



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:11 AM UTC

PDB ID : 1YI8 / pdb_00001yi8
Title : Crystal structure of tryptophanyl trRNA synthetase II from *Deinococcus radiodurans* in complex with L-Trp
Authors : Buddha, M.R.; Crane, B.R.
Deposited on : 2005-01-11
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

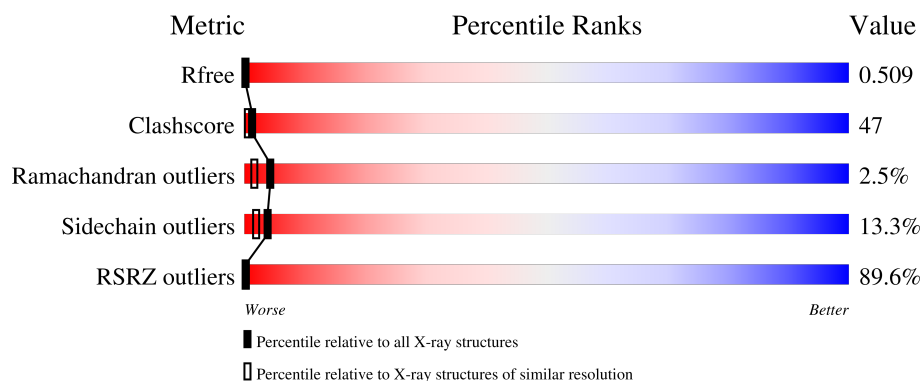
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	351	89% 29% 52% 12% 6%
1	B	351	84% 42% 40% 11% 6%
1	C	351	80% 45% 40% 7% 6%

2 Entry composition [i](#)

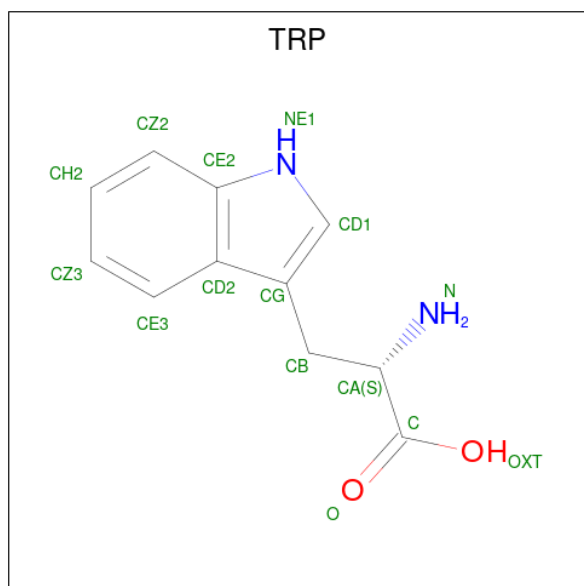
There are 3 unique types of molecules in this entry. The entry contains 8661 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	331	Total	C	N	O	S	2	0	0
			2544	1599	468	471	6			
1	A	331	Total	C	N	O	S	0	0	0
			2511	1581	457	467	6			
1	C	331	Total	C	N	O	S	0	0	0
			2532	1593	462	471	6			

- Molecule 2 is TRYPTOPHAN (CCD ID: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			15	11	2	2		

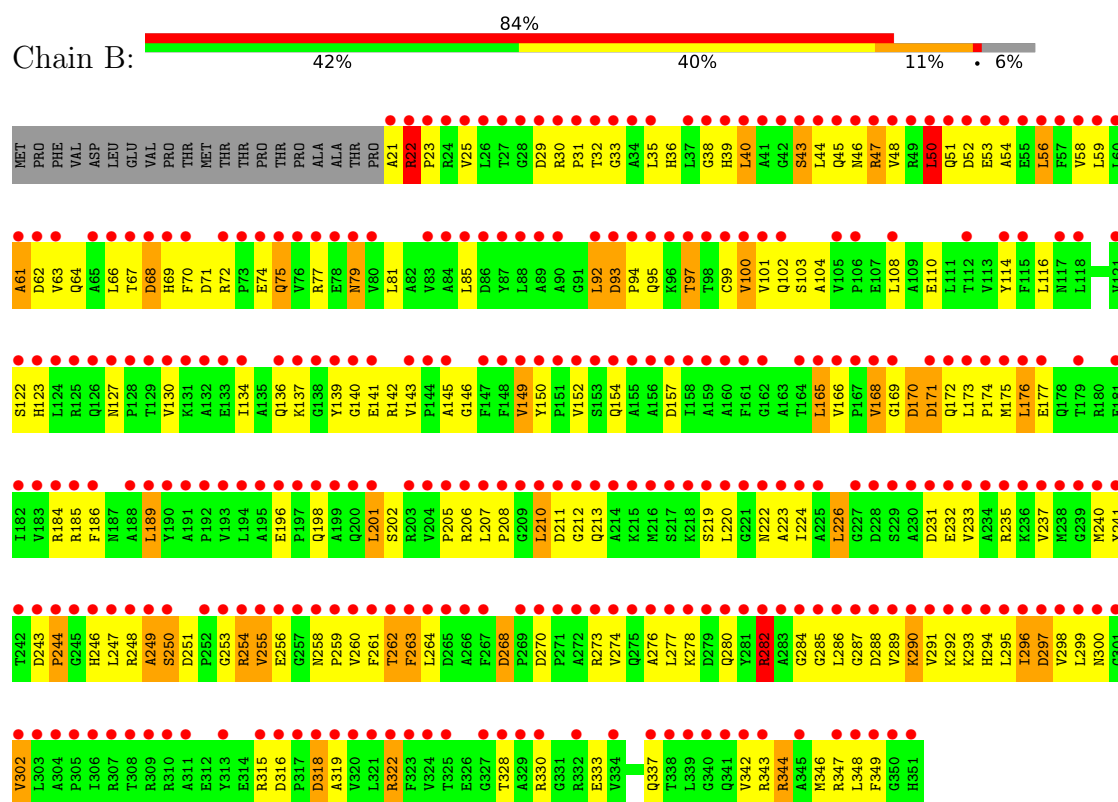
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	308	Total 308	O 308	0	0
3	A	375	Total 375	O 375	0	0
3	C	376	Total 376	O 376	0	0

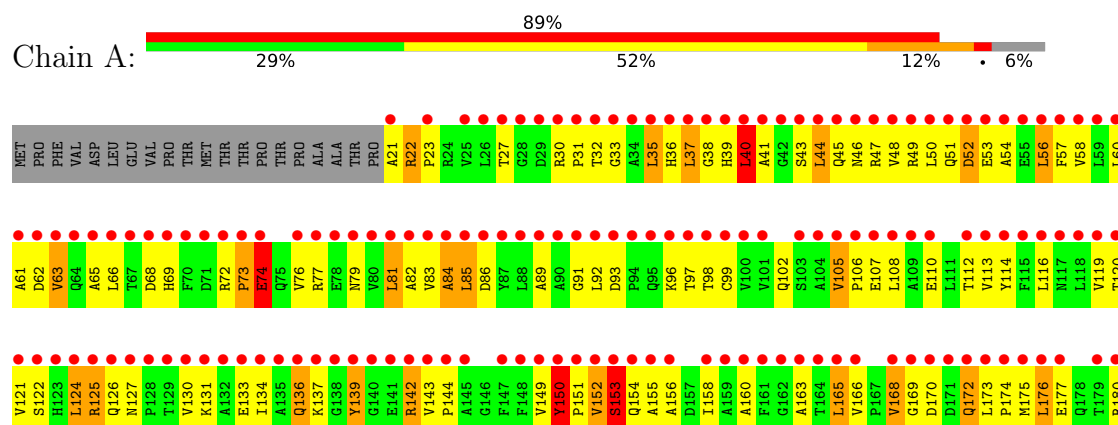
3 Residue-property plots

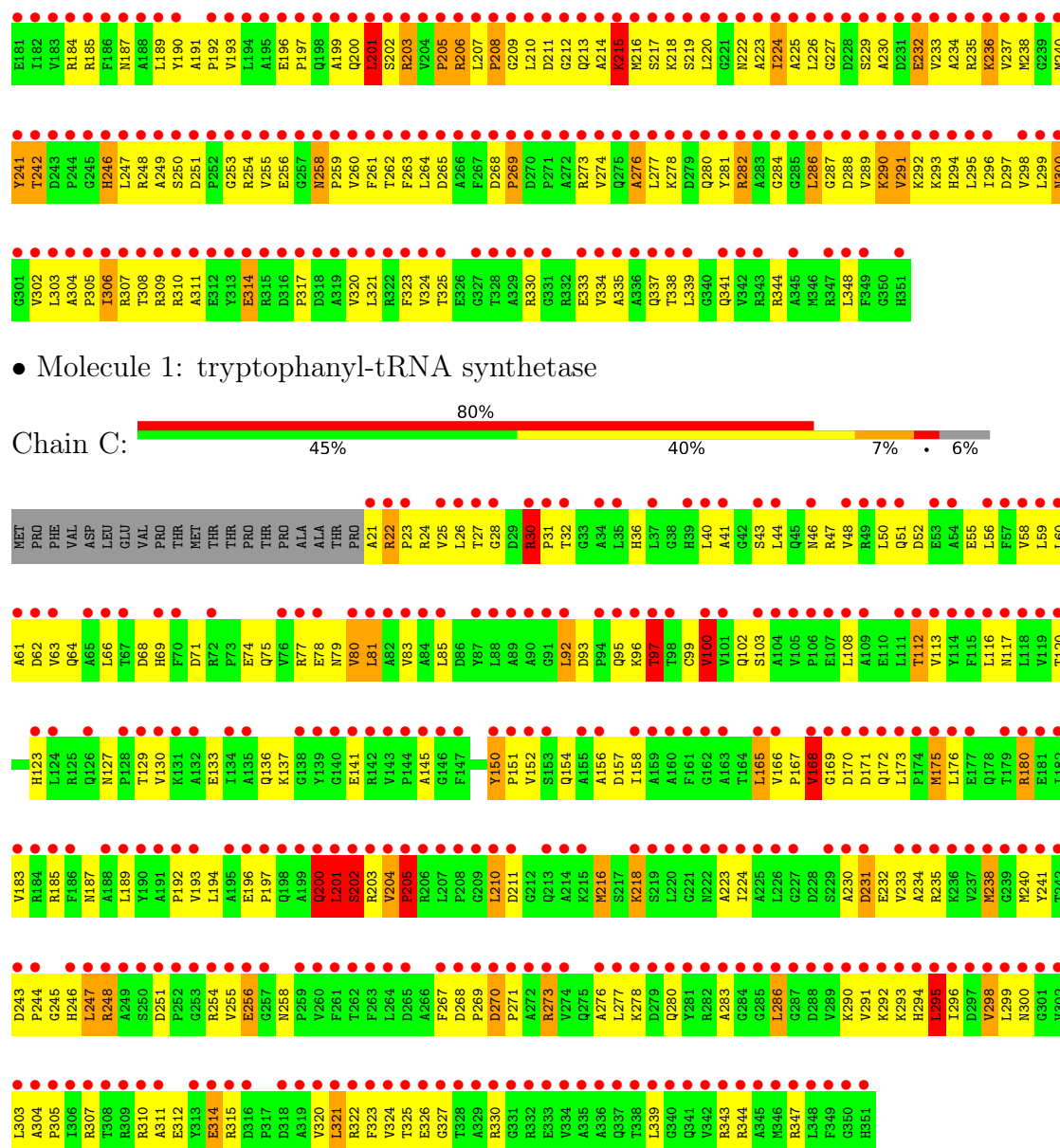
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: tryptophanyl-tRNA synthetase



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	211.80Å 58.50Å 88.90Å 90.00° 100.72° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 50.00 – 2.12	Depositor EDS
% Data completeness (in resolution range)	88.7 (50.00-2.10) 89.3 (50.00-2.12)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.260 , 0.280 0.496 , 0.509	Depositor DCC
R_{free} test set	5520 reflections (10.14%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 34.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	8661	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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	0.47	0/2558	1.11	18/3478 (0.5%)
1	B	0.49	0/2591	1.08	18/3519 (0.5%)
1	C	0.60	1/2579 (0.0%)	1.14	23/3505 (0.7%)
All	All	0.52	1/7728 (0.0%)	1.11	59/10502 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	216	MET	SD-CE	-5.28	1.66	1.79

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	SER	N-CA-C	9.11	121.29	111.36
1	B	268	ASP	CA-C-N	8.13	127.86	119.56
1	B	268	ASP	C-N-CA	8.13	127.86	119.56
1	C	169	GLY	N-CA-C	-7.91	100.45	113.02
1	A	105	VAL	CA-C-N	7.71	127.76	119.28
1	A	105	VAL	C-N-CA	7.71	127.76	119.28
1	A	44	LEU	N-CA-C	7.57	120.42	111.71
1	C	327	GLY	N-CA-C	-7.46	103.78	112.73
1	C	270	ASP	CA-C-N	7.40	127.11	119.56
1	C	270	ASP	C-N-CA	7.40	127.11	119.56
1	C	201	LEU	N-CA-C	7.16	120.34	110.24
1	C	100	VAL	N-CA-C	6.93	118.46	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	212	GLY	N-CA-C	-6.90	105.07	115.00
1	A	215	LYS	N-CA-C	6.87	121.35	108.65
1	A	241	TYR	N-CA-C	6.85	120.86	107.98
1	B	93	ASP	CA-C-N	6.67	127.21	119.47
1	B	93	ASP	C-N-CA	6.67	127.21	119.47
1	C	202	SER	N-CA-C	6.52	124.69	110.80
1	B	244	PRO	N-CA-C	-6.37	102.30	111.22
1	A	155	ALA	N-CA-C	-6.37	104.33	111.28
1	A	236	LYS	N-CA-C	-6.35	103.65	111.40
1	B	263	PHE	N-CA-C	-6.26	105.29	113.12
1	B	100	VAL	N-CA-C	6.17	116.90	107.77
1	A	168	VAL	N-CA-C	6.11	117.16	108.42
1	A	276	ALA	N-CA-C	-6.00	103.50	111.24
1	B	282	ARG	N-CA-C	-5.92	105.15	112.90
1	A	314	GLU	N-CA-C	-5.64	105.13	111.28
1	C	303	LEU	N-CA-C	5.64	119.33	112.23
1	C	295	LEU	N-CA-C	-5.62	105.24	111.36
1	B	157	ASP	N-CA-C	-5.60	104.87	110.97
1	A	84	ALA	N-CA-C	-5.59	104.20	111.02
1	A	153	SER	N-CA-C	-5.58	105.73	112.54
1	B	255	VAL	N-CA-C	5.58	118.06	111.09
1	C	273	ARG	N-CA-C	-5.55	105.15	111.14
1	A	201	LEU	N-CA-C	5.50	117.97	110.55
1	B	291	VAL	N-CA-C	-5.47	105.00	110.30
1	B	171	ASP	N-CA-C	5.46	117.99	111.71
1	C	61	ALA	N-CA-C	5.43	118.03	109.39
1	C	97	THR	N-CA-C	5.37	118.24	109.59
1	A	176	LEU	N-CA-C	-5.37	106.43	112.87
1	B	210	LEU	N-CA-C	-5.36	105.54	111.71
1	C	218	LYS	N-CA-C	-5.35	104.69	111.11
1	B	223	ALA	N-CA-C	5.26	117.82	109.50
1	C	324	VAL	N-CA-C	5.26	116.73	111.00
1	C	200	GLN	N-CA-C	-5.23	96.19	107.49
1	C	168	VAL	N-CA-C	5.22	115.24	108.35
1	C	28	GLY	N-CA-C	5.18	118.14	110.63
1	C	173	LEU	CA-C-N	-5.17	114.34	119.56
1	C	173	LEU	C-N-CA	-5.17	114.34	119.56
1	C	175	MET	N-CA-C	-5.16	105.57	111.14
1	A	91	GLY	N-CA-C	5.13	120.59	114.48
1	B	79	ASN	N-CA-C	5.11	119.39	113.20
1	B	50	LEU	N-CA-C	-5.09	106.84	113.16
1	C	30	ARG	CA-C-N	5.06	126.16	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	30	ARG	C-N-CA	5.06	126.16	119.84
1	B	56	LEU	N-CA-C	5.03	116.93	108.73
1	C	30	ARG	N-CA-C	-5.02	101.98	109.42
1	A	219	SER	N-CA-C	5.02	118.66	112.54
1	A	40	LEU	N-CA-C	-5.01	105.46	111.03

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Sidechain
1	A	150	TYR	Sidechain

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	2511	0	2507	310	15
1	B	2544	0	2568	213	7
1	C	2532	0	2546	205	8
2	C	15	0	9	4	0
3	A	375	0	0	16	6
3	B	308	0	0	7	6
3	C	376	0	0	16	18
All	All	8661	0	7630	713	32

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 47.

All (713) 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:168:VAL:HG23	1:A:172:GLN:HB2	1.20	1.15
1:B:240:MET:HE3	1:B:260:VAL:HG12	1.33	1.09
1:A:226:LEU:HB3	1:A:306:ILE:HD11	1.34	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ARG:HG3	1:C:180:ARG:HH11	1.21	1.03
1:A:207:LEU:HD23	1:A:216:MET:HE1	1.40	1.02
1:B:51:GLN:HE21	1:B:97:THR:HG22	1.18	1.02
1:C:120:THR:HG23	1:C:123:HIS:H	1.22	1.01
1:A:35:LEU:HD11	1:A:86:ASP:HB3	1.39	1.01
1:B:254:ARG:HD3	1:B:256:GLU:HG2	1.46	0.98
1:B:280:GLN:HB2	1:B:286:LEU:HD12	1.45	0.97
1:C:51:GLN:HE22	1:C:93:ASP:H	1.05	0.97
1:C:77:ARG:O	1:C:80:VAL:HG12	1.66	0.96
1:B:50:LEU:HD11	1:B:56:LEU:HD13	1.49	0.92
1:B:168:VAL:HG23	1:B:172:GLN:HB2	1.52	0.92
1:C:204:VAL:HG12	1:C:205:PRO:HD2	1.49	0.92
1:A:73:PRO:O	1:A:76:VAL:HG12	1.70	0.91
1:B:295:LEU:O	1:B:298:VAL:HG12	1.72	0.90
1:B:44:LEU:O	1:B:48:VAL:HG23	1.72	0.90
1:B:47:ARG:HA	1:B:50:LEU:HG	1.54	0.89
1:B:51:GLN:HE22	1:B:93:ASP:N	1.71	0.88
1:B:277:LEU:HD12	1:B:286:LEU:HD11	1.55	0.88
1:C:254:ARG:HD3	1:C:256:GLU:HG2	1.56	0.87
1:A:63:VAL:HG13	1:A:102:GLN:HG2	1.55	0.87
1:A:207:LEU:HD12	1:A:208:PRO:HD2	1.56	0.86
1:C:26:LEU:HD23	1:C:158:ILE:HD13	1.55	0.85
1:B:51:GLN:HE22	1:B:93:ASP:H	0.89	0.85
1:A:35:LEU:CD1	1:A:86:ASP:HB3	2.07	0.84
1:A:193:VAL:HG21	1:A:341:GLN:HB3	1.58	0.84
1:A:226:LEU:HD12	1:A:226:LEU:H	1.43	0.84
1:B:213:GLN:OE1	1:B:220:LEU:HD13	1.79	0.82
1:A:218:LYS:HA	1:A:218:LYS:HE2	1.59	0.82
1:A:127:ASN:HB3	1:A:130:VAL:HG12	1.60	0.82
1:C:180:ARG:HD3	1:C:197:PRO:O	1.80	0.82
1:B:43:SER:O	1:B:47:ARG:HD2	1.79	0.81
1:A:207:LEU:CD1	1:A:208:PRO:HD2	2.10	0.81
1:A:60:LEU:O	1:A:62:ASP:N	2.13	0.81
1:A:139:TYR:O	1:A:142:ARG:HG3	1.81	0.80
1:C:180:ARG:HG3	1:C:180:ARG:NH1	1.97	0.80
1:C:22:ARG:HB2	1:C:23:PRO:CD	2.11	0.79
1:B:68:ASP:HB3	1:B:69:HIS:HD2	1.47	0.79
1:C:211:ASP:HB3	3:C:1003:HOH:O	1.82	0.79
1:A:108:LEU:O	1:A:112:THR:HG23	1.81	0.78
1:B:184:ARG:HG2	1:B:184:ARG:HH21	1.48	0.78
1:C:168:VAL:HG22	1:C:172:GLN:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:THR:O	1:A:58:VAL:HA	1.84	0.78
1:B:36:HIS:HD2	1:B:38:GLY:H	1.30	0.77
1:A:333:GLU:O	1:A:337:GLN:HG2	1.85	0.77
1:C:216:MET:HE3	1:C:223:ALA:HB1	1.67	0.77
1:A:303:LEU:O	1:A:307:ARG:HB2	1.84	0.77
1:C:93:ASP:HB3	1:C:96:LYS:HB2	1.67	0.77
1:A:184:ARG:HD2	1:A:196:GLU:OE1	1.84	0.77
1:C:36:HIS:ND1	1:C:216:MET:HE2	1.99	0.77
1:A:168:VAL:CG2	1:A:172:GLN:HB2	2.10	0.77
1:A:49:ARG:HA	3:A:1677:HOH:O	1.84	0.76
1:A:201:LEU:HD23	1:A:202:SER:H	1.50	0.76
1:C:154:GLN:NE2	2:C:3000:TRP:OXT	2.18	0.76
1:B:51:GLN:NE2	1:B:93:ASP:H	1.75	0.76
1:A:110:GLU:O	1:A:113:VAL:HG12	1.86	0.76
1:A:85:LEU:HD13	1:A:310:ARG:NH2	2.00	0.75
1:B:268:ASP:OD2	1:B:274:VAL:HG23	1.87	0.75
1:C:92:LEU:HG	1:C:97:THR:HG21	1.69	0.75
1:B:51:GLN:NE2	1:B:97:THR:HG22	1.99	0.75
1:A:255:VAL:HG22	1:A:261:PHE:CE1	2.22	0.74
1:C:233:VAL:HG21	1:C:307:ARG:HH21	1.52	0.74
1:B:349:PHE:CD2	1:C:80:VAL:HG11	2.23	0.74
1:A:202:SER:OG	1:A:205:PRO:HB3	1.87	0.74
1:C:56:LEU:HD11	1:C:58:VAL:HG13	1.70	0.73
1:A:291:VAL:HG13	1:A:292:LYS:N	2.02	0.73
1:A:254:ARG:HB2	1:A:256:GLU:OE1	1.88	0.73
1:B:237:VAL:HG13	1:B:240:MET:HE1	1.71	0.72
1:A:30:ARG:HH22	1:A:68:ASP:HB3	1.53	0.72
1:B:22:ARG:HH21	1:B:53:GLU:HG3	1.53	0.72
1:A:127:ASN:HB3	1:A:130:VAL:CG1	2.19	0.72
1:A:201:LEU:CD2	1:A:202:SER:H	2.02	0.72
1:C:24:ARG:HD3	1:C:55:GLU:OE2	1.90	0.72
1:C:40:LEU:HA	1:C:44:LEU:HD12	1.72	0.72
1:A:44:LEU:O	1:A:48:VAL:HG23	1.90	0.72
1:C:273:ARG:HD2	3:C:1520:HOH:O	1.89	0.72
1:A:49:ARG:HD2	3:A:1677:HOH:O	1.90	0.72
1:C:22:ARG:HB2	1:C:23:PRO:HD3	1.71	0.72
1:C:168:VAL:CG2	1:C:172:GLN:HB2	2.20	0.71
1:B:254:ARG:CD	1:B:256:GLU:HG2	2.18	0.71
1:B:43:SER:C	1:B:47:ARG:HD2	2.15	0.71
1:A:291:VAL:HG13	1:A:292:LYS:H	1.55	0.71
1:B:127:ASN:HB3	1:B:130:VAL:HG12	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ASP:OD1	1:B:137:LYS:HE2	1.90	0.71
1:A:169:GLY:H	1:A:172:GLN:HG3	1.54	0.71
1:A:180:ARG:HG2	1:A:196:GLU:HG2	1.73	0.71
1:A:254:ARG:HH11	1:A:256:GLU:HB2	1.56	0.71
1:A:229:SER:O	1:A:233:VAL:HG23	1.91	0.71
1:C:211:ASP:OD1	1:C:211:ASP:O	2.09	0.71
1:C:311:ALA:HA	1:C:314:GLU:HG3	1.71	0.71
1:C:290:LYS:HE2	1:C:290:LYS:HA	1.73	0.70
1:A:173:LEU:N	1:A:174:PRO:HD2	2.05	0.70
1:C:51:GLN:HE21	1:C:97:THR:HG22	1.57	0.70
1:B:277:LEU:CD1	1:B:286:LEU:HD11	2.22	0.69
1:A:230:ALA:HB1	1:A:300:ASN:HD21	1.57	0.69
1:C:108:LEU:O	1:C:112:THR:HG23	1.93	0.69
1:A:273:ARG:O	1:A:277:LEU:HD23	1.91	0.69
1:A:291:VAL:CG1	1:A:292:LYS:H	2.05	0.69
1:B:262:THR:HG21	3:B:1431:HOH:O	1.93	0.69
1:A:112:THR:O	1:A:116:LEU:HG	1.93	0.69
1:B:146:GLY:HA3	1:C:117:ASN:ND2	2.08	0.69
1:A:216:MET:HG3	1:A:223:ALA:HA	1.73	0.69
1:A:337:GLN:HB2	3:A:1490:HOH:O	1.92	0.68
1:B:254:ARG:HD3	1:B:256:GLU:CG	2.22	0.68
1:A:63:VAL:HG13	1:A:102:GLN:CG	2.23	0.68
1:A:305:PRO:HG2	1:A:306:ILE:H	1.59	0.68
1:B:51:GLN:HE21	1:B:97:THR:CG2	1.99	0.68
1:A:168:VAL:HG22	1:A:169:GLY:O	1.93	0.68
1:C:36:HIS:CG	1:C:216:MET:HE2	2.29	0.68
1:A:259:PRO:HA	1:A:262:THR:CG2	2.24	0.68
1:A:168:VAL:HG11	1:A:199:ALA:HB1	1.76	0.67
1:B:259:PRO:HA	1:B:262:THR:CG2	2.25	0.67
1:A:241:TYR:O	1:A:259:PRO:HD2	1.94	0.67
1:A:256:GLU:H	1:A:256:GLU:CD	2.02	0.67
1:A:288:ASP:HA	1:A:291:VAL:HG12	1.75	0.67
1:C:171:ASP:HB2	1:C:172:GLN:NE2	2.09	0.67
1:C:166:VAL:HG21	1:C:176:LEU:HD23	1.76	0.67
1:A:85:LEU:HD13	1:A:310:ARG:HH22	1.58	0.66
1:A:215:LYS:NZ	1:A:217:SER:OG	2.29	0.66
1:A:317:PRO:O	1:A:320:VAL:HG12	1.96	0.66
1:C:234:ALA:O	1:C:238:MET:HG2	1.94	0.66
1:B:273:ARG:O	1:B:276:ALA:HB3	1.96	0.66
1:B:127:ASN:HB3	1:B:130:VAL:CG1	2.25	0.66
1:A:63:VAL:CG1	1:A:102:GLN:HG2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:MET:SD	1:C:175:MET:C	2.79	0.66
1:C:56:LEU:HD12	1:C:97:THR:HB	1.78	0.66
1:B:22:ARG:CB	1:B:23:PRO:HD3	2.26	0.65
1:B:53:GLU:OE1	1:B:53:GLU:HA	1.96	0.65
1:B:122:SER:OG	1:C:141:GLU:HB3	1.97	0.65
1:A:52:ASP:HB3	1:A:96:LYS:NZ	2.12	0.65
1:C:254:ARG:CD	1:C:256:GLU:HG2	2.24	0.65
1:A:254:ARG:HD2	1:A:256:GLU:HB2	1.79	0.65
1:B:322:ARG:HG2	1:B:322:ARG:HH21	1.62	0.65
1:A:190:TYR:O	1:A:191:ALA:C	2.39	0.65
1:A:261:PHE:HA	3:A:1622:HOH:O	1.97	0.65
1:A:41:ALA:CB	1:A:207:LEU:HD22	2.27	0.65
1:C:203:ARG:C	1:C:204:VAL:HG23	2.22	0.65
1:B:35:LEU:HD13	1:B:44:LEU:HD11	1.77	0.64
1:A:130:VAL:O	1:A:134:ILE:HG13	1.97	0.64
1:C:51:GLN:HE22	1:C:93:ASP:N	1.88	0.64
1:B:22:ARG:CG	1:B:23:PRO:HD3	2.28	0.64
1:A:170:ASP:OD1	1:A:203:ARG:NH2	2.31	0.64
1:A:226:LEU:HD23	1:A:306:ILE:CD1	2.27	0.64
1:C:120:THR:CG2	1:C:123:HIS:H	2.04	0.64
1:C:166:VAL:HG23	1:C:166:VAL:O	1.97	0.64
1:B:295:LEU:O	1:B:295:LEU:HD23	1.97	0.64
1:A:99:CYS:SG	1:A:324:VAL:HG12	2.38	0.64
1:A:133:GLU:O	1:A:137:LYS:HG3	1.98	0.63
1:B:40:LEU:HA	1:B:44:LEU:HB2	1.80	0.63
1:A:185:ARG:HD2	1:A:189:LEU:HD22	1.80	0.63
1:B:296:ILE:HG13	1:B:297:ASP:N	2.11	0.63
1:A:139:TYR:CD2	1:A:143:VAL:HG13	2.33	0.63
1:B:233:VAL:O	1:B:237:VAL:HG23	1.98	0.63
1:A:173:LEU:O	1:A:177:GLU:HB2	1.99	0.63
1:B:40:LEU:HD23	1:B:226:LEU:HD21	1.81	0.63
1:A:40:LEU:HA	1:A:44:LEU:HB3	1.79	0.63
1:A:72:ARG:HG2	3:A:1665:HOH:O	1.97	0.63
1:A:130:VAL:HG11	3:A:1543:HOH:O	1.98	0.63
1:C:294:HIS:O	1:C:298:VAL:HG12	1.99	0.63
1:A:30:ARG:HD2	1:A:65:ALA:HA	1.80	0.62
1:A:259:PRO:O	1:A:263:PHE:HB2	1.98	0.62
1:A:160:ALA:HA	1:A:338:THR:HG21	1.82	0.62
1:C:231:ASP:OD1	1:C:235:ARG:NE	2.32	0.62
1:B:101:VAL:HG13	1:B:104:ALA:HB3	1.81	0.62
1:B:255:VAL:HG21	1:B:278:LYS:HG3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:THR:HG22	1:C:156:ALA:CB	2.30	0.62
1:C:254:ARG:HD2	1:C:256:GLU:O	1.99	0.62
1:B:68:ASP:HB3	1:B:69:HIS:CD2	2.31	0.62
1:A:211:ASP:C	1:A:213:GLN:H	2.08	0.62
1:A:269:PRO:HD2	1:A:273:ARG:NH1	2.15	0.62
1:A:253:GLY:O	1:A:282:ARG:HA	1.98	0.62
1:B:289:VAL:O	1:B:293:LYS:HG3	2.00	0.62
1:A:79:ASN:HA	1:A:82:ALA:HB3	1.82	0.62
1:C:56:LEU:CD1	1:C:58:VAL:HG13	2.30	0.61
1:C:64:GLN:H	1:C:102:GLN:HE22	1.47	0.61
1:A:207:LEU:CG	1:A:208:PRO:HD2	2.30	0.61
1:C:295:LEU:HD22	1:C:299:LEU:HG	1.82	0.61
1:C:326:GLU:HG2	3:C:1650:HOH:O	2.00	0.61
1:B:146:GLY:HA3	1:C:117:ASN:HD22	1.64	0.61
1:A:269:PRO:HA	3:A:1293:HOH:O	2.01	0.61
1:C:56:LEU:HD13	1:C:56:LEU:C	2.26	0.61
1:B:248:ARG:HD3	1:B:248:ARG:N	2.15	0.61
1:A:208:PRO:HG2	1:A:263:PHE:CE2	2.35	0.61
1:B:22:ARG:HB2	1:B:23:PRO:HD3	1.81	0.60
1:A:52:ASP:OD2	1:A:52:ASP:N	2.30	0.60
1:A:299:LEU:O	1:A:303:LEU:HD13	2.01	0.60
1:B:173:LEU:N	1:B:174:PRO:HD2	2.16	0.60
1:A:291:VAL:CG1	1:A:292:LYS:N	2.61	0.60
1:B:22:ARG:HH21	1:B:53:GLU:CG	2.15	0.60
1:A:289:VAL:O	1:A:293:LYS:HB2	2.02	0.60
1:B:62:ASP:O	1:B:66:LEU:HD23	2.02	0.60
1:C:201:LEU:HD23	1:C:202:SER:H	1.67	0.60
1:C:256:GLU:H	1:C:256:GLU:CD	2.08	0.60
1:A:232:GLU:O	1:A:236:LYS:HB2	2.02	0.59
1:A:255:VAL:HG22	1:A:261:PHE:CD1	2.36	0.59
1:A:220:LEU:C	1:A:222:ASN:H	2.10	0.59
1:B:40:LEU:O	1:B:45:GLN:HG2	2.03	0.59
1:B:140:GLY:O	1:B:143:VAL:HG23	2.02	0.59
1:B:268:ASP:OD1	1:B:273:ARG:NH2	2.36	0.59
1:A:176:LEU:O	1:A:176:LEU:HD13	2.02	0.59
1:A:294:HIS:HA	1:A:297:ASP:OD2	2.03	0.59
1:A:261:PHE:CE1	1:A:278:LYS:HG2	2.37	0.59
1:A:295:LEU:O	1:A:299:LEU:HG	2.03	0.59
1:B:64:GLN:H	1:B:102:GLN:HE22	1.51	0.59
1:A:210:LEU:HB2	1:A:222:ASN:OD1	2.02	0.59
1:A:229:SER:OG	1:A:232:GLU:HB2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ASN:CB	1:B:130:VAL:HG12	2.32	0.59
1:A:21:ALA:HB3	1:A:53:GLU:O	2.03	0.59
1:A:142:ARG:O	1:A:142:ARG:HD3	2.03	0.59
1:A:254:ARG:HH11	1:A:256:GLU:CB	2.16	0.59
1:C:95:GLN:HA	1:C:95:GLN:NE2	2.17	0.59
1:C:310:ARG:O	1:C:314:GLU:HG2	2.03	0.59
1:A:35:LEU:O	1:A:226:LEU:CD1	2.51	0.58
1:A:35:LEU:HD12	1:A:226:LEU:HD13	1.85	0.58
1:A:304:ALA:N	1:A:305:PRO:HD2	2.18	0.58
1:C:79:ASN:O	1:C:83:VAL:HG22	2.02	0.58
1:C:210:LEU:HD12	1:C:240:MET:HG2	1.84	0.58
1:C:254:ARG:CG	1:C:256:GLU:HG2	2.33	0.58
1:C:310:ARG:O	1:C:314:GLU:CG	2.52	0.58
1:B:295:LEU:HD23	1:B:295:LEU:C	2.28	0.58
1:A:273:ARG:O	1:A:276:ALA:HB3	2.04	0.58
2:C:3000:TRP:OXT	2:C:3000:TRP:CG	2.57	0.58
1:A:237:VAL:O	1:A:240:MET:N	2.30	0.58
1:B:66:LEU:C	1:B:68:ASP:H	2.10	0.58
1:A:208:PRO:HG3	1:A:262:THR:HG23	1.85	0.58
1:B:137:LYS:HD3	1:B:139:TYR:CE2	2.39	0.58
1:C:36:HIS:HB2	1:C:216:MET:CE	2.34	0.57
1:C:68:ASP:OD2	1:C:69:HIS:HD2	1.86	0.57
1:C:293:LYS:HG2	3:C:1361:HOH:O	2.04	0.57
1:B:23:PRO:HD2	1:B:54:ALA:HB2	1.85	0.57
1:A:226:LEU:HD12	1:A:226:LEU:N	2.16	0.57
1:A:305:PRO:HG2	1:A:306:ILE:HG22	1.86	0.57
1:C:48:VAL:O	1:C:51:GLN:HG2	2.04	0.57
1:A:22:ARG:N	1:A:23:PRO:CD	2.67	0.57
1:C:180:ARG:HE	1:C:196:GLU:CD	2.12	0.57
1:B:184:ARG:HG2	1:B:184:ARG:NH2	2.17	0.57
1:C:218:LYS:HB2	3:C:1206:HOH:O	2.04	0.57
1:B:114:TYR:CE1	1:B:346:MET:HE1	2.40	0.57
1:A:98:THR:CG2	1:A:330:ARG:HD2	2.34	0.57
1:C:171:ASP:HB2	1:C:172:GLN:HE22	1.69	0.57
1:A:56:LEU:HD22	1:A:57:PHE:N	2.20	0.57
1:B:231:ASP:O	1:B:235:ARG:HG3	2.05	0.57
1:A:259:PRO:HA	1:A:262:THR:HG22	1.86	0.57
1:A:277:LEU:HD12	1:A:286:LEU:HD11	1.87	0.57
1:A:321:LEU:O	1:A:325:THR:HG23	2.04	0.57
1:B:207:LEU:HD12	1:B:208:PRO:HD2	1.87	0.57
1:C:56:LEU:HD11	1:C:58:VAL:CG1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLU:HG3	3:B:1946:HOH:O	2.05	0.56
1:A:98:THR:OG1	1:A:330:ARG:HD2	2.05	0.56
1:A:296:ILE:HG13	1:A:297:ASP:N	2.20	0.56
1:C:40:LEU:HA	1:C:44:LEU:HB2	1.87	0.56
1:C:133:GLU:O	1:C:136:GLN:HG3	2.04	0.56
1:B:263:PHE:HB3	1:B:295:LEU:HD11	1.86	0.56
1:A:136:GLN:O	1:A:136:GLN:HG3	2.03	0.56
1:C:187:ASN:HB3	1:C:192:PRO:HA	1.86	0.56
1:B:36:HIS:CD2	1:B:38:GLY:H	2.19	0.56
1:B:277:LEU:HD22	1:B:277:LEU:H	1.69	0.56
1:A:246:HIS:NE2	1:A:251:ASP:O	2.33	0.56
1:A:36:HIS:H	1:A:39:HIS:HD2	1.52	0.56
1:C:74:GLU:HB2	3:C:1034:HOH:O	2.05	0.56
1:C:180:ARG:HD2	1:C:196:GLU:HG3	1.87	0.56
1:A:277:LEU:HA	1:A:280:GLN:NE2	2.21	0.56
1:A:302:VAL:O	1:A:305:PRO:HD2	2.06	0.56
1:B:75:GLN:O	1:B:79:ASN:ND2	2.38	0.56
1:A:240:MET:CE	1:A:259:PRO:HB2	2.36	0.56
1:B:44:LEU:HA	1:B:47:ARG:CD	2.35	0.56
1:B:189:LEU:HD21	1:C:71:ASP:HA	1.87	0.55
1:C:166:VAL:HG21	1:C:176:LEU:CD2	2.37	0.55
1:B:93:ASP:OD2	1:B:94:PRO:HD2	2.07	0.55
1:A:149:VAL:O	1:A:149:VAL:HG12	2.07	0.55
1:C:51:GLN:NE2	1:C:97:THR:HG22	2.21	0.55
1:C:204:VAL:HG21	3:C:1173:HOH:O	2.05	0.55
1:B:248:ARG:HD3	1:B:248:ARG:H	1.71	0.55
1:A:112:THR:HG22	1:A:156:ALA:CB	2.36	0.55
1:A:216:MET:HA	1:A:222:ASN:O	2.07	0.55
1:C:254:ARG:HG2	1:C:255:VAL:N	2.20	0.55
1:A:63:VAL:HG13	1:A:102:GLN:CD	2.32	0.55
1:A:220:LEU:C	1:A:222:ASN:N	2.60	0.55
1:A:37:LEU:HG	1:A:224:ILE:HG12	1.88	0.55
1:A:201:LEU:CD2	1:A:202:SER:N	2.70	0.55
1:C:233:VAL:HG21	1:C:307:ARG:NH2	2.22	0.55
1:B:349:PHE:CE2	1:C:81:LEU:HD13	2.42	0.55
1:A:58:VAL:HG13	1:A:58:VAL:O	2.05	0.55
1:A:76:VAL:HG13	1:A:77:ARG:N	2.22	0.55
1:A:218:LYS:HA	1:A:218:LYS:CE	2.34	0.55
1:C:40:LEU:HD12	1:C:44:LEU:HB2	1.87	0.55
1:C:183:VAL:HG13	1:C:194:LEU:HB2	1.89	0.55
1:B:64:GLN:HE22	1:B:154:GLN:CG	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LEU:HD12	1:C:100:VAL:HG22	1.87	0.55
1:B:237:VAL:HG13	1:B:240:MET:CE	2.36	0.55
1:B:134:ILE:HD13	1:B:143:VAL:HG21	1.88	0.54
1:A:35:LEU:O	1:A:226:LEU:HD12	2.07	0.54
1:A:205:PRO:O	1:A:206:ARG:C	2.50	0.54
1:A:260:VAL:O	1:A:264:LEU:HB2	2.07	0.54
1:C:127:ASN:HB3	1:C:130:VAL:HG22	1.89	0.54
1:C:78:GLU:HA	1:C:78:GLU:OE2	2.07	0.54
1:C:175:MET:HB2	3:C:1018:HOH:O	2.07	0.54
1:B:247:LEU:HB2	1:B:248:ARG:HH21	1.72	0.54
1:A:247:LEU:HD22	3:A:1323:HOH:O	2.07	0.54
1:A:288:ASP:O	1:A:292:LYS:HG3	2.07	0.54
1:C:64:GLN:OE1	1:C:154:GLN:HG3	2.08	0.54
1:C:51:GLN:NE2	1:C:93:ASP:H	1.89	0.54
1:A:193:VAL:HG22	1:A:193:VAL:O	2.08	0.54
1:C:339:LEU:O	1:C:343:ARG:HG3	2.08	0.54
1:C:27:THR:HB	3:C:1219:HOH:O	2.07	0.54
1:A:107:GLU:HB3	1:A:339:LEU:HG	1.90	0.54
1:C:187:ASN:CB	1:C:192:PRO:HA	2.37	0.54
1:C:295:LEU:O	1:C:298:VAL:HG13	2.07	0.54
1:B:58:VAL:HG23	1:B:58:VAL:O	2.07	0.54
1:B:168:VAL:HG22	1:B:169:GLY:O	2.07	0.54
1:C:172:GLN:HG2	3:C:1945:HOH:O	2.07	0.54
1:B:296:ILE:HD12	1:B:300:ASN:ND2	2.23	0.54
1:B:22:ARG:NH2	1:B:53:GLU:HG3	2.22	0.53
1:A:248:ARG:HD3	1:A:248:ARG:N	2.23	0.53
1:C:40:LEU:CA	1:C:44:LEU:HD12	2.37	0.53
1:A:249:ALA:HB2	1:A:287:GLY:HA3	1.90	0.53
1:C:216:MET:HE3	1:C:223:ALA:CB	2.37	0.53
1:B:62:ASP:OD1	1:B:103:SER:OG	2.26	0.53
1:B:344:ARG:CG	1:B:344:ARG:HH11	2.21	0.53
1:B:259:PRO:HA	1:B:262:THR:HG23	1.89	0.53
1:A:242:THR:HB	1:A:258:ASN:HD21	1.73	0.53
1:C:243:ASP:OD2	1:C:246:HIS:HB2	2.08	0.53
1:B:237:VAL:O	1:B:240:MET:HE2	2.09	0.53
1:B:23:PRO:O	1:B:54:ALA:HB1	2.09	0.53
1:B:74:GLU:OE1	1:C:347:ARG:NH1	2.42	0.53
1:B:255:VAL:HG13	1:B:261:PHE:CD2	2.43	0.53
1:A:255:VAL:HG13	1:A:261:PHE:CD1	2.44	0.53
1:B:211:ASP:HB3	1:B:213:GLN:HG3	1.90	0.53
1:C:120:THR:HG22	1:C:123:HIS:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:LEU:C	1:B:50:LEU:HD12	2.34	0.52
1:A:175:MET:SD	1:A:175:MET:C	2.92	0.52
1:C:22:ARG:CB	1:C:23:PRO:CD	2.86	0.52
1:A:212:GLY:O	1:A:213:GLN:C	2.53	0.52
1:A:215:LYS:HB3	3:A:2052:HOH:O	2.08	0.52
1:A:237:VAL:HG13	1:A:295:LEU:HD23	1.91	0.52
1:C:286:LEU:HD12	1:C:291:VAL:HG23	1.91	0.52
1:B:127:ASN:CG	1:B:130:VAL:HG12	2.34	0.52
1:A:52:ASP:HB3	1:A:96:LYS:HZ3	1.75	0.52
1:B:299:LEU:HA	1:B:302:VAL:CG1	2.40	0.52
1:A:180:ARG:O	1:A:184:ARG:HD3	2.10	0.52
1:C:180:ARG:NH1	1:C:180:ARG:CG	2.68	0.52
1:B:249:ALA:O	1:B:250:SER:C	2.53	0.52
1:B:202:SER:HB3	3:B:1285:HOH:O	2.09	0.52
1:B:253:GLY:O	1:B:282:ARG:HA	2.09	0.52
1:B:296:ILE:CD1	1:B:300:ASN:ND2	2.73	0.52
1:C:21:ALA:HB2	3:C:1220:HOH:O	2.09	0.52
1:C:154:GLN:CD	2:C:3000:TRP:OXT	2.52	0.52
1:B:102:GLN:HG3	1:B:108:LEU:HD12	1.92	0.52
1:A:180:ARG:HB3	1:A:184:ARG:HH11	1.75	0.52
1:A:207:LEU:HG	1:A:208:PRO:HD2	1.91	0.52
1:A:250:SER:O	1:A:284:GLY:HA2	2.09	0.52
1:C:63:VAL:HB	1:C:102:GLN:NE2	2.25	0.52
1:B:32:THR:O	1:B:75:GLN:NE2	2.43	0.52
1:B:240:MET:CE	1:B:260:VAL:HG12	2.22	0.52
1:A:288:ASP:O	1:A:291:VAL:HG12	2.09	0.52
1:C:216:MET:HE3	1:C:224:ILE:H	1.75	0.52
1:A:116:LEU:HD23	1:A:152:VAL:HG21	1.91	0.52
1:A:261:PHE:CD1	1:A:278:LYS:HG2	2.44	0.52
1:B:299:LEU:HA	1:B:302:VAL:HG12	1.92	0.51
1:A:232:GLU:HB3	3:A:1447:HOH:O	2.10	0.51
1:B:116:LEU:O	1:C:145:ALA:HB3	2.10	0.51
1:B:189:LEU:CD2	1:C:71:ASP:HA	2.40	0.51
1:A:209:GLY:O	1:A:210:LEU:C	2.53	0.51
1:A:255:VAL:HG11	1:A:278:LYS:HE2	1.92	0.51
1:B:211:ASP:OD1	1:B:222:ASN:HB3	2.11	0.51
1:A:23:PRO:O	1:A:54:ALA:HB1	2.09	0.51
1:B:292:LYS:O	1:B:296:ILE:CG2	2.58	0.51
1:A:260:VAL:HG13	1:A:295:LEU:CD2	2.40	0.51
1:B:298:VAL:O	1:B:302:VAL:HG12	2.11	0.51
1:A:234:ALA:HA	1:A:296:ILE:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:LYS:O	1:A:296:ILE:HG12	2.10	0.51
1:C:165:LEU:HD22	1:C:200:GLN:HB2	1.93	0.51
1:C:295:LEU:CD2	1:C:299:LEU:HG	2.40	0.51
1:B:248:ARG:NE	1:B:251:ASP:OD2	2.44	0.51
1:A:41:ALA:HB2	1:A:207:LEU:HD22	1.92	0.51
1:A:66:LEU:HD21	1:A:76:VAL:HG11	1.92	0.51
1:A:208:PRO:HG2	1:A:263:PHE:HE2	1.74	0.51
1:C:258:ASN:C	1:C:258:ASN:HD22	2.18	0.51
1:B:333:GLU:HG3	1:B:337:GLN:HE21	1.74	0.51
1:C:41:ALA:HB2	1:C:267:PHE:CZ	2.46	0.51
1:C:77:ARG:O	1:C:80:VAL:CG1	2.51	0.51
1:C:322:ARG:HD3	3:C:1047:HOH:O	2.10	0.51
1:B:333:GLU:OE2	1:B:333:GLU:HA	2.11	0.50
1:A:215:LYS:O	1:A:222:ASN:ND2	2.44	0.50
1:C:62:ASP:OD2	1:C:103:SER:OG	2.24	0.50
1:A:30:ARG:HH22	1:A:68:ASP:CB	2.21	0.50
1:C:254:ARG:HD3	1:C:256:GLU:CG	2.36	0.50
1:A:150:TYR:CE2	1:A:154:GLN:NE2	2.80	0.50
1:A:256:GLU:CD	1:A:256:GLU:N	2.70	0.50
1:C:120:THR:HG23	1:C:123:HIS:N	2.07	0.50
1:A:193:VAL:HG21	1:A:341:GLN:CB	2.36	0.50
1:C:187:ASN:CG	1:C:192:PRO:HA	2.36	0.50
1:A:74:GLU:HG2	3:A:1380:HOH:O	2.11	0.50
1:A:290:LYS:HE2	1:A:290:LYS:HA	1.93	0.50
1:C:210:LEU:HD12	1:C:240:MET:CG	2.42	0.50
1:B:273:ARG:NH2	1:B:294:HIS:NE2	2.59	0.50
1:A:150:TYR:O	1:A:154:GLN:HG3	2.11	0.50
1:A:276:ALA:O	1:A:280:GLN:HG3	2.12	0.50
1:C:246:HIS:C	1:C:247:LEU:HD12	2.37	0.50
1:C:127:ASN:OD1	1:C:129:THR:HG22	2.12	0.50
1:B:30:ARG:HH22	1:B:68:ASP:HB2	1.76	0.50
1:B:184:ARG:HH21	1:B:184:ARG:CG	2.20	0.50
1:A:110:GLU:O	1:A:113:VAL:CG1	2.58	0.50
1:B:316:ASP:OD2	1:B:319:ALA:HB2	2.11	0.49
1:A:173:LEU:N	1:A:174:PRO:CD	2.75	0.49
1:A:260:VAL:HG13	1:A:295:LEU:HD22	1.92	0.49
1:B:254:ARG:HH11	1:B:256:GLU:CG	2.25	0.49
1:C:256:GLU:HB2	3:C:1723:HOH:O	2.11	0.49
1:B:295:LEU:HA	1:B:298:VAL:HG12	1.94	0.49
1:A:290:LYS:HE2	1:A:290:LYS:CA	2.43	0.49
1:C:133:GLU:O	1:C:137:LYS:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:ALA:HB3	1:C:116:LEU:O	2.13	0.49
1:B:175:MET:SD	1:B:175:MET:C	2.95	0.49
1:C:36:HIS:HB2	1:C:216:MET:HE2	1.94	0.49
1:C:185:ARG:HH11	1:C:189:LEU:HD22	1.77	0.49
1:B:74:GLU:CD	1:C:347:ARG:NH1	2.70	0.49
1:B:169:GLY:O	1:B:170:ASP:C	2.55	0.49
1:B:315:ARG:O	1:B:315:ARG:HG2	2.12	0.49
1:B:349:PHE:CD2	1:C:80:VAL:CG1	2.95	0.49
1:A:237:VAL:O	1:A:240:MET:HB2	2.11	0.49
1:B:25:VAL:HG22	1:B:165:LEU:HB3	1.94	0.49
1:B:292:LYS:O	1:B:296:ILE:HG23	2.12	0.49
1:C:241:TYR:OH	1:C:244:PRO:HD3	2.13	0.49
1:A:134:ILE:HD13	1:A:143:VAL:HG21	1.94	0.49
1:A:218:LYS:NZ	1:A:225:ALA:HB2	2.28	0.49
1:C:23:PRO:HB3	3:C:1304:HOH:O	2.12	0.49
1:A:49:ARG:O	1:A:52:ASP:OD2	2.31	0.49
1:B:23:PRO:HD2	1:B:54:ALA:CB	2.41	0.49
1:B:43:SER:O	1:B:46:ASN:N	2.46	0.49
1:C:60:LEU:HD22	1:C:83:VAL:HG21	1.95	0.49
1:C:254:ARG:CD	1:C:256:GLU:O	2.61	0.49
1:B:66:LEU:C	1:B:68:ASP:N	2.68	0.48
1:A:143:VAL:HG12	1:A:144:PRO:HD2	1.95	0.48
1:A:175:MET:SD	1:A:176:LEU:N	2.86	0.48
1:B:274:VAL:C	1:B:276:ALA:N	2.69	0.48
1:A:211:ASP:O	1:A:213:GLN:N	2.42	0.48
1:A:292:LYS:O	1:A:295:LEU:N	2.47	0.48
1:B:29:ASP:O	1:B:31:PRO:HD3	2.14	0.48
1:C:255:VAL:HG21	1:C:278:LYS:HG2	1.95	0.48
1:A:125:ARG:HG3	1:A:125:ARG:HH21	1.78	0.48
1:C:27:THR:HG22	1:C:167:PRO:HD2	1.94	0.48
1:B:211:ASP:OD1	1:B:213:GLN:NE2	2.47	0.48
1:A:98:THR:OG1	1:A:330:ARG:NH1	2.43	0.48
1:A:112:THR:HG22	1:A:153:SER:HA	1.95	0.48
1:A:158:ILE:HG23	1:A:163:ALA:HB3	1.95	0.48
1:A:105:VAL:HG13	1:A:108:LEU:HG	1.94	0.48
1:A:185:ARG:O	1:A:189:LEU:HB2	2.14	0.48
1:A:308:THR:O	1:A:311:ALA:HB3	2.12	0.48
1:B:270:ASP:O	1:B:273:ARG:HB3	2.14	0.48
1:B:277:LEU:HD13	1:B:280:GLN:NE2	2.29	0.48
1:C:60:LEU:HD22	1:C:83:VAL:CG2	2.43	0.48
1:B:264:LEU:HG	1:B:295:LEU:HD12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:LYS:O	1:C:296:ILE:HG13	2.14	0.48
1:B:68:ASP:OD1	1:B:137:LYS:CE	2.62	0.47
1:B:101:VAL:HG13	1:B:101:VAL:O	2.14	0.47
1:B:255:VAL:HG22	1:B:261:PHE:CE2	2.48	0.47
1:A:253:GLY:HA3	1:A:281:TYR:CE2	2.49	0.47
1:A:291:VAL:O	1:A:292:LYS:C	2.56	0.47
1:B:315:ARG:HG3	3:B:1367:HOH:O	2.13	0.47
1:A:45:GLN:O	1:A:48:VAL:HB	2.14	0.47
1:A:240:MET:HE1	1:A:259:PRO:HB2	1.97	0.47
1:C:276:ALA:O	1:C:280:GLN:HG3	2.13	0.47
1:C:344:ARG:HD3	3:C:1217:HOH:O	2.15	0.47
1:B:36:HIS:CE1	1:B:39:HIS:CE1	3.03	0.47
1:B:77:ARG:NE	1:C:347:ARG:NH2	2.62	0.47
1:C:63:VAL:H	1:C:102:GLN:HE21	1.61	0.47
1:A:32:THR:HG23	1:A:69:HIS:HE1	1.79	0.47
1:A:215:LYS:NZ	1:A:215:LYS:HB2	2.29	0.47
1:A:223:ALA:O	1:A:236:LYS:NZ	2.44	0.47
1:C:201:LEU:HD23	1:C:202:SER:N	2.27	0.47
1:B:92:LEU:HD12	1:B:92:LEU:HA	1.78	0.47
1:B:114:TYR:CD1	1:B:346:MET:HE1	2.49	0.47
1:C:36:HIS:CE1	1:C:216:MET:HG2	2.50	0.47
1:B:22:ARG:HB2	1:B:23:PRO:CD	2.45	0.47
1:B:64:GLN:H	1:B:102:GLN:NE2	2.12	0.47
1:B:149:VAL:O	1:B:149:VAL:CG1	2.63	0.47
1:A:36:HIS:HD2	1:A:38:GLY:H	1.61	0.47
1:A:130:VAL:HG13	1:A:131:LYS:N	2.28	0.47
1:C:171:ASP:CB	1:C:172:GLN:NE2	2.78	0.47
1:C:216:MET:CE	1:C:224:ILE:H	2.27	0.47
1:A:288:ASP:CA	1:A:291:VAL:HG12	2.42	0.47
1:B:316:ASP:OD1	1:B:318:ASP:OD2	2.33	0.47
1:A:241:TYR:O	1:A:259:PRO:CD	2.60	0.47
1:B:71:ASP:OD1	1:B:72:ARG:CD	2.63	0.47
1:A:274:VAL:C	1:A:276:ALA:H	2.22	0.47
1:C:241:TYR:CZ	1:C:244:PRO:HD3	2.50	0.47
1:A:98:THR:HG23	1:A:330:ARG:HD2	1.96	0.46
1:B:241:TYR:O	1:B:259:PRO:HG2	2.14	0.46
1:A:234:ALA:HA	1:A:296:ILE:HG22	1.95	0.46
1:B:110:GLU:OE1	1:B:343:ARG:HD3	2.15	0.46
1:A:214:ALA:C	1:A:215:LYS:HG3	2.40	0.46
1:C:320:VAL:O	1:C:323:PHE:HB3	2.15	0.46
1:B:244:PRO:C	1:B:246:HIS:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LEU:HD13	1:A:97:THR:HG23	1.98	0.46
1:A:288:ASP:HA	1:A:291:VAL:CG1	2.43	0.46
1:A:296:ILE:HG13	1:A:297:ASP:H	1.81	0.46
1:A:32:THR:HG22	1:A:32:THR:O	2.15	0.46
1:A:33:GLY:HA2	1:A:79:ASN:ND2	2.31	0.46
1:A:99:CYS:HB2	1:A:323:PHE:CZ	2.50	0.46
1:A:242:THR:HB	1:A:258:ASN:ND2	2.30	0.46
1:C:310:ARG:O	1:C:314:GLU:HG3	2.15	0.46
1:B:22:ARG:CD	1:B:23:PRO:HD3	2.46	0.46
1:A:32:THR:HG23	1:A:69:HIS:CE1	2.51	0.46
1:A:36:HIS:O	1:A:38:GLY:N	2.49	0.46
1:A:277:LEU:HD13	1:A:280:GLN:NE2	2.31	0.46
1:A:46:ASN:ND2	1:A:50:LEU:HG	2.30	0.46
1:A:255:VAL:HG21	1:A:278:LYS:HD3	1.98	0.46
1:A:290:LYS:HE2	1:A:290:LYS:N	2.30	0.46
1:B:333:GLU:O	1:B:337:GLN:HG3	2.16	0.46
1:A:30:ARG:O	1:A:32:THR:N	2.48	0.46
1:A:335:ALA:O	1:A:339:LEU:HD23	2.16	0.46
1:B:263:PHE:CB	1:B:295:LEU:HD11	2.46	0.46
1:B:344:ARG:HG3	1:B:344:ARG:NH1	2.30	0.46
1:C:311:ALA:CA	1:C:314:GLU:HG3	2.43	0.46
1:C:25:VAL:HG13	1:C:167:PRO:HD3	1.96	0.46
1:B:166:VAL:HB	1:B:176:LEU:HD21	1.98	0.45
1:A:344:ARG:HD3	3:A:1031:HOH:O	2.16	0.45
1:B:22:ARG:CB	1:B:23:PRO:CD	2.94	0.45
1:B:330:ARG:O	1:B:333:GLU:HB3	2.16	0.45
1:B:287:GLY:O	1:B:290:LYS:N	2.49	0.45
1:A:51:GLN:HE22	1:A:92:LEU:HA	1.80	0.45
1:A:180:ARG:HB3	1:A:184:ARG:NH1	2.31	0.45
1:C:270:ASP:OD2	1:C:273:ARG:CZ	2.64	0.45
1:B:51:GLN:NE2	1:B:97:THR:CG2	2.71	0.45
1:B:184:ARG:NH2	1:B:184:ARG:CG	2.76	0.45
1:B:184:ARG:HE	1:B:196:GLU:CD	2.23	0.45
1:A:255:VAL:HG13	1:A:261:PHE:HB3	1.99	0.45
1:C:30:ARG:HD2	1:C:64:GLN:HE21	1.81	0.45
1:C:210:LEU:HD21	1:C:224:ILE:HG13	1.97	0.45
1:C:245:GLY:O	1:C:247:LEU:HD13	2.16	0.45
1:B:219:SER:HA	3:B:1401:HOH:O	2.16	0.45
1:B:264:LEU:O	1:B:268:ASP:HB3	2.17	0.45
1:B:278:LYS:HE3	1:B:278:LYS:HB2	1.76	0.45
1:B:295:LEU:C	1:B:298:VAL:HG12	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ALA:HB1	1:A:23:PRO:HD2	1.98	0.45
1:A:46:ASN:O	1:A:50:LEU:N	2.33	0.45
1:A:187:ASN:OD1	1:A:192:PRO:HA	2.16	0.45
1:A:294:HIS:O	1:A:298:VAL:HG23	2.16	0.45
1:A:296:ILE:O	1:A:300:ASN:HB2	2.15	0.45
1:A:303:LEU:HB3	1:A:307:ARG:NH2	2.31	0.45
1:A:249:ALA:CB	1:A:287:GLY:HA3	2.47	0.45
1:A:265:ASP:HB3	1:A:274:VAL:HG11	1.97	0.45
1:B:74:GLU:OE2	1:C:347:ARG:NH1	2.50	0.45
1:A:226:LEU:HD23	1:A:306:ILE:HD12	1.98	0.45
1:A:277:LEU:O	1:A:281:TYR:N	2.50	0.45
1:A:302:VAL:HG13	1:A:303:LEU:HD13	1.97	0.45
1:B:270:ASP:HB2	1:B:273:ARG:CZ	2.47	0.45
1:C:112:THR:HG22	1:C:156:ALA:HB3	1.98	0.45
1:A:211:ASP:C	1:A:213:GLN:N	2.70	0.44
1:C:51:GLN:NE2	1:C:97:THR:CG2	2.79	0.44
1:C:271:PRO:HG2	3:C:1373:HOH:O	2.17	0.44
1:A:130:VAL:CG1	1:A:131:LYS:N	2.79	0.44
1:C:231:ASP:CG	1:C:232:GLU:N	2.75	0.44
1:B:140:GLY:O	1:B:143:VAL:CG2	2.66	0.44
1:B:165:LEU:HD23	1:B:198:GLN:O	2.18	0.44
1:A:68:ASP:OD2	1:A:137:LYS:NZ	2.45	0.44
1:A:105:VAL:HA	1:A:106:PRO:HD2	1.80	0.44
1:A:293:LYS:HD2	1:A:296:ILE:HD11	1.99	0.44
1:C:185:ARG:O	1:C:189:LEU:HB2	2.16	0.44
1:A:136:GLN:O	1:A:136:GLN:CG	2.66	0.44
1:C:321:LEU:HD22	1:C:325:THR:HG23	2.00	0.44
1:B:346:MET:HE3	1:B:348:LEU:HD11	1.99	0.44
1:B:240:MET:HE3	1:B:260:VAL:CG1	2.23	0.44
1:C:30:ARG:HA	1:C:31:PRO:HD3	1.79	0.44
1:A:205:PRO:HG2	1:A:206:ARG:H	1.82	0.44
1:C:62:ASP:OD2	1:C:103:SER:CB	2.66	0.44
1:C:201:LEU:HD22	1:C:202:SER:HB3	2.00	0.44
1:C:203:ARG:C	1:C:204:VAL:O	2.57	0.44
1:A:119:VAL:HG22	1:A:120:THR:N	2.32	0.44
1:A:149:VAL:O	1:A:152:VAL:HG13	2.17	0.44
1:C:58:VAL:CG2	1:C:99:CYS:HA	2.47	0.44
1:C:92:LEU:HD12	1:C:92:LEU:HA	1.80	0.44
1:B:123:HIS:HE1	3:B:1334:HOH:O	2.01	0.43
1:A:76:VAL:CG1	1:A:77:ARG:N	2.81	0.43
1:A:222:ASN:O	1:A:222:ASN:CG	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG12	1:A:144:PRO:CD	2.49	0.43
1:A:180:ARG:HG2	1:A:197:PRO:HD2	1.99	0.43
1:C:154:GLN:NE2	2:C:3000:TRP:CD2	2.86	0.43
1:C:154:GLN:O	1:C:158:ILE:HG12	2.18	0.43
1:C:166:VAL:O	1:C:166:VAL:CG2	2.66	0.43
1:C:268:ASP:HA	1:C:269:PRO:HD2	1.87	0.43
1:B:346:MET:CE	1:B:348:LEU:HD11	2.49	0.43
1:A:237:VAL:HA	1:A:240:MET:HG3	2.00	0.43
1:C:68:ASP:OD2	1:C:69:HIS:CD2	2.69	0.43
1:A:225:ALA:C	1:A:227:GLY:H	2.26	0.43
1:A:36:HIS:O	1:A:37:LEU:C	2.61	0.43
1:A:168:VAL:CG1	1:A:199:ALA:HB1	2.46	0.43
1:A:294:HIS:HD2	1:A:297:ASP:OD2	2.02	0.43
1:C:136:GLN:CD	1:C:137:LYS:HD2	2.43	0.43
1:B:255:VAL:HG13	1:B:261:PHE:CB	2.48	0.43
1:A:81:LEU:HD12	1:A:81:LEU:HA	1.77	0.43
1:A:250:SER:O	1:A:284:GLY:CA	2.66	0.43
1:A:293:LYS:O	1:A:296:ILE:CG1	2.66	0.43
1:C:204:VAL:HG12	1:C:205:PRO:CD	2.36	0.43
1:C:238:MET:O	1:C:292:LYS:NZ	2.52	0.43
1:A:210:LEU:HD22	1:A:240:MET:HG2	2.01	0.43
1:A:269:PRO:HD2	1:A:273:ARG:HH12	1.84	0.43
1:C:36:HIS:CB	1:C:216:MET:HE2	2.49	0.43
1:C:62:ASP:O	1:C:66:LEU:HG	2.18	0.43
1:B:93:ASP:HA	1:B:94:PRO:HD3	1.86	0.43
1:B:101:VAL:HG12	1:B:328:THR:OG1	2.18	0.43
1:B:348:LEU:O	1:B:349:PHE:C	2.60	0.43
1:B:274:VAL:C	1:B:276:ALA:H	2.25	0.42
1:A:83:VAL:O	1:A:84:ALA:C	2.61	0.42
1:A:210:LEU:HD22	1:A:240:MET:CG	2.49	0.42
1:A:254:ARG:CD	1:A:256:GLU:HB2	2.47	0.42
1:A:334:VAL:HA	1:A:337:GLN:HG3	2.01	0.42
1:C:189:LEU:HD12	1:C:189:LEU:HA	1.87	0.42
1:A:21:ALA:HB1	1:A:23:PRO:CD	2.48	0.42
1:A:121:VAL:O	1:A:125:ARG:HB2	2.19	0.42
1:A:173:LEU:HD13	3:A:2045:HOH:O	2.18	0.42
1:B:58:VAL:HG23	1:B:99:CYS:HA	2.00	0.42
1:A:208:PRO:HG3	1:A:262:THR:CG2	2.48	0.42
1:B:254:ARG:NH1	1:B:256:GLU:HG3	2.34	0.42
1:A:62:ASP:H	1:A:102:GLN:HB3	1.84	0.42
1:A:105:VAL:HG13	1:A:105:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HG13	1:A:108:LEU:CD1	2.49	0.42
1:A:150:TYR:N	1:A:151:PRO:CD	2.83	0.42
1:A:302:VAL:C	1:A:305:PRO:HD2	2.44	0.42
1:C:52:ASP:OD2	1:C:96:LYS:NZ	2.49	0.42
1:B:277:LEU:HA	1:B:286:LEU:HD11	2.01	0.42
1:A:58:VAL:O	1:A:58:VAL:CG1	2.67	0.42
1:A:191:ALA:HA	1:A:192:PRO:HD3	1.80	0.42
1:A:241:TYR:O	1:A:241:TYR:CD1	2.73	0.42
1:B:30:ARG:HH22	1:B:68:ASP:CB	2.33	0.42
1:A:288:ASP:C	1:A:291:VAL:HG12	2.44	0.42
1:C:108:LEU:HD13	1:C:157:ASP:OD1	2.19	0.42
1:C:230:ALA:HB1	1:C:300:ASN:HD21	1.85	0.42
1:B:21:ALA:HA	1:B:54:ALA:HA	2.01	0.42
1:B:232:GLU:O	1:B:233:VAL:C	2.61	0.42
1:B:258:ASN:HA	1:B:259:PRO:HD2	1.97	0.42
1:A:84:ALA:O	1:A:85:LEU:C	2.62	0.42
1:C:231:ASP:OD1	1:C:235:ARG:CZ	2.68	0.42
1:B:211:ASP:CB	1:B:213:GLN:HG3	2.50	0.42
1:C:180:ARG:CD	1:C:197:PRO:O	2.61	0.42
1:B:277:LEU:HA	1:B:286:LEU:CD1	2.50	0.42
1:A:119:VAL:HG21	1:A:124:LEU:HD13	2.02	0.42
1:A:309:ARG:O	1:A:310:ARG:C	2.63	0.42
1:B:59:LEU:HD12	1:B:100:VAL:O	2.19	0.42
1:A:165:LEU:HD22	1:A:166:VAL:N	2.35	0.42
1:C:25:VAL:HG22	1:C:165:LEU:HB3	2.01	0.42
1:C:243:ASP:HA	1:C:244:PRO:HD2	1.87	0.42
1:A:22:ARG:N	1:A:23:PRO:HD2	2.34	0.41
1:A:216:MET:CG	1:A:223:ALA:HA	2.47	0.41
1:A:310:ARG:HG2	1:A:314:GLU:CD	2.45	0.41
1:C:248:ARG:O	1:C:251:ASP:HB2	2.20	0.41
1:B:273:ARG:O	1:B:277:LEU:HD22	2.20	0.41
1:B:278:LYS:HG2	1:B:282:ARG:NH2	2.34	0.41
1:B:344:ARG:CG	1:B:344:ARG:NH1	2.80	0.41
1:A:203:ARG:HD2	3:A:1508:HOH:O	2.20	0.41
1:A:305:PRO:HG2	1:A:306:ILE:N	2.31	0.41
1:C:32:THR:O	1:C:32:THR:HG22	2.19	0.41
1:C:64:GLN:H	1:C:102:GLN:NE2	2.15	0.41
1:C:127:ASN:HB3	1:C:130:VAL:CG2	2.51	0.41
1:B:142:ARG:HA	1:C:120:THR:OG1	2.20	0.41
1:A:47:ARG:O	1:A:51:GLN:N	2.51	0.41
1:A:110:GLU:HG2	1:A:114:TYR:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ARG:HD3	3:A:1187:HOH:O	2.20	0.41
1:C:129:THR:O	1:C:133:GLU:HG3	2.21	0.41
1:B:66:LEU:HD12	1:B:70:PHE:HA	2.01	0.41
1:B:255:VAL:HG22	1:B:261:PHE:CD2	2.56	0.41
1:C:304:ALA:N	1:C:305:PRO:HD2	2.35	0.41
1:A:201:LEU:HD22	1:A:202:SER:N	2.35	0.41
1:C:255:VAL:O	1:C:258:ASN:HB3	2.20	0.41
1:A:51:GLN:OE1	1:A:93:ASP:N	2.43	0.41
1:A:72:ARG:N	1:A:73:PRO:CD	2.83	0.41
1:C:25:VAL:HG11	1:C:50:LEU:HD13	2.02	0.41
1:C:170:ASP:OD1	1:C:170:ASP:N	2.53	0.41
1:C:293:LYS:HD2	1:C:293:LYS:HA	1.93	0.41
1:B:205:PRO:O	1:B:206:ARG:C	2.62	0.41
1:A:32:THR:CG2	1:A:69:HIS:HE1	2.33	0.41
1:A:33:GLY:HA2	1:A:79:ASN:CG	2.46	0.41
1:A:68:ASP:C	1:A:69:HIS:HD2	2.28	0.41
1:A:125:ARG:HG3	1:A:125:ARG:NH2	2.35	0.41
1:A:89:ALA:O	1:A:306:ILE:HB	2.20	0.41
1:A:175:MET:C	1:A:177:GLU:N	2.79	0.41
1:B:63:VAL:H	1:B:102:GLN:HE21	1.67	0.41
1:B:243:ASP:OD1	1:B:244:PRO:O	2.39	0.41
1:B:246:HIS:CE1	1:B:288:ASP:OD2	2.73	0.41
1:A:105:VAL:O	1:A:108:LEU:HG	2.21	0.41
1:A:230:ALA:CB	1:A:300:ASN:HD21	2.28	0.41
1:B:137:LYS:HE3	3:B:1218:HOH:O	2.19	0.41
1:B:210:LEU:HD21	1:B:224:ILE:HG13	2.03	0.41
1:A:36:HIS:O	1:A:39:HIS:N	2.51	0.41
1:C:58:VAL:HG23	1:C:99:CYS:HA	2.02	0.41
1:C:102:GLN:HG3	1:C:108:LEU:HD12	2.02	0.41
1:B:67:THR:HG22	1:C:117:ASN:HD21	1.85	0.40
1:C:150:TYR:CD2	1:C:150:TYR:C	2.99	0.40
1:B:61:ALA:HB1	1:B:64:GLN:HB3	2.04	0.40
1:B:186:PHE:CD1	1:B:186:PHE:C	2.99	0.40
1:A:36:HIS:CE1	1:A:39:HIS:NE2	2.89	0.40
1:A:122:SER:C	1:A:124:LEU:N	2.78	0.40
1:C:258:ASN:C	1:C:258:ASN:ND2	2.80	0.40
1:B:33:GLY:HA2	1:B:79:ASN:OD1	2.21	0.40
1:B:93:ASP:O	1:B:97:THR:CG2	2.69	0.40
1:B:255:VAL:HG13	1:B:261:PHE:CG	2.57	0.40
1:B:342:VAL:HG12	1:B:346:MET:HE2	2.03	0.40
1:A:277:LEU:HA	1:A:280:GLN:HE21	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:VAL:HG13	1:A:303:LEU:CD1	2.51	0.40
1:C:270:ASP:OD2	1:C:273:ARG:NH1	2.54	0.40
1:A:41:ALA:HB1	1:A:207:LEU:HD13	2.04	0.40
1:A:260:VAL:HA	1:A:295:LEU:HD22	2.02	0.40
1:C:62:ASP:OD2	1:C:103:SER:HB2	2.21	0.40
1:C:150:TYR:N	1:C:151:PRO:CD	2.84	0.40
1:B:47:ARG:O	1:B:51:GLN:HB2	2.20	0.40
1:B:254:ARG:NH1	1:B:256:GLU:CG	2.84	0.40
1:B:322:ARG:HG2	1:B:322:ARG:NH2	2.32	0.40
1:A:261:PHE:HZ	1:A:281:TYR:CG	2.40	0.40
1:A:264:LEU:HD22	3:A:1622:HOH:O	2.22	0.40
1:C:32:THR:HG23	1:C:75:GLN:NE2	2.36	0.40
1:C:43:SER:O	1:C:47:ARG:HD3	2.21	0.40

All (32) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:CA	3:C:2021:HOH:O[1_554]	0.49	1.71
3:C:1200:HOH:O	3:C:1789:HOH:O[4_546]	0.74	1.46
1:C:315:ARG:NH1	3:C:1771:HOH:O[4_556]	0.82	1.38
1:A:235:ARG:CZ	3:B:1589:HOH:O[1_554]	0.84	1.36
1:B:322:ARG:NH1	3:A:1468:HOH:O[1_546]	0.88	1.32
1:A:235:ARG:CB	3:C:2021:HOH:O[1_554]	1.14	1.06
1:A:235:ARG:NH2	3:B:1589:HOH:O[1_554]	1.32	0.88
1:A:235:ARG:NH1	3:B:1589:HOH:O[1_554]	1.34	0.86
1:C:315:ARG:NE	3:C:1613:HOH:O[4_556]	1.36	0.84
1:C:315:ARG:CD	3:C:1613:HOH:O[4_556]	1.59	0.61
1:A:235:ARG:CD	3:C:1529:HOH:O[1_554]	1.60	0.60
1:A:235:ARG:NE	3:C:1529:HOH:O[1_554]	1.62	0.58
1:A:235:ARG:N	3:C:2021:HOH:O[1_554]	1.64	0.56
3:A:1790:HOH:O	3:A:1956:HOH:O[2_655]	1.71	0.49
3:C:1118:HOH:O	3:C:1754:HOH:O[4_546]	1.80	0.40
1:B:201:LEU:N	1:A:341:GLN:NE2[2_655]	1.81	0.39
1:C:322:ARG:NH1	3:C:1537:HOH:O[4_546]	1.81	0.39
1:B:201:LEU:O	1:A:341:GLN:OE1[2_655]	1.86	0.34
1:A:235:ARG:C	3:C:2021:HOH:O[1_554]	1.93	0.27
1:B:235:ARG:NH1	1:C:245:GLY:O[4_535]	1.96	0.24
1:A:235:ARG:NE	3:B:1589:HOH:O[1_554]	1.97	0.23
1:B:177:GLU:OE2	1:A:192:PRO:CG[2_655]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ARG:CZ	3:A:1468:HOH:O[1_546]	1.99	0.21
1:C:315:ARG:CZ	3:C:1613:HOH:O[4_556]	2.00	0.20
1:A:235:ARG:CG	3:C:1529:HOH:O[1_554]	2.02	0.18
3:B:1248:HOH:O	3:A:1154:HOH:O[2_655]	2.05	0.15
3:C:1588:HOH:O	3:C:1691:HOH:O[1_545]	2.11	0.09
1:B:170:ASP:OD1	3:A:1031:HOH:O[2_655]	2.12	0.08
1:A:235:ARG:CG	3:C:2021:HOH:O[1_554]	2.12	0.08
1:C:315:ARG:CZ	3:C:1771:HOH:O[4_556]	2.12	0.08
3:B:1371:HOH:O	3:A:1175:HOH:O[2_655]	2.15	0.05
1:C:315:ARG:CA	3:C:1808:HOH:O[4_556]	2.17	0.03

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	329/351 (94%)	278 (84%)	37 (11%)	14 (4%)	2	0
1	B	329/351 (94%)	294 (89%)	28 (8%)	7 (2%)	5	2
1	C	329/351 (94%)	312 (95%)	13 (4%)	4 (1%)	10	7
All	All	987/1053 (94%)	884 (90%)	78 (8%)	25 (2%)	4	1

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	22	ARG
1	A	61	ALA
1	C	22	ARG
1	C	202	SER
1	C	205	PRO
1	B	61	ALA
1	A	37	LEU
1	B	43	SER
1	B	284	GLY

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Mol	Chain	Res	Type
1	A	31	PRO
1	A	205	PRO
1	A	242	THR
1	A	269	PRO
1	B	250	SER
1	A	73	PRO
1	A	74	GLU
1	A	206	ARG
1	A	208	PRO
1	C	283	ALA
1	B	249	ALA
1	A	238	MET
1	B	285	GLY
1	A	258	ASN
1	A	291	VAL
1	A	22	ARG

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	256/282 (91%)	224 (88%)	32 (12%)	4	2
1	B	264/282 (94%)	227 (86%)	37 (14%)	3	2
1	C	262/282 (93%)	227 (87%)	35 (13%)	4	2
All	All	782/846 (92%)	678 (87%)	104 (13%)	4	2

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	ARG
1	B	40	LEU
1	B	47	ARG
1	B	50	LEU
1	B	52	ASP
1	B	68	ASP

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Mol	Chain	Res	Type
1	B	75	GLN
1	B	81	LEU
1	B	85	LEU
1	B	92	LEU
1	B	95	GLN
1	B	97	THR
1	B	136	GLN
1	B	141	GLU
1	B	149	VAL
1	B	150	TYR
1	B	152	VAL
1	B	165	LEU
1	B	168	VAL
1	B	170	ASP
1	B	171	ASP
1	B	176	LEU
1	B	185	ARG
1	B	189	LEU
1	B	201	LEU
1	B	226	LEU
1	B	254	ARG
1	B	262	THR
1	B	282	ARG
1	B	290	LYS
1	B	296	ILE
1	B	297	ASP
1	B	302	VAL
1	B	318	ASP
1	B	322	ARG
1	B	344	ARG
1	B	347	ARG
1	A	35	LEU
1	A	40	LEU
1	A	52	ASP
1	A	56	LEU
1	A	63	VAL
1	A	74	GLU
1	A	81	LEU
1	A	85	LEU
1	A	124	LEU
1	A	125	ARG
1	A	126	GLN

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Mol	Chain	Res	Type
1	A	136	GLN
1	A	142	ARG
1	A	150	TYR
1	A	152	VAL
1	A	153	SER
1	A	165	LEU
1	A	172	GLN
1	A	200	GLN
1	A	201	LEU
1	A	203	ARG
1	A	215	LYS
1	A	224	ILE
1	A	232	GLU
1	A	246	HIS
1	A	268	ASP
1	A	282	ARG
1	A	286	LEU
1	A	290	LYS
1	A	300	ASN
1	A	306	ILE
1	A	348	LEU
1	C	30	ARG
1	C	46	ASN
1	C	80	VAL
1	C	81	LEU
1	C	85	LEU
1	C	92	LEU
1	C	97	THR
1	C	100	VAL
1	C	112	THR
1	C	113	VAL
1	C	150	TYR
1	C	152	VAL
1	C	165	LEU
1	C	168	VAL
1	C	180	ARG
1	C	193	VAL
1	C	200	GLN
1	C	201	LEU
1	C	202	SER
1	C	204	VAL
1	C	205	PRO

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Mol	Chain	Res	Type
1	C	210	LEU
1	C	231	ASP
1	C	238	MET
1	C	247	LEU
1	C	248	ARG
1	C	256	GLU
1	C	277	LEU
1	C	286	LEU
1	C	295	LEU
1	C	298	VAL
1	C	312	GLU
1	C	314	GLU
1	C	321	LEU
1	C	330	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	36	HIS
1	B	46	ASN
1	B	51	GLN
1	B	64	GLN
1	B	69	HIS
1	B	102	GLN
1	B	117	ASN
1	B	136	GLN
1	B	178	GLN
1	B	200	GLN
1	B	300	ASN
1	B	337	GLN
1	A	36	HIS
1	A	46	ASN
1	A	69	HIS
1	A	154	GLN
1	A	172	GLN
1	A	200	GLN
1	A	258	ASN
1	A	280	GLN
1	A	300	ASN
1	A	341	GLN
1	C	46	ASN
1	C	51	GLN

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Mol	Chain	Res	Type
1	C	69	HIS
1	C	95	GLN
1	C	102	GLN
1	C	117	ASN
1	C	126	GLN
1	C	178	GLN
1	C	200	GLN
1	C	213	GLN
1	C	258	ASN
1	C	300	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TRP	C	3000	-	15,16,16	1.17	2 (13%)	18,22,22	0.37	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRP	C	3000	-	-	4/8/8/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3000	TRP	OXT-C	-2.94	1.21	1.30
2	C	3000	TRP	CH2-CZ3	2.06	1.42	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3000	TRP	OXT-C-CA-CB
2	C	3000	TRP	CA-CB-CG-CD2
2	C	3000	TRP	CA-CB-CG-CD1
2	C	3000	TRP	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3000	TRP	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/351 (94%)	4.57	314 (94%) 0 0	37, 72, 96, 99	0
1	B	331/351 (94%)	3.58	294 (88%) 0 0	24, 46, 82, 88	1 (0%)
1	C	331/351 (94%)	3.33	282 (85%) 0 0	16, 31, 56, 65	0
All	All	993/1053 (94%)	3.83	890 (89%) 0 0	16, 46, 91, 99	1 (0%)

All (890) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	267	PHE	12.8
1	A	130	VAL	11.8
1	A	155	ALA	11.5
1	A	249	ALA	10.2
1	A	44	LEU	10.0
1	A	289	VAL	9.6
1	A	287	GLY	9.4
1	A	311	ALA	9.3
1	A	40	LEU	9.3
1	A	239	GLY	9.3
1	A	245	GLY	9.2
1	A	219	SER	9.0
1	C	244	PRO	9.0
1	A	63	VAL	9.0
1	C	271	PRO	8.9
1	A	281	TYR	8.9
1	B	338	THR	8.9
1	A	225	ALA	8.8
1	C	34	ALA	8.7
1	A	48	VAL	8.4
1	A	220	LEU	8.4
1	A	128	PRO	8.4
1	A	50	LEU	8.3

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Mol	Chain	Res	Type	RSRZ
1	C	299	LEU	8.2
1	A	215	LYS	8.0
1	A	204	VAL	8.0
1	A	286	LEU	7.9
1	A	205	PRO	7.9
1	C	253	GLY	7.9
1	A	307	ARG	7.8
1	A	92	LEU	7.8
1	B	266	ALA	7.8
1	A	263	PHE	7.8
1	B	173	LEU	7.7
1	C	321	LEU	7.7
1	A	224	ILE	7.7
1	A	264	LEU	7.7
1	A	252	PRO	7.7
1	A	88	LEU	7.5
1	A	91	GLY	7.5
1	C	165	LEU	7.5
1	C	293	LYS	7.4
1	A	89	ALA	7.4
1	B	321	LEU	7.3
1	A	69	HIS	7.2
1	A	226	LEU	7.2
1	A	260	VAL	7.1
1	A	97	THR	7.1
1	A	35	LEU	7.0
1	A	254	ARG	7.0
1	B	257	GLY	7.0
1	A	269	PRO	7.0
1	A	232	GLU	6.9
1	B	105	VAL	6.9
1	C	160	ALA	6.8
1	B	264	LEU	6.8
1	B	322	ARG	6.7
1	B	261	PHE	6.7
1	B	247	LEU	6.6
1	A	161	PHE	6.6
1	B	40	LEU	6.6
1	A	85	LEU	6.6
1	B	204	VAL	6.6
1	A	253	GLY	6.6
1	A	234	ALA	6.5

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Mol	Chain	Res	Type	RSRZ
1	B	152	VAL	6.5
1	B	245	GLY	6.5
1	B	279	ASP	6.5
1	B	89	ALA	6.4
1	B	182	ILE	6.4
1	A	255	VAL	6.4
1	C	255	VAL	6.4
1	C	286	LEU	6.4
1	A	243	ASP	6.3
1	A	134	ILE	6.3
1	B	54	ALA	6.3
1	A	222	ASN	6.3
1	C	239	GLY	6.2
1	A	256	GLU	6.2
1	B	66	LEU	6.2
1	B	224	ILE	6.2
1	A	80	VAL	6.2
1	A	36	HIS	6.2
1	A	276	ALA	6.2
1	A	37	LEU	6.2
1	B	98	THR	6.2
1	A	107	GLU	6.2
1	A	238	MET	6.1
1	B	97	THR	6.1
1	B	189	LEU	6.1
1	C	177	GLU	6.1
1	A	57	PHE	6.1
1	A	324	VAL	6.1
1	B	241	TYR	6.1
1	C	273	ARG	6.0
1	B	281	TYR	6.0
1	B	263	PHE	6.0
1	A	313	TYR	6.0
1	C	22	ARG	6.0
1	A	244	PRO	6.0
1	B	42	GLY	6.0
1	B	32	THR	5.9
1	A	207	LEU	5.9
1	A	271	PRO	5.9
1	A	272	ALA	5.9
1	A	237	VAL	5.9
1	A	39	HIS	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	233	VAL	5.8
1	A	261	PHE	5.8
1	B	277	LEU	5.8
1	A	257	GLY	5.8
1	A	277	LEU	5.8
1	B	150	TYR	5.8
1	B	320	VAL	5.8
1	C	139	TYR	5.7
1	A	262	THR	5.7
1	C	281	TYR	5.7
1	B	253	GLY	5.7
1	A	115	PHE	5.7
1	A	310	ARG	5.7
1	B	138	GLY	5.7
1	A	42	GLY	5.7
1	A	211	ASP	5.7
1	C	143	VAL	5.7
1	A	230	ALA	5.7
1	A	210	LEU	5.7
1	A	247	LEU	5.7
1	C	28	GLY	5.6
1	B	280	GLN	5.6
1	A	82	ALA	5.6
1	A	233	VAL	5.6
1	C	324	VAL	5.6
1	A	148	PHE	5.6
1	C	202	SER	5.6
1	B	44	LEU	5.6
1	C	175	MET	5.6
1	A	67	THR	5.6
1	A	98	THR	5.6
1	B	246	HIS	5.6
1	A	295	LEU	5.6
1	A	125	ARG	5.6
1	C	135	ALA	5.6
1	A	296	ILE	5.5
1	B	156	ALA	5.5
1	C	80	VAL	5.5
1	A	135	ALA	5.5
1	B	118	LEU	5.5
1	C	105	VAL	5.5
1	A	285	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	301	GLY	5.4
1	B	158	ILE	5.4
1	A	34	ALA	5.4
1	A	320	VAL	5.4
1	A	123	HIS	5.4
1	B	262	THR	5.4
1	C	88	LEU	5.4
1	B	298	VAL	5.4
1	C	280	GLN	5.4
1	A	221	GLY	5.4
1	B	220	LEU	5.3
1	A	54	ALA	5.3
1	A	145	ALA	5.3
1	A	176	LEU	5.3
1	A	241	TYR	5.3
1	A	268	ASP	5.3
1	A	279	ASP	5.3
1	A	283	ALA	5.3
1	A	227	GLY	5.3
1	A	290	LYS	5.3
1	B	286	LEU	5.3
1	B	295	LEU	5.3
1	C	51	GLN	5.2
1	B	267	PHE	5.2
1	A	94	PRO	5.2
1	A	303	LEU	5.2
1	A	242	THR	5.2
1	A	294	HIS	5.2
1	A	138	GLY	5.2
1	A	160	ALA	5.2
1	B	302	VAL	5.2
1	C	300	ASN	5.2
1	B	306	ILE	5.2
1	A	21	ALA	5.2
1	A	250	SER	5.1
1	B	56	LEU	5.1
1	B	201	LEU	5.1
1	C	277	LEU	5.1
1	A	240	MET	5.1
1	B	90	ALA	5.1
1	C	132	ALA	5.1
1	C	272	ALA	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	81	LEU	5.1
1	C	97	THR	5.1
1	A	90	ALA	5.1
1	C	269	PRO	5.1
1	C	21	ALA	5.0
1	C	308	THR	5.0
1	A	298	VAL	5.0
1	B	203	ARG	5.0
1	B	41	ALA	5.0
1	A	199	ALA	5.0
1	A	299	LEU	5.0
1	A	86	ASP	5.0
1	B	38	GLY	5.0
1	A	156	ALA	5.0
1	A	195	ALA	5.0
1	A	58	VAL	5.0
1	A	273	ARG	5.0
1	B	129	THR	5.0
1	A	202	SER	4.9
1	B	236	LYS	4.9
1	B	278	LYS	4.9
1	B	276	ALA	4.9
1	A	26	LEU	4.9
1	C	108	LEU	4.9
1	B	209	GLY	4.9
1	B	300	ASN	4.9
1	B	329	ALA	4.9
1	B	210	LEU	4.9
1	A	165	LEU	4.9
1	A	201	LEU	4.9
1	A	175	MET	4.9
1	C	138	GLY	4.9
1	A	214	ALA	4.9
1	C	230	ALA	4.9
1	B	50	LEU	4.9
1	B	296	ILE	4.9
1	A	197	PRO	4.9
1	A	162	GLY	4.9
1	B	85	LEU	4.8
1	A	66	LEU	4.8
1	B	219	SER	4.8
1	A	212	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	333	GLU	4.8
1	A	293	LYS	4.8
1	A	173	LEU	4.8
1	C	261	PHE	4.8
1	B	230	ALA	4.8
1	B	325	THR	4.8
1	A	55	GLU	4.7
1	A	182	ILE	4.7
1	B	239	GLY	4.7
1	C	315	ARG	4.7
1	C	171	ASP	4.7
1	B	27	THR	4.7
1	B	92	LEU	4.7
1	A	306	ILE	4.7
1	C	323	PHE	4.7
1	B	255	VAL	4.7
1	C	101	VAL	4.7
1	A	266	ALA	4.7
1	B	37	LEU	4.7
1	B	51	GLN	4.7
1	A	108	LEU	4.7
1	A	169	GLY	4.7
1	A	216	MET	4.7
1	B	83	VAL	4.7
1	B	289	VAL	4.7
1	A	99	CYS	4.7
1	A	64	GLN	4.7
1	A	319	ALA	4.7
1	B	237	VAL	4.6
1	C	307	ARG	4.6
1	B	134	ILE	4.6
1	C	306	ILE	4.6
1	A	126	GLN	4.6
1	C	49	ARG	4.6
1	B	242	THR	4.6
1	A	121	VAL	4.6
1	B	234	ALA	4.6
1	C	241	TYR	4.6
1	B	175	MET	4.6
1	B	265	ASP	4.6
1	A	171	ASP	4.6
1	B	198	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	95	GLN	4.6
1	B	342	VAL	4.6
1	A	166	VAL	4.6
1	A	84	ALA	4.6
1	A	208	PRO	4.6
1	C	59	LEU	4.6
1	C	270	ASP	4.6
1	C	25	VAL	4.5
1	C	335	ALA	4.5
1	B	254	ARG	4.5
1	C	150	TYR	4.5
1	B	258	ASN	4.5
1	A	113	VAL	4.5
1	A	274	VAL	4.5
1	C	203	ARG	4.5
1	A	194	LEU	4.5
1	B	87	TYR	4.5
1	C	336	ALA	4.5
1	A	270	ASP	4.5
1	C	289	VAL	4.5
1	C	345	ALA	4.5
1	B	303	LEU	4.5
1	C	46	ASN	4.5
1	C	72	ARG	4.4
1	A	93	ASP	4.4
1	A	177	GLU	4.4
1	A	291	VAL	4.4
1	C	48	VAL	4.4
1	A	132	ALA	4.4
1	A	158	ILE	4.4
1	A	129	THR	4.4
1	B	274	VAL	4.4
1	C	276	ALA	4.4
1	C	298	VAL	4.4
1	C	56	LEU	4.4
1	B	115	PHE	4.4
1	B	132	ALA	4.4
1	C	283	ALA	4.4
1	B	26	LEU	4.4
1	B	88	LEU	4.4
1	C	303	LEU	4.4
1	B	125	ARG	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	349	PHE	4.3
1	B	136	GLN	4.3
1	A	71	ASP	4.3
1	B	256	GLU	4.3
1	C	134	ILE	4.3
1	A	315	ARG	4.3
1	A	305	PRO	4.3
1	B	215	LYS	4.3
1	B	76	VAL	4.3
1	B	176	LEU	4.3
1	A	68	ASP	4.3
1	C	238	MET	4.3
1	A	316	ASP	4.3
1	A	339	LEU	4.3
1	C	142	ARG	4.3
1	B	238	MET	4.3
1	B	341	GLN	4.3
1	C	174	PRO	4.3
1	C	259	PRO	4.3
1	C	234	ALA	4.2
1	A	248	ARG	4.2
1	A	246	HIS	4.2
1	C	192	PRO	4.2
1	A	51	GLN	4.2
1	A	278	LYS	4.2
1	C	285	GLY	4.2
1	C	184	ARG	4.2
1	C	103	SER	4.2
1	C	84	ALA	4.2
1	B	130	VAL	4.2
1	A	131	LYS	4.2
1	A	27	THR	4.2
1	A	164	THR	4.2
1	A	309	ARG	4.2
1	A	217	SER	4.2
1	A	288	ASP	4.2
1	A	200	GLN	4.2
1	B	214	ALA	4.2
1	B	260	VAL	4.2
1	C	274	VAL	4.2
1	B	67	THR	4.1
1	A	179	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	98	THR	4.1
1	A	23	PRO	4.1
1	A	151	PRO	4.1
1	A	275	GLN	4.1
1	B	195	ALA	4.1
1	B	58	VAL	4.1
1	C	209	GLY	4.1
1	B	252	PRO	4.1
1	C	200	GLN	4.1
1	B	21	ALA	4.1
1	B	315	ARG	4.1
1	A	41	ALA	4.1
1	A	61	ALA	4.1
1	C	328	THR	4.1
1	C	254	ARG	4.1
1	A	139	TYR	4.1
1	C	243	ASP	4.1
1	C	129	THR	4.1
1	B	244	PRO	4.1
1	C	197	PRO	4.1
1	C	249	ALA	4.0
1	A	114	TYR	4.0
1	C	313	TYR	4.0
1	B	101	VAL	4.0
1	A	110	GLU	4.0
1	C	237	VAL	4.0
1	A	330	ARG	4.0
1	B	212	GLY	4.0
1	A	218	LYS	4.0
1	C	172	GLN	4.0
1	C	350	GLY	4.0
1	B	309	ARG	4.0
1	A	142	ARG	4.0
1	A	308	THR	4.0
1	A	76	VAL	4.0
1	C	117	ASN	4.0
1	B	293	LYS	4.0
1	C	314	GLU	4.0
1	B	340	GLY	4.0
1	A	140	GLY	4.0
1	C	140	GLY	4.0
1	C	251	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	268	ASP	4.0
1	C	309	ARG	4.0
1	A	43	SER	3.9
1	C	262	THR	3.9
1	B	259	PRO	3.9
1	C	252	PRO	3.9
1	A	318	ASP	3.9
1	C	191	ALA	3.9
1	B	124	LEU	3.9
1	A	258	ASN	3.9
1	B	96	LYS	3.9
1	A	143	VAL	3.9
1	A	282	ARG	3.9
1	A	302	VAL	3.9
1	A	284	GLY	3.9
1	C	162	GLY	3.9
1	C	204	VAL	3.8
1	C	334	VAL	3.8
1	B	350	GLY	3.8
1	B	43	SER	3.8
1	B	250	SER	3.8
1	C	159	ALA	3.8
1	C	319	ALA	3.8
1	A	321	LEU	3.8
1	B	31	PRO	3.8
1	B	94	PRO	3.8
1	A	259	PRO	3.8
1	A	149	VAL	3.8
1	C	318	ASP	3.8
1	B	323	PHE	3.8
1	C	57	PHE	3.8
1	A	292	LYS	3.8
1	A	153	SER	3.8
1	C	229	SER	3.8
1	A	180	ARG	3.8
1	A	65	ALA	3.8
1	C	199	ALA	3.8
1	A	193	VAL	3.8
1	C	147	PHE	3.8
1	A	133	GLU	3.8
1	A	53	GLU	3.8
1	C	95	GLN	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	284	GLY	3.8
1	C	257	GLY	3.8
1	A	186	PHE	3.8
1	C	186	PHE	3.8
1	B	73	PRO	3.7
1	A	119	VAL	3.7
1	C	113	VAL	3.7
1	C	35	LEU	3.7
1	C	78	GLU	3.7
1	C	215	LYS	3.7
1	C	287	GLY	3.7
1	B	304	ALA	3.7
1	A	25	VAL	3.7
1	C	294	HIS	3.7
1	A	185	ARG	3.7
1	B	45	GLN	3.7
1	B	272	ALA	3.7
1	B	271	PRO	3.6
1	A	127	ASN	3.6
1	B	161	PHE	3.6
1	B	318	ASP	3.6
1	A	159	ALA	3.6
1	B	165	LEU	3.6
1	B	205	PRO	3.6
1	A	124	LEU	3.6
1	C	210	LEU	3.6
1	A	150	TYR	3.6
1	C	123	HIS	3.6
1	A	103	SER	3.6
1	B	57	PHE	3.6
1	B	199	ALA	3.6
1	A	109	ALA	3.6
1	A	189	LEU	3.6
1	B	141	GLU	3.6
1	C	344	ARG	3.6
1	A	104	ALA	3.6
1	A	73	PRO	3.6
1	A	317	PRO	3.6
1	C	66	LEU	3.6
1	B	301	GLY	3.6
1	A	251	ASP	3.5
1	B	100	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	291	VAL	3.5
1	C	338	THR	3.5
1	B	39	HIS	3.5
1	B	290	LYS	3.5
1	A	46	ASN	3.5
1	A	174	PRO	3.5
1	A	300	ASN	3.5
1	C	302	VAL	3.5
1	B	248	ARG	3.5
1	B	172	GLN	3.5
1	B	275	GLN	3.5
1	C	44	LEU	3.5
1	C	207	LEU	3.5
1	B	33	GLY	3.5
1	B	347	ARG	3.5
1	A	312	GLU	3.5
1	C	130	VAL	3.5
1	C	224	ILE	3.5
1	B	147	PHE	3.5
1	C	54	ALA	3.5
1	C	90	ALA	3.5
1	B	299	LEU	3.5
1	C	37	LEU	3.5
1	C	62	ASP	3.5
1	A	322	ARG	3.5
1	C	332	ARG	3.5
1	A	172	GLN	3.5
1	C	320	VAL	3.5
1	B	70	PHE	3.4
1	B	186	PHE	3.4
1	A	147	PHE	3.4
1	C	267	PHE	3.4
1	B	288	ASP	3.4
1	C	248	ARG	3.4
1	B	294	HIS	3.4
1	B	168	VAL	3.4
1	B	151	PRO	3.4
1	C	182	ILE	3.4
1	A	231	ASP	3.4
1	B	235	ARG	3.4
1	A	347	ARG	3.4
1	C	26	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	181	GLU	3.4
1	B	337	GLN	3.4
1	A	100	VAL	3.4
1	C	158	ILE	3.4
1	C	211	ASP	3.4
1	B	311	ALA	3.4
1	B	319	ALA	3.4
1	B	137	LYS	3.4
1	A	56	LEU	3.4
1	A	116	LEU	3.4
1	C	92	LEU	3.4
1	C	173	LEU	3.4
1	C	242	THR	3.4
1	A	78	GLU	3.4
1	B	167	PRO	3.4
1	C	170	ASP	3.4
1	C	40	LEU	3.4
1	C	351	HIS	3.3
1	A	117	ASN	3.3
1	B	48	VAL	3.3
1	B	192	PRO	3.3
1	A	45	GLN	3.3
1	C	264	LEU	3.3
1	C	23	PRO	3.3
1	C	169	GLY	3.3
1	C	337	GLN	3.3
1	C	58	VAL	3.3
1	C	260	VAL	3.3
1	B	206	ARG	3.3
1	B	282	ARG	3.3
1	B	74	GLU	3.3
1	B	216	MET	3.3
1	B	218	LYS	3.3
1	A	236	LYS	3.3
1	A	228	ASP	3.3
1	B	75	GLN	3.3
1	C	282	ARG	3.3
1	A	33	GLY	3.2
1	A	106	PRO	3.2
1	B	283	ALA	3.2
1	A	190	TYR	3.2
1	B	240	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	59	LEU	3.2
1	C	341	GLN	3.2
1	B	328	THR	3.2
1	A	112	THR	3.2
1	C	27	THR	3.2
1	C	112	THR	3.2
1	B	63	VAL	3.2
1	B	183	VAL	3.2
1	A	105	VAL	3.2
1	A	152	VAL	3.2
1	A	79	ASN	3.2
1	A	60	LEU	3.2
1	C	124	LEU	3.2
1	C	176	LEU	3.2
1	A	213	GLN	3.2
1	A	323	PHE	3.2
1	B	49	ARG	3.2
1	B	273	ARG	3.2
1	A	338	THR	3.2
1	B	227	GLY	3.2
1	C	305	PRO	3.2
1	A	96	LYS	3.2
1	B	222	ASN	3.2
1	A	101	VAL	3.2
1	C	83	VAL	3.2
1	C	163	ALA	3.2
1	C	223	ALA	3.2
1	A	29	ASP	3.2
1	B	310	ARG	3.2
1	B	285	GLY	3.2
1	C	128	PRO	3.2
1	B	166	VAL	3.1
1	B	324	VAL	3.1
1	A	83	VAL	3.1
1	A	163	ALA	3.1
1	A	74	GLU	3.1
1	C	326	GLU	3.1
1	A	229	SER	3.1
1	B	287	GLY	3.1
1	C	67	THR	3.1
1	B	61	ALA	3.1
1	A	334	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	119	VAL	3.1
1	C	288	ASP	3.1
1	B	59	LEU	3.1
1	B	196	GLU	3.1
1	C	349	PHE	3.1
1	C	205	PRO	3.1
1	A	235	ARG	3.1
1	C	63	VAL	3.1
1	B	348	LEU	3.1
1	A	87	TYR	3.1
1	C	340	GLY	3.1
1	B	23	PRO	3.1
1	C	94	PRO	3.1
1	C	30	ARG	3.1
1	B	65	ALA	3.1
1	B	249	ALA	3.1
1	A	335	ALA	3.1
1	C	50	LEU	3.1
1	B	126	GLN	3.1
1	C	87	TYR	3.0
1	C	32	THR	3.0
1	B	330	ARG	3.0
1	B	157	ASP	3.0
1	B	188	ALA	3.0
1	C	61	ALA	3.0
1	C	226	LEU	3.0
1	A	38	GLY	3.0
1	C	347	ARG	3.0
1	B	78	GLU	3.0
1	C	141	GLU	3.0
1	B	231	ASP	3.0
1	B	143	VAL	3.0
1	A	168	VAL	3.0
1	A	342	VAL	3.0
1	C	118	LEU	3.0
1	C	250	SER	3.0
1	C	208	PRO	3.0
1	B	93	ASP	3.0
1	A	265	ASP	3.0
1	C	81	LEU	3.0
1	B	28	GLY	3.0
1	A	209	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	179	THR	3.0
1	B	29	ASP	3.0
1	B	211	ASP	3.0
1	B	153	SER	2.9
1	C	195	ALA	2.9
1	B	35	LEU	2.9
1	C	152	VAL	2.9
1	B	270	ASP	2.9
1	B	139	TYR	2.9
1	B	313	TYR	2.9
1	C	333	GLU	2.9
1	A	223	ALA	2.9
1	A	28	GLY	2.9
1	C	284	GLY	2.9
1	C	193	VAL	2.9
1	A	70	PHE	2.9
1	B	345	ALA	2.9
1	B	221	GLY	2.9
1	C	331	GLY	2.9
1	A	183	VAL	2.9
1	B	53	GLU	2.9
1	C	190	TYR	2.9
1	B	223	ALA	2.9
1	C	145	ALA	2.9
1	C	311	ALA	2.9
1	B	60	LEU	2.8
1	A	154	GLN	2.8
1	B	232	GLU	2.8
1	A	314	GLU	2.8
1	B	114	TYR	2.8
1	B	243	ASP	2.8
1	A	170	ASP	2.8
1	A	203	ARG	2.8
1	C	221	GLY	2.8
1	C	60	LEU	2.8
1	C	342	VAL	2.8
1	C	31	PRO	2.8
1	C	236	LYS	2.8
1	B	160	ALA	2.8
1	C	188	ALA	2.8
1	C	111	LEU	2.8
1	B	197	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	137	LYS	2.8
1	A	30	ARG	2.8
1	B	200	GLN	2.8
1	B	140	GLY	2.8
1	A	349	PHE	2.8
1	C	89	ALA	2.8
1	C	104	ALA	2.8
1	C	201	LEU	2.8
1	C	295	LEU	2.8
1	B	269	PRO	2.8
1	A	144	PRO	2.8
1	C	151	PRO	2.8
1	B	334	VAL	2.8
1	B	72	ARG	2.7
1	A	47	ARG	2.7
1	A	280	GLN	2.7
1	B	171	ASP	2.7
1	C	114	TYR	2.7
1	A	120	THR	2.7
1	C	183	VAL	2.7
1	C	153	SER	2.7
1	B	228	ASP	2.7
1	C	146	GLY	2.7
1	C	290	LYS	2.7
1	C	263	PHE	2.7
1	B	47	ARG	2.7
1	B	77	ARG	2.7
1	B	184	ARG	2.7
1	A	343	ARG	2.7
1	A	32	THR	2.7
1	A	325	THR	2.7
1	B	317	PRO	2.7
1	B	121	VAL	2.7
1	B	181	GLU	2.7
1	C	100	VAL	2.7
1	C	233	VAL	2.7
1	A	122	SER	2.7
1	B	297	ASP	2.7
1	B	162	GLY	2.7
1	A	49	ARG	2.7
1	A	184	ARG	2.7
1	A	304	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	136	GLN	2.7
1	B	144	PRO	2.7
1	A	141	GLU	2.7
1	B	229	SER	2.7
1	B	291	VAL	2.7
1	C	278	LYS	2.7
1	B	225	ALA	2.6
1	B	112	THR	2.6
1	B	62	ASP	2.6
1	C	297	ASP	2.6
1	C	96	LYS	2.6
1	C	343	ARG	2.6
1	C	327	GLY	2.6
1	C	213	GLN	2.6
1	B	55	GLU	2.6
1	A	345	ALA	2.6
1	C	41	ALA	2.6
1	B	339	LEU	2.6
1	A	52	ASP	2.6
1	C	168	VAL	2.6
1	A	331	GLY	2.6
1	B	191	ALA	2.6
1	B	52	ASP	2.6
1	B	316	ASP	2.6
1	A	62	ASP	2.6
1	C	220	LEU	2.6
1	C	247	LEU	2.6
1	B	307	ARG	2.6
1	A	198	GLN	2.6
1	C	227	GLY	2.6
1	A	206	ARG	2.6
1	A	118	LEU	2.6
1	C	116	LEU	2.6
1	C	115	PHE	2.5
1	A	341	GLN	2.5
1	B	177	GLU	2.5
1	B	190	TYR	2.5
1	C	246	HIS	2.5
1	B	127	ASN	2.5
1	B	30	ARG	2.5
1	C	77	ARG	2.5
1	A	328	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	279	ASP	2.5
1	B	174	PRO	2.5
1	C	329	ALA	2.5
1	B	193	VAL	2.5
1	A	187	ASN	2.5
1	C	185	ARG	2.5
1	B	194	LEU	2.5
1	C	346	MET	2.5
1	C	76	VAL	2.5
1	C	265	ASP	2.5
1	C	219	SER	2.5
1	B	145	ALA	2.5
1	C	109	ALA	2.5
1	C	144	PRO	2.5
1	C	304	ALA	2.5
1	B	207	LEU	2.5
1	C	189	LEU	2.5
1	B	292	LYS	2.5
1	B	332	ARG	2.5
1	A	72	ARG	2.5
1	C	70	PHE	2.5
1	C	206	ARG	2.5
1	B	169	GLY	2.5
1	B	308	THR	2.4
1	B	84	ALA	2.4
1	C	156	ALA	2.4
1	B	95	GLN	2.4
1	C	126	GLN	2.4
1	C	296	ILE	2.4
1	C	240	MET	2.4
1	B	24	ARG	2.4
1	C	82	ALA	2.4
1	C	225	ALA	2.4
1	B	69	HIS	2.4
1	B	149	VAL	2.4
1	B	131	LYS	2.4
1	B	305	PRO	2.4
1	A	329	ALA	2.4
1	A	336	ALA	2.4
1	A	196	GLU	2.4
1	C	222	ASN	2.4
1	B	148	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	80	VAL	2.4
1	B	122	SER	2.4
1	B	106	PRO	2.4
1	C	39	HIS	2.4
1	C	53	GLU	2.3
1	C	65	ALA	2.3
1	C	155	ALA	2.3
1	C	181	GLU	2.3
1	C	310	ARG	2.3
1	B	34	ALA	2.3
1	A	327	GLY	2.3
1	B	68	ASP	2.3
1	B	123	HIS	2.3
1	C	166	VAL	2.3
1	C	179	THR	2.3
1	B	99	CYS	2.3
1	C	85	LEU	2.3
1	C	91	GLY	2.3
1	C	196	GLU	2.3
1	B	128	PRO	2.3
1	A	192	PRO	2.3
1	B	117	ASN	2.3
1	C	131	LYS	2.3
1	B	351	HIS	2.2
1	C	256	GLU	2.2
1	C	43	SER	2.2
1	B	79	ASN	2.2
1	C	218	LYS	2.2
1	B	133	GLU	2.2
1	B	343	ARG	2.2
1	C	161	PHE	2.2
1	B	25	VAL	2.2
1	B	208	PRO	2.2
1	C	106	PRO	2.2
1	C	325	THR	2.2
1	B	108	LEU	2.2
1	A	348	LEU	2.2
1	B	213	GLN	2.2
1	A	337	GLN	2.2
1	C	235	ARG	2.2
1	B	159	ALA	2.2
1	B	185	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	31	PRO	2.1
1	C	231	ASP	2.2
1	B	22	ARG	2.1
1	C	330	ARG	2.1
1	A	351	HIS	2.1
1	C	301	GLY	2.1
1	C	214	ALA	2.1
1	C	339	LEU	2.1
1	C	348	LEU	2.1
1	A	77	ARG	2.1
1	C	180	ARG	2.1
1	C	322	ARG	2.1
1	A	188	ALA	2.1
1	C	107	GLU	2.1
1	B	86	ASP	2.1
1	B	102	GLN	2.1
1	C	198	GLN	2.1
1	C	69	HIS	2.1
1	C	120	THR	2.1
1	C	292	LYS	2.1
1	B	155	ALA	2.1
1	B	154	GLN	2.0
1	C	316	ASP	2.0
1	B	217	SER	2.0
1	B	46	ASN	2.0
1	B	164	THR	2.0
1	B	327	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TRP	C	3000	15/15	0.43	0.29	52,54,57,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.