLY	2.2
1	C	415	PRO	2.2
1	A	576	VAL	2.2
1	B	506	ALA	2.2
1	D	164	ARG	2.2
1	B	495	ARG	2.2
1	C	421	ARG	2.2
1	D	158	TYR	2.2
1	D	503	SER	2.2
1	B	94	ILE	2.2
1	B	115	ILE	2.2
1	C	323	LEU	2.2
1	C	177	ALA	2.2
1	D	229	ASP	2.2
1	A	412	ASP	2.2
1	B	589	LYS	2.2
1	A	245	ARG	2.2
1	D	585	TYR	2.2
1	A	558	SER	2.2
1	B	450	ALA	2.2
1	B	453	ARG	2.2
1	D	150	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	402	ASP	2.2
1	A	7	PHE	2.2
1	A	247	ASP	2.2
1	D	468	HIS	2.2
1	D	525	TYR	2.1
1	D	563	GLN	2.1
1	C	52	LEU	2.1
1	D	155	GLU	2.1
1	D	161	ARG	2.1
1	C	343	GLU	2.1
1	A	457	GLY	2.1
1	A	410	VAL	2.1
1	C	186	TYR	2.1
1	C	406	TYR	2.1
1	C	570	TYR	2.1
1	C	285	LYS	2.1
1	D	152	ARG	2.1
1	A	266	ALA	2.1
1	B	464	ARG	2.1
1	D	270	SER	2.1
1	D	393	GLY	2.1
1	A	353	GLU	2.1
1	C	605	PRO	2.1
1	A	276	VAL	2.1
1	A	359	ASP	2.1
1	D	604	THR	2.1
1	D	434	TYR	2.1
1	B	190	TYR	2.1
1	B	322	ALA	2.1
1	D	514	SER	2.1
1	C	471	VAL	2.1
1	C	472	VAL	2.1
1	D	560	LEU	2.1
1	C	132	CYS	2.1
1	C	392	ASP	2.1
1	C	402	ASP	2.1
1	B	116	ARG	2.1
1	B	380	THR	2.1
1	B	599	ALA	2.1
1	D	154	GLY	2.1
1	A	58	PHE	2.1
1	B	336	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	469	ASP	2.1
1	A	158	TYR	2.1
1	A	525	TYR	2.1
1	D	64	PHE	2.1
1	D	486	SER	2.0
1	D	517	SER	2.0
1	A	408	ARG	2.0
1	C	65	LEU	2.0
1	C	71	LEU	2.0
1	C	75	ASN	2.0
1	C	152	ARG	2.0
1	B	456	ALA	2.0
1	B	580	ALA	2.0
1	A	360	VAL	2.0
1	A	384	LEU	2.0
1	B	6	ILE	2.0
1	A	67	THR	2.0
1	A	315	TYR	2.0
1	B	331	THR	2.0
1	D	345	GLY	2.0
1	D	516	GLY	2.0
1	A	453	ARG	2.0
1	C	117	VAL	2.0
1	D	62	ILE	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.