



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:56 AM UTC

PDB ID : 2XQ5 / pdb_00002xq5
Title : Pentameric ligand gated ion channel GLIC in complex with tetraethylarsonium (TEAs)
Authors : Hilf, R.J.C.; Bertozzi, C.; Zimmermann, I.; Reiter, A.; Trauner, D.; Dutzler, R.
Deposited on : 2010-09-01
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

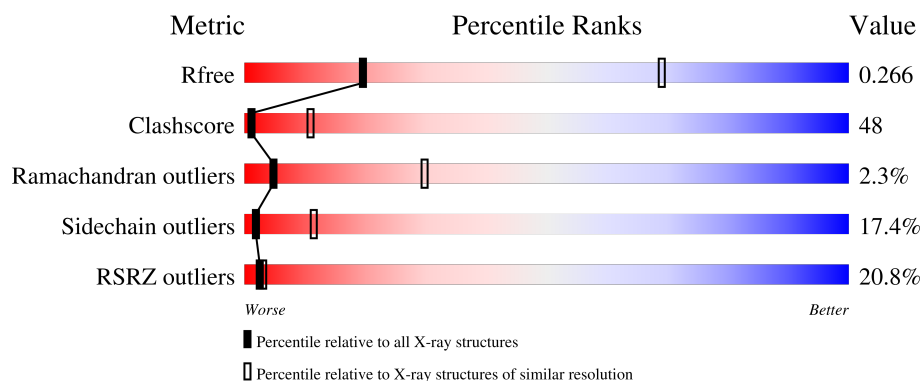
1 Overall quality at a glance

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	317	18% 30% 51% 16% .
1	B	317	21% 30% 53% 15% .
1	C	317	19% 33% 51% 13% .
1	D	317	24% 31% 51% 16% .
1	E	317	20% 33% 50% 15% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12606 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 GLR4197 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	B	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	C	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	D	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	E	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			

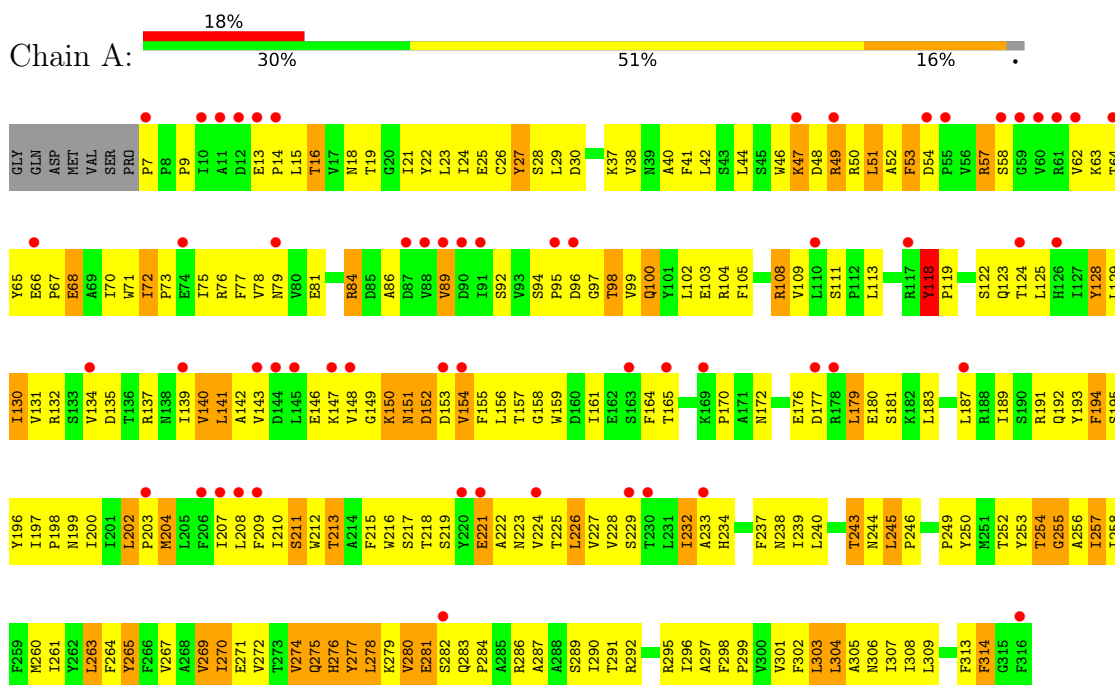
- Molecule 2 is ARSENIC (CCD ID: ARS) (formula: As).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	As	0	0
			1	1		

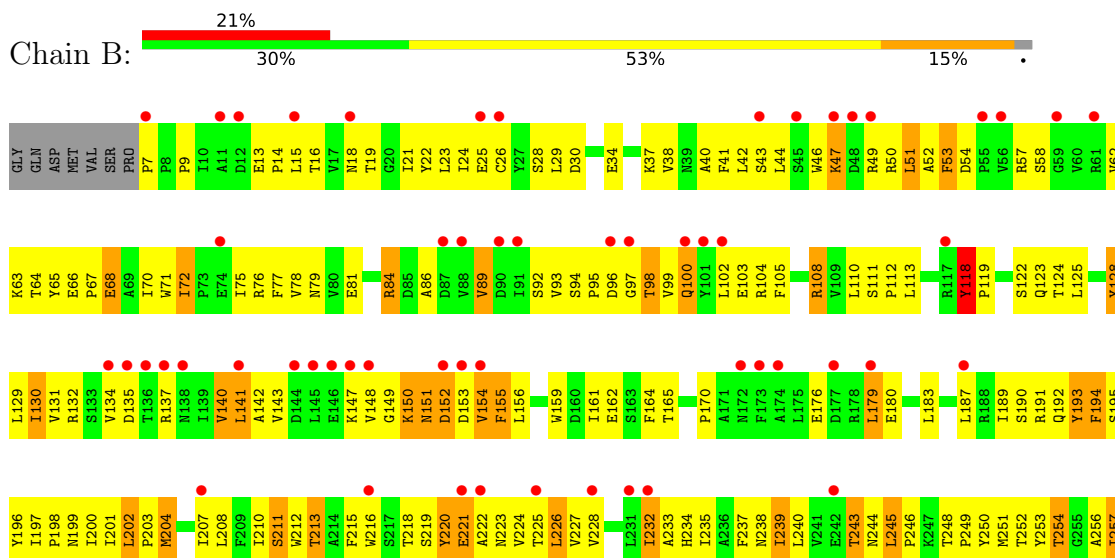
3 Residue-property plots [i](#)

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: GLR4197 PROTEIN

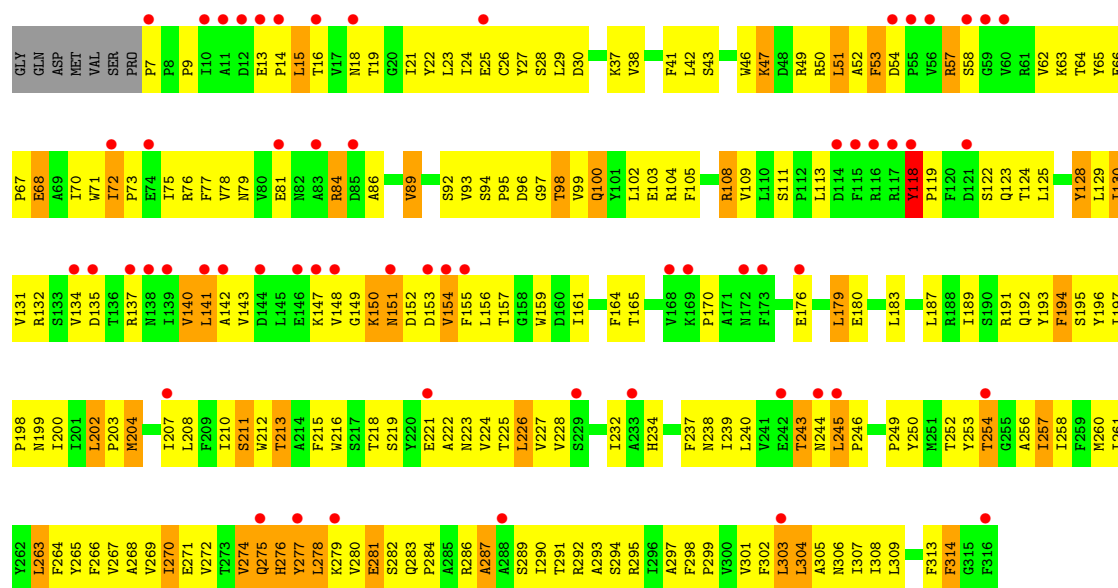


• Molecule 1: GLR4197 PROTEIN

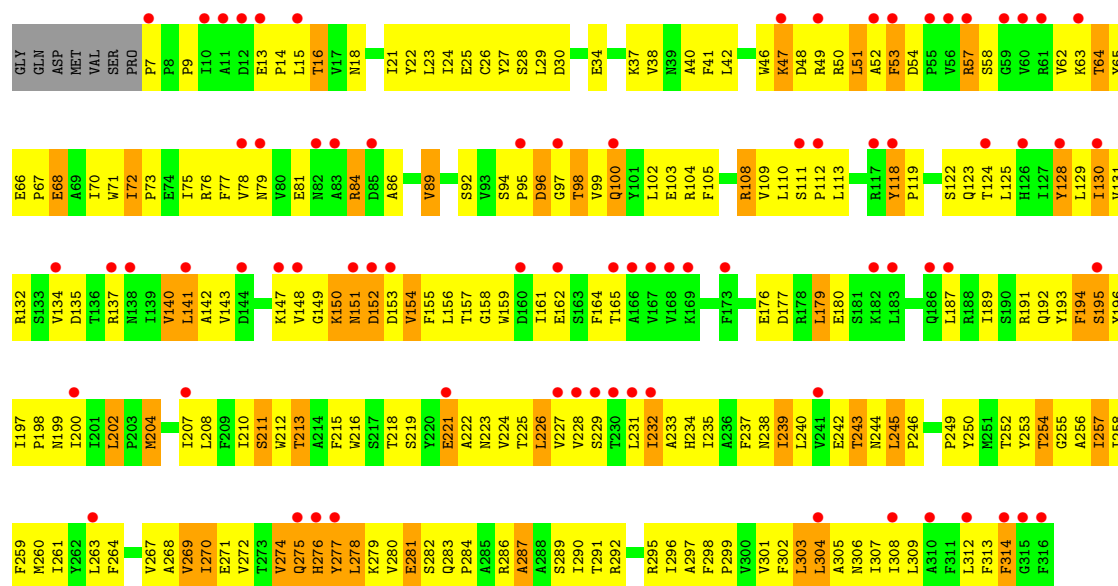




• Molecule 1: GLR4197 PROTEIN

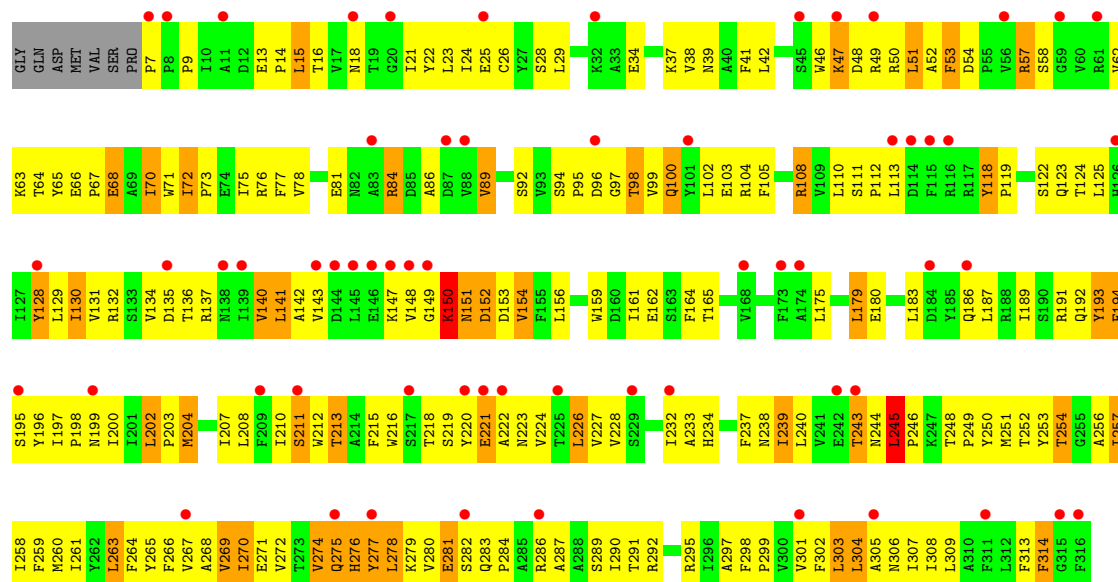


• Molecule 1: GLR4197 PROTEIN



• Molecule 1: GLR4197 PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.31Å 128.31Å 164.37Å 90.00° 104.04° 90.00°	Depositor
Resolution (Å)	40.20 – 3.50 40.20 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.20-3.50) 97.6 (40.20-3.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 3.40Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.249 , 0.266 0.247 , 0.266	Depositor DCC
R_{free} test set	2591 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	98.3	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 98.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	12606	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ARS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.60	0/2589	1.02	15/3535 (0.4%)
1	B	0.61	0/2589	1.03	13/3535 (0.4%)
1	C	0.62	0/2589	1.01	10/3535 (0.3%)
1	D	0.64	1/2589 (0.0%)	1.03	13/3535 (0.4%)
1	E	0.61	0/2589	1.03	17/3535 (0.5%)
All	All	0.62	1/12945 (0.0%)	1.02	68/17675 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	57	ARG	C-N	-6.05	1.26	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	128	TYR	N-CA-C	7.81	122.83	112.13
1	C	135	ASP	N-CA-CB	-7.69	100.82	110.98
1	B	128	TYR	N-CA-C	7.67	122.63	112.13
1	C	281	GLU	N-CA-C	-7.47	98.61	109.59
1	A	281	GLU	N-CA-C	-7.46	98.63	109.59
1	E	281	GLU	N-CA-C	-7.46	98.63	109.59
1	B	281	GLU	N-CA-C	-7.45	98.64	109.59
1	D	281	GLU	N-CA-C	-7.42	98.68	109.59
1	A	280	VAL	N-CA-C	-7.37	105.59	112.96
1	E	128	TYR	N-CA-C	7.35	122.20	112.13
1	E	135	ASP	N-CA-CB	-7.31	101.33	110.98
1	D	135	ASP	N-CA-CB	-7.18	101.50	110.98
1	B	135	ASP	N-CA-CB	-6.76	102.05	110.98
1	A	128	TYR	N-CA-C	6.66	121.26	112.13
1	D	128	TYR	N-CA-C	6.66	121.25	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	111	SER	CA-C-N	6.58	126.55	120.03
1	E	111	SER	C-N-CA	6.58	126.55	120.03
1	D	118	TYR	CA-C-N	-6.47	113.03	119.56
1	D	118	TYR	C-N-CA	-6.47	113.03	119.56
1	C	278	LEU	N-CA-CB	-6.44	100.58	111.27
1	B	278	LEU	N-CA-CB	-6.42	100.61	111.27
1	D	278	LEU	N-CA-CB	-6.42	100.61	111.27
1	A	278	LEU	N-CA-CB	-6.41	100.63	111.27
1	E	278	LEU	N-CA-CB	-6.41	100.63	111.27
1	B	152	ASP	N-CA-C	-6.39	105.44	112.72
1	D	111	SER	CA-C-N	6.38	126.29	119.85
1	D	111	SER	C-N-CA	6.38	126.29	119.85
1	C	111	SER	CA-C-N	6.34	126.30	120.03
1	C	111	SER	C-N-CA	6.34	126.30	120.03
1	A	118	TYR	CA-C-N	-6.26	113.24	119.56
1	A	118	TYR	C-N-CA	-6.26	113.24	119.56
1	E	134	VAL	CB-CA-C	6.22	121.49	111.29
1	D	134	VAL	CB-CA-C	6.20	121.46	111.29
1	C	118	TYR	CA-C-N	-6.20	113.30	119.56
1	C	118	TYR	C-N-CA	-6.20	113.30	119.56
1	B	134	VAL	CB-CA-C	6.19	121.45	111.29
1	A	134	VAL	CB-CA-C	6.18	121.42	111.29
1	B	118	TYR	CA-C-N	-6.11	113.39	119.56
1	B	118	TYR	C-N-CA	-6.11	113.39	119.56
1	B	111	SER	CA-C-N	6.10	126.01	119.85
1	B	111	SER	C-N-CA	6.10	126.01	119.85
1	A	135	ASP	N-CA-CB	-6.06	101.42	111.06
1	C	134	VAL	CB-CA-C	6.06	121.23	111.29
1	D	255	GLY	N-CA-C	-6.03	107.19	114.66
1	A	152	ASP	N-CA-C	-6.01	105.86	112.72
1	A	111	SER	CA-C-N	5.95	125.86	119.85
1	A	111	SER	C-N-CA	5.95	125.86	119.85
1	D	152	ASP	N-CA-C	-5.95	105.94	112.72
1	E	152	ASP	N-CA-C	-5.88	106.01	112.72
1	B	193	TYR	N-CA-C	-5.69	102.61	110.35
1	E	118	TYR	CA-C-N	-5.68	113.82	119.56
1	E	118	TYR	C-N-CA	-5.68	113.82	119.56
1	E	150	LYS	N-CA-C	-5.44	99.21	110.80
1	D	195	SER	N-CA-C	-5.33	106.47	112.87
1	A	255	GLY	N-CA-C	-5.15	106.13	113.86
1	E	193	TYR	N-CA-C	-5.15	102.76	110.23
1	E	245	LEU	CA-C-N	5.15	125.15	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	245	LEU	C-N-CA	5.15	125.15	120.21
1	A	27	TYR	N-CA-C	5.12	115.10	107.88
1	B	220	TYR	N-CA-C	-5.12	105.70	111.28
1	E	70	ILE	CB-CA-C	-5.09	105.74	111.45
1	B	276	HIS	N-CA-CB	-5.05	101.95	110.49
1	E	136	THR	N-CA-C	-5.05	101.47	109.59
1	D	276	HIS	N-CA-CB	-5.04	101.98	110.49
1	A	276	HIS	N-CA-CB	-5.03	101.98	110.49
1	C	276	HIS	N-CA-CB	-5.03	101.98	110.49
1	E	276	HIS	N-CA-CB	-5.02	102.00	110.49
1	A	265	TYR	N-CA-C	-5.01	107.56	113.97

There are no chirality outliers.

There are no planarity outliers.

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	2521	0	2537	291	0
1	B	2521	0	2537	279	0
1	C	2521	0	2537	243	0
1	D	2521	0	2537	278	0
1	E	2521	0	2537	254	0
2	C	1	0	0	0	0
All	All	12606	0	12685	1220	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 48.

All (1220) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:LEU:HD23	1:B:224:VAL:HB	1.33	1.06
1:D:155:PHE:CE1	1:E:112:PRO:HB3	1.92	1.03
1:A:155:PHE:CE1	1:B:112:PRO:HB3	1.94	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ALA:HB2	1:B:221:GLU:HA	1.42	1.01
1:A:27:TYR:HB3	1:B:110:LEU:HD11	1.42	0.99
1:D:210:ILE:HG23	1:E:269:VAL:HG11	1.44	0.97
1:A:155:PHE:CZ	1:B:112:PRO:HB3	1.98	0.97
1:D:76:ARG:NH2	1:D:130:ILE:HD12	1.81	0.95
1:B:89:VAL:HG11	1:B:102:LEU:HD23	1.48	0.95
1:A:76:ARG:NH2	1:A:130:ILE:HD12	1.82	0.95
1:B:76:ARG:NH2	1:B:130:ILE:HD12	1.81	0.95
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.50	0.94
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.50	0.93
1:E:76:ARG:NH2	1:E:130:ILE:HD12	1.84	0.93
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.50	0.92
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.51	0.92
1:C:22:TYR:HA	1:C:149:GLY:HA3	1.51	0.92
1:B:147:LYS:C	1:B:149:GLY:H	1.77	0.92
1:E:147:LYS:C	1:E:149:GLY:H	1.76	0.92
1:A:27:TYR:CB	1:B:110:LEU:HD11	1.99	0.91
1:C:22:TYR:HA	1:C:149:GLY:CA	2.02	0.90
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.53	0.90
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.52	0.90
1:B:76:ARG:HH22	1:B:130:ILE:HD12	1.33	0.90
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.50	0.90
1:A:78:VAL:HG22	1:A:130:ILE:HG12	1.52	0.90
1:C:76:ARG:NH2	1:C:130:ILE:HD12	1.86	0.90
1:D:76:ARG:HH22	1:D:130:ILE:HD12	1.37	0.89
1:C:27:TYR:HB3	1:D:110:LEU:HD11	1.55	0.88
1:C:147:LYS:C	1:C:149:GLY:H	1.79	0.88
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.56	0.88
1:E:76:ARG:HH22	1:E:130:ILE:HD12	1.38	0.88
1:D:22:TYR:HA	1:D:149:GLY:CA	2.04	0.87
1:D:147:LYS:C	1:D:149:GLY:H	1.80	0.87
1:A:147:LYS:C	1:A:149:GLY:H	1.81	0.87
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.57	0.87
1:A:22:TYR:HA	1:A:149:GLY:HA3	1.56	0.86
1:A:22:TYR:HA	1:A:149:GLY:CA	2.04	0.86
1:B:22:TYR:HA	1:B:149:GLY:CA	2.06	0.85
1:A:104:ARG:HH22	1:B:78:VAL:HA	1.38	0.85
1:C:234:HIS:CE1	1:C:261:ILE:HG21	2.12	0.85
1:D:253:TYR:HA	1:D:313:PHE:CE2	2.11	0.84
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.58	0.84
1:A:226:LEU:CD2	1:B:224:VAL:HB	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.41	0.83
1:E:253:TYR:HA	1:E:313:PHE:CE2	2.13	0.83
1:D:253:TYR:HA	1:D:313:PHE:HE2	1.41	0.83
1:E:253:TYR:HA	1:E:313:PHE:HE2	1.43	0.83
1:C:253:TYR:HA	1:C:313:PHE:CE2	2.14	0.83
1:B:253:TYR:HA	1:B:313:PHE:CE2	2.14	0.83
1:A:76:ARG:HH22	1:A:130:ILE:HD12	1.40	0.82
1:A:253:TYR:HA	1:A:313:PHE:CE2	2.14	0.82
1:B:253:TYR:HA	1:B:313:PHE:HE2	1.44	0.82
1:A:202:LEU:HD12	1:B:259:PHE:CZ	2.16	0.81
1:C:253:TYR:HA	1:C:313:PHE:HE2	1.45	0.81
1:E:22:TYR:HA	1:E:149:GLY:CA	2.09	0.81
1:A:253:TYR:HA	1:A:313:PHE:HE2	1.45	0.80
1:E:22:TYR:HA	1:E:149:GLY:HA3	1.61	0.80
1:A:210:ILE:HG23	1:B:269:VAL:HG11	1.61	0.80
1:A:202:LEU:HD12	1:B:259:PHE:HZ	1.46	0.80
1:A:221:GLU:HB3	1:B:221:GLU:HG2	1.63	0.80
1:E:234:HIS:CE1	1:E:261:ILE:HG21	2.17	0.79
1:A:234:HIS:CE1	1:A:261:ILE:HG21	2.18	0.79
1:C:131:VAL:HG11	1:C:140:VAL:HG13	1.65	0.78
1:A:104:ARG:NH2	1:B:78:VAL:HA	1.98	0.78
1:D:155:PHE:CZ	1:E:112:PRO:HB3	2.18	0.77
1:A:219:SER:OG	1:A:222:ALA:HB3	1.85	0.77
1:B:22:TYR:CD1	1:B:149:GLY:HA2	2.20	0.77
1:B:131:VAL:HG11	1:B:140:VAL:HG13	1.66	0.76
1:A:77:PHE:H	1:A:84:ARG:HD3	1.48	0.76
1:B:234:HIS:CE1	1:B:261:ILE:HG21	2.21	0.76
1:D:77:PHE:H	1:D:84:ARG:HD3	1.50	0.76
1:A:131:VAL:HG11	1:A:140:VAL:HG13	1.67	0.75
1:A:132:ARG:HA	1:A:180:GLU:HG2	1.69	0.75
1:E:131:VAL:HG11	1:E:140:VAL:HG13	1.67	0.75
1:A:128:TYR:O	1:A:129:LEU:HB2	1.86	0.75
1:B:257:ILE:O	1:B:261:ILE:HG12	1.86	0.75
1:D:22:TYR:CD1	1:D:149:GLY:HA2	2.22	0.75
1:C:199:ASN:HB3	1:D:242:GLU:CD	2.11	0.74
1:C:219:SER:OG	1:C:222:ALA:HB3	1.87	0.74
1:C:77:PHE:H	1:C:84:ARG:HD3	1.52	0.74
1:A:77:PHE:CD1	1:A:84:ARG:HD2	2.23	0.74
1:D:54:ASP:HB2	1:D:57:ARG:HG3	1.69	0.74
1:D:128:TYR:O	1:D:129:LEU:HB2	1.87	0.73
1:D:47:LYS:HD2	1:D:49:ARG:HH21	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLY:O	1:A:164:PHE:HD1	1.71	0.73
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.24	0.73
1:B:54:ASP:HB2	1:B:57:ARG:HG3	1.70	0.73
1:C:22:TYR:CD1	1:C:149:GLY:HA2	2.23	0.73
1:C:149:GLY:O	1:C:164:PHE:HD1	1.72	0.73
1:D:234:HIS:CE1	1:D:261:ILE:HG21	2.24	0.73
1:C:94:SER:OG	1:C:95:PRO:HD2	1.89	0.73
1:D:131:VAL:HG11	1:D:140:VAL:HG13	1.71	0.73
1:C:157:THR:HG21	1:D:34:GLU:HG3	1.71	0.73
1:D:149:GLY:O	1:D:164:PHE:HD1	1.72	0.72
1:B:77:PHE:H	1:B:84:ARG:HD3	1.54	0.72
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.71	0.72
1:E:149:GLY:O	1:E:164:PHE:HD1	1.71	0.72
1:C:226:LEU:CD2	1:D:224:VAL:HB	2.19	0.72
1:B:47:LYS:HD2	1:B:49:ARG:HH21	1.55	0.72
1:D:77:PHE:CD1	1:D:84:ARG:HD2	2.25	0.72
1:E:54:ASP:HB2	1:E:57:ARG:HG3	1.71	0.72
1:E:147:LYS:C	1:E:149:GLY:N	2.43	0.72
1:A:147:LYS:C	1:A:149:GLY:N	2.48	0.71
1:C:222:ALA:HB2	1:D:221:GLU:HA	1.70	0.71
1:E:238:ASN:HA	1:E:258:ILE:HD11	1.71	0.71
1:D:229:SER:CB	1:E:228:VAL:HG11	2.20	0.71
1:E:22:TYR:CD1	1:E:149:GLY:HA2	2.25	0.71
1:C:128:TYR:O	1:C:129:LEU:HB2	1.90	0.71
1:C:147:LYS:C	1:C:149:GLY:N	2.46	0.71
1:D:141:LEU:HD23	1:D:142:ALA:H	1.55	0.71
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.72	0.71
1:A:283:GLN:N	1:A:284:PRO:HD3	2.05	0.71
1:D:221:GLU:OE2	1:E:221:GLU:CD	2.34	0.71
1:B:149:GLY:O	1:B:164:PHE:HD1	1.73	0.70
1:A:21:ILE:O	1:A:149:GLY:HA3	1.92	0.70
1:B:238:ASN:HA	1:B:258:ILE:HD11	1.73	0.70
1:B:89:VAL:CG1	1:B:102:LEU:HD23	2.20	0.70
1:D:257:ILE:O	1:D:261:ILE:HG12	1.91	0.70
1:E:257:ILE:O	1:E:261:ILE:HG12	1.91	0.70
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.73	0.70
1:D:198:PRO:CG	1:E:251:MET:HE1	2.22	0.70
1:B:254:THR:O	1:B:258:ILE:HB	1.91	0.70
1:A:198:PRO:CG	1:B:251:MET:HE1	2.22	0.70
1:D:283:GLN:N	1:D:284:PRO:HD3	2.06	0.70
1:C:21:ILE:O	1:C:149:GLY:HA3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLN:N	1:B:284:PRO:HD3	2.07	0.69
1:C:42:LEU:HB3	1:C:103:GLU:HG3	1.74	0.69
1:C:213:THR:HG22	1:C:226:LEU:HD11	1.73	0.69
1:D:21:ILE:O	1:D:149:GLY:HA3	1.92	0.69
1:E:47:LYS:HD2	1:E:49:ARG:HH21	1.57	0.69
1:E:254:THR:O	1:E:258:ILE:HB	1.93	0.69
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.27	0.69
1:E:42:LEU:HB3	1:E:103:GLU:HG3	1.75	0.69
1:B:77:PHE:CD1	1:B:84:ARG:HD2	2.27	0.69
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.27	0.69
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.73	0.69
1:C:84:ARG:HB2	1:C:84:ARG:HH11	1.57	0.69
1:E:128:TYR:O	1:E:129:LEU:HB2	1.90	0.69
1:E:283:GLN:N	1:E:284:PRO:HD3	2.07	0.69
1:A:22:TYR:CD1	1:A:149:GLY:HA2	2.27	0.69
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.27	0.69
1:A:94:SER:OG	1:A:95:PRO:HD2	1.91	0.69
1:E:13:GLU:HB3	1:E:14:PRO:HD2	1.74	0.69
1:E:77:PHE:CD1	1:E:84:ARG:HD2	2.27	0.69
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.27	0.69
1:D:276:HIS:O	1:D:280:VAL:HG22	1.93	0.69
1:A:42:LEU:HB3	1:A:103:GLU:HG3	1.75	0.69
1:A:257:ILE:O	1:A:261:ILE:HG12	1.93	0.69
1:C:257:ILE:O	1:C:261:ILE:HG12	1.93	0.69
1:D:254:THR:O	1:D:258:ILE:HB	1.92	0.69
1:B:81:GLU:HG3	1:B:108:ARG:HG2	1.75	0.68
1:B:47:LYS:HD2	1:B:49:ARG:NH2	2.08	0.68
1:B:147:LYS:C	1:B:149:GLY:N	2.44	0.68
1:C:77:PHE:CD1	1:C:84:ARG:HD2	2.27	0.68
1:C:84:ARG:HB2	1:C:84:ARG:NH1	2.07	0.68
1:D:94:SER:OG	1:D:95:PRO:HD2	1.93	0.68
1:B:276:HIS:O	1:B:280:VAL:HG22	1.93	0.68
1:C:47:LYS:HD2	1:C:49:ARG:HH21	1.59	0.68
1:D:13:GLU:HB3	1:D:14:PRO:HD2	1.75	0.68
1:E:77:PHE:H	1:E:84:ARG:HD3	1.56	0.68
1:E:21:ILE:O	1:E:149:GLY:HA3	1.93	0.68
1:C:132:ARG:HA	1:C:180:GLU:HG2	1.75	0.68
1:D:238:ASN:HA	1:D:258:ILE:HD11	1.74	0.68
1:E:276:HIS:O	1:E:280:VAL:HG22	1.94	0.68
1:E:89:VAL:CG1	1:E:102:LEU:HD23	2.22	0.68
1:A:240:LEU:HD13	1:B:239:ILE:HG12	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:GLU:HB3	1:C:14:PRO:HD2	1.74	0.68
1:C:283:GLN:N	1:C:284:PRO:HD3	2.09	0.68
1:D:225:THR:HG21	1:E:224:VAL:HG23	1.76	0.68
1:B:132:ARG:HA	1:B:180:GLU:HG2	1.75	0.67
1:D:84:ARG:NH1	1:D:84:ARG:HB2	2.08	0.67
1:D:225:THR:CG2	1:E:224:VAL:HG23	2.25	0.67
1:C:84:ARG:HH11	1:C:84:ARG:CB	2.07	0.67
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.29	0.67
1:B:141:LEU:HD23	1:B:142:ALA:H	1.59	0.67
1:D:81:GLU:HG3	1:D:108:ARG:HG2	1.76	0.67
1:E:94:SER:OG	1:E:95:PRO:HD2	1.94	0.67
1:A:226:LEU:HD22	1:B:228:VAL:HG21	1.77	0.67
1:D:147:LYS:C	1:D:149:GLY:N	2.48	0.67
1:E:84:ARG:HB2	1:E:84:ARG:NH1	2.09	0.67
1:A:229:SER:HB2	1:B:228:VAL:HG11	1.76	0.67
1:C:238:ASN:HA	1:C:258:ILE:HD11	1.76	0.67
1:C:276:HIS:O	1:C:280:VAL:HG22	1.95	0.67
1:D:89:VAL:CG1	1:D:102:LEU:HD23	2.24	0.67
1:D:132:ARG:HA	1:D:180:GLU:HG2	1.75	0.67
1:E:238:ASN:HA	1:E:258:ILE:CD1	2.24	0.67
1:B:53:PHE:CE1	1:B:95:PRO:HA	2.30	0.67
1:D:53:PHE:CE1	1:D:95:PRO:HA	2.29	0.67
1:E:84:ARG:HB2	1:E:84:ARG:HH11	1.60	0.67
1:A:254:THR:O	1:A:258:ILE:HB	1.94	0.67
1:D:47:LYS:HD2	1:D:49:ARG:NH2	2.10	0.67
1:A:81:GLU:HG3	1:A:108:ARG:HG2	1.76	0.66
1:A:276:HIS:O	1:A:280:VAL:HG22	1.95	0.66
1:B:21:ILE:O	1:B:149:GLY:HA3	1.94	0.66
1:B:100:GLN:HE21	1:B:100:GLN:HA	1.60	0.66
1:A:84:ARG:NH1	1:A:84:ARG:HB2	2.10	0.66
1:D:42:LEU:HB3	1:D:103:GLU:HG3	1.77	0.66
1:A:155:PHE:CE1	1:B:112:PRO:CB	2.75	0.66
1:B:42:LEU:HB3	1:B:103:GLU:HG3	1.78	0.66
1:C:226:LEU:HD23	1:D:224:VAL:HB	1.77	0.66
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.30	0.66
1:B:84:ARG:CB	1:B:84:ARG:HH11	2.09	0.66
1:B:128:TYR:O	1:B:129:LEU:HB2	1.95	0.66
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.76	0.66
1:C:200:ILE:HD11	1:C:240:LEU:HD23	1.78	0.66
1:E:84:ARG:HH11	1:E:84:ARG:CB	2.07	0.66
1:E:132:ARG:HA	1:E:180:GLU:HG2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ASN:HA	1:A:258:ILE:HD11	1.78	0.66
1:B:84:ARG:NH1	1:B:84:ARG:HB2	2.11	0.65
1:C:238:ASN:HA	1:C:258:ILE:CD1	2.26	0.65
1:D:84:ARG:HB2	1:D:84:ARG:HH11	1.61	0.65
1:D:304:LEU:O	1:D:308:ILE:HG12	1.97	0.65
1:B:94:SER:OG	1:B:95:PRO:HD2	1.97	0.65
1:A:213:THR:HG22	1:A:226:LEU:HD11	1.79	0.65
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.78	0.65
1:C:254:THR:O	1:C:258:ILE:HB	1.95	0.65
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.79	0.65
1:C:53:PHE:CE1	1:C:95:PRO:HA	2.31	0.65
1:B:191:ARG:HG3	1:B:192:GLN:N	2.12	0.65
1:A:47:LYS:HD2	1:A:49:ARG:HH21	1.61	0.65
1:D:104:ARG:HH22	1:E:78:VAL:HA	1.61	0.64
1:A:22:TYR:HA	1:A:149:GLY:HA2	1.78	0.64
1:E:53:PHE:HE2	1:E:63:LYS:HB3	1.62	0.64
1:B:249:PRO:HD2	1:B:250:TYR:CD1	2.31	0.64
1:D:84:ARG:HH11	1:D:84:ARG:CB	2.09	0.64
1:A:53:PHE:CE1	1:A:95:PRO:HA	2.31	0.64
1:D:22:TYR:HA	1:D:149:GLY:HA2	1.78	0.64
1:E:81:GLU:HG3	1:E:108:ARG:HG2	1.79	0.64
1:A:226:LEU:HD23	1:B:224:VAL:CB	2.20	0.64
1:B:22:TYR:HA	1:B:149:GLY:HA2	1.80	0.64
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.27	0.64
1:A:84:ARG:HB2	1:A:84:ARG:HH11	1.63	0.64
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.80	0.64
1:C:81:GLU:HG3	1:C:108:ARG:HG2	1.78	0.63
1:E:249:PRO:HD2	1:E:250:TYR:CD1	2.33	0.63
1:A:198:PRO:HG3	1:B:251:MET:HE1	1.79	0.63
1:C:53:PHE:HE2	1:C:63:LYS:HB3	1.63	0.63
1:E:219:SER:OG	1:E:222:ALA:HB3	1.98	0.63
1:C:22:TYR:HA	1:C:149:GLY:HA2	1.78	0.63
1:E:22:TYR:HA	1:E:149:GLY:HA2	1.80	0.63
1:A:303:LEU:O	1:A:307:ILE:HD12	1.99	0.63
1:B:53:PHE:HE2	1:B:63:LYS:HB3	1.64	0.63
1:B:123:GLN:HA	1:B:123:GLN:NE2	2.12	0.63
1:C:215:PHE:O	1:C:291:THR:HG22	1.98	0.63
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.34	0.63
1:A:215:PHE:HZ	1:A:298:PHE:CE1	2.17	0.63
1:A:84:ARG:HH11	1:A:84:ARG:CB	2.10	0.63
1:C:213:THR:HG22	1:C:226:LEU:CD1	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:LEU:O	1:E:211:SER:HB3	1.99	0.63
1:E:276:HIS:C	1:E:278:LEU:H	2.07	0.63
1:E:100:GLN:HA	1:E:100:GLN:HE21	1.64	0.63
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.80	0.63
1:D:276:HIS:C	1:D:278:LEU:H	2.07	0.63
1:A:53:PHE:HE2	1:A:63:LYS:HB3	1.64	0.62
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.29	0.62
1:B:213:THR:HG22	1:B:226:LEU:HD11	1.81	0.62
1:D:123:GLN:HA	1:D:123:GLN:NE2	2.14	0.62
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.34	0.62
1:E:303:LEU:O	1:E:307:ILE:HD12	2.00	0.62
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.80	0.62
1:B:200:ILE:HD11	1:B:240:LEU:HD23	1.79	0.62
1:C:276:HIS:C	1:C:278:LEU:H	2.07	0.62
1:D:219:SER:OG	1:D:222:ALA:HB3	2.00	0.62
1:A:229:SER:HB3	1:B:228:VAL:CG1	2.29	0.62
1:A:276:HIS:C	1:A:278:LEU:H	2.07	0.62
1:B:238:ASN:HA	1:B:258:ILE:CD1	2.28	0.62
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.82	0.62
1:C:47:LYS:HD2	1:C:49:ARG:NH2	2.15	0.62
1:D:210:ILE:HG13	1:E:266:PHE:CE1	2.34	0.62
1:D:215:PHE:HZ	1:D:298:PHE:CE1	2.18	0.62
1:B:215:PHE:HZ	1:B:298:PHE:CE1	2.18	0.62
1:E:47:LYS:HD2	1:E:49:ARG:NH2	2.13	0.62
1:D:100:GLN:HE21	1:D:100:GLN:HA	1.64	0.62
1:A:229:SER:CB	1:B:228:VAL:HG11	2.29	0.62
1:C:89:VAL:CG1	1:C:102:LEU:HD23	2.28	0.62
1:E:200:ILE:HD11	1:E:240:LEU:HD23	1.81	0.62
1:B:208:LEU:O	1:B:211:SER:HB3	2.00	0.62
1:D:191:ARG:HG3	1:D:192:GLN:N	2.15	0.62
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.29	0.62
1:A:89:VAL:CG1	1:A:102:LEU:HD23	2.27	0.61
1:A:217:SER:OG	1:B:220:TYR:CE2	2.51	0.61
1:C:297:ALA:O	1:C:301:VAL:HG23	2.00	0.61
1:E:215:PHE:O	1:E:291:THR:HG22	2.00	0.61
1:B:42:LEU:HB3	1:B:103:GLU:CG	2.30	0.61
1:C:29:LEU:C	1:C:29:LEU:HD23	2.25	0.61
1:C:234:HIS:CE1	1:C:261:ILE:CG2	2.82	0.61
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.35	0.61
1:E:147:LYS:O	1:E:149:GLY:N	2.33	0.61
1:A:213:THR:HG22	1:A:226:LEU:CD1	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LYS:HE2	1:C:165:THR:HA	1.82	0.61
1:C:215:PHE:HZ	1:C:298:PHE:CE1	2.18	0.61
1:D:53:PHE:HE2	1:D:63:LYS:HB3	1.63	0.61
1:D:238:ASN:HA	1:D:258:ILE:CD1	2.30	0.61
1:B:84:ARG:HH11	1:B:84:ARG:HB2	1.64	0.61
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.82	0.61
1:B:147:LYS:O	1:B:149:GLY:N	2.33	0.61
1:A:47:LYS:HD2	1:A:49:ARG:NH2	2.16	0.61
1:A:238:ASN:HA	1:A:258:ILE:CD1	2.31	0.61
1:A:297:ALA:O	1:A:301:VAL:HG23	2.00	0.61
1:B:276:HIS:C	1:B:278:LEU:H	2.07	0.61
1:D:229:SER:HB3	1:E:228:VAL:CG1	2.31	0.61
1:E:215:PHE:HZ	1:E:298:PHE:CE1	2.19	0.61
1:C:42:LEU:HB3	1:C:103:GLU:CG	2.31	0.60
1:E:24:ILE:HD13	1:E:104:ARG:HE	1.67	0.60
1:D:194:PHE:C	1:D:196:TYR:N	2.57	0.60
1:D:202:LEU:HD12	1:E:259:PHE:HZ	1.66	0.60
1:D:229:SER:HB3	1:E:228:VAL:HG11	1.83	0.60
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.83	0.60
1:E:54:ASP:HB2	1:E:57:ARG:CG	2.30	0.60
1:E:150:LYS:CG	1:E:154:VAL:HG21	2.31	0.60
1:A:157:THR:CG2	1:B:34:GLU:OE1	2.50	0.60
1:B:223:ASN:O	1:B:227:VAL:HG23	2.01	0.60
1:B:245:LEU:HD12	1:B:246:PRO:HD2	1.83	0.60
1:E:213:THR:HG22	1:E:226:LEU:HD11	1.84	0.60
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.31	0.60
1:A:141:LEU:HD23	1:A:142:ALA:H	1.67	0.60
1:A:277:TYR:O	1:A:281:GLU:CG	2.50	0.60
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.82	0.60
1:D:29:LEU:HD23	1:D:29:LEU:C	2.27	0.60
1:D:194:PHE:C	1:D:196:TYR:H	2.09	0.60
1:D:277:TYR:O	1:D:281:GLU:CG	2.50	0.60
1:A:29:LEU:C	1:A:29:LEU:HD23	2.26	0.60
1:A:229:SER:CB	1:B:228:VAL:CG1	2.80	0.60
1:B:303:LEU:O	1:B:307:ILE:HD12	2.02	0.60
1:C:249:PRO:HD2	1:C:250:TYR:CD1	2.37	0.60
1:E:304:LEU:O	1:E:308:ILE:HG12	2.01	0.60
1:B:29:LEU:HD23	1:B:29:LEU:C	2.27	0.60
1:B:213:THR:HG22	1:B:226:LEU:CD1	2.32	0.60
1:D:223:ASN:O	1:D:227:VAL:HG23	2.02	0.60
1:A:233:ALA:HB1	1:B:235:ILE:CD1	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:PHE:C	1:C:196:TYR:H	2.09	0.60
1:E:151:ASN:HD22	1:E:152:ASP:H	1.49	0.60
1:E:277:TYR:O	1:E:281:GLU:CG	2.50	0.60
1:A:147:LYS:HE2	1:A:165:THR:HA	1.83	0.59
1:A:223:ASN:O	1:A:227:VAL:HG23	2.01	0.59
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.32	0.59
1:B:219:SER:OG	1:B:222:ALA:HB3	2.03	0.59
1:C:29:LEU:HB2	1:C:156:LEU:HD11	1.83	0.59
1:A:27:TYR:HB3	1:B:110:LEU:CD1	2.24	0.59
1:A:221:GLU:OE2	1:B:221:GLU:OE2	2.21	0.59
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.83	0.59
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.37	0.59
1:C:25:GLU:OE1	1:C:25:GLU:HA	2.01	0.59
1:C:194:PHE:C	1:C:196:TYR:N	2.59	0.59
1:A:192:GLN:CD	1:B:249:PRO:HB3	2.27	0.59
1:C:65:TYR:CD2	1:C:70:ILE:HD11	2.37	0.59
1:C:147:LYS:HG2	1:C:147:LYS:O	2.01	0.59
1:A:208:LEU:O	1:A:211:SER:HB3	2.02	0.59
1:A:249:PRO:HD2	1:A:250:TYR:CD1	2.38	0.59
1:E:194:PHE:C	1:E:196:TYR:H	2.11	0.59
1:E:213:THR:HG22	1:E:226:LEU:CD1	2.33	0.59
1:C:303:LEU:O	1:C:307:ILE:HD12	2.02	0.59
1:D:192:GLN:CD	1:E:249:PRO:HB3	2.27	0.59
1:E:218:THR:HG22	1:E:279:LYS:HE2	1.84	0.59
1:B:29:LEU:HB2	1:B:156:LEU:HD11	1.84	0.59
1:B:297:ALA:O	1:B:301:VAL:HG23	2.03	0.59
1:D:15:LEU:HD11	1:D:46:TRP:HB2	1.85	0.59
1:E:141:LEU:HD23	1:E:142:ALA:H	1.68	0.59
1:B:277:TYR:O	1:B:281:GLU:CG	2.50	0.59
1:C:151:ASN:HD22	1:C:152:ASP:H	1.49	0.59
1:C:245:LEU:HD12	1:C:246:PRO:HD2	1.85	0.59
1:D:212:TRP:HZ3	1:D:264:PHE:HD2	1.50	0.59
1:A:191:ARG:HG3	1:A:192:GLN:N	2.18	0.59
1:C:223:ASN:O	1:C:227:VAL:HG23	2.02	0.59
1:E:245:LEU:HD12	1:E:246:PRO:HD2	1.85	0.59
1:A:215:PHE:O	1:A:291:THR:HG22	2.03	0.58
1:C:225:THR:HG21	1:D:225:THR:OG1	2.03	0.58
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.69	0.58
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.86	0.58
1:A:245:LEU:HD12	1:A:246:PRO:HD2	1.84	0.58
1:C:150:LYS:CG	1:C:154:VAL:HG21	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ILE:CD1	1:C:240:LEU:HD23	2.33	0.58
1:D:42:LEU:HB3	1:D:103:GLU:CG	2.33	0.58
1:D:200:ILE:HD11	1:D:240:LEU:HD23	1.85	0.58
1:E:42:LEU:HB3	1:E:103:GLU:CG	2.32	0.58
1:B:215:PHE:O	1:B:291:THR:HG22	2.02	0.58
1:C:100:GLN:HE21	1:C:100:GLN:HA	1.69	0.58
1:C:277:TYR:O	1:C:281:GLU:CG	2.50	0.58
1:D:253:TYR:HD1	1:D:313:PHE:CD2	2.21	0.58
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.34	0.58
1:C:314:PHE:CD1	1:C:314:PHE:N	2.71	0.58
1:D:24:ILE:HD13	1:D:104:ARG:HE	1.69	0.58
1:E:223:ASN:O	1:E:227:VAL:HG23	2.03	0.58
1:A:13:GLU:HB3	1:A:14:PRO:CD	2.33	0.58
1:E:297:ALA:O	1:E:301:VAL:HG23	2.04	0.58
1:B:304:LEU:O	1:B:308:ILE:HG12	2.04	0.58
1:C:191:ARG:HG3	1:C:192:GLN:N	2.17	0.58
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.85	0.58
1:A:218:THR:HG22	1:A:279:LYS:HE2	1.86	0.58
1:D:215:PHE:O	1:D:291:THR:HG22	2.03	0.58
1:E:194:PHE:C	1:E:196:TYR:N	2.60	0.58
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.86	0.58
1:A:24:ILE:HD13	1:A:104:ARG:HE	1.69	0.58
1:D:155:PHE:HE1	1:E:112:PRO:HB3	1.59	0.58
1:A:222:ALA:O	1:A:226:LEU:HB2	2.03	0.58
1:A:42:LEU:HB3	1:A:103:GLU:CG	2.33	0.57
1:A:212:TRP:HZ3	1:A:264:PHE:HD2	1.52	0.57
1:A:314:PHE:CD1	1:A:314:PHE:N	2.71	0.57
1:D:147:LYS:O	1:D:149:GLY:N	2.37	0.57
1:A:151:ASN:HD22	1:A:152:ASP:H	1.51	0.57
1:A:157:THR:HG21	1:B:34:GLU:OE1	2.04	0.57
1:A:298:PHE:HB2	1:A:299:PRO:HD3	1.87	0.57
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.35	0.57
1:D:215:PHE:CZ	1:D:298:PHE:CD1	2.92	0.57
1:D:297:ALA:O	1:D:301:VAL:HG23	2.04	0.57
1:E:29:LEU:HB2	1:E:156:LEU:HD11	1.85	0.57
1:A:215:PHE:CZ	1:A:298:PHE:CD1	2.91	0.57
1:B:281:GLU:O	1:B:283:GLN:N	2.36	0.57
1:E:123:GLN:NE2	1:E:123:GLN:HA	2.19	0.57
1:A:314:PHE:N	1:A:314:PHE:HD1	2.03	0.57
1:C:147:LYS:O	1:C:149:GLY:N	2.37	0.57
1:D:18:ASN:HB3	1:D:143:VAL:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.40	0.57
1:E:234:HIS:CE1	1:E:261:ILE:CG2	2.87	0.57
1:A:200:ILE:HD11	1:A:240:LEU:HD23	1.86	0.57
1:A:281:GLU:O	1:A:283:GLN:N	2.36	0.57
1:B:218:THR:HG22	1:B:279:LYS:HE2	1.86	0.57
1:B:200:ILE:O	1:B:204:MET:HB2	2.05	0.57
1:C:202:LEU:HD12	1:D:259:PHE:CE1	2.40	0.57
1:C:212:TRP:HZ3	1:C:264:PHE:HD2	1.52	0.57
1:D:218:THR:HG22	1:D:279:LYS:HE2	1.86	0.57
1:A:150:LYS:CG	1:A:154:VAL:HG21	2.35	0.57
1:B:151:ASN:HD22	1:B:152:ASP:H	1.52	0.57
1:E:212:TRP:HZ3	1:E:264:PHE:HD2	1.52	0.57
1:A:194:PHE:C	1:A:196:TYR:N	2.62	0.57
1:C:24:ILE:HD13	1:C:104:ARG:HE	1.69	0.57
1:C:226:LEU:HD21	1:D:224:VAL:HB	1.86	0.57
1:A:65:TYR:CD2	1:A:70:ILE:HD11	2.40	0.56
1:B:159:TRP:CE3	1:B:189:ILE:HD12	2.39	0.56
1:C:215:PHE:CZ	1:C:298:PHE:CD1	2.93	0.56
1:E:29:LEU:C	1:E:29:LEU:HD23	2.30	0.56
1:A:234:HIS:CE1	1:A:261:ILE:CG2	2.89	0.56
1:A:277:TYR:O	1:A:281:GLU:HG3	2.05	0.56
1:A:290:ILE:HG22	1:A:291:THR:N	2.19	0.56
1:C:208:LEU:O	1:C:211:SER:HB3	2.05	0.56
1:D:68:GLU:CD	1:D:68:GLU:H	2.11	0.56
1:D:245:LEU:HD12	1:D:246:PRO:HD2	1.87	0.56
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.87	0.56
1:A:159:TRP:CE3	1:A:189:ILE:HD12	2.40	0.56
1:B:277:TYR:O	1:B:281:GLU:HG3	2.06	0.56
1:D:208:LEU:O	1:D:211:SER:HB3	2.05	0.56
1:D:213:THR:HG22	1:D:226:LEU:CD1	2.35	0.56
1:D:277:TYR:O	1:D:281:GLU:HG3	2.05	0.56
1:D:298:PHE:HB2	1:D:299:PRO:HD3	1.87	0.56
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.87	0.56
1:C:253:TYR:O	1:C:256:ALA:HB3	2.05	0.56
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.87	0.56
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.35	0.56
1:E:65:TYR:CD2	1:E:70:ILE:HD11	2.40	0.56
1:E:147:LYS:HE2	1:E:165:THR:HA	1.87	0.56
1:B:194:PHE:C	1:B:196:TYR:N	2.61	0.56
1:D:54:ASP:HB2	1:D:57:ARG:HB2	1.88	0.56
1:A:147:LYS:O	1:A:149:GLY:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:ALA:HA	1:D:95:PRO:O	2.06	0.56
1:E:137:ARG:HD2	1:E:179:LEU:HG	1.88	0.56
1:B:150:LYS:CG	1:B:154:VAL:HG21	2.36	0.56
1:B:194:PHE:C	1:B:196:TYR:H	2.13	0.56
1:B:212:TRP:HZ3	1:B:264:PHE:HD2	1.51	0.56
1:C:277:TYR:O	1:C:281:GLU:HG3	2.06	0.56
1:C:314:PHE:N	1:C:314:PHE:HD1	2.04	0.56
1:D:290:ILE:HG22	1:D:291:THR:N	2.21	0.56
1:D:303:LEU:O	1:D:307:ILE:HD12	2.06	0.56
1:A:222:ALA:HA	1:B:221:GLU:OE1	2.06	0.56
1:B:24:ILE:HD13	1:B:104:ARG:HE	1.69	0.56
1:C:150:LYS:HG3	1:C:154:VAL:HG21	1.88	0.56
1:C:218:THR:HG22	1:C:279:LYS:HE2	1.87	0.56
1:D:213:THR:HG22	1:D:226:LEU:HD11	1.87	0.56
1:B:215:PHE:CZ	1:B:298:PHE:CD1	2.93	0.56
1:B:298:PHE:HB2	1:B:299:PRO:HD3	1.87	0.56
1:D:29:LEU:HB2	1:D:156:LEU:HD11	1.88	0.56
1:E:147:LYS:O	1:E:147:LYS:HG2	2.06	0.56
1:B:54:ASP:HB2	1:B:57:ARG:HB2	1.88	0.55
1:B:253:TYR:O	1:B:256:ALA:HB3	2.07	0.55
1:E:275:GLN:HG3	1:E:291:THR:OG1	2.06	0.55
1:D:147:LYS:O	1:D:147:LYS:HG2	2.07	0.55
1:E:277:TYR:O	1:E:281:GLU:HG3	2.06	0.55
1:C:46:TRP:HH2	1:C:72:ILE:HG23	1.69	0.55
1:A:194:PHE:C	1:A:196:TYR:H	2.13	0.55
1:E:25:GLU:OE1	1:E:25:GLU:HA	2.04	0.55
1:A:275:GLN:HG3	1:A:291:THR:OG1	2.07	0.55
1:C:53:PHE:CD1	1:C:53:PHE:C	2.85	0.55
1:C:274:VAL:C	1:C:276:HIS:H	2.15	0.55
1:B:274:VAL:C	1:B:276:HIS:H	2.15	0.55
1:C:68:GLU:H	1:C:68:GLU:CD	2.14	0.55
1:C:195:SER:O	1:C:199:ASN:HB2	2.07	0.55
1:C:290:ILE:HG22	1:C:291:THR:N	2.22	0.55
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.89	0.55
1:A:123:GLN:HA	1:A:123:GLN:NE2	2.22	0.55
1:B:53:PHE:CD1	1:B:53:PHE:C	2.85	0.55
1:B:234:HIS:CE1	1:B:261:ILE:CG2	2.90	0.55
1:D:283:GLN:N	1:D:284:PRO:CD	2.70	0.55
1:A:51:LEU:CD1	1:A:70:ILE:HD12	2.37	0.55
1:A:53:PHE:CD1	1:A:53:PHE:C	2.85	0.55
1:A:75:ILE:HD13	1:A:131:VAL:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:PHE:N	1:B:314:PHE:CD1	2.75	0.55
1:D:53:PHE:CD1	1:D:53:PHE:C	2.85	0.55
1:D:275:GLN:HG3	1:D:291:THR:OG1	2.06	0.55
1:A:147:LYS:O	1:A:147:LYS:HG2	2.07	0.54
1:A:215:PHE:HZ	1:A:298:PHE:CD1	2.25	0.54
1:A:274:VAL:C	1:A:276:HIS:H	2.15	0.54
1:C:281:GLU:O	1:C:283:GLN:N	2.38	0.54
1:D:159:TRP:CE3	1:D:189:ILE:HD12	2.43	0.54
1:E:314:PHE:CD1	1:E:314:PHE:N	2.74	0.54
1:A:253:TYR:O	1:A:256:ALA:HB3	2.07	0.54
1:B:65:TYR:CD2	1:B:70:ILE:HD11	2.42	0.54
1:B:290:ILE:HG22	1:B:291:THR:N	2.22	0.54
1:C:141:LEU:HD23	1:C:142:ALA:H	1.71	0.54
1:D:253:TYR:O	1:D:256:ALA:HB3	2.06	0.54
1:B:51:LEU:CD1	1:B:70:ILE:HD12	2.38	0.54
1:B:275:GLN:HG3	1:B:291:THR:OG1	2.08	0.54
1:D:149:GLY:O	1:D:150:LYS:HB2	2.07	0.54
1:E:75:ILE:HD13	1:E:131:VAL:HB	1.88	0.54
1:E:191:ARG:HG3	1:E:192:GLN:N	2.21	0.54
1:A:304:LEU:O	1:A:308:ILE:HG12	2.06	0.54
1:C:256:ALA:HB1	1:C:309:LEU:HD21	1.90	0.54
1:C:271:GLU:O	1:C:272:VAL:C	2.50	0.54
1:A:29:LEU:HB2	1:A:156:LEU:HD11	1.90	0.54
1:C:54:ASP:HB2	1:C:57:ARG:HB2	1.90	0.54
1:B:267:VAL:HA	1:B:270:ILE:HB	1.90	0.54
1:D:215:PHE:HZ	1:D:298:PHE:CD1	2.26	0.54
1:D:275:GLN:O	1:D:275:GLN:HG2	2.08	0.54
1:A:68:GLU:H	1:A:68:GLU:CD	2.15	0.54
1:A:283:GLN:N	1:A:284:PRO:CD	2.70	0.54
1:B:283:GLN:N	1:B:284:PRO:CD	2.71	0.54
1:D:193:TYR:O	1:D:194:PHE:HB2	2.06	0.54
1:D:274:VAL:C	1:D:276:HIS:H	2.15	0.54
1:E:53:PHE:CD1	1:E:53:PHE:C	2.85	0.54
1:E:275:GLN:O	1:E:275:GLN:HG2	2.08	0.54
1:B:68:GLU:CD	1:B:68:GLU:H	2.16	0.54
1:A:193:TYR:O	1:A:194:PHE:HB2	2.06	0.54
1:D:51:LEU:CD1	1:D:70:ILE:HD12	2.38	0.54
1:D:192:GLN:OE1	1:E:249:PRO:HB3	2.07	0.54
1:E:215:PHE:CZ	1:E:298:PHE:CD1	2.95	0.54
1:E:267:VAL:HA	1:E:270:ILE:HB	1.88	0.54
1:B:25:GLU:HA	1:B:25:GLU:OE1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:GLN:HA	1:C:123:GLN:NE2	2.22	0.54
1:C:275:GLN:O	1:C:275:GLN:HG2	2.08	0.54
1:D:53:PHE:CD1	1:D:95:PRO:HA	2.43	0.54
1:D:222:ALA:O	1:D:226:LEU:HB2	2.07	0.54
1:C:275:GLN:HG3	1:C:291:THR:OG1	2.08	0.53
1:E:150:LYS:HG3	1:E:154:VAL:HG21	1.89	0.53
1:A:209:PHE:HB2	1:B:266:PHE:CE1	2.43	0.53
1:B:147:LYS:HE2	1:B:165:THR:HA	1.90	0.53
1:B:305:ALA:O	1:B:309:LEU:HB2	2.08	0.53
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.90	0.53
1:C:215:PHE:HZ	1:C:298:PHE:CD1	2.26	0.53
1:A:150:LYS:HG3	1:A:154:VAL:HG21	1.89	0.53
1:B:275:GLN:HG2	1:B:275:GLN:O	2.08	0.53
1:D:65:TYR:CD2	1:D:70:ILE:HD11	2.43	0.53
1:E:53:PHE:CD1	1:E:95:PRO:HA	2.44	0.53
1:E:54:ASP:HB2	1:E:57:ARG:HB2	1.90	0.53
1:E:222:ALA:O	1:E:226:LEU:HB2	2.09	0.53
1:B:147:LYS:O	1:B:147:LYS:HG2	2.08	0.53
1:E:22:TYR:HB3	1:E:41:PHE:HB2	1.90	0.53
1:A:46:TRP:HH2	1:A:72:ILE:HG23	1.72	0.53
1:C:199:ASN:HB3	1:D:242:GLU:OE2	2.08	0.53
1:E:290:ILE:HG22	1:E:291:THR:N	2.22	0.53
1:A:225:THR:HG21	1:B:225:THR:OG1	2.09	0.53
1:B:215:PHE:HZ	1:B:298:PHE:CD1	2.27	0.53
1:C:193:TYR:O	1:C:194:PHE:HB2	2.08	0.53
1:C:283:GLN:N	1:C:284:PRO:CD	2.71	0.53
1:E:274:VAL:C	1:E:276:HIS:H	2.15	0.53
1:E:281:GLU:O	1:E:283:GLN:N	2.39	0.53
1:A:298:PHE:CB	1:A:299:PRO:HD3	2.39	0.53
1:B:125:LEU:HB2	1:B:187:LEU:HB3	1.90	0.53
1:B:200:ILE:CD1	1:B:240:LEU:HD23	2.39	0.53
1:B:298:PHE:CB	1:B:299:PRO:HD3	2.39	0.53
1:C:215:PHE:HB2	1:C:216:TRP:CZ3	2.43	0.53
1:C:267:VAL:HA	1:C:270:ILE:HB	1.91	0.53
1:E:147:LYS:CE	1:E:165:THR:HA	2.39	0.53
1:C:237:PHE:HE1	1:D:235:ILE:HD13	1.74	0.52
1:D:281:GLU:O	1:D:283:GLN:N	2.36	0.52
1:E:51:LEU:CD1	1:E:70:ILE:HD12	2.38	0.52
1:E:298:PHE:CB	1:E:299:PRO:HD3	2.39	0.52
1:C:51:LEU:CD1	1:C:70:ILE:HD12	2.40	0.52
1:D:221:GLU:OE2	1:E:221:GLU:OE2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:PHE:CD1	1:D:314:PHE:N	2.76	0.52
1:E:68:GLU:CD	1:E:68:GLU:H	2.17	0.52
1:E:305:ALA:O	1:E:309:LEU:HB2	2.08	0.52
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.91	0.52
1:C:304:LEU:O	1:C:308:ILE:HG12	2.08	0.52
1:D:157:THR:HG21	1:E:34:GLU:OE1	2.10	0.52
1:D:298:PHE:CB	1:D:299:PRO:HD3	2.39	0.52
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.91	0.52
1:D:25:GLU:HA	1:D:25:GLU:OE1	2.08	0.52
1:E:200:ILE:O	1:E:204:MET:HB2	2.08	0.52
1:B:7:PRO:O	1:B:50:ARG:NH2	2.43	0.52
1:D:198:PRO:HG2	1:E:251:MET:HE1	1.91	0.52
1:E:18:ASN:HB3	1:E:143:VAL:HG23	1.90	0.52
1:E:200:ILE:CD1	1:E:240:LEU:HD23	2.38	0.52
1:E:253:TYR:HD1	1:E:313:PHE:CD2	2.27	0.52
1:A:53:PHE:CD1	1:A:53:PHE:O	2.63	0.52
1:A:221:GLU:HB3	1:B:221:GLU:CG	2.37	0.52
1:A:275:GLN:O	1:A:275:GLN:HG2	2.08	0.52
1:B:53:PHE:CD1	1:B:53:PHE:O	2.63	0.52
1:B:53:PHE:CD1	1:B:95:PRO:HA	2.44	0.52
1:D:53:PHE:CD1	1:D:53:PHE:O	2.63	0.52
1:D:193:TYR:O	1:D:194:PHE:CB	2.56	0.52
1:A:7:PRO:O	1:A:50:ARG:NH2	2.42	0.52
1:A:25:GLU:OE1	1:A:25:GLU:HA	2.09	0.52
1:C:222:ALA:HA	1:D:221:GLU:OE1	2.10	0.52
1:E:314:PHE:N	1:E:314:PHE:HD1	2.07	0.52
1:A:27:TYR:CG	1:B:110:LEU:CD1	2.92	0.52
1:B:123:GLN:HB2	1:B:189:ILE:HG13	1.92	0.52
1:D:267:VAL:HA	1:D:270:ILE:HB	1.90	0.52
1:A:193:TYR:O	1:A:194:PHE:CB	2.57	0.52
1:B:161:ILE:HA	1:B:189:ILE:HG22	1.92	0.52
1:B:243:THR:HG22	1:B:244:ASN:ND2	2.25	0.52
1:C:298:PHE:CB	1:C:299:PRO:HD3	2.39	0.52
1:E:52:ALA:HA	1:E:95:PRO:O	2.09	0.52
1:E:53:PHE:CD1	1:E:53:PHE:O	2.63	0.52
1:A:27:TYR:CB	1:B:110:LEU:CD1	2.82	0.52
1:B:215:PHE:HB2	1:B:216:TRP:CZ3	2.45	0.52
1:C:53:PHE:CD1	1:C:53:PHE:O	2.63	0.52
1:D:210:ILE:CG2	1:E:269:VAL:HG11	2.29	0.52
1:D:150:LYS:CG	1:D:154:VAL:HG21	2.40	0.51
1:A:137:ARG:HD2	1:A:179:LEU:HG	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ALA:CB	1:B:221:GLU:HA	2.27	0.51
1:D:75:ILE:HD13	1:D:131:VAL:HB	1.93	0.51
1:C:222:ALA:O	1:C:226:LEU:HB2	2.11	0.51
1:E:283:GLN:N	1:E:284:PRO:CD	2.71	0.51
1:A:195:SER:O	1:A:199:ASN:HB2	2.10	0.51
1:C:193:TYR:O	1:C:194:PHE:CB	2.58	0.51
1:C:210:ILE:CD1	1:D:231:LEU:HD22	2.41	0.51
1:C:222:ALA:CB	1:D:221:GLU:HA	2.40	0.51
1:D:240:LEU:HD13	1:E:239:ILE:HG12	1.92	0.51
1:D:305:ALA:O	1:D:309:LEU:HB2	2.10	0.51
1:A:53:PHE:HE2	1:A:63:LYS:CB	2.24	0.51
1:C:159:TRP:CE3	1:C:189:ILE:HD12	2.45	0.51
1:E:161:ILE:HA	1:E:189:ILE:HG22	1.93	0.51
1:E:216:TRP:CZ2	1:E:295:ARG:HB3	2.46	0.51
1:A:104:ARG:HH22	1:B:78:VAL:CA	2.17	0.51
1:A:277:TYR:O	1:A:281:GLU:HG2	2.11	0.51
1:B:46:TRP:HH2	1:B:72:ILE:HG23	1.75	0.51
1:D:277:TYR:O	1:D:281:GLU:HG2	2.11	0.51
1:A:54:ASP:HB2	1:A:57:ARG:HB2	1.93	0.51
1:A:305:ALA:O	1:A:309:LEU:HB2	2.11	0.51
1:B:193:TYR:O	1:B:194:PHE:HB2	2.10	0.51
1:C:75:ILE:HD13	1:C:131:VAL:HB	1.92	0.51
1:D:147:LYS:HE2	1:D:165:THR:HA	1.92	0.51
1:D:151:ASN:HD22	1:D:152:ASP:H	1.56	0.51
1:A:253:TYR:HD1	1:A:313:PHE:CD2	2.29	0.51
1:E:125:LEU:HB2	1:E:187:LEU:HB3	1.93	0.51
1:B:277:TYR:O	1:B:281:GLU:HG2	2.11	0.51
1:B:314:PHE:N	1:B:314:PHE:HD1	2.07	0.51
1:C:53:PHE:HE2	1:C:63:LYS:CB	2.24	0.51
1:D:53:PHE:HE2	1:D:63:LYS:CB	2.24	0.51
1:D:210:ILE:HG13	1:E:266:PHE:HE1	1.76	0.51
1:D:225:THR:O	1:D:225:THR:HG22	2.11	0.51
1:A:37:LYS:CG	1:A:108:ARG:HB2	2.40	0.50
1:A:51:LEU:HD13	1:A:70:ILE:HD12	1.93	0.50
1:C:271:GLU:OE2	1:C:272:VAL:N	2.44	0.50
1:D:22:TYR:HB3	1:D:41:PHE:HB2	1.93	0.50
1:D:96:ASP:OD1	1:D:98:THR:HB	2.12	0.50
1:D:257:ILE:HG22	1:D:309:LEU:HD23	1.94	0.50
1:E:7:PRO:O	1:E:50:ARG:NH2	2.44	0.50
1:E:243:THR:HG22	1:E:244:ASN:ND2	2.26	0.50
1:A:216:TRP:CZ2	1:A:295:ARG:HB3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLU:O	1:A:272:VAL:C	2.53	0.50
1:A:53:PHE:CD1	1:A:95:PRO:HA	2.47	0.50
1:C:123:GLN:HB2	1:C:189:ILE:HG13	1.94	0.50
1:C:204:MET:O	1:C:207:ILE:HG12	2.12	0.50
1:D:123:GLN:HB2	1:D:189:ILE:HG13	1.93	0.50
1:E:37:LYS:HG3	1:E:108:ARG:HB2	1.94	0.50
1:E:193:TYR:O	1:E:194:PHE:HB2	2.10	0.50
1:A:53:PHE:CE2	1:A:63:LYS:HB3	2.47	0.50
1:A:78:VAL:HB	1:A:128:TYR:HB2	1.93	0.50
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.94	0.50
1:C:264:PHE:CE2	1:C:302:PHE:HB2	2.47	0.50
1:E:215:PHE:HB2	1:E:216:TRP:CZ3	2.46	0.50
1:E:224:VAL:C	1:E:226:LEU:H	2.19	0.50
1:E:277:TYR:O	1:E:281:GLU:HG2	2.11	0.50
1:D:215:PHE:HB2	1:D:216:TRP:CZ3	2.45	0.50
1:E:46:TRP:HH2	1:E:72:ILE:HG23	1.76	0.50
1:E:215:PHE:HZ	1:E:298:PHE:CD1	2.30	0.50
1:D:104:ARG:NH2	1:E:78:VAL:HA	2.26	0.50
1:B:52:ALA:HA	1:B:95:PRO:O	2.12	0.50
1:B:53:PHE:O	1:B:54:ASP:C	2.55	0.50
1:C:46:TRP:CH2	1:C:72:ILE:HG23	2.47	0.50
1:C:51:LEU:HD13	1:C:70:ILE:HD12	1.94	0.50
1:D:81:GLU:HG3	1:D:108:ARG:CG	2.42	0.50
1:B:23:LEU:HD22	1:B:38:VAL:HG21	1.93	0.50
1:B:222:ALA:O	1:B:226:LEU:HB2	2.11	0.50
1:C:155:PHE:CZ	1:D:112:PRO:HB3	2.47	0.50
1:D:95:PRO:C	1:D:97:GLY:H	2.20	0.50
1:E:204:MET:O	1:E:207:ILE:HG12	2.11	0.50
1:A:23:LEU:HG	1:A:164:PHE:CE1	2.47	0.49
1:A:151:ASN:HB3	1:A:153:ASP:H	1.77	0.49
1:B:224:VAL:O	1:B:228:VAL:HB	2.12	0.49
1:C:53:PHE:O	1:C:54:ASP:C	2.55	0.49
1:C:53:PHE:CE2	1:C:63:LYS:HB3	2.46	0.49
1:D:314:PHE:N	1:D:314:PHE:HD1	2.10	0.49
1:B:271:GLU:O	1:B:272:VAL:C	2.53	0.49
1:C:42:LEU:HD23	1:C:103:GLU:OE1	2.11	0.49
1:C:52:ALA:HA	1:C:95:PRO:O	2.12	0.49
1:D:198:PRO:HG3	1:E:251:MET:HE1	1.93	0.49
1:D:234:HIS:CE1	1:D:261:ILE:CG2	2.94	0.49
1:D:264:PHE:CE2	1:D:302:PHE:HB2	2.47	0.49
1:E:159:TRP:CE3	1:E:189:ILE:HD12	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:PHE:HE2	1:E:63:LYS:CB	2.25	0.49
1:A:204:MET:O	1:A:207:ILE:HG12	2.12	0.49
1:B:75:ILE:HD13	1:B:131:VAL:HB	1.93	0.49
1:C:119:PRO:O	1:C:193:TYR:HB3	2.13	0.49
1:D:195:SER:O	1:D:199:ASN:HB2	2.13	0.49
1:D:216:TRP:CZ2	1:D:295:ARG:HB3	2.47	0.49
1:A:37:LYS:HG2	1:A:108:ARG:HB2	1.95	0.49
1:C:23:LEU:HB2	1:C:150:LYS:HA	1.95	0.49
1:D:23:LEU:HB2	1:D:150:LYS:HA	1.95	0.49
1:D:27:TYR:CB	1:E:110:LEU:HD11	2.43	0.49
1:A:53:PHE:O	1:A:54:ASP:C	2.55	0.49
1:A:147:LYS:CE	1:A:165:THR:HA	2.42	0.49
1:A:149:GLY:O	1:A:150:LYS:HB2	2.13	0.49
1:A:215:PHE:HB2	1:A:216:TRP:CZ3	2.47	0.49
1:A:267:VAL:HA	1:A:270:ILE:HB	1.93	0.49
1:B:81:GLU:HG3	1:B:108:ARG:CG	2.42	0.49
1:B:224:VAL:C	1:B:226:LEU:H	2.21	0.49
1:C:213:THR:CG2	1:C:226:LEU:HD11	2.42	0.49
1:C:243:THR:HG22	1:C:244:ASN:ND2	2.28	0.49
1:C:277:TYR:O	1:C:281:GLU:HG2	2.11	0.49
1:A:200:ILE:CD1	1:A:240:LEU:HD23	2.43	0.49
1:A:200:ILE:O	1:A:204:MET:HB2	2.12	0.49
1:A:282:SER:C	1:A:284:PRO:HD3	2.38	0.49
1:C:15:LEU:O	1:C:15:LEU:HG	2.10	0.49
1:D:7:PRO:O	1:D:50:ARG:NH2	2.43	0.49
1:D:27:TYR:HB3	1:E:110:LEU:HD11	1.94	0.49
1:D:161:ILE:HA	1:D:189:ILE:HG22	1.94	0.49
1:D:200:ILE:O	1:D:204:MET:HB2	2.13	0.49
1:E:149:GLY:O	1:E:150:LYS:HB2	2.13	0.49
1:A:271:GLU:OE2	1:A:272:VAL:N	2.46	0.49
1:B:76:ARG:HH12	1:B:130:ILE:HD11	1.78	0.49
1:B:119:PRO:O	1:B:193:TYR:HB3	2.12	0.49
1:B:149:GLY:O	1:B:150:LYS:HB2	2.12	0.49
1:B:224:VAL:C	1:B:226:LEU:N	2.69	0.49
1:B:264:PHE:CE2	1:B:302:PHE:HB2	2.47	0.49
1:C:253:TYR:HD1	1:C:313:PHE:CD2	2.30	0.49
1:A:119:PRO:O	1:A:193:TYR:HB3	2.12	0.49
1:A:264:PHE:CE2	1:A:302:PHE:HB2	2.48	0.49
1:C:23:LEU:HG	1:C:164:PHE:CE1	2.48	0.49
1:C:202:LEU:HD12	1:D:259:PHE:CZ	2.48	0.49
1:D:37:LYS:CG	1:D:108:ARG:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ALA:CB	1:E:220:TYR:CD2	2.96	0.49
1:E:23:LEU:HD22	1:E:38:VAL:HG21	1.94	0.49
1:A:224:VAL:C	1:A:226:LEU:N	2.69	0.48
1:B:216:TRP:CZ2	1:B:295:ARG:HB3	2.48	0.48
1:C:155:PHE:CE1	1:D:112:PRO:HB3	2.48	0.48
1:C:305:ALA:O	1:C:309:LEU:HB2	2.13	0.48
1:D:243:THR:HG22	1:D:244:ASN:ND2	2.28	0.48
1:E:193:TYR:O	1:E:194:PHE:CB	2.60	0.48
1:E:264:PHE:CE2	1:E:302:PHE:HB2	2.48	0.48
1:A:72:ILE:HG22	1:A:73:PRO:HD2	1.95	0.48
1:A:157:THR:HG21	1:B:34:GLU:HG3	1.94	0.48
1:B:53:PHE:HE2	1:B:63:LYS:CB	2.25	0.48
1:B:271:GLU:OE2	1:B:272:VAL:N	2.46	0.48
1:C:53:PHE:CD1	1:C:95:PRO:HA	2.48	0.48
1:E:76:ARG:HH12	1:E:130:ILE:HD11	1.78	0.48
1:E:264:PHE:O	1:E:268:ALA:HB2	2.13	0.48
1:B:193:TYR:O	1:B:194:PHE:CB	2.59	0.48
1:C:200:ILE:O	1:C:204:MET:HB2	2.12	0.48
1:E:81:GLU:HG3	1:E:108:ARG:CG	2.44	0.48
1:A:9:PRO:HD3	1:A:71:TRP:CE3	2.49	0.48
1:A:276:HIS:C	1:A:278:LEU:N	2.71	0.48
1:D:53:PHE:O	1:D:54:ASP:C	2.55	0.48
1:E:53:PHE:O	1:E:54:ASP:C	2.55	0.48
1:E:215:PHE:HB3	1:E:295:ARG:HG2	1.95	0.48
1:A:253:TYR:CA	1:A:313:PHE:HE2	2.22	0.48
1:E:224:VAL:C	1:E:226:LEU:N	2.69	0.48
1:E:271:GLU:O	1:E:272:VAL:C	2.54	0.48
1:C:7:PRO:O	1:C:50:ARG:NH2	2.45	0.48
1:C:65:TYR:CD1	1:C:70:ILE:HD11	2.48	0.48
1:D:65:TYR:CD1	1:D:70:ILE:HD11	2.48	0.48
1:A:123:GLN:HB2	1:A:189:ILE:HG13	1.94	0.48
1:A:243:THR:HG22	1:A:244:ASN:ND2	2.29	0.48
1:B:282:SER:C	1:B:284:PRO:HD3	2.39	0.48
1:A:23:LEU:HD22	1:A:38:VAL:HG21	1.94	0.48
1:A:52:ALA:HA	1:A:95:PRO:O	2.13	0.48
1:A:96:ASP:OD1	1:A:98:THR:HB	2.12	0.48
1:D:137:ARG:HD2	1:D:179:LEU:HG	1.94	0.48
1:D:202:LEU:HD12	1:E:259:PHE:CZ	2.47	0.48
1:E:70:ILE:HD13	1:E:70:ILE:N	2.27	0.48
1:B:9:PRO:HD3	1:B:71:TRP:CE3	2.49	0.48
1:C:125:LEU:HB2	1:C:187:LEU:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ILE:HG13	1:E:266:PHE:CD1	2.48	0.48
1:A:137:ARG:HA	1:A:137:ARG:HD3	1.57	0.48
1:A:192:GLN:CG	1:B:249:PRO:HB3	2.44	0.48
1:C:81:GLU:HG3	1:C:108:ARG:CG	2.44	0.48
1:C:215:PHE:HB2	1:C:216:TRP:CE3	2.49	0.48
1:C:215:PHE:HB3	1:C:295:ARG:HG2	1.95	0.48
1:D:41:PHE:HE2	1:E:175:LEU:CD2	2.27	0.48
1:D:271:GLU:OE2	1:D:272:VAL:N	2.46	0.48
1:A:25:GLU:HG3	1:B:79:ASN:HA	1.95	0.47
1:B:179:LEU:HD12	1:B:179:LEU:O	2.14	0.47
1:D:158:GLY:HA2	1:D:192:GLN:OE1	2.14	0.47
1:D:271:GLU:O	1:D:272:VAL:C	2.56	0.47
1:E:70:ILE:HG22	1:E:71:TRP:N	2.29	0.47
1:A:104:ARG:NH1	1:B:77:PHE:O	2.44	0.47
1:A:146:GLU:HG3	1:B:176:GLU:CD	2.39	0.47
1:A:232:ILE:HG22	1:A:233:ALA:N	2.30	0.47
1:B:215:PHE:HB3	1:B:295:ARG:HG2	1.95	0.47
1:B:253:TYR:CA	1:B:313:PHE:HE2	2.22	0.47
1:C:257:ILE:HG22	1:C:309:LEU:HD23	1.96	0.47
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.45	0.47
1:E:86:ALA:HB2	1:E:105:PHE:HB3	1.96	0.47
1:B:261:ILE:HD13	1:B:302:PHE:HE1	1.80	0.47
1:C:147:LYS:CE	1:C:165:THR:HA	2.43	0.47
1:C:179:LEU:O	1:C:179:LEU:HD12	2.14	0.47
1:D:210:ILE:CG1	1:E:266:PHE:CD1	2.97	0.47
1:D:256:ALA:HB1	1:D:309:LEU:HD21	1.97	0.47
1:E:151:ASN:HB3	1:E:153:ASP:H	1.78	0.47
1:B:253:TYR:HD1	1:B:313:PHE:CD2	2.32	0.47
1:C:23:LEU:HD22	1:C:38:VAL:HG21	1.97	0.47
1:C:78:VAL:HB	1:C:128:TYR:HB2	1.97	0.47
1:C:137:ARG:HD2	1:C:179:LEU:HG	1.95	0.47
1:D:179:LEU:HD12	1:D:179:LEU:O	2.14	0.47
1:E:282:SER:C	1:E:284:PRO:HD3	2.38	0.47
1:B:233:ALA:O	1:B:237:PHE:HD1	1.97	0.47
1:D:210:ILE:O	1:D:211:SER:C	2.58	0.47
1:E:23:LEU:HG	1:E:164:PHE:CE1	2.49	0.47
1:E:53:PHE:C	1:E:53:PHE:HD1	2.22	0.47
1:A:132:ARG:HH22	1:A:176:GLU:HB2	1.80	0.47
1:A:179:LEU:C	1:A:179:LEU:HD12	2.40	0.47
1:B:150:LYS:HG3	1:B:154:VAL:HG21	1.95	0.47
1:B:151:ASN:HB3	1:B:153:ASP:H	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:LEU:HD12	1:B:179:LEU:C	2.40	0.47
1:C:224:VAL:C	1:C:226:LEU:N	2.71	0.47
1:D:23:LEU:HD22	1:D:38:VAL:HG21	1.97	0.47
1:D:78:VAL:HB	1:D:128:TYR:HB2	1.95	0.47
1:E:62:VAL:HG11	1:E:92:SER:HB3	1.97	0.47
1:E:137:ARG:HD3	1:E:137:ARG:HA	1.60	0.47
1:E:179:LEU:HD12	1:E:179:LEU:O	2.14	0.47
1:E:195:SER:O	1:E:199:ASN:HB2	2.15	0.47
1:A:125:LEU:HB2	1:A:187:LEU:HB3	1.96	0.47
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.50	0.47
1:B:276:HIS:C	1:B:278:LEU:N	2.71	0.47
1:C:179:LEU:HD12	1:C:179:LEU:C	2.40	0.47
1:E:95:PRO:C	1:E:97:GLY:H	2.23	0.47
1:C:132:ARG:HH22	1:C:176:GLU:HB2	1.80	0.47
1:C:151:ASN:HB3	1:C:153:ASP:H	1.80	0.47
1:D:70:ILE:HG22	1:D:71:TRP:N	2.29	0.47
1:D:151:ASN:HB3	1:D:153:ASP:H	1.80	0.47
1:A:132:ARG:CA	1:A:180:GLU:HG2	2.43	0.47
1:D:150:LYS:HG3	1:D:154:VAL:HG21	1.98	0.47
1:E:37:LYS:CG	1:E:108:ARG:HB2	2.45	0.47
1:E:76:ARG:CZ	1:E:130:ILE:HD12	2.44	0.47
1:E:253:TYR:O	1:E:256:ALA:HB3	2.14	0.47
1:A:53:PHE:C	1:A:53:PHE:HD1	2.23	0.46
1:C:149:GLY:O	1:C:150:LYS:HB2	2.15	0.46
1:D:215:PHE:HB3	1:D:295:ARG:HG2	1.97	0.46
1:E:233:ALA:O	1:E:237:PHE:HD1	1.98	0.46
1:A:179:LEU:HD12	1:A:179:LEU:O	2.14	0.46
1:B:65:TYR:CD1	1:B:70:ILE:HD11	2.50	0.46
1:B:232:ILE:HG22	1:B:233:ALA:N	2.30	0.46
1:D:232:ILE:HG22	1:D:233:ALA:N	2.30	0.46
1:E:96:ASP:OD1	1:E:98:THR:HB	2.15	0.46
1:A:27:TYR:CG	1:B:110:LEU:HD11	2.50	0.46
1:A:196:TYR:N	1:A:196:TYR:HD1	2.13	0.46
1:A:225:THR:CG2	1:B:224:VAL:HG23	2.46	0.46
1:A:256:ALA:HB1	1:A:309:LEU:HD21	1.97	0.46
1:E:23:LEU:HB2	1:E:150:LYS:HA	1.96	0.46
1:A:15:LEU:HD12	1:A:16:THR:N	2.30	0.46
1:A:46:TRP:CH2	1:A:72:ILE:HG23	2.49	0.46
1:A:157:THR:HG22	1:B:34:GLU:OE1	2.15	0.46
1:A:221:GLU:OE1	1:A:221:GLU:HA	2.14	0.46
1:E:9:PRO:HD3	1:E:71:TRP:CE3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:179:LEU:HD12	1:E:179:LEU:C	2.40	0.46
1:A:19:THR:HG22	1:A:44:LEU:CD2	2.46	0.46
1:A:23:LEU:HB2	1:A:150:LYS:HA	1.97	0.46
1:B:53:PHE:C	1:B:53:PHE:HD1	2.23	0.46
1:B:204:MET:O	1:B:207:ILE:HG12	2.16	0.46
1:B:215:PHE:HB2	1:B:216:TRP:CE3	2.50	0.46
1:D:270:ILE:HD13	1:D:270:ILE:HA	1.62	0.46
1:E:151:ASN:ND2	1:E:152:ASP:H	2.13	0.46
1:B:226:LEU:HD22	1:B:226:LEU:HA	1.71	0.46
1:D:41:PHE:HE2	1:E:175:LEU:HD23	1.80	0.46
1:A:210:ILE:O	1:A:211:SER:C	2.59	0.46
1:B:23:LEU:HB2	1:B:150:LYS:HA	1.97	0.46
1:B:195:SER:O	1:B:199:ASN:HB2	2.16	0.46
1:D:23:LEU:HG	1:D:164:PHE:CE1	2.50	0.46
1:D:119:PRO:O	1:D:193:TYR:HB3	2.15	0.46
1:D:131:VAL:CG1	1:D:140:VAL:HG13	2.44	0.46
1:D:179:LEU:HD12	1:D:179:LEU:C	2.40	0.46
1:D:215:PHE:HB2	1:D:216:TRP:CE3	2.51	0.46
1:E:51:LEU:HD13	1:E:70:ILE:HD12	1.97	0.46
1:A:224:VAL:C	1:A:226:LEU:H	2.23	0.46
1:C:72:ILE:HG22	1:C:73:PRO:HD2	1.97	0.46
1:C:151:ASN:ND2	1:C:152:ASP:H	2.14	0.46
1:D:53:PHE:C	1:D:53:PHE:HD1	2.22	0.46
1:D:224:VAL:C	1:D:226:LEU:H	2.24	0.46
1:D:282:SER:C	1:D:284:PRO:HD3	2.40	0.46
1:E:123:GLN:HB2	1:E:189:ILE:HG13	1.96	0.46
1:B:204:MET:HE2	1:B:204:MET:HB3	1.80	0.46
1:D:54:ASP:HB2	1:D:57:ARG:CB	2.44	0.46
1:A:196:TYR:N	1:A:196:TYR:CD1	2.84	0.46
1:A:215:PHE:HB2	1:A:216:TRP:CE3	2.51	0.46
1:C:224:VAL:C	1:C:226:LEU:H	2.23	0.46
1:D:53:PHE:CE2	1:D:63:LYS:HB3	2.47	0.46
1:D:200:ILE:CD1	1:D:240:LEU:HD23	2.46	0.46
1:D:253:TYR:CA	1:D:313:PHE:HE2	2.20	0.46
1:C:29:LEU:HD23	1:C:30:ASP:N	2.31	0.45
1:D:196:TYR:N	1:D:196:TYR:HD1	2.14	0.45
1:E:119:PRO:O	1:E:193:TYR:HB3	2.16	0.45
1:A:257:ILE:HG22	1:A:309:LEU:HD23	1.97	0.45
1:B:53:PHE:CE2	1:B:63:LYS:HB3	2.48	0.45
1:B:54:ASP:HB2	1:B:57:ARG:CB	2.46	0.45
1:B:264:PHE:O	1:B:268:ALA:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:TYR:CD1	1:A:70:ILE:HD11	2.50	0.45
1:B:86:ALA:HB2	1:B:105:PHE:HB3	1.98	0.45
1:C:204:MET:HE2	1:C:204:MET:HB3	1.74	0.45
1:C:224:VAL:O	1:C:228:VAL:HB	2.15	0.45
1:C:282:SER:C	1:C:284:PRO:HD3	2.41	0.45
1:D:79:ASN:OD1	1:D:109:VAL:HG12	2.16	0.45
1:A:131:VAL:CG1	1:A:140:VAL:HG13	2.41	0.45
1:A:161:ILE:HA	1:A:189:ILE:HG22	1.99	0.45
1:C:95:PRO:C	1:C:97:GLY:H	2.25	0.45
1:C:96:ASP:OD1	1:C:98:THR:HB	2.17	0.45
1:C:216:TRP:CZ2	1:C:295:ARG:HB3	2.51	0.45
1:D:76:ARG:HH12	1:D:130:ILE:HD11	1.82	0.45
1:E:256:ALA:HB1	1:E:309:LEU:HD21	1.97	0.45
1:A:215:PHE:HB3	1:A:295:ARG:HG2	1.98	0.45
1:B:137:ARG:HD2	1:B:179:LEU:HG	1.98	0.45
1:D:29:LEU:HD23	1:D:30:ASP:N	2.31	0.45
1:D:224:VAL:O	1:D:228:VAL:HB	2.16	0.45
1:A:225:THR:O	1:A:225:THR:HG22	2.17	0.45
1:B:137:ARG:HA	1:B:137:ARG:HD3	1.58	0.45
1:C:37:LYS:CG	1:C:108:ARG:HB2	2.46	0.45
1:C:76:ARG:HH12	1:C:130:ILE:HD11	1.82	0.45
1:D:76:ARG:CZ	1:D:130:ILE:HD12	2.44	0.45
1:B:270:ILE:HD13	1:B:270:ILE:HA	1.64	0.45
1:C:253:TYR:HB2	1:C:313:PHE:HD2	1.82	0.45
1:D:196:TYR:N	1:D:196:TYR:CD1	2.84	0.45
1:E:65:TYR:CD1	1:E:70:ILE:HD11	2.51	0.45
1:E:210:ILE:O	1:E:211:SER:C	2.60	0.45
1:E:215:PHE:HB2	1:E:216:TRP:CE3	2.52	0.45
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.98	0.45
1:A:47:LYS:HB3	1:A:47:LYS:HE2	1.75	0.45
1:A:224:VAL:O	1:A:228:VAL:HB	2.16	0.45
1:C:21:ILE:HA	1:C:41:PHE:O	2.17	0.45
1:D:276:HIS:C	1:D:278:LEU:N	2.71	0.45
1:E:78:VAL:HB	1:E:128:TYR:HB2	1.97	0.45
1:A:255:GLY:O	1:A:258:ILE:HG22	2.17	0.45
1:C:54:ASP:HB2	1:C:57:ARG:CB	2.47	0.45
1:C:226:LEU:HD22	1:C:226:LEU:HA	1.66	0.45
1:C:276:HIS:C	1:C:278:LEU:N	2.71	0.45
1:D:195:SER:HB3	1:E:248:THR:O	2.17	0.45
1:A:213:THR:CG2	1:A:226:LEU:HD11	2.46	0.45
1:C:28:SER:HB2	1:C:37:LYS:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ALA:HB2	1:C:105:PHE:HB3	1.97	0.45
1:D:51:LEU:HD13	1:D:70:ILE:HD12	1.99	0.45
1:E:54:ASP:HB2	1:E:57:ARG:CB	2.47	0.45
1:A:204:MET:HE2	1:A:204:MET:HB3	1.74	0.44
1:A:270:ILE:HD13	1:A:270:ILE:HA	1.63	0.44
1:B:70:ILE:HG22	1:B:71:TRP:N	2.32	0.44
1:B:78:VAL:HB	1:B:128:TYR:HB2	1.97	0.44
1:B:179:LEU:C	1:B:179:LEU:CD1	2.90	0.44
1:D:204:MET:O	1:D:207:ILE:HG12	2.17	0.44
1:E:119:PRO:HB3	1:E:196:TYR:HD2	1.82	0.44
1:A:62:VAL:HG11	1:A:92:SER:HB3	1.98	0.44
1:A:76:ARG:CZ	1:A:130:ILE:HD12	2.45	0.44
1:A:253:TYR:HB2	1:A:313:PHE:HD2	1.81	0.44
1:C:53:PHE:C	1:C:53:PHE:HD1	2.23	0.44
1:D:37:LYS:HG3	1:D:108:ARG:HB2	1.99	0.44
1:D:179:LEU:C	1:D:179:LEU:CD1	2.90	0.44
1:B:86:ALA:HA	1:B:105:PHE:HA	1.98	0.44
1:D:132:ARG:CA	1:D:180:GLU:HG2	2.47	0.44
1:E:179:LEU:C	1:E:179:LEU:CD1	2.90	0.44
1:A:179:LEU:C	1:A:179:LEU:CD1	2.90	0.44
1:B:76:ARG:CZ	1:B:130:ILE:HD12	2.45	0.44
1:D:46:TRP:HH2	1:D:72:ILE:HG23	1.82	0.44
1:D:68:GLU:CD	1:D:68:GLU:N	2.75	0.44
1:E:271:GLU:OE2	1:E:272:VAL:N	2.50	0.44
1:A:79:ASN:OD1	1:A:109:VAL:HG12	2.18	0.44
1:B:147:LYS:CE	1:B:165:THR:HA	2.47	0.44
1:B:210:ILE:O	1:B:211:SER:C	2.59	0.44
1:D:64:THR:O	1:D:64:THR:HG22	2.17	0.44
1:D:125:LEU:HB2	1:D:187:LEU:HB3	1.99	0.44
1:D:212:TRP:HB2	1:D:215:PHE:CE1	2.52	0.44
1:C:89:VAL:CG2	1:D:76:ARG:HD3	2.48	0.44
1:D:48:ASP:C	1:D:50:ARG:N	2.74	0.44
1:D:132:ARG:HH22	1:D:176:GLU:HB2	1.83	0.44
1:D:224:VAL:C	1:D:226:LEU:N	2.73	0.44
1:D:226:LEU:HD23	1:E:224:VAL:HB	1.99	0.44
1:D:261:ILE:HD13	1:D:302:PHE:HE1	1.82	0.44
1:A:151:ASN:ND2	1:A:152:ASP:H	2.15	0.44
1:C:118:TYR:HB3	1:C:119:PRO:HD3	1.99	0.44
1:C:240:LEU:HD22	1:D:239:ILE:HG12	1.99	0.44
1:A:42:LEU:HD23	1:A:103:GLU:OE1	2.17	0.44
1:A:202:LEU:HD12	1:B:259:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ALA:HB1	1:B:309:LEU:HD21	1.99	0.44
1:C:105:PHE:HD1	1:C:105:PHE:H	1.64	0.44
1:C:155:PHE:HD1	1:D:110:LEU:HD22	1.83	0.44
1:C:179:LEU:C	1:C:179:LEU:CD1	2.90	0.44
1:D:48:ASP:O	1:D:50:ARG:N	2.51	0.44
1:D:226:LEU:HD22	1:D:226:LEU:HA	1.67	0.44
1:B:37:LYS:CG	1:B:108:ARG:HB2	2.48	0.44
1:C:70:ILE:HG22	1:C:71:TRP:N	2.33	0.44
1:C:161:ILE:HA	1:C:189:ILE:HG22	1.99	0.44
1:D:149:GLY:O	1:D:150:LYS:CB	2.66	0.44
1:A:202:LEU:O	1:A:203:PRO:C	2.61	0.43
1:B:131:VAL:CG1	1:B:140:VAL:HG13	2.41	0.43
1:B:257:ILE:HG22	1:B:309:LEU:HD23	2.00	0.43
1:C:86:ALA:HA	1:C:105:PHE:HA	2.00	0.43
1:A:29:LEU:HD23	1:A:30:ASP:N	2.33	0.43
1:A:81:GLU:HG3	1:A:108:ARG:CG	2.45	0.43
1:A:118:TYR:HB3	1:A:119:PRO:HD3	1.99	0.43
1:A:215:PHE:CE1	1:A:298:PHE:CD1	3.07	0.43
1:A:222:ALA:HB2	1:B:221:GLU:CA	2.30	0.43
1:B:19:THR:HA	1:B:43:SER:O	2.17	0.43
1:B:196:TYR:N	1:B:196:TYR:HD1	2.16	0.43
1:C:27:TYR:CE1	1:D:81:GLU:OE1	2.72	0.43
1:E:291:THR:O	1:E:295:ARG:HG3	2.18	0.43
1:A:170:PRO:HB3	1:A:183:LEU:CD2	2.48	0.43
1:A:260:MET:HE2	1:A:309:LEU:HD22	2.00	0.43
1:B:96:ASP:OD1	1:B:98:THR:HB	2.17	0.43
1:D:79:ASN:OD1	1:D:109:VAL:CG1	2.66	0.43
1:E:46:TRP:CH2	1:E:72:ILE:HG23	2.53	0.43
1:A:86:ALA:HA	1:A:105:PHE:HA	2.00	0.43
1:B:47:LYS:HB3	1:B:47:LYS:HE2	1.73	0.43
1:B:249:PRO:HD2	1:B:250:TYR:CE1	2.53	0.43
1:D:86:ALA:HA	1:D:105:PHE:HA	2.00	0.43
1:D:86:ALA:HB2	1:D:105:PHE:HB3	2.00	0.43
1:D:260:MET:HE2	1:D:309:LEU:HD22	2.01	0.43
1:E:72:ILE:HG22	1:E:73:PRO:HD2	2.00	0.43
1:E:196:TYR:N	1:E:196:TYR:HD1	2.17	0.43
1:E:204:MET:HE2	1:E:204:MET:HB3	1.75	0.43
1:A:226:LEU:CD2	1:B:228:VAL:HG21	2.47	0.43
1:B:23:LEU:HA	1:B:40:ALA:HB2	2.00	0.43
1:B:28:SER:HB2	1:B:37:LYS:HD2	2.00	0.43
1:C:264:PHE:O	1:C:268:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:PHE:HB2	1:D:84:ARG:HD2	2.00	0.43
1:D:155:PHE:CE1	1:E:112:PRO:CB	2.83	0.43
1:E:86:ALA:HA	1:E:105:PHE:HA	2.00	0.43
1:A:70:ILE:HG22	1:A:71:TRP:N	2.33	0.43
1:A:86:ALA:HB2	1:A:105:PHE:HB3	2.00	0.43
1:C:37:LYS:HG2	1:C:108:ARG:HB2	1.99	0.43
1:C:131:VAL:CG1	1:C:140:VAL:HG13	2.43	0.43
1:E:276:HIS:C	1:E:278:LEU:N	2.71	0.43
1:A:78:VAL:CG2	1:A:130:ILE:HG12	2.37	0.43
1:A:139:ILE:HG12	1:A:172:ASN:HD21	1.84	0.43
1:A:194:PHE:HE2	1:B:250:TYR:O	2.01	0.43
1:B:95:PRO:C	1:B:97:GLY:H	2.27	0.43
1:C:157:THR:HG22	1:D:34:GLU:OE1	2.19	0.43
1:D:233:ALA:O	1:D:237:PHE:HD1	2.02	0.43
1:D:286:ARG:O	1:D:289:SER:HB3	2.18	0.43
1:E:212:TRP:HB2	1:E:215:PHE:CE1	2.53	0.43
1:B:76:ARG:NH1	1:B:130:ILE:HD11	2.33	0.43
1:E:131:VAL:CG1	1:E:140:VAL:HG13	2.42	0.43
1:E:283:GLN:O	1:E:283:GLN:HG2	2.19	0.43
1:A:28:SER:HB2	1:A:37:LYS:HD2	2.01	0.43
1:D:157:THR:CG2	1:E:34:GLU:OE1	2.66	0.43
1:E:28:SER:HB2	1:E:37:LYS:HD2	2.01	0.43
1:E:70:ILE:HG22	1:E:71:TRP:O	2.18	0.43
1:A:76:ARG:HH12	1:A:130:ILE:HD11	1.83	0.42
1:A:261:ILE:HD13	1:A:302:PHE:HE1	1.84	0.42
1:C:238:ASN:HA	1:C:258:ILE:HD13	2.00	0.42
1:D:28:SER:HB2	1:D:37:LYS:HD2	2.01	0.42
1:E:238:ASN:HA	1:E:258:ILE:HD13	2.01	0.42
1:A:155:PHE:CZ	1:B:112:PRO:CB	2.87	0.42
1:B:29:LEU:HD23	1:B:30:ASP:N	2.34	0.42
1:B:51:LEU:HD13	1:B:70:ILE:HD12	2.00	0.42
1:C:132:ARG:CA	1:C:180:GLU:HG2	2.45	0.42
1:C:291:THR:O	1:C:295:ARG:HG3	2.19	0.42
1:D:215:PHE:CE1	1:D:298:PHE:CD1	3.08	0.42
1:E:25:GLU:HB2	1:E:39:ASN:HB3	2.01	0.42
1:E:268:ALA:HA	1:E:298:PHE:HE1	1.85	0.42
1:A:21:ILE:HA	1:A:41:PHE:O	2.19	0.42
1:A:286:ARG:O	1:A:289:SER:HB3	2.19	0.42
1:B:23:LEU:HG	1:B:164:PHE:CE1	2.55	0.42
1:E:150:LYS:HG2	1:E:154:VAL:HG21	2.01	0.42
1:E:224:VAL:O	1:E:228:VAL:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:HG3	1:B:176:GLU:CG	2.50	0.42
1:B:293:ALA:O	1:B:294:SER:C	2.62	0.42
1:C:119:PRO:HB3	1:C:196:TYR:HD2	1.84	0.42
1:C:210:ILE:O	1:C:211:SER:C	2.63	0.42
1:B:42:LEU:HD23	1:B:103:GLU:OE1	2.19	0.42
1:B:170:PRO:HB3	1:B:183:LEU:CD2	2.49	0.42
1:B:291:THR:O	1:B:295:ARG:HG3	2.20	0.42
1:C:78:VAL:CG2	1:C:130:ILE:HG12	2.36	0.42
1:D:54:ASP:CB	1:D:57:ARG:HG3	2.44	0.42
1:D:291:THR:O	1:D:295:ARG:HG3	2.19	0.42
1:A:15:LEU:O	1:A:15:LEU:HG	2.20	0.42
1:A:198:PRO:HG2	1:B:251:MET:HE1	1.99	0.42
1:B:196:TYR:N	1:B:196:TYR:CD1	2.87	0.42
1:C:79:ASN:OD1	1:C:109:VAL:HG12	2.19	0.42
1:D:105:PHE:HD1	1:D:105:PHE:H	1.66	0.42
1:A:291:THR:O	1:A:295:ARG:HG3	2.20	0.42
1:B:13:GLU:OE1	1:B:14:PRO:HD3	2.19	0.42
1:B:213:THR:CG2	1:B:226:LEU:HD11	2.48	0.42
1:C:62:VAL:HG13	1:C:93:VAL:O	2.20	0.42
1:C:261:ILE:HD13	1:C:302:PHE:HE1	1.84	0.42
1:E:47:LYS:HE2	1:E:47:LYS:HB3	1.71	0.42
1:E:215:PHE:CE1	1:E:298:PHE:CD1	3.07	0.42
1:A:203:PRO:HB3	1:B:262:TYR:CZ	2.55	0.42
1:B:253:TYR:HB2	1:B:313:PHE:HD2	1.85	0.42
1:B:286:ARG:O	1:B:289:SER:HB3	2.20	0.42
1:C:202:LEU:HD22	1:C:202:LEU:HA	1.86	0.42
1:D:62:VAL:HG11	1:D:92:SER:HB3	2.01	0.42
1:D:95:PRO:O	1:D:97:GLY:N	2.53	0.42
1:E:76:ARG:NH1	1:E:130:ILE:HD11	2.34	0.42
1:E:261:ILE:HD13	1:E:302:PHE:HE1	1.84	0.42
1:B:62:VAL:HG11	1:B:92:SER:HB3	2.02	0.42
1:C:202:LEU:O	1:C:203:PRO:C	2.62	0.42
1:A:105:PHE:HD1	1:A:105:PHE:H	1.67	0.41
1:B:155:PHE:HB3	1:B:156:LEU:H	1.68	0.41
1:B:225:THR:HG21	1:C:224:VAL:HG23	2.02	0.41
1:C:9:PRO:HD3	1:C:71:TRP:CE3	2.54	0.41
1:D:312:LEU:HD12	1:D:312:LEU:HA	1.86	0.41
1:E:196:TYR:N	1:E:196:TYR:CD1	2.87	0.41
1:E:270:ILE:HD13	1:E:270:ILE:HA	1.60	0.41
1:A:48:ASP:C	1:A:50:ARG:N	2.78	0.41
1:B:132:ARG:HH22	1:B:176:GLU:HB2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:PHE:CD1	1:D:110:LEU:CD2	3.02	0.41
1:D:156:LEU:HD12	1:D:156:LEU:HA	1.87	0.41
1:D:278:LEU:HD23	1:D:287:ALA:HA	2.02	0.41
1:E:226:LEU:HD22	1:E:226:LEU:HA	1.67	0.41
1:B:23:LEU:HD22	1:B:38:VAL:CG2	2.49	0.41
1:B:118:TYR:HB3	1:B:119:PRO:HD3	2.01	0.41
1:C:196:TYR:O	1:C:200:ILE:HB	2.20	0.41
1:C:263:LEU:C	1:C:265:TYR:H	2.27	0.41
1:C:278:LEU:HD23	1:C:287:ALA:HA	2.02	0.41
1:D:42:LEU:HD23	1:D:103:GLU:OE1	2.20	0.41
1:E:164:PHE:HD2	1:E:186:GLN:O	2.02	0.41
1:A:240:LEU:HD22	1:B:239:ILE:HG12	2.02	0.41
1:B:37:LYS:HG3	1:B:108:ARG:HB2	2.02	0.41
1:B:151:ASN:ND2	1:B:152:ASP:H	2.16	0.41
1:C:19:THR:HA	1:C:43:SER:O	2.20	0.41
1:C:27:TYR:CE1	1:D:81:GLU:CD	2.99	0.41
1:C:70:ILE:HD13	1:C:70:ILE:N	2.35	0.41
1:D:23:LEU:HD22	1:D:38:VAL:CG2	2.51	0.41
1:D:72:ILE:HG22	1:D:73:PRO:HD2	2.02	0.41
1:E:21:ILE:HA	1:E:41:PHE:O	2.20	0.41
1:E:253:TYR:CA	1:E:313:PHE:HE2	2.22	0.41
1:A:77:PHE:CG	1:A:84:ARG:HD2	2.54	0.41
1:C:170:PRO:HB3	1:C:183:LEU:CD2	2.50	0.41
1:E:274:VAL:C	1:E:276:HIS:N	2.79	0.41
1:A:54:ASP:HB2	1:A:57:ARG:CB	2.50	0.41
1:A:269:VAL:HA	1:A:272:VAL:HG22	2.02	0.41
1:A:278:LEU:HD23	1:A:287:ALA:HA	2.02	0.41
1:B:46:TRP:CH2	1:B:72:ILE:HG23	2.54	0.41
1:B:294:SER:C	1:B:296:ILE:N	2.77	0.41
1:E:128:TYR:O	1:E:183:LEU:O	2.39	0.41
1:A:23:LEU:HD22	1:A:38:VAL:CG2	2.51	0.41
1:A:157:THR:HG21	1:B:34:GLU:CD	2.44	0.41
1:A:158:GLY:HA2	1:A:192:GLN:OE1	2.21	0.41
1:C:62:VAL:HG11	1:C:92:SER:HB3	2.03	0.41
1:C:212:TRP:HB2	1:C:215:PHE:CE1	2.55	0.41
1:C:286:ARG:O	1:C:289:SER:HB3	2.21	0.41
1:C:293:ALA:O	1:C:294:SER:C	2.63	0.41
1:E:42:LEU:HD23	1:E:103:GLU:OE1	2.21	0.41
1:E:260:MET:HE2	1:E:309:LEU:HD22	2.02	0.41
1:A:149:GLY:O	1:A:150:LYS:CB	2.68	0.41
1:D:9:PRO:HD3	1:D:71:TRP:CE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:ARG:O	1:E:289:SER:HB3	2.21	0.41
1:A:23:LEU:HA	1:A:40:ALA:HB2	2.03	0.41
1:A:68:GLU:CD	1:A:68:GLU:N	2.79	0.41
1:A:76:ARG:NH1	1:A:130:ILE:HD11	2.36	0.41
1:A:95:PRO:C	1:A:97:GLY:H	2.29	0.41
1:B:70:ILE:HG22	1:B:71:TRP:O	2.21	0.41
1:B:132:ARG:CA	1:B:180:GLU:HG2	2.47	0.41
1:B:196:TYR:O	1:B:201:ILE:HG12	2.19	0.41
1:B:215:PHE:CE1	1:B:298:PHE:CD1	3.08	0.41
1:C:215:PHE:CE1	1:C:298:PHE:CD1	3.09	0.41
1:C:270:ILE:HD13	1:C:270:ILE:HA	1.66	0.41
1:D:269:VAL:HA	1:D:272:VAL:HG22	2.02	0.41
1:E:23:LEU:HD22	1:E:38:VAL:CG2	2.51	0.41
1:E:249:PRO:HD2	1:E:250:TYR:CE1	2.56	0.41
1:A:119:PRO:HB3	1:A:196:TYR:HD2	1.86	0.41
1:A:195:SER:HB3	1:B:248:THR:O	2.20	0.41
1:A:225:THR:HG22	1:B:224:VAL:HG23	2.03	0.41
1:B:202:LEU:O	1:B:203:PRO:C	2.62	0.41
1:C:137:ARG:HD3	1:C:137:ARG:HA	1.55	0.41
1:D:23:LEU:HA	1:D:40:ALA:HB2	2.02	0.41
1:E:202:LEU:O	1:E:203:PRO:C	2.64	0.41
1:A:140:VAL:HG22	1:A:181:SER:CB	2.51	0.40
1:B:19:THR:HG22	1:B:44:LEU:CD2	2.51	0.40
1:B:210:ILE:HG13	1:C:266:PHE:HE1	1.85	0.40
1:C:23:LEU:HD22	1:C:38:VAL:CG2	2.51	0.40
1:C:197:ILE:CB	1:C:198:PRO:HD3	2.49	0.40
1:D:94:SER:OG	1:D:95:PRO:CD	2.67	0.40
1:D:204:MET:HE2	1:D:204:MET:HB3	1.72	0.40
1:D:296:ILE:HD13	1:D:296:ILE:HA	1.93	0.40
1:E:263:LEU:C	1:E:265:TYR:H	2.28	0.40
1:B:149:GLY:O	1:B:150:LYS:CB	2.70	0.40
1:B:290:ILE:O	1:B:291:THR:C	2.64	0.40
1:D:15:LEU:HD12	1:D:16:THR:N	2.36	0.40
1:D:47:LYS:HE2	1:D:47:LYS:HB3	1.70	0.40
1:D:264:PHE:O	1:D:268:ALA:HB2	2.22	0.40
1:E:132:ARG:CA	1:E:180:GLU:HG2	2.46	0.40
1:E:278:LEU:HD23	1:E:287:ALA:HA	2.02	0.40
1:A:118:TYR:CZ	1:A:196:TYR:HE2	2.40	0.40
1:A:140:VAL:HG22	1:A:181:SER:HB3	2.03	0.40
1:A:194:PHE:CE2	1:B:250:TYR:C	3.00	0.40
1:A:233:ALA:O	1:A:237:PHE:HD1	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:TRP:HB2	1:B:215:PHE:CE1	2.56	0.40
1:C:118:TYR:CZ	1:C:196:TYR:HE2	2.40	0.40
1:D:287:ALA:C	1:D:289:SER:H	2.29	0.40
1:E:290:ILE:O	1:E:291:THR:C	2.64	0.40
1:A:70:ILE:HG22	1:A:71:TRP:O	2.21	0.40
1:A:140:VAL:HG22	1:A:181:SER:OG	2.21	0.40
1:A:155:PHE:HE1	1:B:112:PRO:CA	2.34	0.40
1:A:217:SER:OG	1:B:220:TYR:HE2	1.96	0.40
1:A:260:MET:CE	1:A:309:LEU:HD22	2.51	0.40
1:A:263:LEU:C	1:A:265:TYR:H	2.29	0.40
1:A:296:ILE:HD13	1:A:296:ILE:HA	1.95	0.40
1:C:47:LYS:HE2	1:C:47:LYS:HB3	1.72	0.40
1:C:68:GLU:CD	1:C:68:GLU:N	2.79	0.40
1:C:170:PRO:HB3	1:C:183:LEU:HD23	2.03	0.40
1:C:210:ILE:HD12	1:D:231:LEU:CD2	2.51	0.40
1:C:253:TYR:CA	1:C:313:PHE:HE2	2.23	0.40
1:D:76:ARG:NH1	1:D:130:ILE:HD11	2.37	0.40
1:E:15:LEU:O	1:E:15:LEU:HG	2.16	0.40
1:E:105:PHE:H	1:E:105:PHE:HD1	1.67	0.40
1:E:269:VAL:HA	1:E:272:VAL:HG22	2.03	0.40
1:E:287:ALA:C	1:E:289:SER:H	2.27	0.40
1:A:37:LYS:HG3	1:A:108:ARG:HB2	2.02	0.40
1:B:62:VAL:HG13	1:B:93:VAL:O	2.22	0.40
1:B:70:ILE:N	1:B:70:ILE:HD13	2.35	0.40
1:B:150:LYS:HG2	1:B:154:VAL:HG21	2.03	0.40
1:C:151:ASN:HD22	1:C:152:ASP:N	2.18	0.40
1:D:222:ALA:HB3	1:E:220:TYR:CD2	2.56	0.40
1:E:48:ASP:C	1:E:50:ARG:N	2.80	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	308/317 (97%)	245 (80%)	56 (18%)	7 (2%)	5	30
1	B	308/317 (97%)	250 (81%)	51 (17%)	7 (2%)	5	30
1	C	308/317 (97%)	249 (81%)	52 (17%)	7 (2%)	5	30
1	D	308/317 (97%)	253 (82%)	47 (15%)	8 (3%)	4	27
1	E	308/317 (97%)	250 (81%)	52 (17%)	6 (2%)	6	33
All	All	1540/1585 (97%)	1247 (81%)	258 (17%)	35 (2%)	5	30

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	TYR
1	A	150	LYS
1	A	194	PHE
1	B	118	TYR
1	B	150	LYS
1	B	194	PHE
1	C	118	TYR
1	C	150	LYS
1	C	194	PHE
1	D	118	TYR
1	D	148	VAL
1	D	150	LYS
1	D	194	PHE
1	E	118	TYR
1	E	148	VAL
1	E	150	LYS
1	E	194	PHE
1	A	148	VAL
1	A	277	TYR
1	B	148	VAL
1	B	277	TYR
1	C	148	VAL
1	C	277	TYR
1	D	277	TYR
1	E	277	TYR
1	A	275	GLN
1	B	275	GLN
1	C	275	GLN
1	D	96	ASP
1	D	275	GLN
1	E	275	GLN

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Mol	Chain	Res	Type
1	A	49	ARG
1	B	155	PHE
1	C	287	ALA
1	D	287	ALA

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	278/284 (98%)	230 (83%)	48 (17%)	2	11
1	B	278/284 (98%)	230 (83%)	48 (17%)	2	11
1	C	278/284 (98%)	229 (82%)	49 (18%)	2	11
1	D	278/284 (98%)	230 (83%)	48 (17%)	2	11
1	E	278/284 (98%)	229 (82%)	49 (18%)	2	11
All	All	1390/1420 (98%)	1148 (83%)	242 (17%)	2	11

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	26	CYS
1	A	47	LYS
1	A	51	LEU
1	A	53	PHE
1	A	57	ARG
1	A	58	SER
1	A	64	THR
1	A	68	GLU
1	A	72	ILE
1	A	84	ARG
1	A	89	VAL
1	A	98	THR
1	A	99	VAL
1	A	100	GLN

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Mol	Chain	Res	Type
1	A	108	ARG
1	A	113	LEU
1	A	122	SER
1	A	124	THR
1	A	130	ILE
1	A	140	VAL
1	A	141	LEU
1	A	151	ASN
1	A	154	VAL
1	A	177	ASP
1	A	179	LEU
1	A	202	LEU
1	A	204	MET
1	A	211	SER
1	A	213	THR
1	A	221	GLU
1	A	226	LEU
1	A	232	ILE
1	A	239	ILE
1	A	243	THR
1	A	245	LEU
1	A	252	THR
1	A	254	THR
1	A	257	ILE
1	A	263	LEU
1	A	269	VAL
1	A	270	ILE
1	A	274	VAL
1	A	292	ARG
1	A	303	LEU
1	A	304	LEU
1	A	306	ASN
1	A	314	PHE
1	B	16	THR
1	B	26	CYS
1	B	47	LYS
1	B	51	LEU
1	B	53	PHE
1	B	58	SER
1	B	64	THR
1	B	68	GLU
1	B	72	ILE

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Mol	Chain	Res	Type
1	B	84	ARG
1	B	89	VAL
1	B	98	THR
1	B	99	VAL
1	B	100	GLN
1	B	108	ARG
1	B	113	LEU
1	B	122	SER
1	B	124	THR
1	B	130	ILE
1	B	140	VAL
1	B	141	LEU
1	B	151	ASN
1	B	154	VAL
1	B	162	GLU
1	B	179	LEU
1	B	190	SER
1	B	202	LEU
1	B	204	MET
1	B	211	SER
1	B	213	THR
1	B	221	GLU
1	B	226	LEU
1	B	232	ILE
1	B	239	ILE
1	B	243	THR
1	B	245	LEU
1	B	252	THR
1	B	254	THR
1	B	257	ILE
1	B	263	LEU
1	B	269	VAL
1	B	270	ILE
1	B	274	VAL
1	B	292	ARG
1	B	303	LEU
1	B	304	LEU
1	B	306	ASN
1	B	314	PHE
1	C	15	LEU
1	C	16	THR
1	C	26	CYS

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Mol	Chain	Res	Type
1	C	47	LYS
1	C	51	LEU
1	C	53	PHE
1	C	57	ARG
1	C	58	SER
1	C	64	THR
1	C	68	GLU
1	C	72	ILE
1	C	84	ARG
1	C	89	VAL
1	C	98	THR
1	C	99	VAL
1	C	100	GLN
1	C	108	ARG
1	C	113	LEU
1	C	122	SER
1	C	124	THR
1	C	130	ILE
1	C	140	VAL
1	C	141	LEU
1	C	151	ASN
1	C	154	VAL
1	C	179	LEU
1	C	202	LEU
1	C	204	MET
1	C	211	SER
1	C	213	THR
1	C	221	GLU
1	C	226	LEU
1	C	232	ILE
1	C	239	ILE
1	C	243	THR
1	C	245	LEU
1	C	252	THR
1	C	254	THR
1	C	257	ILE
1	C	260	MET
1	C	263	LEU
1	C	269	VAL
1	C	270	ILE
1	C	274	VAL
1	C	292	ARG

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Mol	Chain	Res	Type
1	C	303	LEU
1	C	304	LEU
1	C	306	ASN
1	C	314	PHE
1	D	16	THR
1	D	26	CYS
1	D	47	LYS
1	D	51	LEU
1	D	53	PHE
1	D	58	SER
1	D	64	THR
1	D	68	GLU
1	D	72	ILE
1	D	84	ARG
1	D	89	VAL
1	D	98	THR
1	D	99	VAL
1	D	100	GLN
1	D	108	ARG
1	D	113	LEU
1	D	122	SER
1	D	124	THR
1	D	130	ILE
1	D	140	VAL
1	D	141	LEU
1	D	151	ASN
1	D	154	VAL
1	D	162	GLU
1	D	177	ASP
1	D	179	LEU
1	D	202	LEU
1	D	204	MET
1	D	211	SER
1	D	213	THR
1	D	221	GLU
1	D	226	LEU
1	D	232	ILE
1	D	239	ILE
1	D	243	THR
1	D	245	LEU
1	D	252	THR
1	D	254	THR

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Mol	Chain	Res	Type
1	D	257	ILE
1	D	263	LEU
1	D	269	VAL
1	D	270	ILE
1	D	274	VAL
1	D	292	ARG
1	D	303	LEU
1	D	304	LEU
1	D	306	ASN
1	D	314	PHE
1	E	15	LEU
1	E	16	THR
1	E	26	CYS
1	E	47	LYS
1	E	51	LEU
1	E	53	PHE
1	E	57	ARG
1	E	58	SER
1	E	64	THR
1	E	68	GLU
1	E	72	ILE
1	E	84	ARG
1	E	89	VAL
1	E	98	THR
1	E	99	VAL
1	E	100	GLN
1	E	108	ARG
1	E	113	LEU
1	E	122	SER
1	E	124	THR
1	E	130	ILE
1	E	140	VAL
1	E	141	LEU
1	E	151	ASN
1	E	154	VAL
1	E	162	GLU
1	E	179	LEU
1	E	202	LEU
1	E	204	MET
1	E	211	SER
1	E	213	THR
1	E	221	GLU

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Mol	Chain	Res	Type
1	E	226	LEU
1	E	232	ILE
1	E	239	ILE
1	E	243	THR
1	E	245	LEU
1	E	252	THR
1	E	254	THR
1	E	257	ILE
1	E	263	LEU
1	E	269	VAL
1	E	270	ILE
1	E	274	VAL
1	E	292	ARG
1	E	303	LEU
1	E	304	LEU
1	E	306	ASN
1	E	314	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	100	GLN
1	A	151	ASN
1	A	238	ASN
1	A	244	ASN
1	B	18	ASN
1	B	100	GLN
1	B	151	ASN
1	B	238	ASN
1	B	244	ASN
1	C	18	ASN
1	C	100	GLN
1	C	151	ASN
1	C	238	ASN
1	C	244	ASN
1	D	100	GLN
1	D	151	ASN
1	D	244	ASN
1	E	100	GLN
1	E	151	ASN
1	E	238	ASN

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Mol	Chain	Res	Type
1	E	244	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	310/317 (97%)	1.20	58 (18%) 3 4	64, 106, 164, 215	0
1	B	310/317 (97%)	1.17	66 (21%) 2 3	69, 106, 164, 215	0
1	C	310/317 (97%)	1.07	60 (19%) 3 3	66, 106, 163, 215	0
1	D	310/317 (97%)	1.31	77 (24%) 2 2	66, 105, 164, 215	0
1	E	310/317 (97%)	1.24	62 (20%) 3 3	70, 106, 164, 215	0
All	All	1550/1585 (97%)	1.20	323 (20%) 2 3	64, 106, 164, 215	0

All (323) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	VAL	8.8
1	B	152	ASP	7.8
1	D	153	ASP	7.8
1	E	144	ASP	7.7
1	C	144	ASP	7.3
1	D	11	ALA	7.3
1	B	144	ASP	7.0
1	E	147	LYS	6.9
1	A	153	ASP	6.7
1	C	60	VAL	6.4
1	A	144	ASP	6.1
1	A	206	PHE	5.8
1	B	148	VAL	5.7
1	A	59	GLY	5.4
1	A	11	ALA	5.4
1	A	58	SER	5.4
1	D	144	ASP	5.4
1	A	74	GLU	5.2
1	B	231	LEU	5.2
1	B	47	LYS	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	49	ARG	5.1
1	D	263	LEU	5.0
1	E	148	VAL	4.9
1	C	59	GLY	4.9
1	E	149	GLY	4.8
1	B	153	ASP	4.6
1	C	83	ALA	4.5
1	B	100	GLN	4.5
1	C	153	ASP	4.5
1	A	221	GLU	4.5
1	E	114	ASP	4.5
1	D	112	PRO	4.4
1	D	148	VAL	4.4
1	B	232	ILE	4.4
1	C	147	LYS	4.3
1	D	117	ARG	4.3
1	D	78	VAL	4.3
1	A	13	GLU	4.3
1	B	117	ARG	4.2
1	D	83	ALA	4.1
1	A	88	VAL	4.1
1	B	90	ASP	4.1
1	C	221	GLU	4.1
1	C	85	ASP	4.0
1	D	57	ARG	4.0
1	D	60	VAL	4.0
1	D	187	LEU	3.9
1	D	304	LEU	3.9
1	A	134	VAL	3.9
1	C	229	SER	3.9
1	B	11	ALA	3.9
1	E	232	ILE	3.9
1	E	11	ALA	3.9
1	C	13	GLU	3.8
1	A	230	THR	3.8
1	C	11	ALA	3.8
1	C	233	ALA	3.8
1	D	128	TYR	3.8
1	A	229	SER	3.8
1	C	114	ASP	3.8
1	E	47	LYS	3.7
1	A	224	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	231	LEU	3.7
1	D	316	PHE	3.7
1	E	222	ALA	3.7
1	A	148	VAL	3.7
1	B	101	TYR	3.7
1	D	85	ASP	3.6
1	E	7	PRO	3.6
1	B	74	GLU	3.6
1	C	117	ARG	3.6
1	D	111	SER	3.6
1	D	126	HIS	3.6
1	B	136	THR	3.5
1	A	7	PRO	3.5
1	C	55	PRO	3.5
1	D	100	GLN	3.5
1	A	117	ARG	3.5
1	B	7	PRO	3.5
1	D	241	VAL	3.5
1	E	20	GLY	3.5
1	A	208	LEU	3.4
1	D	134	VAL	3.4
1	A	79	ASN	3.4
1	D	7	PRO	3.4
1	E	45	SER	3.4
1	E	282	SER	3.4
1	A	12	ASP	3.4
1	B	135	ASP	3.4
1	B	88	VAL	3.3
1	C	279	LYS	3.3
1	D	227	VAL	3.3
1	E	88	VAL	3.3
1	E	61	ARG	3.3
1	E	18	ASN	3.3
1	C	242	GLU	3.3
1	A	207	ILE	3.2
1	A	177	ASP	3.2
1	B	314	PHE	3.2
1	E	83	ALA	3.2
1	E	184	ASP	3.2
1	D	277	TYR	3.2
1	A	233	ALA	3.2
1	E	315	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	59	GLY	3.1
1	A	64	THR	3.1
1	C	288	ALA	3.1
1	D	169	LYS	3.1
1	D	56	VAL	3.1
1	D	82	ASN	3.1
1	B	222	ALA	3.1
1	C	138	ASN	3.1
1	B	96	ASP	3.1
1	E	174	ALA	3.0
1	E	139	ILE	3.0
1	E	146	GLU	3.0
1	A	90	ASP	3.0
1	D	12	ASP	3.0
1	D	230	THR	3.0
1	A	145	LEU	3.0
1	A	187	LEU	3.0
1	C	121	ASP	3.0
1	C	18	ASN	3.0
1	B	97	GLY	3.0
1	B	177	ASP	3.0
1	E	116	ARG	2.9
1	E	277	TYR	2.9
1	A	87	ASP	2.9
1	E	173	PHE	2.9
1	B	315	GLY	2.9
1	B	26	CYS	2.9
1	A	203	PRO	2.9
1	E	59	GLY	2.9
1	C	139	ILE	2.9
1	E	126	HIS	2.8
1	E	128	TYR	2.8
1	B	301	VAL	2.8
1	C	176	GLU	2.8
1	C	141	LEU	2.8
1	A	169	LYS	2.8
1	C	169	LYS	2.8
1	A	143	VAL	2.8
1	B	138	ASN	2.8
1	B	221	GLU	2.8
1	B	173	PHE	2.8
1	E	316	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	55	PRO	2.8
1	E	195	SER	2.8
1	A	126	HIS	2.8
1	B	187	LEU	2.8
1	D	49	ARG	2.7
1	A	165	THR	2.7
1	D	308	ILE	2.7
1	B	154	VAL	2.7
1	D	79	ASN	2.7
1	B	216	TRP	2.7
1	D	195	SER	2.7
1	B	266	PHE	2.7
1	C	168	VAL	2.7
1	B	277	TYR	2.7
1	E	32	LYS	2.7
1	E	311	PHE	2.7
1	B	12	ASP	2.7
1	B	174	ALA	2.7
1	C	137	ARG	2.7
1	D	310	ALA	2.7
1	A	139	ILE	2.7
1	D	162	GLU	2.7
1	E	56	VAL	2.7
1	E	49	ARG	2.7
1	A	10	ILE	2.7
1	C	277	TYR	2.7
1	C	151	ASN	2.7
1	B	61	ARG	2.6
1	C	116	ARG	2.6
1	A	14	PRO	2.6
1	B	305	ALA	2.6
1	D	124	THR	2.6
1	B	45	SER	2.6
1	D	130	ILE	2.6
1	E	96	ASP	2.6
1	A	62	VAL	2.6
1	E	301	VAL	2.6
1	A	95	PRO	2.6
1	B	316	PHE	2.6
1	E	221	GLU	2.5
1	B	304	LEU	2.5
1	E	113	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	178	ARG	2.5
1	A	282	SER	2.5
1	B	25	GLU	2.5
1	C	74	GLU	2.5
1	E	242	GLU	2.5
1	D	147	LYS	2.5
1	C	58	SER	2.5
1	D	55	PRO	2.5
1	B	91	ILE	2.5
1	C	10	ILE	2.5
1	C	316	PHE	2.5
1	C	7	PRO	2.5
1	C	14	PRO	2.5
1	C	135	ASP	2.5
1	D	61	ARG	2.5
1	D	63	LYS	2.5
1	D	182	LYS	2.5
1	C	54	ASP	2.5
1	E	243	THR	2.5
1	A	209	PHE	2.4
1	B	146	GLU	2.4
1	D	13	GLU	2.4
1	D	151	ASN	2.4
1	B	56	VAL	2.4
1	A	220	TYR	2.4
1	D	186	GLN	2.4
1	A	91	ILE	2.4
1	B	207	ILE	2.4
1	C	244	ASN	2.4
1	D	152	ASP	2.4
1	C	25	GLU	2.4
1	C	81	GLU	2.4
1	E	305	ALA	2.4
1	B	225	THR	2.4
1	E	87	ASP	2.4
1	E	101	TYR	2.4
1	A	110	LEU	2.4
1	B	48	ASP	2.4
1	B	87	ASP	2.4
1	E	25	GLU	2.4
1	E	186	GLN	2.3
1	C	16	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	225	THR	2.3
1	A	163	SER	2.3
1	D	168	VAL	2.3
1	A	316	PHE	2.3
1	B	179	LEU	2.3
1	D	276	HIS	2.3
1	B	228	VAL	2.3
1	D	52	ALA	2.3
1	D	118	TYR	2.3
1	A	66	GLU	2.3
1	C	118	TYR	2.3
1	D	53	PHE	2.3
1	C	275	GLN	2.3
1	C	148	VAL	2.3
1	D	47	LYS	2.3
1	C	172	ASN	2.3
1	D	173	PHE	2.3
1	E	115	PHE	2.3
1	D	166	ALA	2.3
1	E	275	GLN	2.3
1	C	146	GLU	2.3
1	A	154	VAL	2.3
1	B	55	PRO	2.3
1	D	315	GLY	2.3
1	A	61	ARG	2.3
1	B	137	ARG	2.3
1	C	303	LEU	2.2
1	D	221	GLU	2.2
1	B	141	LEU	2.2
1	D	183	LEU	2.2
1	C	155	PHE	2.2
1	D	95	PRO	2.2
1	C	173	PHE	2.2
1	B	134	VAL	2.2
1	E	145	LEU	2.2
1	E	286	ARG	2.2
1	B	308	ILE	2.2
1	D	232	ILE	2.2
1	D	160	ASP	2.2
1	D	167	VAL	2.2
1	B	59	GLY	2.2
1	B	242	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	165	THR	2.2
1	B	18	ASN	2.2
1	A	54	ASP	2.2
1	A	96	ASP	2.2
1	C	142	ALA	2.2
1	E	135	ASP	2.2
1	D	275	GLN	2.2
1	C	154	VAL	2.2
1	B	172	ASN	2.2
1	D	138	ASN	2.2
1	E	211	SER	2.1
1	D	207	ILE	2.1
1	B	102	LEU	2.1
1	D	15	LEU	2.1
1	E	143	VAL	2.1
1	B	147	LYS	2.1
1	C	115	PHE	2.1
1	B	145	LEU	2.1
1	B	310	ALA	2.1
1	E	199	ASN	2.1
1	D	229	SER	2.1
1	E	217	SER	2.1
1	D	200	ILE	2.1
1	A	47	LYS	2.1
1	A	89	VAL	2.1
1	C	56	VAL	2.1
1	C	12	ASP	2.1
1	D	314	PHE	2.1
1	E	8	PRO	2.1
1	A	49	ARG	2.1
1	E	168	VAL	2.1
1	D	97	GLY	2.1
1	D	10	ILE	2.1
1	E	229	SER	2.1
1	C	134	VAL	2.1
1	A	124	THR	2.1
1	C	207	ILE	2.1
1	B	43	SER	2.1
1	E	209	PHE	2.1
1	B	15	LEU	2.1
1	D	141	LEU	2.0
1	E	267	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	254	THR	2.0
1	C	245	LEU	2.0
1	D	312	LEU	2.0
1	E	138	ASN	2.0
1	A	147	LYS	2.0
1	C	72	ILE	2.0
1	D	137	ARG	2.0
1	E	220	TYR	2.0
1	D	228	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ARS	C	1317	1/1	0.79	0.19	144,144,144,144	0

6.5 Other polymers [i](#)

There are no such residues in this entry.