



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:33 AM UTC

PDB ID : 1EQR / pdb_00001eqr
Title : CRYSTAL STRUCTURE OF FREE ASPARTYL-TRNA SYNTHETASE
FROM ESCHERICHIA COLI
Authors : Rees, B.; Webster, G.; Delarue, M.; Boeglin, M.; Moras, D.
Deposited on : 2000-04-06
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

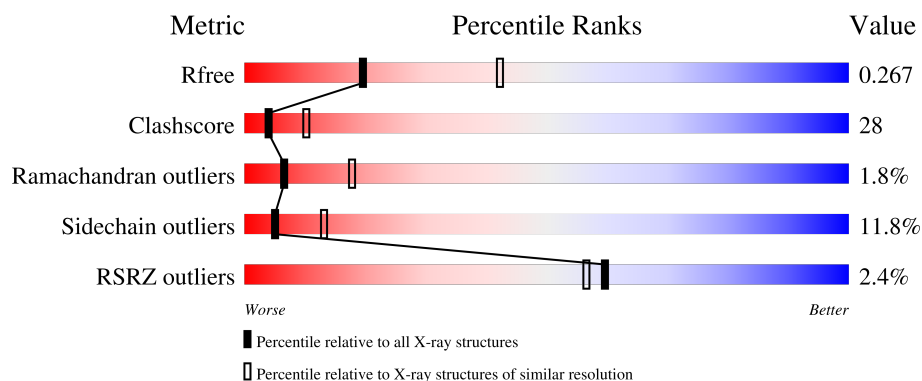
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	590	2% 51% 40% 9%
1	B	590	2% 50% 41% 8%
1	C	590	3% 48% 43% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14323 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 ASPARTYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	590	Total	C	N	O	S	0	0	0
			4631	2922	812	871	26			
1	B	590	Total	C	N	O	S	0	0	0
			4631	2922	812	871	26			
1	C	590	Total	C	N	O	S	0	0	0
			4631	2922	812	871	26			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

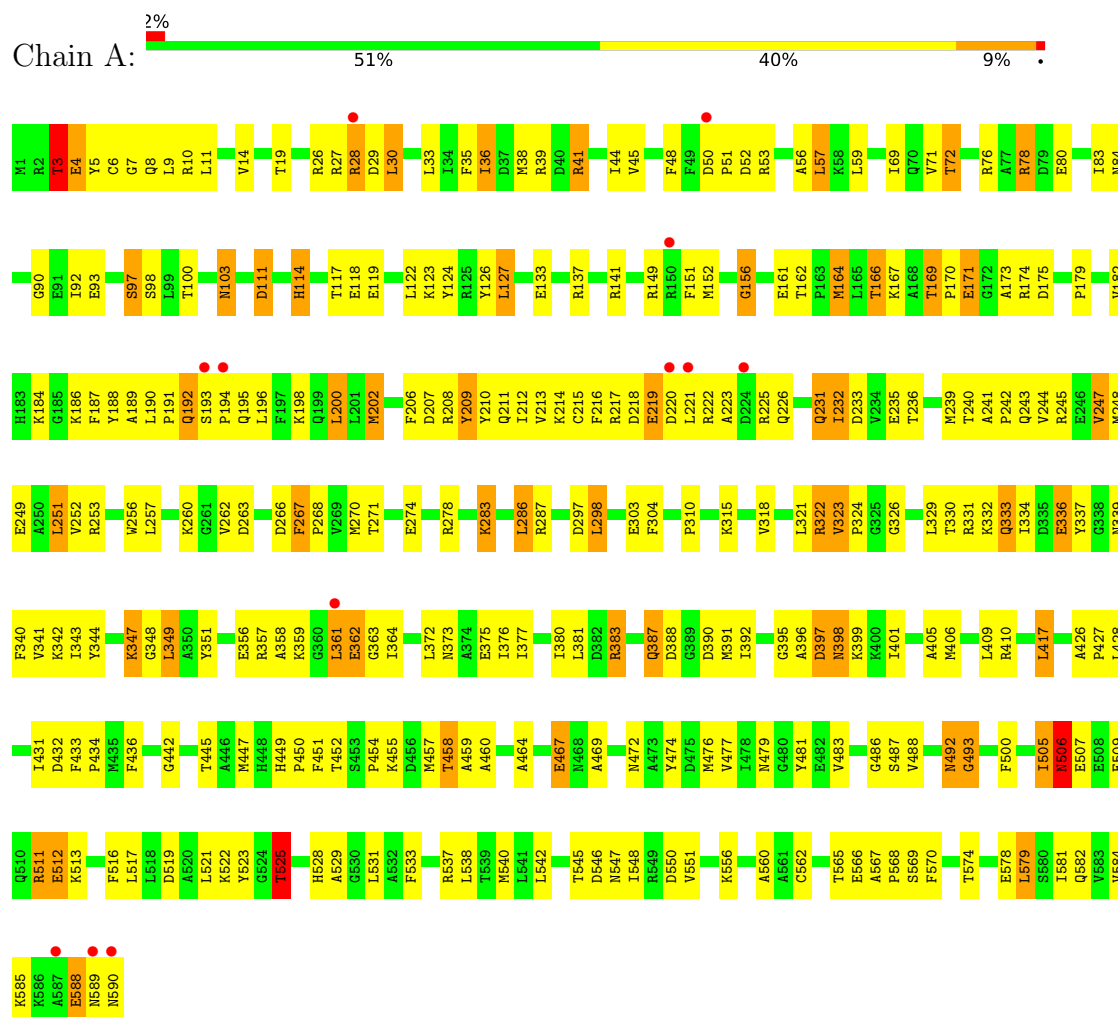
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	148	Total	O	0	0
			148	148		
3	B	131	Total	O	0	0
			131	131		
3	C	148	Total	O	0	0
			148	148		

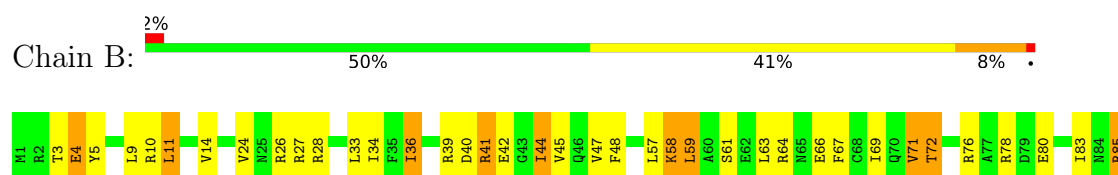
3 Residue-property plots [i](#)

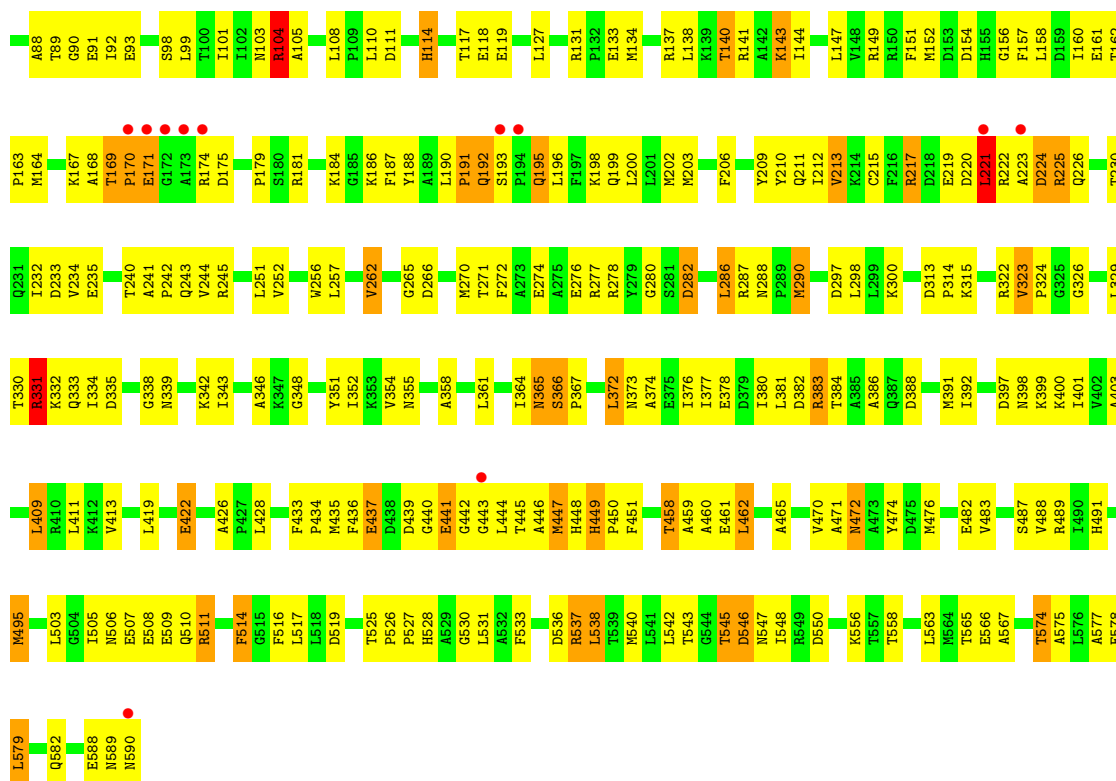
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

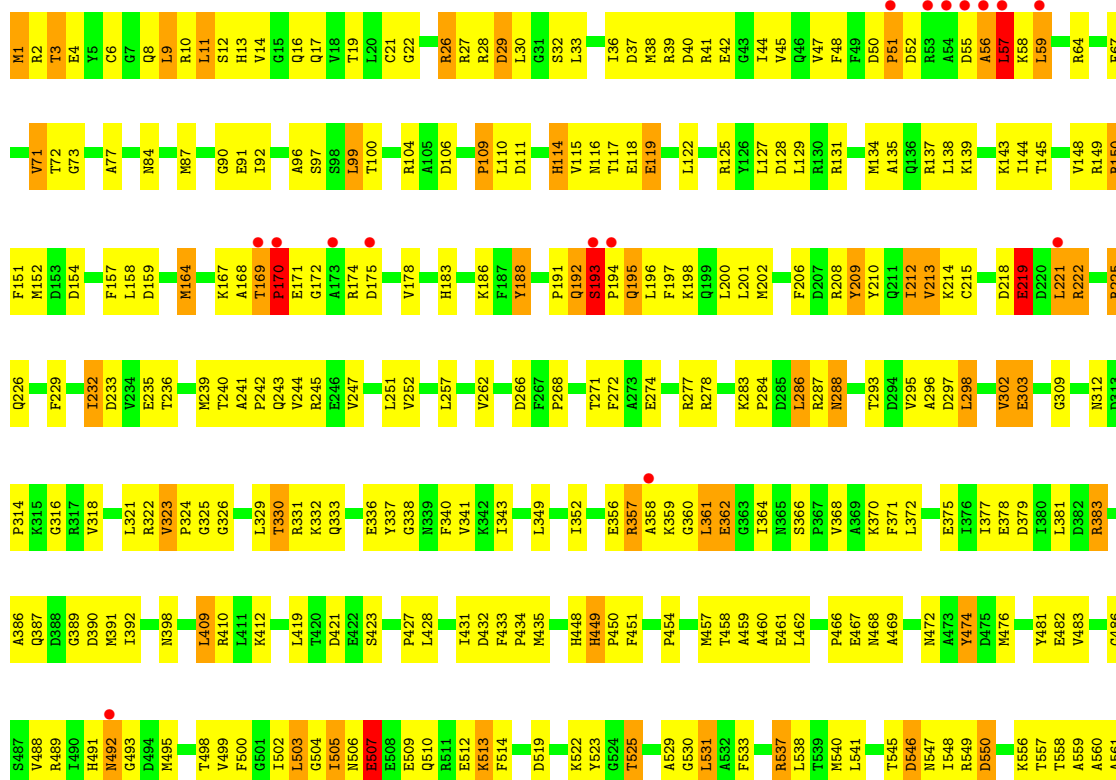


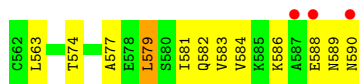
• Molecule 1: ASPARTYL-TRNA SYNTHETASE





• Molecule 1: ASPARTYL-TRNA SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.75Å 161.96Å 131.60Å 90.00° 110.36° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	90.2 (20.00-2.70) 90.1 (20.00-2.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 2.64Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.269 0.197 , 0.267	Depositor DCC
R_{free} test set	2958 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14323	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: MG

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	0.68	1/4717 (0.0%)	1.11	25/6372 (0.4%)
1	B	0.66	0/4717	1.13	30/6372 (0.5%)
1	C	0.61	0/4717	1.12	35/6372 (0.5%)
All	All	0.65	1/14151 (0.0%)	1.12	90/19116 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	525	THR	CA-CB	5.34	1.61	1.53

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	PHE	N-CA-C	-10.69	95.81	110.35
1	A	192	GLN	N-CA-C	-9.43	100.35	112.23
1	A	190	LEU	N-CA-C	-9.28	98.04	109.83
1	A	206	PHE	N-CA-C	-8.78	98.41	110.35
1	B	287	ARG	N-CA-C	-8.62	102.75	113.18
1	C	206	PHE	N-CA-C	-8.53	97.86	110.23
1	C	507	GLU	N-CA-C	8.32	120.35	111.28
1	A	278	ARG	N-CA-C	8.01	123.16	113.23
1	C	29	ASP	N-CA-C	7.72	121.20	111.24
1	C	449	HIS	CA-C-N	7.72	127.38	119.82
1	C	449	HIS	C-N-CA	7.72	127.38	119.82
1	B	213	VAL	N-CA-C	7.41	120.94	108.86
1	A	78	ARG	N-CA-C	-7.35	101.05	110.53
1	B	188	TYR	N-CA-C	-7.10	99.73	109.95
1	A	523	TYR	N-CA-C	7.05	119.12	109.11
1	C	164	MET	N-CA-C	-6.98	104.92	113.50
1	B	192	GLN	N-CA-C	-6.96	103.74	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	419	LEU	N-CA-C	-6.94	104.28	112.89
1	C	188	TYR	N-CA-C	-6.79	99.13	109.85
1	C	523	TYR	N-CA-C	6.74	120.93	111.30
1	C	109	PRO	N-CA-C	-6.68	104.44	113.40
1	C	195	GLN	N-CA-C	6.67	122.38	111.37
1	B	331	ARG	N-CA-C	-6.66	104.02	111.28
1	A	472	ASN	N-CA-C	-6.66	99.64	109.62
1	C	192	GLN	N-CA-C	-6.65	105.16	113.20
1	B	482	GLU	N-CA-C	-6.61	100.11	109.96
1	C	361	LEU	N-CA-C	-6.56	105.14	113.01
1	B	232	ILE	N-CA-C	-6.49	97.61	107.73
1	A	169	THR	CA-C-N	6.45	126.21	119.76
1	A	169	THR	C-N-CA	6.45	126.21	119.76
1	B	234	VAL	N-CA-C	6.38	117.97	108.46
1	A	212	ILE	N-CA-C	-6.37	97.80	106.85
1	A	188	TYR	N-CA-C	-6.37	100.52	109.69
1	C	433	PHE	CA-C-N	-6.37	113.73	120.03
1	C	433	PHE	C-N-CA	-6.37	113.73	120.03
1	C	3	THR	N-CA-C	-6.16	106.30	113.88
1	C	459	ALA	N-CA-C	-6.14	104.59	111.28
1	A	3	THR	N-CA-C	-5.97	106.61	114.31
1	B	465	ALA	CA-C-N	5.96	125.51	119.19
1	B	465	ALA	C-N-CA	5.96	125.51	119.19
1	A	97	SER	N-CA-C	-5.96	105.58	114.64
1	B	190	LEU	N-CA-C	-5.89	100.83	109.50
1	C	39	ARG	N-CA-C	5.87	119.03	109.24
1	C	97	SER	N-CA-C	-5.83	105.94	114.39
1	A	202	MET	N-CA-C	-5.83	105.67	112.89
1	C	213	VAL	N-CA-C	5.76	118.25	108.86
1	B	527	PRO	N-CA-C	-5.76	102.11	110.80
1	B	191	PRO	N-CA-C	5.70	120.14	111.19
1	B	156	GLY	N-CA-C	5.67	123.63	114.90
1	A	44	ILE	N-CA-C	5.66	116.74	108.53
1	C	287	ARG	N-CA-C	-5.63	105.91	112.89
1	A	506	ASN	N-CA-C	5.63	118.15	110.55
1	B	206	PHE	CA-C-N	-5.62	112.69	122.36
1	B	206	PHE	C-N-CA	-5.62	112.69	122.36
1	C	202	MET	N-CA-C	-5.62	104.77	111.69
1	A	232	ILE	N-CA-C	-5.60	97.30	106.32
1	C	309	GLY	CA-C-N	5.58	125.20	119.56
1	C	309	GLY	C-N-CA	5.58	125.20	119.56
1	B	545	THR	N-CA-C	-5.57	101.96	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	PRO	N-CA-C	5.53	119.87	111.19
1	A	156	GLY	N-CA-C	5.51	123.57	115.08
1	B	449	HIS	CA-C-N	5.46	125.17	119.82
1	B	449	HIS	C-N-CA	5.46	125.17	119.82
1	B	470	VAL	N-CA-C	5.44	115.93	107.99
1	A	493	GLY	N-CA-C	5.41	118.78	112.50
1	C	288	ASN	CA-C-N	5.38	124.89	119.19
1	C	288	ASN	C-N-CA	5.38	124.89	119.19
1	C	472	ASN	N-CA-C	-5.33	101.63	109.62
1	C	232	ILE	N-CA-C	-5.30	98.83	106.88
1	A	336	GLU	N-CA-C	-5.30	105.40	111.07
1	C	9	LEU	N-CA-C	5.28	118.13	110.42
1	B	366	SER	CA-C-N	5.22	124.84	119.56
1	B	366	SER	C-N-CA	5.22	124.84	119.56
1	C	423	SER	N-CA-C	-5.17	106.97	113.28
1	B	282	ASP	N-CA-C	-5.17	106.56	112.92
1	B	290	MET	N-CA-C	5.16	116.99	110.33
1	A	464	ALA	N-CA-C	5.14	116.69	111.14
1	A	39	ARG	N-CA-C	5.14	117.95	109.72
1	B	118	GLU	N-CA-C	-5.10	106.89	113.01
1	C	378	GLU	N-CA-C	-5.09	105.81	111.36
1	B	44	ILE	N-CA-C	5.09	116.29	108.71
1	A	488	VAL	N-CA-C	-5.07	102.20	108.89
1	B	472	ASN	N-CA-C	-5.07	104.27	110.65
1	C	283	LYS	CA-C-N	5.05	125.06	119.90
1	C	283	LYS	C-N-CA	5.05	125.06	119.90
1	C	52	ASP	N-CA-C	5.04	119.14	112.89
1	C	212	ILE	N-CA-C	-5.02	99.25	106.88
1	B	546	ASP	N-CA-C	-5.01	107.12	114.39
1	A	267	PHE	CA-C-N	-5.01	114.50	120.11
1	A	267	PHE	C-N-CA	-5.01	114.50	120.11

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	4631	0	4626	270	0
1	B	4631	0	4626	267	0
1	C	4631	0	4626	264	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	148	0	0	13	0
3	B	131	0	0	13	0
3	C	148	0	0	14	0
All	All	14323	0	13878	777	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (777) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ASP:O	1:C:57:LEU:HG	1.47	1.15
1:A:51:PRO:HA	1:A:57:LEU:HD12	1.29	1.12
1:B:511:ARG:HG3	1:B:511:ARG:HH11	1.17	1.07
1:A:585:LYS:HB2	1:A:588:GLU:HB3	1.35	1.04
1:C:236:THR:HB	1:C:239:MET:HE3	1.40	0.99
1:B:240:THR:H	1:B:243:GLN:HE21	1.06	0.96
1:B:462:LEU:HD12	1:B:495:MET:HE1	1.47	0.96
1:B:69:ILE:HG22	1:B:101:ILE:HA	1.46	0.94
1:B:226:GLN:HE22	1:B:556:LYS:H	1.10	0.93
1:C:240:THR:H	1:C:243:GLN:HE21	1.08	0.93
1:C:59:LEU:H	1:C:59:LEU:CD1	1.81	0.92
1:B:171:GLU:CG	1:B:192:GLN:HG3	2.01	0.91
1:C:225:ARG:HH11	1:C:225:ARG:HB3	1.34	0.91
1:A:347:LYS:HG3	1:A:348:GLY:H	1.33	0.91
1:A:170:PRO:HD3	1:A:513:LYS:HD2	1.53	0.91
1:A:240:THR:H	1:A:243:GLN:HE21	1.15	0.91
1:A:357:ARG:HB3	1:A:357:ARG:NH1	1.87	0.90
1:A:398:ASN:HD22	1:A:401:ILE:HG12	1.35	0.90
1:A:248:MET:HE2	1:A:248:MET:HA	1.52	0.88
1:C:505:ILE:HG13	1:C:509:GLU:HG3	1.56	0.88
1:B:330:THR:HG22	1:B:332:LYS:H	1.36	0.88
1:B:161:GLU:HA	1:B:211:GLN:NE2	1.88	0.87
1:C:55:ASP:O	1:C:59:LEU:HD13	1.76	0.86
1:C:356:GLU:OE1	1:C:359:LYS:HD2	1.74	0.86
1:A:222:ARG:HB2	1:A:225:ARG:HG3	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:H	1:A:243:GLN:NE2	1.73	0.84
1:C:170:PRO:HB3	3:C:1016:HOH:O	1.77	0.84
1:B:511:ARG:HG3	1:B:511:ARG:NH1	1.87	0.83
1:B:27:ARG:HG3	1:B:36:ILE:HG13	1.57	0.83
1:C:171:GLU:HG2	1:C:172:GLY:H	1.43	0.82
1:A:182:VAL:HG21	1:B:221:LEU:HD11	1.60	0.81
1:A:186:LYS:HE3	1:C:303:GLU:HG3	1.61	0.81
1:A:236:THR:HB	1:A:239:MET:HE3	1.63	0.81
1:B:240:THR:H	1:B:243:GLN:NE2	1.78	0.80
1:A:434:PRO:HG2	1:A:447:MET:HG3	1.62	0.80
1:C:458:THR:HB	1:C:461:GLU:HG3	1.60	0.80
1:A:226:GLN:HE22	1:A:556:LYS:H	1.28	0.80
1:A:333:GLN:O	1:A:336:GLU:HG2	1.81	0.80
1:C:226:GLN:HE22	1:C:556:LYS:H	1.26	0.80
1:A:506:ASN:C	1:A:506:ASN:HD22	1.90	0.80
1:A:151:PHE:HD1	1:A:152:MET:HE2	1.46	0.79
1:A:166:THR:HG23	1:A:167:LYS:N	1.97	0.79
1:C:236:THR:CB	1:C:239:MET:HE3	2.11	0.79
1:C:271:THR:OG1	1:C:274:GLU:HG3	1.81	0.79
1:B:329:LEU:HA	3:B:979:HOH:O	1.80	0.79
1:A:78:ARG:HD2	1:A:92:ILE:O	1.82	0.79
1:B:36:ILE:HG22	1:B:47:VAL:CG1	2.12	0.78
1:B:331:ARG:HH22	1:C:118:GLU:HB3	1.48	0.78
1:C:59:LEU:H	1:C:59:LEU:HD13	1.48	0.78
1:C:482:GLU:OE2	3:C:1042:HOH:O	2.00	0.78
1:B:64:ARG:HB2	1:B:67:PHE:CE1	2.18	0.78
1:A:141:ARG:HD3	3:B:911:HOH:O	1.81	0.78
1:C:149:ARG:NH1	1:C:212:ILE:HD12	1.99	0.78
1:B:458:THR:HG22	1:B:460:ALA:H	1.49	0.78
1:A:357:ARG:HB3	1:A:357:ARG:HH11	1.49	0.77
1:C:359:LYS:O	1:C:362:GLU:HG3	1.84	0.77
1:B:252:VAL:HG21	1:B:476:MET:SD	2.24	0.77
1:B:192:GLN:O	1:B:215:CYS:HB3	1.85	0.77
1:B:240:THR:HG23	1:B:243:GLN:NE2	1.99	0.77
1:C:330:THR:HG22	1:C:333:GLN:H	1.46	0.77
1:A:192:GLN:O	1:A:215:CYS:HB3	1.84	0.76
1:B:342:LYS:NZ	1:B:348:GLY:HA2	2.01	0.76
1:A:506:ASN:ND2	1:A:509:GLU:H	1.84	0.76
1:A:221:LEU:HD11	1:A:560:ALA:HB2	1.67	0.76
1:B:85:ARG:HB2	1:B:85:ARG:NH1	2.01	0.76
1:C:225:ARG:HB3	1:C:225:ARG:NH1	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ASN:ND2	1:A:509:GLU:HG3	2.00	0.76
1:C:329:LEU:HD21	1:C:337:TYR:HE2	1.50	0.76
1:C:458:THR:HG22	1:C:460:ALA:H	1.50	0.76
1:B:169:THR:N	1:B:170:PRO:HD3	2.01	0.75
1:C:194:PRO:HG2	1:C:213:VAL:HG11	1.68	0.75
1:A:357:ARG:HH11	1:A:357:ARG:CB	1.99	0.75
1:B:169:THR:HG23	1:B:169:THR:O	1.85	0.75
1:B:545:THR:HG22	1:B:547:ASN:H	1.50	0.75
1:C:169:THR:HB	1:C:170:PRO:CD	2.16	0.75
1:A:174:ARG:HB2	1:A:219:GLU:OE2	1.87	0.74
1:A:174:ARG:HH22	1:B:579:LEU:HD22	1.52	0.74
1:C:330:THR:HG23	1:C:332:LYS:H	1.51	0.74
1:A:166:THR:HG23	1:A:167:LYS:H	1.52	0.74
1:B:59:LEU:HB2	1:B:99:LEU:HD23	1.68	0.74
1:A:72:THR:HG23	1:A:98:SER:HB3	1.70	0.74
1:B:241:ALA:HB3	1:B:242:PRO:HD3	1.69	0.74
1:C:59:LEU:CD1	1:C:59:LEU:N	2.51	0.74
1:A:26:ARG:NH1	1:A:28:ARG:HB2	2.02	0.73
1:A:166:THR:CG2	1:A:167:LYS:N	2.51	0.73
1:B:171:GLU:HG3	1:B:192:GLN:HG3	1.67	0.73
1:C:509:GLU:O	1:C:513:LYS:HG3	1.89	0.73
1:B:223:ALA:O	1:B:224:ASP:HB3	1.87	0.73
1:C:170:PRO:CG	1:C:513:LYS:HD2	2.19	0.73
1:B:111:ASP:HB3	1:B:114:HIS:ND1	2.04	0.72
1:B:72:THR:HG23	1:B:98:SER:HB3	1.72	0.72
1:B:240:THR:N	1:B:243:GLN:HE21	1.84	0.72
1:A:540:MET:HE2	1:A:548:ILE:HG13	1.70	0.72
1:B:119:GLU:HG2	3:C:1019:HOH:O	1.88	0.72
1:C:64:ARG:HB2	1:C:67:PHE:CE1	2.25	0.71
1:A:151:PHE:CD1	1:A:152:MET:HE2	2.26	0.71
1:C:192:GLN:O	1:C:193:SER:OG	2.07	0.71
1:A:3:THR:HG22	1:A:4:GLU:OE1	1.91	0.71
1:B:346:ALA:HA	3:B:924:HOH:O	1.91	0.71
1:A:589:ASN:O	1:A:590:ASN:HB2	1.91	0.70
1:C:492:ASN:C	1:C:492:ASN:HD22	1.98	0.70
1:B:324:PRO:HG2	1:B:419:LEU:HD13	1.73	0.70
1:B:221:LEU:HB2	1:B:558:THR:O	1.92	0.69
1:C:55:ASP:O	1:C:56:ALA:O	2.09	0.69
1:C:498:THR:O	1:C:502:ILE:HG13	1.92	0.69
1:B:545:THR:HG21	1:B:550:ASP:HB2	1.74	0.69
1:C:150:ARG:O	1:C:154:ASP:HB2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:ARG:HH22	1:B:278:ARG:HH21	1.40	0.69
1:B:33:LEU:HD13	1:B:48:PHE:HZ	1.58	0.69
1:B:330:THR:O	1:B:334:ILE:HG13	1.92	0.69
1:A:588:GLU:HG3	1:A:589:ASN:H	1.59	0.68
1:B:36:ILE:HG22	1:B:47:VAL:HG12	1.75	0.68
1:C:547:ASN:O	1:C:550:ASP:HB2	1.93	0.68
1:C:333:GLN:O	1:C:336:GLU:HG2	1.93	0.68
1:C:506:ASN:HB2	3:C:958:HOH:O	1.92	0.68
1:B:219:GLU:HG2	1:B:220:ASP:H	1.58	0.68
1:C:296:ALA:HB2	3:C:911:HOH:O	1.91	0.68
1:C:505:ILE:HD12	1:C:513:LYS:HE2	1.75	0.68
1:B:33:LEU:HB3	1:B:48:PHE:HE1	1.59	0.68
1:B:240:THR:O	1:B:244:VAL:HG23	1.94	0.68
1:B:27:ARG:HG3	1:B:36:ILE:CG1	2.23	0.68
1:A:53:ARG:HD2	1:A:97:SER:HA	1.76	0.68
1:A:492:ASN:HD22	1:A:493:GLY:N	1.92	0.67
1:A:506:ASN:HD21	1:A:509:GLU:HG3	1.59	0.67
1:B:330:THR:HG22	1:B:332:LYS:N	2.07	0.67
1:A:356:GLU:HG2	1:A:358:ALA:HB3	1.77	0.67
1:A:545:THR:HG22	1:A:547:ASN:H	1.59	0.67
1:B:4:GLU:HG3	3:B:928:HOH:O	1.94	0.67
1:B:286:LEU:HD22	1:B:428:LEU:HD22	1.75	0.67
1:B:11:LEU:O	1:B:14:VAL:HG23	1.95	0.66
1:B:226:GLN:HE22	1:B:556:LYS:N	1.90	0.66
1:B:574:THR:O	1:B:577:ALA:HB3	1.94	0.66
1:B:511:ARG:HH11	1:B:511:ARG:CG	2.03	0.66
1:A:198:LYS:HE3	1:A:235:GLU:OE1	1.95	0.66
1:A:321:LEU:HD23	1:A:409:LEU:HD12	1.76	0.66
1:B:193:SER:C	1:B:195:GLN:H	2.03	0.66
1:B:588:GLU:O	1:B:590:ASN:N	2.27	0.66
1:B:588:GLU:C	1:B:590:ASN:H	2.03	0.66
1:B:459:ALA:HA	1:B:495:MET:HE3	1.77	0.66
1:C:169:THR:HB	1:C:170:PRO:HD2	1.77	0.66
1:A:226:GLN:NE2	1:A:556:LYS:H	1.93	0.66
1:A:240:THR:N	1:A:243:GLN:HE21	1.92	0.66
1:B:210:TYR:HA	1:B:233:ASP:O	1.94	0.66
1:B:458:THR:HG22	1:B:460:ALA:N	2.11	0.66
1:A:51:PRO:CA	1:A:57:LEU:HD12	2.18	0.66
1:B:459:ALA:HA	1:B:495:MET:CE	2.26	0.65
1:C:56:ALA:O	1:C:58:LYS:N	2.29	0.65
1:C:51:PRO:HA	1:C:57:LEU:CD1	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:GLU:HG2	1:C:172:GLY:N	2.10	0.65
1:C:241:ALA:HB3	1:C:242:PRO:HD3	1.79	0.65
1:A:7:GLY:O	1:A:10:ARG:NH2	2.30	0.65
1:A:56:ALA:HB3	3:A:969:HOH:O	1.96	0.65
1:A:481:TYR:HB3	1:A:537:ARG:HD3	1.78	0.65
1:A:588:GLU:HG3	1:A:589:ASN:N	2.11	0.65
1:C:208:ARG:HE	1:C:239:MET:HE2	1.62	0.65
1:A:565:THR:HG22	1:B:516:PHE:CE1	2.31	0.64
1:B:59:LEU:H	1:B:59:LEU:HD12	1.63	0.64
1:C:59:LEU:N	1:C:59:LEU:HD12	2.11	0.64
1:C:170:PRO:CD	1:C:513:LYS:HD2	2.26	0.64
1:C:361:LEU:HD23	1:C:361:LEU:H	1.61	0.64
1:A:111:ASP:HB3	1:A:114:HIS:CD2	2.33	0.64
1:A:240:THR:O	1:A:244:VAL:HG23	1.97	0.64
1:B:326:GLY:O	1:B:329:LEU:HB2	1.98	0.64
1:C:193:SER:HA	1:C:215:CYS:SG	2.38	0.64
1:C:492:ASN:C	1:C:492:ASN:ND2	2.55	0.64
1:A:341:VAL:HG11	1:A:349:LEU:HD13	1.80	0.64
1:B:352:ILE:HA	1:B:366:SER:HB2	1.80	0.63
1:C:323:VAL:CG2	1:C:326:GLY:HA3	2.28	0.63
1:A:356:GLU:O	1:A:363:GLY:HA3	1.99	0.63
1:B:274:GLU:HG2	1:B:278:ARG:NH2	2.13	0.63
1:C:9:LEU:HD12	1:C:45:VAL:HG21	1.80	0.63
1:A:347:LYS:HG3	1:A:348:GLY:N	2.10	0.63
1:C:499:VAL:HG12	1:C:503:LEU:HD22	1.80	0.63
1:A:585:LYS:HB2	1:A:588:GLU:CB	2.22	0.63
1:B:169:THR:O	1:B:169:THR:CG2	2.47	0.63
3:A:930:HOH:O	1:B:141:ARG:HD3	1.98	0.62
1:A:33:LEU:HD22	1:A:48:PHE:HE1	1.64	0.62
1:A:409:LEU:HD13	1:A:409:LEU:O	1.99	0.62
1:B:26:ARG:NH2	1:B:28:ARG:HG3	2.13	0.62
1:C:547:ASN:OD1	1:C:549:ARG:NH1	2.32	0.62
1:A:537:ARG:HA	1:A:540:MET:HE3	1.80	0.62
1:B:240:THR:OG1	1:B:243:GLN:HG3	2.00	0.62
1:C:170:PRO:HB3	1:C:174:ARG:HH12	1.64	0.62
1:C:325:GLY:HA2	1:C:389:GLY:O	1.99	0.62
1:C:340:PHE:CE2	1:C:412:LYS:HD2	2.35	0.62
1:A:3:THR:HB	1:A:19:THR:H	1.63	0.61
1:B:324:PRO:HG2	1:B:419:LEU:CD1	2.30	0.61
1:C:119:GLU:HG3	1:C:563:LEU:CD1	2.30	0.61
1:A:248:MET:HE2	1:A:248:MET:CA	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HE	1:B:28:ARG:NH1	1.98	0.61
1:B:168:ALA:O	1:B:169:THR:HG22	2.01	0.61
1:B:174:ARG:NH1	1:B:219:GLU:HA	2.15	0.61
1:A:33:LEU:HD22	1:A:48:PHE:CE1	2.35	0.61
1:A:179:PRO:HG3	1:A:187:PHE:CE2	2.36	0.61
1:A:519:ASP:HA	1:A:522:LYS:HE2	1.81	0.61
1:A:9:LEU:HD12	1:A:45:VAL:HG21	1.83	0.61
1:A:215:CYS:SG	1:A:231:GLN:HG3	2.39	0.61
1:C:11:LEU:HD12	1:C:91:GLU:OE1	2.00	0.61
1:C:449:HIS:HB2	1:C:450:PRO:HD2	1.83	0.61
1:A:38:MET:HE3	1:A:69:ILE:HG13	1.82	0.61
1:B:33:LEU:HB3	1:B:48:PHE:CE1	2.36	0.61
1:C:171:GLU:CG	1:C:172:GLY:H	2.14	0.61
1:B:169:THR:N	1:B:170:PRO:CD	2.64	0.60
1:B:409:LEU:HD22	1:B:413:VAL:HG23	1.83	0.60
1:B:439:ASP:OD2	1:B:445:THR:HB	2.00	0.60
1:A:565:THR:O	1:A:566:GLU:HB2	1.99	0.60
1:B:361:LEU:HD21	1:B:374:ALA:HA	1.83	0.60
1:C:584:VAL:HG23	1:C:584:VAL:O	2.02	0.60
1:B:439:ASP:O	1:B:441:GLU:N	2.35	0.60
1:A:588:GLU:CG	1:A:589:ASN:N	2.63	0.60
1:C:6:CYS:N	1:C:40:ASP:OD2	2.35	0.60
1:C:29:ASP:O	1:C:33:LEU:O	2.19	0.60
1:B:170:PRO:HG2	1:B:171:GLU:H	1.65	0.59
1:C:329:LEU:HD21	1:C:337:TYR:CE2	2.35	0.59
1:A:359:LYS:HB3	1:A:362:GLU:HB2	1.85	0.59
1:C:111:ASP:OD2	1:C:114:HIS:HB3	2.02	0.59
1:C:193:SER:C	1:C:195:GLN:H	2.08	0.59
1:A:361:LEU:O	1:A:364:ILE:HG13	2.03	0.59
1:A:361:LEU:CD2	1:A:377:ILE:HD12	2.33	0.59
1:C:244:VAL:O	1:C:247:VAL:HG12	2.03	0.59
1:A:322:ARG:O	1:A:322:ARG:HD3	2.03	0.59
1:C:586:LYS:HE2	1:C:588:GLU:OE1	2.03	0.59
1:A:194:PRO:HG2	1:A:213:VAL:HG11	1.84	0.59
1:B:339:ASN:O	1:B:342:LYS:HB2	2.02	0.59
1:B:11:LEU:HD13	1:B:92:ILE:HG23	1.85	0.58
1:C:240:THR:N	1:C:243:GLN:HE21	1.91	0.58
1:C:545:THR:HG21	1:C:550:ASP:HB2	1.85	0.58
1:A:249:GLU:O	1:A:253:ARG:HG3	2.03	0.58
1:A:326:GLY:O	1:A:329:LEU:HD13	2.02	0.58
1:A:387:GLN:HB2	1:A:390:ASP:OD1	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:ASN:OD1	1:C:509:GLU:HG2	2.03	0.58
1:C:183:HIS:HB3	1:C:186:LYS:HD2	1.85	0.58
1:A:585:LYS:HA	3:A:967:HOH:O	2.02	0.58
1:B:342:LYS:HZ1	1:B:348:GLY:HA2	1.68	0.58
1:B:443:GLY:O	1:B:444:LEU:HG	2.02	0.58
1:C:109:PRO:HG2	1:C:110:LEU:H	1.67	0.58
1:A:232:ILE:HB	1:A:533:PHE:HB2	1.85	0.58
1:B:161:GLU:HA	1:B:211:GLN:HE22	1.66	0.58
1:B:196:LEU:HG	1:B:517:LEU:HD22	1.85	0.58
1:B:78:ARG:HD2	1:B:92:ILE:O	2.04	0.58
1:A:174:ARG:HH22	1:B:579:LEU:CD2	2.15	0.57
1:A:398:ASN:ND2	1:A:401:ILE:HG12	2.14	0.57
1:B:83:ILE:HG23	1:B:91:GLU:HG2	1.85	0.57
1:B:342:LYS:HZ2	1:B:348:GLY:HA2	1.68	0.57
1:A:359:LYS:O	1:A:362:GLU:HG2	2.05	0.57
1:C:26:ARG:HD2	1:C:37:ASP:OD2	2.04	0.57
1:C:505:ILE:HG12	1:C:505:ILE:O	2.03	0.57
1:A:248:MET:HA	1:A:248:MET:CE	2.27	0.57
1:A:449:HIS:HD2	1:A:451:PHE:H	1.51	0.57
1:A:123:LYS:HD3	1:A:123:LYS:C	2.30	0.57
1:A:344:TYR:HB2	1:A:405:ALA:HB2	1.87	0.57
1:C:3:THR:HG23	1:C:19:THR:HB	1.87	0.57
1:C:286:LEU:HD22	1:C:428:LEU:HD22	1.86	0.57
1:A:123:LYS:HD3	1:A:123:LYS:O	2.04	0.57
1:A:240:THR:OG1	1:A:243:GLN:HG3	2.05	0.57
1:A:512:GLU:HG2	1:A:512:GLU:O	2.05	0.57
1:C:58:LYS:HB3	1:C:59:LEU:HD12	1.86	0.57
1:C:375:GLU:O	1:C:379:ASP:OD1	2.22	0.57
1:C:557:THR:HG23	1:C:561:ALA:O	2.05	0.57
1:A:156:GLY:O	1:B:41:ARG:NH2	2.38	0.57
1:C:145:THR:O	1:C:149:ARG:HG3	2.05	0.57
1:A:540:MET:HB3	3:A:939:HOH:O	2.05	0.57
1:C:454:PRO:CD	1:C:495:MET:HE3	2.35	0.57
1:C:352:ILE:HA	1:C:366:SER:HB2	1.87	0.56
1:B:144:ILE:HD13	1:B:542:LEU:HD12	1.86	0.56
1:B:300:LYS:HD2	1:C:590:ASN:O	2.05	0.56
1:B:10:ARG:NH2	1:B:88:ALA:HB1	2.21	0.56
1:B:174:ARG:HG3	1:B:174:ARG:HH11	1.69	0.56
1:C:364:ILE:HD13	1:C:377:ILE:HG21	1.86	0.56
1:B:449:HIS:HB2	1:B:450:PRO:HD2	1.87	0.56
1:C:92:ILE:HD12	1:C:92:ILE:C	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:ALA:O	1:C:139:LYS:HG3	2.05	0.56
1:A:545:THR:HG21	1:A:550:ASP:HB2	1.87	0.56
1:B:149:ARG:NH1	1:B:212:ILE:HG13	2.20	0.56
1:A:164:MET:O	1:A:191:PRO:HD3	2.06	0.56
1:A:126:TYR:CE2	1:A:127:LEU:HD22	2.41	0.56
1:A:458:THR:HG22	1:A:460:ALA:H	1.69	0.56
1:B:27:ARG:HG3	1:B:36:ILE:CD1	2.35	0.56
1:B:83:ILE:CG2	1:B:91:GLU:HG2	2.35	0.56
1:C:330:THR:CG2	1:C:332:LYS:H	2.19	0.56
1:B:588:GLU:C	1:B:590:ASN:N	2.64	0.56
1:C:59:LEU:H	1:C:59:LEU:HD12	1.62	0.56
1:C:454:PRO:HD2	1:C:495:MET:HE3	1.86	0.56
1:A:26:ARG:HH11	1:A:26:ARG:HG2	1.70	0.56
1:C:150:ARG:HG2	1:C:150:ARG:HH11	1.71	0.56
1:A:256:TRP:HD1	1:A:262:VAL:CG2	2.18	0.56
1:B:24:VAL:HG13	1:B:36:ILE:HG12	1.88	0.56
1:C:312:ASN:O	1:C:314:PRO:HD3	2.06	0.56
1:B:545:THR:HG22	1:B:546:ASP:H	1.72	0.55
1:A:547:ASN:O	1:A:550:ASP:HB2	2.07	0.55
1:C:167:LYS:HD2	1:C:169:THR:HG23	1.89	0.55
1:A:245:ARG:NH1	3:A:914:HOH:O	2.31	0.55
1:B:476:MET:O	1:B:483:VAL:HG22	2.06	0.55
1:A:323:VAL:HG22	1:A:323:VAL:O	2.06	0.55
1:B:152:MET:HE3	1:B:157:PHE:CG	2.41	0.55
1:B:545:THR:HG22	1:B:546:ASP:N	2.22	0.55
1:A:247:VAL:HG22	1:A:248:MET:CE	2.37	0.55
1:A:356:GLU:C	1:A:358:ALA:H	2.15	0.55
1:B:85:ARG:HB2	1:B:85:ARG:CZ	2.36	0.55
1:B:277:ARG:NH2	1:B:278:ARG:HH21	2.05	0.54
1:B:439:ASP:HB3	1:B:445:THR:HG21	1.89	0.54
1:C:193:SER:O	1:C:195:GLN:HG2	2.08	0.54
1:A:35:PHE:O	1:A:36:ILE:HD12	2.08	0.54
1:A:161:GLU:HA	1:A:211:GLN:NE2	2.22	0.54
1:B:89:THR:HB	1:B:92:ILE:HD11	1.87	0.54
1:A:167:LYS:HB2	1:B:567:ALA:HB2	1.90	0.54
1:A:570:PHE:CE2	1:B:186:LYS:HE2	2.42	0.54
1:B:179:PRO:HB3	1:B:187:PHE:CE2	2.42	0.54
1:B:505:ILE:HG23	1:B:509:GLU:HB3	1.89	0.54
1:C:92:ILE:HD12	1:C:92:ILE:O	2.07	0.54
1:A:256:TRP:HD1	1:A:262:VAL:HG21	1.72	0.54
1:A:351:TYR:HA	1:A:392:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:GLU:CD	1:A:467:GLU:H	2.14	0.54
1:B:403:ALA:HB2	3:B:986:HOH:O	2.08	0.54
1:C:11:LEU:HD23	1:C:14:VAL:HG21	1.87	0.54
1:C:491:HIS:HB2	1:C:525:THR:OG1	2.08	0.54
1:B:199:GLN:O	1:B:203:MET:HG2	2.08	0.54
1:C:119:GLU:HG3	1:C:563:LEU:HD11	1.90	0.54
1:C:506:ASN:OD1	1:C:509:GLU:OE2	2.26	0.54
1:C:333:GLN:O	1:C:336:GLU:CG	2.56	0.54
1:C:492:ASN:HD22	1:C:493:GLY:N	2.05	0.54
1:A:179:PRO:HB2	1:A:579:LEU:HG	1.88	0.54
1:A:209:TYR:CD1	1:A:209:TYR:C	2.86	0.54
1:C:458:THR:HG22	1:C:460:ALA:N	2.20	0.54
1:C:498:THR:HG22	1:C:502:ILE:HD11	1.88	0.54
1:C:357:ARG:C	1:C:359:LYS:H	2.15	0.54
1:B:111:ASP:HB3	1:B:114:HIS:HD1	1.73	0.53
1:B:540:MET:HE2	1:B:548:ILE:HG13	1.89	0.53
1:B:225:ARG:HB3	1:B:225:ARG:HH11	1.73	0.53
1:A:326:GLY:C	1:A:391:MET:HB2	2.33	0.53
1:B:9:LEU:HD12	1:B:45:VAL:HG21	1.90	0.53
1:C:326:GLY:O	1:C:329:LEU:HB2	2.08	0.53
1:C:387:GLN:N	1:C:390:ASP:OD2	2.41	0.53
1:A:474:TYR:CE1	1:A:487:SER:HA	2.44	0.53
1:A:171:GLU:HG2	3:A:1040:HOH:O	2.07	0.53
1:A:474:TYR:N	1:A:474:TYR:CD1	2.76	0.53
1:A:505:ILE:HG13	1:A:509:GLU:HB2	1.89	0.53
1:B:211:GLN:HG2	1:B:213:VAL:HB	1.91	0.53
1:C:131:ARG:NH1	1:C:134:MET:CG	2.71	0.53
1:C:244:VAL:O	1:C:245:ARG:C	2.51	0.53
1:C:486:GLY:HA3	1:C:531:LEU:HA	1.91	0.53
1:A:216:PHE:CD1	1:A:216:PHE:N	2.77	0.53
1:B:330:THR:HG21	1:B:332:LYS:HB3	1.91	0.53
1:A:133:GLU:HG2	1:A:137:ARG:NH2	2.24	0.53
1:A:283:LYS:HA	1:A:477:VAL:HG21	1.90	0.53
1:A:387:GLN:HE21	1:A:387:GLN:HA	1.74	0.53
1:B:458:THR:CG2	1:B:460:ALA:H	2.22	0.53
1:C:99:LEU:HG	1:C:100:THR:N	2.24	0.53
1:A:51:PRO:HA	1:A:57:LEU:CD1	2.21	0.52
1:C:27:ARG:O	1:C:28:ARG:HD3	2.09	0.52
1:A:537:ARG:HD2	3:A:970:HOH:O	2.08	0.52
1:A:298:LEU:HD22	1:A:383:ARG:NH2	2.25	0.52
1:C:545:THR:HG21	1:C:550:ASP:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:VAL:HG22	1:A:248:MET:HE3	1.91	0.52
1:A:476:MET:O	1:A:483:VAL:HG22	2.09	0.52
1:B:164:MET:HE2	3:B:934:HOH:O	2.08	0.52
1:B:326:GLY:C	1:B:391:MET:HB2	2.34	0.52
1:C:152:MET:O	1:C:157:PHE:HB2	2.09	0.52
1:C:251:LEU:C	1:C:251:LEU:HD13	2.34	0.52
1:A:50:ASP:OD2	1:A:52:ASP:HB2	2.08	0.52
1:B:27:ARG:CG	1:B:36:ILE:HG13	2.34	0.52
1:C:125:ARG:O	1:C:129:LEU:HG	2.10	0.52
1:C:451:PHE:HZ	1:C:514:PHE:CE1	2.28	0.52
1:B:439:ASP:HB3	1:B:445:THR:CG2	2.40	0.52
1:A:342:LYS:C	1:A:342:LYS:HD3	2.34	0.52
1:A:492:ASN:C	1:A:492:ASN:ND2	2.68	0.52
1:A:310:PRO:HG3	1:A:396:ALA:HB1	1.92	0.52
1:C:357:ARG:O	1:C:359:LYS:N	2.43	0.52
1:C:232:ILE:HB	1:C:533:PHE:HB2	1.92	0.51
1:C:505:ILE:HD11	1:C:510:GLN:HA	1.92	0.51
1:B:313:ASP:OD1	1:B:314:PRO:HD2	2.09	0.51
1:B:198:LYS:HE3	1:B:235:GLU:OE1	2.10	0.51
1:B:330:THR:CG2	1:B:332:LYS:HB3	2.40	0.51
1:C:109:PRO:HG2	1:C:110:LEU:N	2.26	0.51
1:C:192:GLN:C	1:C:193:SER:OG	2.53	0.51
1:A:179:PRO:HG3	1:A:187:PHE:HE2	1.72	0.51
1:A:322:ARG:NH2	1:A:387:GLN:HG2	2.25	0.51
1:B:537:ARG:NH2	1:B:540:MET:SD	2.83	0.51
1:C:213:VAL:HG22	1:C:214:LYS:O	2.10	0.51
1:A:152:MET:CE	1:A:251:LEU:HG	2.41	0.51
1:C:218:ASP:C	1:C:219:GLU:O	2.52	0.51
1:C:474:TYR:CD1	1:C:474:TYR:N	2.78	0.51
1:A:322:ARG:HE	1:A:324:PRO:HG3	1.76	0.51
1:A:458:THR:HG22	1:A:460:ALA:N	2.25	0.51
1:C:67:PHE:CE2	1:C:104:ARG:HG2	2.46	0.51
1:A:118:GLU:O	1:A:122:LEU:HG	2.11	0.51
1:C:1:MET:HB2	1:C:21:CYS:SG	2.51	0.51
1:A:5:TYR:O	1:A:8:GLN:HG2	2.10	0.51
1:A:193:SER:C	1:A:195:GLN:H	2.17	0.51
1:C:209:TYR:CD1	1:C:209:TYR:C	2.89	0.51
1:A:521:LEU:HA	1:A:525:THR:HG21	1.93	0.51
1:B:85:ARG:HB2	1:B:85:ARG:HH11	1.75	0.51
1:C:386:ALA:HB2	1:C:392:ILE:HD11	1.92	0.51
1:C:387:GLN:O	1:C:390:ASP:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG21	1:A:529:ALA:HB3	1.94	0.50
1:A:506:ASN:HD22	1:A:509:GLU:H	1.54	0.50
1:C:505:ILE:HG12	1:C:510:GLN:HG3	1.93	0.50
1:B:39:ARG:HG2	1:B:40:ASP:N	2.27	0.50
1:C:58:LYS:HB3	1:C:59:LEU:CD1	2.41	0.50
1:C:77:ALA:HB1	3:C:986:HOH:O	2.11	0.50
1:A:321:LEU:HD21	1:A:410:ARG:HA	1.93	0.50
1:A:270:MET:HG2	1:A:274:GLU:HB2	1.93	0.50
1:A:436:PHE:HA	1:A:445:THR:O	2.11	0.50
1:C:33:LEU:HD22	1:C:48:PHE:CZ	2.47	0.50
1:C:284:PRO:HG2	1:C:428:LEU:HD11	1.94	0.50
1:C:330:THR:CG2	1:C:332:LYS:HB2	2.42	0.50
1:A:492:ASN:HD22	1:A:492:ASN:C	2.19	0.50
1:B:256:TRP:HD1	1:B:262:VAL:HG22	1.77	0.50
1:A:208:ARG:HE	1:A:239:MET:CE	2.25	0.50
1:A:528:HIS:HA	3:A:924:HOH:O	2.11	0.50
1:B:171:GLU:HG2	1:B:192:GLN:HG3	1.89	0.50
1:B:66:GLU:HG2	1:B:108:LEU:HD11	1.93	0.50
1:B:141:ARG:NH2	1:B:536:ASP:OD1	2.45	0.50
1:C:537:ARG:HH11	1:C:537:ARG:CG	2.25	0.50
1:B:164:MET:O	1:B:191:PRO:HD3	2.12	0.49
1:B:196:LEU:HD21	1:B:514:PHE:HB3	1.92	0.49
1:C:431:ILE:HG22	1:C:474:TYR:HB3	1.93	0.49
1:B:5:TYR:CZ	1:B:41:ARG:NH1	2.80	0.49
1:B:226:GLN:HB3	3:B:996:HOH:O	2.11	0.49
1:C:303:GLU:CD	1:C:303:GLU:H	2.20	0.49
1:B:563:LEU:HD22	1:C:370:LYS:HE2	1.94	0.49
1:A:213:VAL:HG22	1:A:214:LYS:N	2.28	0.49
1:B:381:LEU:HD22	1:B:386:ALA:HB3	1.95	0.49
1:B:437:GLU:HG3	1:B:445:THR:HG23	1.94	0.49
1:B:437:GLU:OE1	1:B:447:MET:HG2	2.12	0.49
1:B:134:MET:HE3	3:B:989:HOH:O	2.13	0.49
1:C:209:TYR:CG	1:C:210:TYR:N	2.81	0.49
1:A:339:ASN:O	1:A:342:LYS:HB3	2.13	0.49
1:C:167:LYS:HD3	1:C:168:ALA:N	2.28	0.49
1:A:584:VAL:HG11	1:B:582:GLN:NE2	2.27	0.49
1:A:241:ALA:N	1:A:242:PRO:CD	2.76	0.49
1:B:511:ARG:NH2	1:B:519:ASP:OD1	2.46	0.49
1:C:210:TYR:HA	1:C:233:ASP:O	2.12	0.49
1:C:545:THR:HG22	1:C:547:ASN:H	1.78	0.49
1:B:151:PHE:CD1	1:B:251:LEU:HD23	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:O	1:B:558:THR:HG23	2.12	0.48
1:B:222:ARG:O	1:B:225:ARG:HB2	2.13	0.48
1:B:256:TRP:HD1	1:B:262:VAL:CG2	2.27	0.48
1:B:34:ILE:CD1	1:B:61:SER:HA	2.44	0.48
1:B:131:ARG:NH2	1:B:133:GLU:OE1	2.46	0.48
1:B:354:VAL:HG12	1:B:388:ASP:HA	1.94	0.48
1:C:30:LEU:HD23	1:C:30:LEU:O	2.13	0.48
1:B:297:ASP:CG	1:B:383:ARG:HH22	2.20	0.48
1:A:409:LEU:HD13	1:A:409:LEU:C	2.39	0.48
1:B:462:LEU:CD1	1:B:495:MET:HE1	2.33	0.48
1:C:150:ARG:HG2	1:C:150:ARG:NH1	2.29	0.48
1:C:278:ARG:HG2	3:C:1033:HOH:O	2.13	0.48
1:B:472:ASN:HD22	1:B:488:VAL:HB	1.79	0.48
1:C:540:MET:HE2	1:C:548:ILE:HG13	1.96	0.48
1:B:240:THR:HG23	1:B:243:GLN:HE21	1.77	0.48
1:B:276:GLU:O	1:B:280:GLY:HA2	2.13	0.48
1:C:149:ARG:CZ	1:C:212:ILE:HD12	2.44	0.48
1:C:170:PRO:HG2	1:C:513:LYS:NZ	2.29	0.48
1:C:360:GLY:C	1:C:362:GLU:N	2.72	0.48
1:A:329:LEU:HD21	1:A:337:TYR:HE2	1.77	0.48
1:C:170:PRO:CB	1:C:174:ARG:HH12	2.27	0.48
1:B:436:PHE:O	1:B:437:GLU:HB3	2.13	0.48
1:B:489:ARG:HG3	1:B:528:HIS:CD2	2.48	0.48
1:C:559:ALA:O	1:C:560:ALA:HB3	2.13	0.48
1:B:331:ARG:HH22	1:C:118:GLU:CB	2.23	0.47
1:A:336:GLU:HG3	1:A:337:TYR:N	2.29	0.47
1:B:282:ASP:OD1	1:B:282:ASP:C	2.57	0.47
1:B:315:LYS:O	1:B:399:LYS:HG2	2.14	0.47
1:B:575:ALA:O	1:B:579:LEU:HD22	2.14	0.47
1:B:11:LEU:CD1	1:B:92:ILE:HG23	2.45	0.47
1:B:386:ALA:HB2	1:B:392:ILE:HD11	1.96	0.47
1:B:373:ASN:OD1	1:B:373:ASN:C	2.56	0.47
1:C:338:GLY:O	1:C:341:VAL:HG22	2.13	0.47
1:A:30:LEU:O	1:A:33:LEU:HB2	2.14	0.47
1:A:207:ASP:HB2	3:A:920:HOH:O	2.13	0.47
1:B:174:ARG:NH1	1:B:174:ARG:HG3	2.30	0.47
1:C:114:HIS:CE1	1:C:116:ASN:HA	2.50	0.47
1:A:486:GLY:HA3	1:A:531:LEU:HA	1.95	0.47
1:A:26:ARG:HG2	1:A:27:ARG:N	2.29	0.47
1:A:252:VAL:HG21	1:A:476:MET:SD	2.55	0.47
1:B:171:GLU:CD	1:B:192:GLN:HG3	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ASP:OD1	1:B:297:ASP:N	2.47	0.47
1:C:109:PRO:CG	1:C:110:LEU:H	2.27	0.47
1:C:360:GLY:C	1:C:362:GLU:H	2.21	0.47
1:A:333:GLN:HA	1:A:333:GLN:OE1	2.14	0.47
1:B:41:ARG:HD2	1:B:42:GLU:OE2	2.15	0.47
1:C:208:ARG:HE	1:C:239:MET:CE	2.26	0.47
1:B:458:THR:HB	1:B:461:GLU:HG3	1.97	0.47
1:C:221:LEU:O	1:C:222:ARG:CB	2.63	0.47
1:B:217:ARG:NH1	1:B:225:ARG:HD2	2.30	0.47
1:C:84:ASN:CG	1:C:87:MET:HG3	2.40	0.47
1:C:466:PRO:O	1:C:467:GLU:C	2.58	0.47
1:A:202:MET:HE2	1:A:202:MET:HA	1.97	0.46
1:A:263:ASP:HA	3:A:906:HOH:O	2.14	0.46
1:B:354:VAL:HG21	1:B:381:LEU:HD22	1.97	0.46
1:C:51:PRO:HA	1:C:57:LEU:HD12	1.96	0.46
1:C:322:ARG:NH2	1:C:387:GLN:HG3	2.29	0.46
1:B:331:ARG:NH2	1:C:118:GLU:HB3	2.24	0.46
1:B:351:TYR:CD1	1:B:351:TYR:C	2.92	0.46
1:C:8:GLN:HG3	1:C:42:GLU:HG2	1.97	0.46
1:C:225:ARG:NH1	1:C:225:ARG:CB	2.75	0.46
1:C:323:VAL:HG22	1:C:391:MET:HB3	1.97	0.46
1:C:519:ASP:HA	1:C:522:LYS:HE2	1.97	0.46
1:B:193:SER:C	1:B:195:GLN:N	2.72	0.46
1:A:192:GLN:O	1:A:215:CYS:CB	2.59	0.46
1:A:548:ILE:O	1:A:551:VAL:HG22	2.15	0.46
1:B:117:THR:C	1:B:119:GLU:H	2.21	0.46
1:C:272:PHE:CD2	1:C:434:PRO:HD3	2.50	0.46
1:C:558:THR:HG22	1:C:558:THR:O	2.15	0.46
1:C:277:ARG:NE	3:C:937:HOH:O	2.33	0.46
1:A:347:LYS:CG	1:A:348:GLY:H	2.10	0.46
1:B:111:ASP:HB3	1:B:114:HIS:CG	2.51	0.46
1:A:174:ARG:HD3	3:A:1021:HOH:O	2.14	0.46
1:B:78:ARG:HG3	1:B:93:GLU:HG2	1.98	0.46
1:B:222:ARG:HG2	1:B:223:ALA:N	2.31	0.46
1:A:84:ASN:O	1:A:90:GLY:HA3	2.16	0.46
1:A:184:LYS:O	1:C:303:GLU:HB3	2.15	0.46
1:A:218:ASP:CG	1:A:218:ASP:O	2.58	0.46
1:B:198:LYS:O	1:B:202:MET:HG2	2.16	0.46
1:C:50:ASP:OD1	1:C:96:ALA:O	2.33	0.46
1:C:481:TYR:CD2	1:C:541:LEU:HD21	2.51	0.46
1:C:579:LEU:HB3	1:C:581:ILE:HG12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:THR:HG22	1:A:331:ARG:H	1.80	0.45
1:B:245:ARG:NH1	3:B:938:HOH:O	2.48	0.45
1:C:448:HIS:HB2	3:C:1050:HOH:O	2.15	0.45
1:A:351:TYR:CD1	1:A:351:TYR:C	2.94	0.45
1:C:151:PHE:CD1	1:C:151:PHE:C	2.94	0.45
1:A:340:PHE:HA	1:A:343:ILE:HD13	1.98	0.45
1:A:442:GLY:HA3	3:A:976:HOH:O	2.15	0.45
1:B:398:ASN:ND2	1:B:400:LYS:HB3	2.31	0.45
1:C:324:PRO:HA	1:C:390:ASP:OD1	2.17	0.45
1:A:260:LYS:HD3	1:A:542:LEU:O	2.16	0.45
1:B:474:TYR:CE2	1:B:487:SER:HA	2.51	0.45
1:C:333:GLN:C	1:C:336:GLU:HG2	2.42	0.45
1:B:14:VAL:HG13	1:B:76:ARG:HA	1.98	0.45
1:B:270:MET:HE3	1:B:270:MET:HB2	1.74	0.45
1:B:397:ASP:HB3	1:B:401:ILE:HB	1.98	0.45
1:A:6:CYS:O	1:A:45:VAL:HB	2.17	0.45
1:A:569:SER:C	1:B:186:LYS:HD2	2.42	0.45
1:C:170:PRO:HD2	1:C:513:LYS:HD2	1.97	0.45
1:A:103:ASN:OD1	1:B:525:THR:HG23	2.17	0.45
1:A:417:LEU:HD23	1:A:417:LEU:N	2.32	0.45
1:A:492:ASN:ND2	1:A:493:GLY:N	2.63	0.45
1:B:225:ARG:HH11	1:B:225:ARG:CG	2.29	0.45
1:B:322:ARG:HD2	1:B:384:THR:O	2.17	0.45
1:B:367:PRO:HA	1:C:119:GLU:OE2	2.17	0.45
1:B:439:ASP:OD1	1:B:442:GLY:O	2.35	0.45
1:C:341:VAL:HG11	1:C:349:LEU:HD13	1.98	0.45
1:A:184:LYS:NZ	1:A:578:GLU:O	2.48	0.45
1:A:358:ALA:O	1:A:359:LYS:HD2	2.17	0.45
1:A:458:THR:CG2	1:A:460:ALA:H	2.30	0.45
1:B:271:THR:O	1:B:272:PHE:C	2.57	0.45
1:A:111:ASP:HB3	1:A:114:HIS:HD2	1.77	0.45
1:A:208:ARG:HE	1:A:239:MET:HE2	1.82	0.45
1:A:318:VAL:N	3:A:913:HOH:O	2.40	0.45
1:C:178:VAL:HB	1:C:188:TYR:HB2	1.99	0.45
1:C:303:GLU:CD	1:C:303:GLU:N	2.75	0.45
1:C:323:VAL:HG22	1:C:326:GLY:HA3	1.99	0.45
1:C:330:THR:HG23	1:C:332:LYS:N	2.26	0.45
1:B:149:ARG:HH22	1:B:212:ILE:HB	1.82	0.45
1:A:117:THR:C	1:A:119:GLU:N	2.73	0.44
1:A:341:VAL:HG21	1:A:348:GLY:O	2.18	0.44
1:B:117:THR:C	1:B:119:GLU:N	2.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ASN:HD22	1:A:103:ASN:HA	1.65	0.44
1:A:196:LEU:HD23	1:A:516:PHE:CZ	2.51	0.44
1:A:297:ASP:CG	1:A:383:ARG:HH22	2.25	0.44
1:A:454:PRO:O	1:A:455:LYS:C	2.60	0.44
1:B:69:ILE:HD13	1:B:71:VAL:CG1	2.47	0.44
1:C:33:LEU:HD22	1:C:48:PHE:CE1	2.52	0.44
1:A:376:ILE:O	1:A:380:ILE:HG13	2.17	0.44
1:B:143:LYS:O	1:B:147:LEU:HG	2.17	0.44
1:B:226:GLN:NE2	3:B:996:HOH:O	2.43	0.44
1:C:194:PRO:HG3	3:C:968:HOH:O	2.18	0.44
1:C:235:GLU:HA	1:C:530:GLY:HA3	1.99	0.44
1:C:321:LEU:HD23	1:C:409:LEU:HD13	1.99	0.44
1:C:588:GLU:C	1:C:590:ASN:N	2.73	0.44
1:A:377:ILE:O	1:A:381:LEU:HG	2.18	0.44
1:C:330:THR:CG2	1:C:332:LYS:N	2.81	0.44
1:A:286:LEU:HB2	1:A:426:ALA:HB1	1.98	0.44
1:A:481:TYR:CB	1:A:537:ARG:HD3	2.44	0.44
1:B:290:MET:HE2	1:B:419:LEU:HD12	1.98	0.44
1:C:71:VAL:HG12	1:C:99:LEU:HD12	2.00	0.44
1:B:137:ARG:NE	1:B:545:THR:OG1	2.50	0.44
1:B:447:MET:HB3	1:B:448:HIS:CE1	2.53	0.44
1:C:13:HIS:O	1:C:16:GLN:HG3	2.18	0.44
1:C:59:LEU:HD23	1:C:99:LEU:HD23	1.99	0.44
1:B:437:GLU:O	1:B:444:LEU:HA	2.18	0.44
1:C:17:GLN:HA	1:C:73:GLY:O	2.18	0.44
1:C:333:GLN:HA	1:C:336:GLU:HG2	2.00	0.44
1:A:208:ARG:NE	1:A:239:MET:HE1	2.33	0.44
1:A:357:ARG:NH1	1:A:357:ARG:CB	2.61	0.44
1:A:387:GLN:O	1:A:390:ASP:HB2	2.18	0.44
1:A:579:LEU:O	1:A:581:ILE:HG23	2.18	0.44
1:B:235:GLU:OE1	1:B:530:GLY:HA3	2.17	0.44
1:A:11:LEU:O	1:A:14:VAL:HG23	2.18	0.44
1:A:286:LEU:HD21	1:A:428:LEU:HD13	1.99	0.44
1:B:92:ILE:C	1:B:92:ILE:HD12	2.43	0.44
1:C:149:ARG:NH2	1:C:212:ILE:HB	2.32	0.44
1:C:271:THR:HA	1:C:431:ILE:O	2.17	0.44
1:C:330:THR:HG23	1:C:331:ARG:N	2.33	0.44
1:C:583:VAL:HB	3:C:1031:HOH:O	2.18	0.44
1:A:28:ARG:HD3	1:A:29:ASP:O	2.18	0.43
1:A:161:GLU:OE1	1:B:230:THR:OG1	2.33	0.43
1:C:109:PRO:CG	1:C:110:LEU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:PRO:HG3	1:B:245:ARG:NH2	2.32	0.43
1:C:431:ILE:O	1:C:432:ASP:HB2	2.17	0.43
1:A:240:THR:CB	1:A:242:PRO:HD2	2.49	0.43
1:A:322:ARG:NH2	1:A:387:GLN:CG	2.81	0.43
1:A:210:TYR:HA	1:A:233:ASP:O	2.18	0.43
1:A:315:LYS:C	1:A:399:LYS:HG3	2.44	0.43
1:B:104:ARG:HG2	1:B:104:ARG:HH11	1.82	0.43
1:B:110:LEU:HD12	1:B:110:LEU:HA	1.90	0.43
1:B:330:THR:HB	1:B:333:GLN:HG3	1.99	0.43
1:C:137:ARG:HD3	1:C:545:THR:OG1	2.18	0.43
1:B:181:ARG:HE	1:B:181:ARG:HB3	1.47	0.43
1:C:13:HIS:O	1:C:14:VAL:C	2.61	0.43
1:A:26:ARG:HH12	1:A:28:ARG:HB2	1.78	0.43
1:A:92:ILE:HD12	1:A:92:ILE:C	2.44	0.43
1:A:133:GLU:CD	1:A:137:ARG:HH22	2.26	0.43
1:B:57:LEU:O	1:B:58:LYS:C	2.61	0.43
1:B:225:ARG:HH11	1:B:225:ARG:CB	2.31	0.43
1:C:50:ASP:OD1	1:C:50:ASP:N	2.52	0.43
1:C:144:ILE:O	1:C:148:VAL:HG23	2.18	0.43
1:C:297:ASP:CG	1:C:383:ARG:HH22	2.26	0.43
1:A:342:LYS:HD3	1:A:342:LYS:O	2.19	0.43
1:B:160:ILE:HG12	3:B:914:HOH:O	2.19	0.43
1:B:397:ASP:OD1	1:B:398:ASN:N	2.48	0.43
1:C:500:PHE:CD2	1:C:510:GLN:HG2	2.54	0.43
1:A:330:THR:O	1:A:334:ILE:HG13	2.19	0.43
1:A:364:ILE:HD12	1:A:364:ILE:C	2.43	0.43
1:A:457:MET:SD	1:A:469:ALA:HB2	2.58	0.43
1:C:11:LEU:HD23	1:C:14:VAL:CG2	2.47	0.43
1:A:152:MET:HE3	1:A:251:LEU:HG	2.01	0.43
1:B:162:THR:H	1:B:211:GLN:HE22	1.66	0.43
1:B:355:ASN:O	1:B:388:ASP:HB3	2.19	0.43
1:C:293:THR:HG21	1:C:383:ARG:HG2	1.99	0.43
1:A:202:MET:HG3	1:A:235:GLU:HG3	2.01	0.43
1:B:226:GLN:NE2	1:B:556:LYS:H	1.93	0.43
1:C:229:PHE:CD1	1:C:229:PHE:N	2.87	0.43
1:A:117:THR:O	1:A:118:GLU:C	2.62	0.42
1:B:533:PHE:HB3	1:B:538:LEU:CD2	2.49	0.42
1:A:170:PRO:HD3	1:A:513:LYS:CD	2.35	0.42
1:B:33:LEU:HD13	1:B:48:PHE:CZ	2.46	0.42
1:B:433:PHE:O	1:B:434:PRO:C	2.61	0.42
1:B:451:PHE:CE2	1:B:517:LEU:HD23	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:GLU:H	1:C:219:GLU:HG3	1.44	0.42
1:C:410:ARG:HD3	3:C:941:HOH:O	2.20	0.42
1:C:574:THR:O	1:C:577:ALA:HB3	2.19	0.42
1:A:359:LYS:HB2	1:A:363:GLY:CA	2.49	0.42
1:A:452:THR:HG23	1:A:487:SER:HB2	2.01	0.42
1:B:184:LYS:HE2	3:B:917:HOH:O	2.19	0.42
1:B:265:GLY:O	1:B:266:ASP:C	2.60	0.42
1:B:365:ASN:HD22	1:B:365:ASN:HA	1.59	0.42
1:C:99:LEU:HD23	1:C:99:LEU:C	2.44	0.42
1:C:131:ARG:NH1	1:C:134:MET:HG2	2.33	0.42
1:C:221:LEU:O	1:C:222:ARG:HG3	2.18	0.42
1:C:336:GLU:HG3	1:C:337:TYR:H	1.84	0.42
1:C:368:VAL:O	1:C:372:LEU:HD13	2.19	0.42
1:B:151:PHE:CD1	1:B:151:PHE:C	2.97	0.42
1:B:343:ILE:HG23	1:C:343:ILE:HG23	2.01	0.42
1:B:436:PHE:HB3	1:B:444:LEU:HD22	2.02	0.42
1:C:159:ASP:HB2	1:C:210:TYR:CE1	2.55	0.42
1:A:500:PHE:O	1:A:505:ILE:HG23	2.19	0.42
1:B:372:LEU:HB3	1:B:373:ASN:H	1.62	0.42
1:B:435:MET:HG2	1:B:471:ALA:CA	2.49	0.42
1:C:240:THR:OG1	1:C:243:GLN:HG3	2.20	0.42
1:A:200:LEU:HD12	1:A:200:LEU:HA	1.81	0.42
1:A:226:GLN:HE22	1:A:556:LYS:N	2.06	0.42
1:B:323:VAL:HA	1:B:324:PRO:HD2	1.85	0.42
1:B:411:LEU:HD23	1:B:411:LEU:HA	1.88	0.42
1:C:240:THR:H	1:C:243:GLN:NE2	1.93	0.42
1:C:252:VAL:HG21	1:C:476:MET:SD	2.59	0.42
1:C:488:VAL:HA	1:C:529:ALA:HB2	2.01	0.42
1:A:167:LYS:CB	1:B:567:ALA:HB2	2.49	0.42
1:A:271:THR:HA	1:A:431:ILE:O	2.19	0.42
1:A:303:GLU:HG3	1:A:304:PHE:N	2.35	0.42
1:A:356:GLU:C	1:A:358:ALA:N	2.74	0.42
1:B:364:ILE:HD13	1:B:377:ILE:HG21	2.02	0.42
1:B:437:GLU:CG	1:B:445:THR:HG23	2.49	0.42
1:C:545:THR:HG22	1:C:546:ASP:N	2.33	0.42
1:B:221:LEU:CB	1:B:558:THR:O	2.64	0.42
1:B:506:ASN:ND2	1:B:508:GLU:H	2.17	0.42
1:C:295:VAL:O	1:C:298:LEU:HB2	2.20	0.42
1:C:316:GLY:HA2	1:C:398:ASN:HA	2.01	0.42
1:C:435:MET:HE2	1:C:454:PRO:HG3	2.01	0.42
1:A:240:THR:OG1	1:A:242:PRO:HD2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:HIS:HB2	1:A:450:PRO:CD	2.50	0.42
1:B:288:ASN:OD1	1:B:288:ASN:C	2.63	0.42
1:B:330:THR:HB	1:B:333:GLN:H	1.85	0.42
1:B:451:PHE:CZ	1:B:517:LEU:HD23	2.55	0.42
1:C:38:MET:O	1:C:44:ILE:HA	2.20	0.42
1:A:373:ASN:HD21	1:A:375:GLU:HB3	1.85	0.42
1:A:395:GLY:N	1:A:406:MET:HE2	2.35	0.42
1:A:565:THR:HG22	1:B:516:PHE:CZ	2.54	0.42
1:B:202:MET:HA	1:B:202:MET:HE2	2.02	0.42
1:C:371:PHE:C	1:C:372:LEU:HD12	2.44	0.42
1:C:449:HIS:HE1	1:C:489:ARG:NH1	2.17	0.42
1:A:268:PRO:HD2	1:A:427:PRO:O	2.20	0.41
1:A:458:THR:CG2	1:A:459:ALA:N	2.81	0.41
1:A:540:MET:SD	1:A:548:ILE:HA	2.60	0.41
1:B:34:ILE:HD11	1:B:61:SER:HA	2.02	0.41
1:C:164:MET:O	1:C:191:PRO:HD3	2.20	0.41
1:C:288:ASN:O	1:C:410:ARG:NH2	2.53	0.41
1:C:357:ARG:C	1:C:359:LYS:N	2.78	0.41
1:C:537:ARG:CG	1:C:537:ARG:NH1	2.82	0.41
1:A:187:PHE:N	1:A:187:PHE:CD1	2.87	0.41
1:A:196:LEU:HD21	1:A:517:LEU:HD22	2.02	0.41
1:A:361:LEU:O	1:A:361:LEU:HD13	2.21	0.41
1:B:66:GLU:CG	1:B:108:LEU:HD11	2.49	0.41
1:B:184:LYS:HD2	1:B:184:LYS:N	2.34	0.41
1:C:221:LEU:O	1:C:222:ARG:CG	2.68	0.41
1:A:59:LEU:HA	1:A:59:LEU:HD23	1.84	0.41
1:A:195:GLN:HG3	1:A:196:LEU:H	1.85	0.41
1:A:222:ARG:HB2	1:A:225:ARG:CG	2.41	0.41
1:A:297:ASP:OD1	1:A:383:ARG:NH2	2.53	0.41
1:A:322:ARG:HH11	1:A:322:ARG:HG3	1.86	0.41
1:B:224:ASP:O	1:B:224:ASP:CG	2.62	0.41
1:B:323:VAL:O	1:B:323:VAL:CG2	2.68	0.41
1:C:457:MET:HG2	3:C:974:HOH:O	2.19	0.41
1:B:63:LEU:CD2	1:B:69:ILE:HG21	2.50	0.41
1:A:76:ARG:NE	1:A:93:GLU:OE2	2.51	0.41
1:A:80:GLU:HA	1:A:83:ILE:HD12	2.02	0.41
1:A:521:LEU:HA	1:A:525:THR:CG2	2.50	0.41
1:A:562:CYS:SG	1:A:565:THR:OG1	2.76	0.41
1:B:286:LEU:HB2	1:B:426:ALA:HB1	2.02	0.41
1:B:323:VAL:O	1:B:323:VAL:HG22	2.19	0.41
1:B:351:TYR:HA	1:B:392:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:MET:HE3	1:B:436:PHE:CZ	2.55	0.41
1:A:336:GLU:HG3	1:A:337:TYR:H	1.86	0.41
1:A:522:LYS:O	1:B:105:ALA:HA	2.20	0.41
1:A:540:MET:HE2	1:A:548:ILE:CG1	2.44	0.41
1:B:331:ARG:HG3	1:B:335:ASP:OD2	2.19	0.41
1:B:376:ILE:O	1:B:380:ILE:HG13	2.20	0.41
1:B:537:ARG:HG3	3:B:1015:HOH:O	2.21	0.41
1:C:295:VAL:HG23	1:C:318:VAL:HG12	2.02	0.41
1:A:162:THR:H	1:A:211:GLN:HE22	1.69	0.41
1:A:388:ASP:OD1	1:A:388:ASP:N	2.53	0.41
1:A:567:ALA:HB2	1:B:167:LYS:HA	2.02	0.41
1:C:10:ARG:C	1:C:12:SER:N	2.76	0.41
1:C:208:ARG:NE	1:C:239:MET:CE	2.84	0.41
1:C:377:ILE:O	1:C:381:LEU:HG	2.21	0.41
1:C:502:ILE:C	1:C:504:GLY:H	2.29	0.41
1:A:217:ARG:NH1	1:A:225:ARG:NH1	2.68	0.41
1:A:357:ARG:HB3	1:A:357:ARG:CZ	2.49	0.41
1:B:437:GLU:HG3	1:B:445:THR:CG2	2.51	0.41
1:C:340:PHE:CD1	1:C:340:PHE:C	2.99	0.41
1:C:421:ASP:HB3	3:C:947:HOH:O	2.20	0.41
1:C:588:GLU:C	1:C:590:ASN:H	2.29	0.41
1:A:166:THR:HG22	1:A:189:ALA:HB3	2.03	0.41
1:B:140:THR:HG21	1:B:543:THR:HG22	2.02	0.41
1:B:338:GLY:O	1:B:342:LYS:HD3	2.20	0.41
1:B:505:ILE:HG22	1:B:510:GLN:HG3	2.03	0.41
1:C:29:ASP:O	1:C:30:LEU:HB3	2.20	0.41
1:C:87:MET:HE2	1:C:87:MET:HB3	1.85	0.41
1:C:128:ASP:OD1	1:C:131:ARG:HD3	2.21	0.41
1:C:167:LYS:HD3	1:C:168:ALA:H	1.85	0.41
1:C:198:LYS:HE2	1:C:235:GLU:OE1	2.20	0.41
1:C:268:PRO:HD2	1:C:427:PRO:O	2.21	0.41
1:C:507:GLU:HA	1:C:510:GLN:HB2	2.02	0.41
1:A:333:GLN:O	1:A:336:GLU:CG	2.61	0.41
1:A:507:GLU:OE2	1:A:511:ARG:HG2	2.21	0.41
1:B:565:THR:O	1:B:566:GLU:HB2	2.21	0.41
1:A:433:PHE:HD2	1:A:447:MET:HE2	1.86	0.40
1:A:545:THR:HG22	1:A:547:ASN:N	2.32	0.40
1:A:567:ALA:HA	1:A:568:PRO:C	2.45	0.40
1:B:334:ILE:O	1:B:334:ILE:HG22	2.21	0.40
1:B:446:ALA:HB1	1:B:448:HIS:O	2.21	0.40
1:A:267:PHE:N	1:A:267:PHE:CD1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:TYR:O	1:C:483:VAL:HG13	2.22	0.40
1:A:222:ARG:N	1:A:225:ARG:HB2	2.36	0.40
1:A:240:THR:HB	1:A:242:PRO:HD2	2.03	0.40
1:B:297:ASP:OD1	1:B:383:ARG:NH2	2.55	0.40
1:C:2:ARG:HA	1:C:19:THR:O	2.20	0.40
1:A:123:LYS:HD2	1:A:124:TYR:CZ	2.57	0.40
1:A:287:ARG:HD3	1:A:479:ASN:ND2	2.36	0.40
1:A:431:ILE:O	1:A:432:ASP:HB2	2.21	0.40
1:C:197:PHE:O	1:C:201:LEU:HG	2.22	0.40
1:C:336:GLU:HG3	1:C:337:TYR:N	2.36	0.40
1:C:468:ASN:O	1:C:469:ALA:C	2.64	0.40
1:A:169:THR:HB	1:A:170:PRO:HD2	2.04	0.40
1:C:22:GLY:N	1:C:38:MET:HE2	2.37	0.40
1:C:118:GLU:O	1:C:122:LEU:HG	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:GLN:NE2	1:C:582:GLN:NE2[2_654]	1.92	0.28

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	588/590 (100%)	540 (92%)	41 (7%)	7 (1%)	10	27
1	B	588/590 (100%)	529 (90%)	48 (8%)	11 (2%)	6	17
1	C	588/590 (100%)	520 (88%)	54 (9%)	14 (2%)	4	12
All	All	1764/1770 (100%)	1589 (90%)	143 (8%)	32 (2%)	6	18

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	588	GLU
1	B	58	LYS
1	B	221	LEU
1	B	440	GLY
1	B	589	ASN
1	C	56	ALA
1	C	57	LEU
1	C	169	THR
1	C	170	PRO
1	C	222	ARG
1	A	223	ALA
1	B	80	GLU
1	B	170	PRO
1	C	90	GLY
1	C	302	VAL
1	C	358	ALA
1	A	347	LYS
1	A	397	ASP
1	B	358	ALA
1	C	193	SER
1	C	219	GLU
1	C	221	LEU
1	A	41	ARG
1	A	173	ALA
1	A	349	LEU
1	B	104	ARG
1	B	422	GLU
1	C	357	ARG
1	B	437	GLU
1	C	51	PRO
1	B	90	GLY
1	C	115	VAL

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	490/490 (100%)	434 (89%)	56 (11%)	5	14
1	B	490/490 (100%)	431 (88%)	59 (12%)	5	12
1	C	490/490 (100%)	432 (88%)	58 (12%)	5	13
All	All	1470/1470 (100%)	1297 (88%)	173 (12%)	5	13

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	4	GLU
1	A	28	ARG
1	A	30	LEU
1	A	36	ILE
1	A	41	ARG
1	A	57	LEU
1	A	71	VAL
1	A	72	THR
1	A	100	THR
1	A	103	ASN
1	A	111	ASP
1	A	114	HIS
1	A	127	LEU
1	A	149	ARG
1	A	164	MET
1	A	166	THR
1	A	171	GLU
1	A	175	ASP
1	A	200	LEU
1	A	209	TYR
1	A	219	GLU
1	A	220	ASP
1	A	231	GLN
1	A	247	VAL
1	A	251	LEU
1	A	257	LEU
1	A	266	ASP
1	A	283	LYS
1	A	286	LEU
1	A	298	LEU
1	A	322	ARG
1	A	323	VAL
1	A	332	LYS

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Mol	Chain	Res	Type
1	A	333	GLN
1	A	361	LEU
1	A	362	GLU
1	A	372	LEU
1	A	383	ARG
1	A	387	GLN
1	A	397	ASP
1	A	398	ASN
1	A	417	LEU
1	A	458	THR
1	A	467	GLU
1	A	492	ASN
1	A	505	ILE
1	A	506	ASN
1	A	511	ARG
1	A	512	GLU
1	A	525	THR
1	A	538	LEU
1	A	546	ASP
1	A	574	THR
1	A	579	LEU
1	A	582	GLN
1	B	3	THR
1	B	4	GLU
1	B	11	LEU
1	B	36	ILE
1	B	41	ARG
1	B	44	ILE
1	B	59	LEU
1	B	71	VAL
1	B	72	THR
1	B	85	ARG
1	B	103	ASN
1	B	104	ARG
1	B	114	HIS
1	B	127	LEU
1	B	138	LEU
1	B	140	THR
1	B	143	LYS
1	B	154	ASP
1	B	158	LEU
1	B	169	THR

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Mol	Chain	Res	Type
1	B	171	GLU
1	B	175	ASP
1	B	195	GLN
1	B	200	LEU
1	B	209	TYR
1	B	217	ARG
1	B	221	LEU
1	B	224	ASP
1	B	225	ARG
1	B	257	LEU
1	B	262	VAL
1	B	286	LEU
1	B	298	LEU
1	B	323	VAL
1	B	331	ARG
1	B	365	ASN
1	B	372	LEU
1	B	378	GLU
1	B	382	ASP
1	B	383	ARG
1	B	409	LEU
1	B	422	GLU
1	B	441	GLU
1	B	447	MET
1	B	458	THR
1	B	462	LEU
1	B	491	HIS
1	B	495	MET
1	B	503	LEU
1	B	507	GLU
1	B	511	ARG
1	B	514	PHE
1	B	526	PRO
1	B	531	LEU
1	B	537	ARG
1	B	538	LEU
1	B	574	THR
1	B	578	GLU
1	B	579	LEU
1	C	1	MET
1	C	4	GLU
1	C	11	LEU

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Mol	Chain	Res	Type
1	C	26	ARG
1	C	32	SER
1	C	36	ILE
1	C	41	ARG
1	C	47	VAL
1	C	57	LEU
1	C	59	LEU
1	C	71	VAL
1	C	72	THR
1	C	99	LEU
1	C	106	ASP
1	C	114	HIS
1	C	117	THR
1	C	119	GLU
1	C	127	LEU
1	C	138	LEU
1	C	143	LYS
1	C	150	ARG
1	C	158	LEU
1	C	170	PRO
1	C	175	ASP
1	C	193	SER
1	C	196	LEU
1	C	200	LEU
1	C	209	TYR
1	C	219	GLU
1	C	225	ARG
1	C	257	LEU
1	C	262	VAL
1	C	266	ASP
1	C	286	LEU
1	C	298	LEU
1	C	302	VAL
1	C	303	GLU
1	C	323	VAL
1	C	330	THR
1	C	362	GLU
1	C	383	ARG
1	C	409	LEU
1	C	462	LEU
1	C	474	TYR
1	C	492	ASN

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Mol	Chain	Res	Type
1	C	503	LEU
1	C	505	ILE
1	C	507	GLU
1	C	512	GLU
1	C	513	LYS
1	C	525	THR
1	C	531	LEU
1	C	537	ARG
1	C	538	LEU
1	C	546	ASP
1	C	550	ASP
1	C	579	LEU
1	C	589	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	70	GLN
1	A	103	ASN
1	A	155	HIS
1	A	211	GLN
1	A	226	GLN
1	A	231	GLN
1	A	243	GLN
1	A	339	ASN
1	A	387	GLN
1	A	398	ASN
1	A	448	HIS
1	A	449	HIS
1	A	492	ASN
1	A	497	GLN
1	A	506	ASN
1	A	510	GLN
1	A	547	ASN
1	A	590	ASN
1	B	16	GLN
1	B	46	GLN
1	B	65	ASN
1	B	70	GLN
1	B	211	GLN
1	B	226	GLN

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Mol	Chain	Res	Type
1	B	243	GLN
1	B	365	ASN
1	B	398	ASN
1	B	472	ASN
1	B	506	ASN
1	B	582	GLN
1	B	590	ASN
1	C	16	GLN
1	C	65	ASN
1	C	70	GLN
1	C	116	ASN
1	C	192	GLN
1	C	195	GLN
1	C	211	GLN
1	C	226	GLN
1	C	243	GLN
1	C	365	ASN
1	C	449	HIS
1	C	472	ASN
1	C	492	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	590/590 (100%)	-0.32	12 (2%) 65 62	9, 31, 75, 101	0
1	B	590/590 (100%)	-0.31	11 (1%) 66 63	10, 33, 73, 101	0
1	C	590/590 (100%)	-0.19	19 (3%) 50 46	15, 37, 82, 101	0
All	All	1770/1770 (100%)	-0.27	42 (2%) 59 56	9, 34, 78, 101	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	194	PRO	4.9
1	B	173	ALA	4.6
1	C	57	LEU	4.5
1	C	56	ALA	4.3
1	B	170	PRO	4.2
1	A	587	ALA	4.1
1	A	193	SER	3.8
1	C	221	LEU	3.6
1	C	590	ASN	3.6
1	C	170	PRO	3.2
1	B	172	GLY	3.2
1	C	54	ALA	3.1
1	A	589	ASN	3.1
1	C	358	ALA	3.1
1	C	59	LEU	3.0
1	C	173	ALA	3.0
1	B	194	PRO	3.0
1	C	193	SER	3.0
1	C	175	ASP	2.9
1	B	193	SER	2.8
1	C	588	GLU	2.7
1	A	221	LEU	2.6
1	B	443	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	590	ASN	2.5
1	A	224	ASP	2.5
1	C	194	PRO	2.4
1	B	223	ALA	2.4
1	C	53	ARG	2.4
1	B	171	GLU	2.4
1	A	220	ASP	2.4
1	C	169	THR	2.3
1	C	492	ASN	2.2
1	B	174	ARG	2.2
1	C	55	ASP	2.2
1	C	51	PRO	2.2
1	B	221	LEU	2.2
1	A	361	LEU	2.2
1	A	50	ASP	2.1
1	C	587	ALA	2.1
1	B	590	ASN	2.0
1	A	28	ARG	2.0
1	A	150	ARG	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	MG	A	901	1/1	0.97	0.23	2,2,2,2	0
2	MG	C	903	1/1	0.97	0.25	2,2,2,2	0
2	MG	B	902	1/1	0.98	0.20	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.