



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:50 PM UTC

PDB ID : 2HN2 / pdb_00002hn2
Title : Crystal structure of the CorA Mg²⁺ transporter homologue from *T. maritima*
in complex with divalent cations
Authors : Payandeh, J.; Pai, E.F.
Deposited on : 2006-07-11
Resolution : 3.70 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

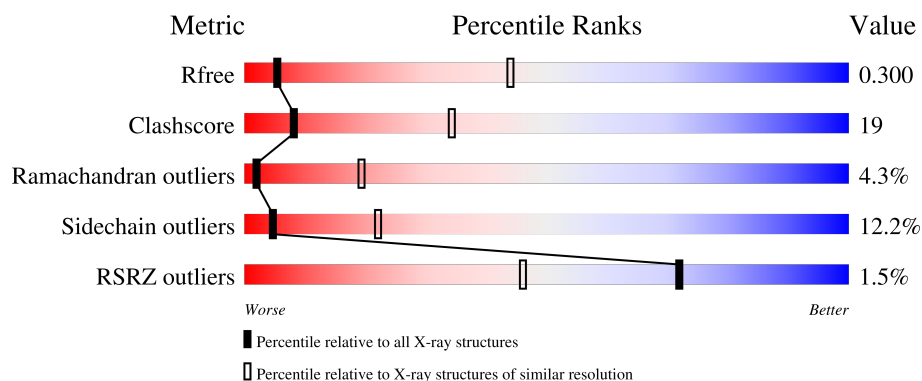
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	354	% 52% 35% 6% • 6%
1	B	354	2% 52% 35% 6% • 6%
1	C	354	2% 53% 34% 6% • 6%
1	D	354	% 51% 36% 6% • 6%
1	E	354	% 53% 34% 6% • 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13698 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 Magnesium transport protein corA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2737	1782	445	501	9			
1	B	331	Total	C	N	O	S	0	0	0
			2737	1782	445	501	9			
1	C	331	Total	C	N	O	S	0	0	0
			2737	1782	445	501	9			
1	D	331	Total	C	N	O	S	0	0	0
			2737	1782	445	501	9			
1	E	331	Total	C	N	O	S	0	0	0
			2737	1782	445	501	9			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	998	GLY	-	cloning artifact	UNP Q9WZ31
A	999	SER	-	cloning artifact	UNP Q9WZ31
A	1000	HIS	-	cloning artifact	UNP Q9WZ31
B	1998	GLY	-	cloning artifact	UNP Q9WZ31
B	1999	SER	-	cloning artifact	UNP Q9WZ31
B	2000	HIS	-	cloning artifact	UNP Q9WZ31
C	2998	GLY	-	cloning artifact	UNP Q9WZ31
C	2999	SER	-	cloning artifact	UNP Q9WZ31
C	3000	HIS	-	cloning artifact	UNP Q9WZ31
D	3998	GLY	-	cloning artifact	UNP Q9WZ31
D	3999	SER	-	cloning artifact	UNP Q9WZ31
D	4000	HIS	-	cloning artifact	UNP Q9WZ31
E	4998	GLY	-	cloning artifact	UNP Q9WZ31
E	4999	SER	-	cloning artifact	UNP Q9WZ31
E	5000	HIS	-	cloning artifact	UNP Q9WZ31

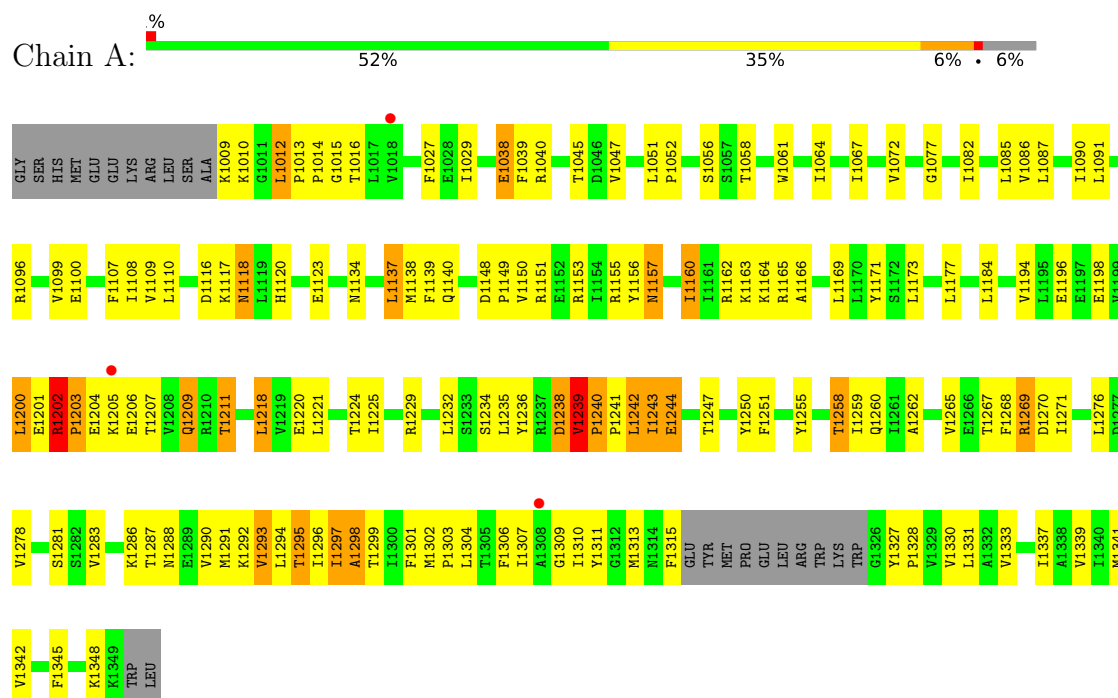
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total 4	Ca 4	0	0
2	B	3	Total 3	Ca 3	0	0
2	C	2	Total 2	Ca 2	0	0
2	D	3	Total 3	Ca 3	0	0
2	E	1	Total 1	Ca 1	0	0

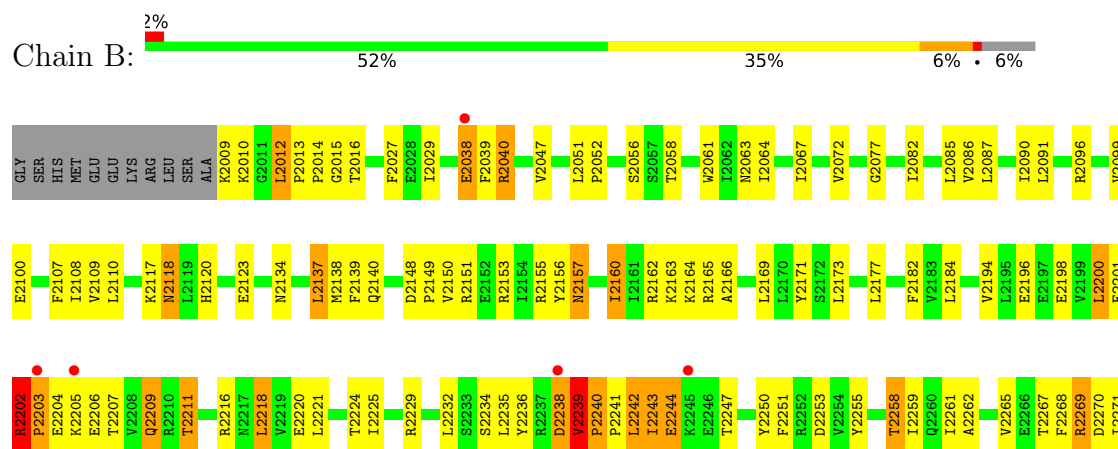
3 Residue-property plots

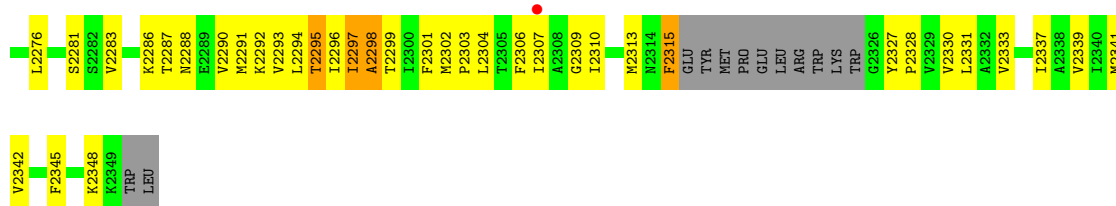
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

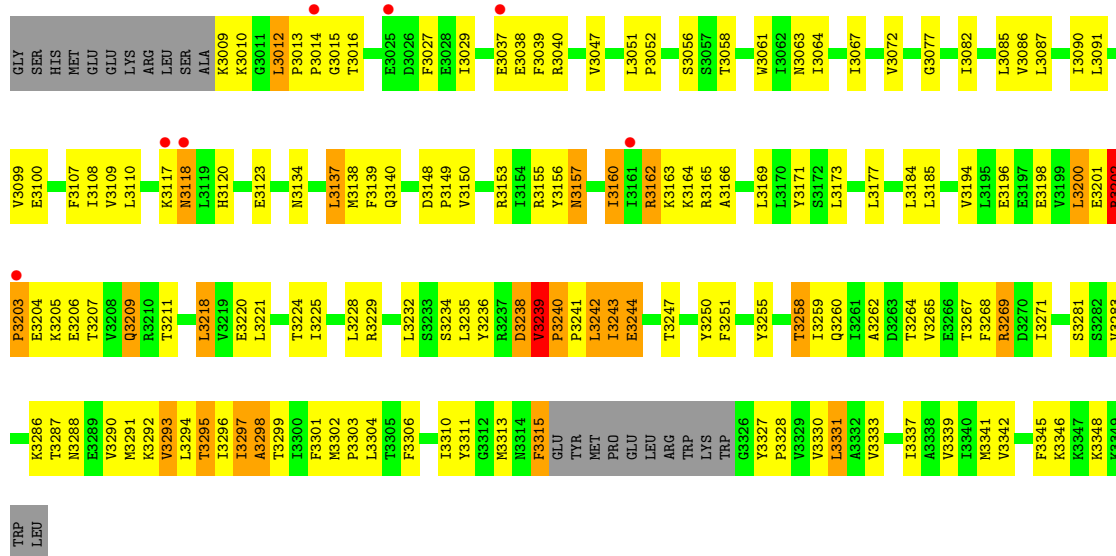


• Molecule 1: Magnesium transport protein corA

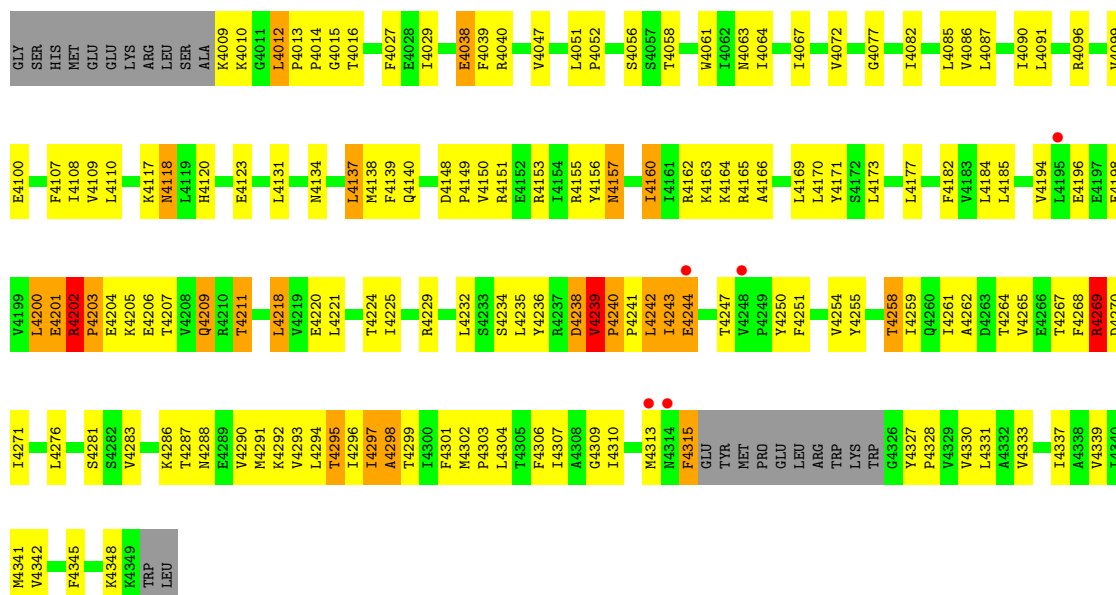




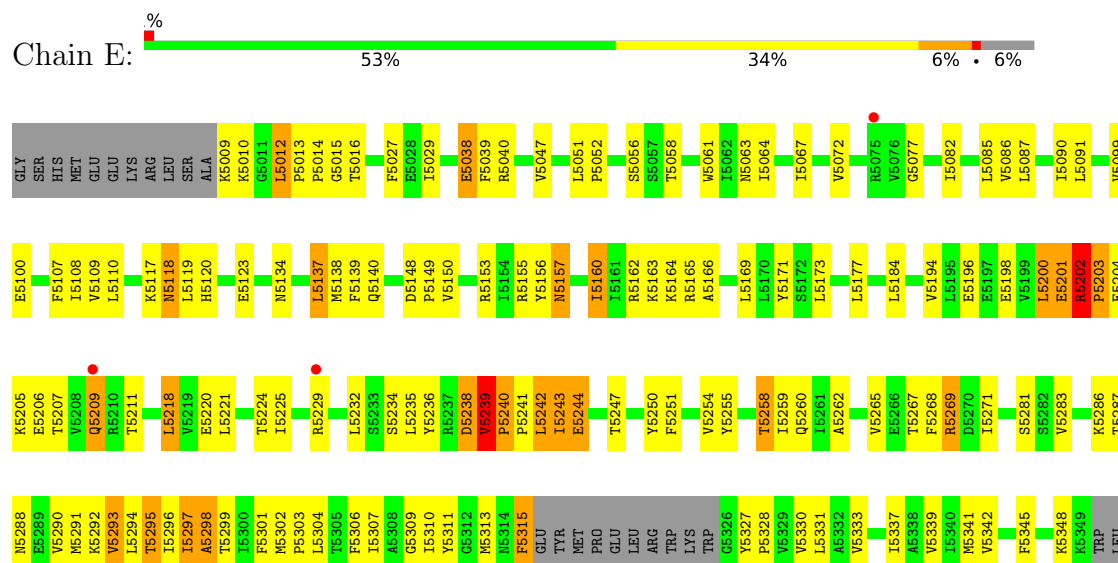
• Molecule 1: Magnesium transport protein corA



• Molecule 1: Magnesium transport protein corA



● Molecule 1: Magnesium transport protein corA



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.25Å 86.30Å 181.53Å 90.00° 112.23° 90.00°	Depositor
Resolution (Å)	20.00 – 3.70 20.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-3.70) 91.4 (20.00-3.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 3.67Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.295 , 0.316 0.294 , 0.300	Depositor DCC
R_{free} test set	1562 reflections (3.36%)	wwPDB-VP
Wilson B-factor (Å ²)	120.5	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 107.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13698	wwPDB-VP
Average B, all atoms (Å ²)	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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: CA

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	0/2794	0.83	1/3785 (0.0%)
1	B	0.47	0/2794	0.84	2/3785 (0.1%)
1	C	0.47	0/2794	0.84	0/3785
1	D	0.47	0/2794	0.86	4/3785 (0.1%)
1	E	0.47	0/2794	0.83	1/3785 (0.0%)
All	All	0.47	0/13970	0.84	8/18925 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4269	ARG	NE-CZ-NH2	-8.62	111.44	119.20
1	D	4269	ARG	CD-NE-CZ	7.83	135.36	124.40
1	D	4269	ARG	NE-CZ-NH1	7.40	128.90	121.50
1	D	4038	GLU	N-CA-C	6.24	117.35	108.74
1	E	5038	GLU	N-CA-C	6.07	117.12	108.74
1	A	1038	GLU	N-CA-C	5.91	116.89	108.74
1	B	2038	GLU	CA-CB-CG	5.21	124.52	114.10
1	B	2038	GLU	N-CA-CB	-5.10	103.61	111.46

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	2737	0	2790	118	1
1	B	2737	0	2790	128	1
1	C	2737	0	2790	122	1
1	D	2737	0	2790	124	0
1	E	2737	0	2790	120	1
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	3	0	0	0	0
2	E	1	0	0	0	0
All	All	13698	0	13950	535	3

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 19.

All (535) 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:E:5240:PRO:HB2	1:E:5241:PRO:HD3	1.33	1.10
1:A:1240:PRO:HB2	1:A:1241:PRO:HD3	1.33	1.09
1:D:4240:PRO:HB2	1:D:4241:PRO:HD3	1.33	1.08
1:B:2240:PRO:HB2	1:B:2241:PRO:HD3	1.33	1.07
1:C:3240:PRO:HB2	1:C:3241:PRO:HD3	1.33	1.07
1:B:2012:LEU:H	1:B:2013:PRO:HD3	1.22	1.04
1:E:5310:ILE:O	1:E:5313:MET:HG2	1.58	1.04
1:C:3012:LEU:H	1:C:3013:PRO:HD3	1.22	1.04
1:D:4310:ILE:O	1:D:4313:MET:HG2	1.58	1.04
1:C:3310:ILE:O	1:C:3313:MET:HG2	1.58	1.03
1:B:2310:ILE:O	1:B:2313:MET:HG2	1.58	1.02
1:A:1012:LEU:H	1:A:1013:PRO:HD3	1.22	1.02
1:A:1310:ILE:O	1:A:1313:MET:HG2	1.58	1.01
1:D:4012:LEU:H	1:D:4013:PRO:HD3	1.22	1.01
1:E:5012:LEU:H	1:E:5013:PRO:HD3	1.22	1.01
1:B:2303:PRO:HA	1:C:3301:PHE:CD2	1.98	0.99
1:B:2306:PHE:CE1	1:C:3304:LEU:HB3	2.02	0.95
1:B:2236:TYR:HA	1:B:2251:PHE:HZ	1.33	0.94
1:E:5236:TYR:HA	1:E:5251:PHE:HZ	1.33	0.92
1:A:1236:TYR:HA	1:A:1251:PHE:HZ	1.33	0.92
1:C:3236:TYR:HA	1:C:3251:PHE:HZ	1.33	0.91
1:D:4236:TYR:HA	1:D:4251:PHE:HZ	1.33	0.91
1:B:2303:PRO:HA	1:C:3301:PHE:HD2	1.34	0.90
1:A:1304:LEU:HB3	1:E:5306:PHE:CE1	2.08	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1301:PHE:CD2	1:E:5303:PRO:HA	2.09	0.87
1:A:1301:PHE:HD2	1:E:5303:PRO:HA	1.42	0.85
1:D:4303:PRO:HA	1:E:5301:PHE:CD2	2.12	0.84
1:D:4306:PHE:CE1	1:E:5304:LEU:HB3	2.11	0.83
1:B:2240:PRO:HB2	1:B:2241:PRO:CD	2.12	0.79
1:D:4303:PRO:HA	1:E:5301:PHE:HD2	1.45	0.79
1:C:3240:PRO:HB2	1:C:3241:PRO:CD	2.12	0.78
1:A:1012:LEU:H	1:A:1013:PRO:CD	1.97	0.78
1:B:2012:LEU:N	1:B:2013:PRO:HD3	1.99	0.77
1:E:5012:LEU:N	1:E:5013:PRO:HD3	1.99	0.77
1:D:4240:PRO:HB2	1:D:4241:PRO:CD	2.12	0.77
1:E:5240:PRO:HB2	1:E:5241:PRO:CD	2.12	0.77
1:D:4302:MET:H	1:D:4303:PRO:HD2	1.50	0.77
1:B:2302:MET:H	1:B:2303:PRO:HD2	1.49	0.77
1:A:1302:MET:H	1:A:1303:PRO:HD2	1.50	0.77
1:D:4012:LEU:H	1:D:4013:PRO:CD	1.97	0.77
1:D:4012:LEU:N	1:D:4013:PRO:HD3	1.99	0.77
1:C:3012:LEU:H	1:C:3013:PRO:CD	1.98	0.76
1:A:1240:PRO:HB2	1:A:1241:PRO:CD	2.12	0.76
1:C:3302:MET:H	1:C:3303:PRO:HD2	1.50	0.76
1:B:2012:LEU:H	1:B:2013:PRO:CD	1.97	0.76
1:A:1260:GLN:HG3	1:B:2096:ARG:HG2	1.68	0.75
1:A:1306:PHE:CE1	1:B:2304:LEU:HB3	2.22	0.75
1:E:5302:MET:H	1:E:5303:PRO:HD2	1.50	0.75
1:A:1012:LEU:N	1:A:1013:PRO:HD3	1.99	0.74
1:D:4202:ARG:H	1:D:4203:PRO:HD3	1.53	0.74
1:E:5012:LEU:H	1:E:5013:PRO:CD	1.97	0.74
1:C:3202:ARG:H	1:C:3203:PRO:HD3	1.53	0.73
1:E:5202:ARG:H	1:E:5203:PRO:HD3	1.53	0.72
1:C:3303:PRO:HA	1:D:4301:PHE:CD2	2.25	0.72
1:A:1202:ARG:H	1:A:1203:PRO:HD3	1.53	0.72
1:B:2202:ARG:H	1:B:2203:PRO:HD3	1.53	0.72
1:B:2302:MET:N	1:B:2303:PRO:HD2	2.05	0.72
1:A:1303:PRO:HA	1:B:2301:PHE:HD2	1.54	0.71
1:E:5302:MET:N	1:E:5303:PRO:HD2	2.05	0.71
1:A:1302:MET:N	1:A:1303:PRO:HD2	2.06	0.71
1:C:3012:LEU:N	1:C:3013:PRO:HD3	1.99	0.71
1:C:3225:ILE:HG22	1:C:3262:ALA:HB2	1.71	0.71
1:D:4302:MET:N	1:D:4303:PRO:HD2	2.06	0.71
1:A:1303:PRO:HA	1:B:2301:PHE:CD2	2.25	0.70
1:B:2299:THR:HG23	1:C:3297:ILE:HD13	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3306:PHE:CE1	1:D:4304:LEU:HB3	2.26	0.70
1:C:3302:MET:N	1:C:3303:PRO:HD2	2.06	0.69
1:E:5012:LEU:N	1:E:5013:PRO:CD	2.55	0.69
1:B:2012:LEU:N	1:B:2013:PRO:CD	2.55	0.68
1:C:3012:LEU:N	1:C:3013:PRO:CD	2.56	0.68
1:C:3303:PRO:HA	1:D:4301:PHE:HD2	1.57	0.68
1:B:2303:PRO:HA	1:C:3301:PHE:CE2	2.29	0.67
1:D:4012:LEU:N	1:D:4013:PRO:CD	2.55	0.66
1:B:2295:THR:HA	1:C:3294:LEU:HD13	1.77	0.66
1:A:1202:ARG:N	1:A:1203:PRO:HD3	2.11	0.65
1:D:4202:ARG:N	1:D:4203:PRO:HD3	2.11	0.65
1:D:4225:ILE:HD13	1:D:4265:VAL:HG21	1.79	0.65
1:A:1012:LEU:N	1:A:1013:PRO:CD	2.55	0.65
1:C:3202:ARG:N	1:C:3203:PRO:HD3	2.11	0.65
1:A:1225:ILE:HG22	1:A:1262:ALA:HB2	1.79	0.64
1:B:2202:ARG:N	1:B:2203:PRO:HD3	2.11	0.64
1:E:5202:ARG:N	1:E:5203:PRO:HD3	2.11	0.64
1:C:3225:ILE:HD13	1:C:3265:VAL:HG21	1.80	0.64
1:B:2225:ILE:HG22	1:B:2262:ALA:HB2	1.80	0.63
1:D:4221:LEU:HG	1:D:4225:ILE:HD11	1.80	0.63
1:A:1287:THR:HG22	1:A:1287:THR:O	1.98	0.63
1:C:3287:THR:HG22	1:C:3287:THR:O	1.98	0.63
1:B:2221:LEU:HG	1:B:2225:ILE:HD11	1.81	0.63
1:E:5287:THR:HG22	1:E:5287:THR:O	1.99	0.63
1:C:3221:LEU:HG	1:C:3225:ILE:HD11	1.80	0.63
1:D:4287:THR:HG22	1:D:4287:THR:O	1.98	0.63
1:B:2039:PHE:CZ	1:B:2155:ARG:HA	2.34	0.62
1:D:4085:LEU:H	1:D:4085:LEU:HD23	1.64	0.62
1:C:3085:LEU:H	1:C:3085:LEU:HD23	1.64	0.62
1:E:5171:TYR:OH	1:E:5235:LEU:HG	1.99	0.62
1:E:5221:LEU:HG	1:E:5225:ILE:HD11	1.80	0.62
1:A:1221:LEU:HG	1:A:1225:ILE:HD11	1.80	0.62
1:D:4171:TYR:OH	1:D:4235:LEU:HG	1.99	0.62
1:C:3171:TYR:O	1:C:3250:TYR:CE2	2.53	0.62
1:B:2287:THR:HG22	1:B:2287:THR:O	1.99	0.62
1:C:3171:TYR:OH	1:C:3235:LEU:HG	2.00	0.62
1:B:2303:PRO:CA	1:C:3301:PHE:CD2	2.80	0.62
1:A:1085:LEU:H	1:A:1085:LEU:HD23	1.64	0.62
1:A:1218:LEU:HD21	1:A:1268:PHE:HB3	1.82	0.62
1:B:2171:TYR:OH	1:B:2235:LEU:HG	1.99	0.62
1:C:3218:LEU:HD21	1:C:3268:PHE:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4067:ILE:HG22	1:D:4091:LEU:HD23	1.81	0.61
1:D:4236:TYR:HA	1:D:4251:PHE:CZ	2.25	0.61
1:C:3039:PHE:CZ	1:C:3155:ARG:HA	2.35	0.61
1:C:3171:TYR:CD1	1:C:3251:PHE:HB3	2.35	0.61
1:D:4171:TYR:O	1:D:4250:TYR:CE2	2.53	0.61
1:D:4171:TYR:CD1	1:D:4251:PHE:HB3	2.35	0.61
1:E:5171:TYR:CD1	1:E:5251:PHE:HB3	2.36	0.61
1:D:4295:THR:HA	1:E:5294:LEU:HD13	1.80	0.61
1:E:5171:TYR:O	1:E:5250:TYR:CE2	2.53	0.61
1:C:3232:LEU:HB3	1:C:3255:TYR:HB2	1.82	0.61
1:E:5085:LEU:H	1:E:5085:LEU:HD23	1.65	0.61
1:A:1171:TYR:OH	1:A:1235:LEU:HG	2.00	0.60
1:A:1297:ILE:HD13	1:E:5299:THR:HG23	1.83	0.60
1:B:2171:TYR:CD1	1:B:2251:PHE:HB3	2.35	0.60
1:E:5067:ILE:HG22	1:E:5091:LEU:HD23	1.83	0.60
1:A:1171:TYR:O	1:A:1250:TYR:CE2	2.54	0.60
1:D:4225:ILE:HG22	1:D:4262:ALA:HB2	1.83	0.60
1:A:1171:TYR:CD1	1:A:1251:PHE:HB3	2.36	0.60
1:B:2171:TYR:O	1:B:2250:TYR:CE2	2.53	0.60
1:B:2138:MET:HE3	1:B:2140:GLN:HE21	1.67	0.60
1:B:2085:LEU:H	1:B:2085:LEU:HD23	1.65	0.60
1:E:5218:LEU:HD21	1:E:5268:PHE:HB3	1.83	0.60
1:D:4051:LEU:N	1:D:4052:PRO:HD2	2.17	0.60
1:D:4138:MET:HE3	1:D:4140:GLN:HE21	1.66	0.59
1:E:5117:LYS:O	1:E:5118:ASN:HB2	2.00	0.59
1:A:1138:MET:HE3	1:A:1140:GLN:HE21	1.66	0.59
1:E:5061:TRP:HB2	1:E:5169:LEU:HD21	1.84	0.59
1:B:2299:THR:CG2	1:C:3297:ILE:HD13	2.32	0.59
1:B:2315:PHE:CZ	1:C:3327:TYR:HA	2.37	0.59
1:A:1225:ILE:HD13	1:A:1265:VAL:HG21	1.84	0.59
1:B:2236:TYR:HA	1:B:2251:PHE:CZ	2.25	0.59
1:C:3067:ILE:HG22	1:C:3091:LEU:HD23	1.84	0.59
1:E:5051:LEU:N	1:E:5052:PRO:HD2	2.18	0.59
1:B:2067:ILE:HG22	1:B:2091:LEU:HD23	1.85	0.59
1:C:3061:TRP:HB2	1:C:3169:LEU:HD21	1.83	0.59
1:C:3138:MET:HE3	1:C:3140:GLN:HE21	1.67	0.59
1:D:4218:LEU:HD21	1:D:4268:PHE:HB3	1.84	0.59
1:E:5138:MET:HE3	1:E:5140:GLN:HE21	1.67	0.59
1:D:4027:PHE:CZ	1:D:4072:VAL:HG21	2.38	0.59
1:E:5027:PHE:CZ	1:E:5072:VAL:HG21	2.38	0.59
1:A:1067:ILE:HG22	1:A:1091:LEU:HD23	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2051:LEU:N	1:B:2052:PRO:HD2	2.17	0.58
1:C:3051:LEU:N	1:C:3052:PRO:HD2	2.17	0.58
1:B:2225:ILE:HD13	1:B:2265:VAL:HG21	1.84	0.58
1:B:2027:PHE:CZ	1:B:2072:VAL:HG21	2.38	0.58
1:A:1051:LEU:N	1:A:1052:PRO:HD2	2.17	0.58
1:A:1150:VAL:HG11	1:A:1173:LEU:HD23	1.85	0.58
1:A:1027:PHE:CZ	1:A:1072:VAL:HG21	2.38	0.58
1:B:2150:VAL:HG11	1:B:2173:LEU:HD23	1.86	0.57
1:B:2218:LEU:HD21	1:B:2268:PHE:HB3	1.86	0.57
1:D:4150:VAL:HG11	1:D:4173:LEU:HD23	1.86	0.57
1:C:3027:PHE:CZ	1:C:3072:VAL:HG21	2.38	0.57
1:A:1117:LYS:O	1:A:1118:ASN:HB2	2.04	0.57
1:A:1236:TYR:HA	1:A:1251:PHE:CZ	2.25	0.57
1:B:2117:LYS:O	1:B:2118:ASN:HB2	2.04	0.57
1:E:5150:VAL:HG11	1:E:5173:LEU:HD23	1.86	0.57
1:D:4203:PRO:HG2	1:D:4286:LYS:HE3	1.87	0.57
1:C:3117:LYS:O	1:C:3118:ASN:HB2	2.04	0.56
1:D:4315:PHE:CZ	1:E:5327:TYR:HA	2.41	0.56
1:A:1196:GLU:O	1:A:1200:LEU:HD22	2.06	0.56
1:C:3150:VAL:HG11	1:C:3173:LEU:HD23	1.85	0.56
1:C:3225:ILE:CG2	1:C:3262:ALA:HB2	2.35	0.56
1:D:4218:LEU:HB3	1:D:4269:ARG:HG3	1.87	0.56
1:E:5039:PHE:CZ	1:E:5155:ARG:HA	2.40	0.56
1:E:5225:ILE:HG22	1:E:5262:ALA:HB2	1.87	0.56
1:E:5236:TYR:HA	1:E:5251:PHE:CZ	2.25	0.56
1:A:1294:LEU:HD13	1:E:5295:THR:HA	1.85	0.56
1:D:4299:THR:HG23	1:E:5297:ILE:HD13	1.88	0.56
1:E:5100:GLU:HB2	1:E:5107:PHE:HB3	1.88	0.56
1:B:2077:GLY:HA2	1:B:2082:ILE:HD12	1.88	0.56
1:C:3196:GLU:O	1:C:3200:LEU:HD22	2.06	0.56
1:E:5077:GLY:HA2	1:E:5082:ILE:HD12	1.88	0.56
1:E:5196:GLU:O	1:E:5200:LEU:HD22	2.06	0.56
1:A:1099:VAL:HG21	1:A:1235:LEU:HD13	1.88	0.55
1:C:3077:GLY:HA2	1:C:3082:ILE:HD12	1.88	0.55
1:C:3099:VAL:HG21	1:C:3235:LEU:HD13	1.88	0.55
1:D:4117:LYS:O	1:D:4118:ASN:HB2	2.05	0.55
1:E:5302:MET:N	1:E:5303:PRO:CD	2.69	0.55
1:B:2100:GLU:HB2	1:B:2107:PHE:HB3	1.89	0.55
1:D:4100:GLU:HB2	1:D:4107:PHE:HB3	1.88	0.55
1:B:2165:ARG:HD3	1:B:2243:ILE:HD11	1.89	0.55
1:C:3302:MET:N	1:C:3303:PRO:CD	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4061:TRP:HB2	1:D:4169:LEU:HD21	1.87	0.55
1:D:4302:MET:N	1:D:4303:PRO:CD	2.69	0.55
1:A:1061:TRP:HB2	1:A:1169:LEU:HD21	1.88	0.55
1:A:1077:GLY:HA2	1:A:1082:ILE:HD12	1.88	0.55
1:A:1255:TYR:O	1:A:1258:THR:HG22	2.07	0.55
1:A:1302:MET:N	1:A:1303:PRO:CD	2.69	0.55
1:B:2196:GLU:O	1:B:2200:LEU:HD22	2.06	0.55
1:C:3165:ARG:HD3	1:C:3243:ILE:HD11	1.89	0.55
1:E:5099:VAL:HG21	1:E:5235:LEU:HD13	1.88	0.55
1:B:2236:TYR:CA	1:B:2251:PHE:HZ	2.15	0.55
1:D:4099:VAL:HG21	1:D:4235:LEU:HD13	1.88	0.55
1:E:5225:ILE:HD13	1:E:5265:VAL:HG21	1.88	0.55
1:B:2087:LEU:HA	1:B:2090:ILE:HD12	1.89	0.55
1:C:3327:TYR:HB3	1:C:3328:PRO:HD3	1.89	0.55
1:D:4196:GLU:O	1:D:4200:LEU:HD22	2.06	0.55
1:D:4165:ARG:HD3	1:D:4243:ILE:HD11	1.89	0.54
1:D:4327:TYR:HB3	1:D:4328:PRO:HD3	1.89	0.54
1:B:2067:ILE:HG13	1:B:2140:GLN:O	2.07	0.54
1:A:1039:PHE:CZ	1:A:1155:ARG:HA	2.41	0.54
1:A:1100:GLU:HB2	1:A:1107:PHE:HB3	1.88	0.54
1:E:5165:ARG:HD3	1:E:5243:ILE:HD11	1.89	0.54
1:E:5255:TYR:O	1:E:5258:THR:HG22	2.07	0.54
1:A:1301:PHE:CE2	1:E:5303:PRO:HA	2.42	0.54
1:B:2099:VAL:HG21	1:B:2235:LEU:HD13	1.89	0.54
1:B:2255:TYR:O	1:B:2258:THR:HG22	2.08	0.54
1:B:2302:MET:N	1:B:2303:PRO:CD	2.69	0.54
1:E:5327:TYR:HB3	1:E:5328:PRO:HD3	1.89	0.54
1:A:1067:ILE:HG13	1:A:1140:GLN:O	2.07	0.54
1:C:3100:GLU:HB2	1:C:3107:PHE:HB3	1.88	0.54
1:B:2240:PRO:CB	1:B:2241:PRO:HD3	2.23	0.54
1:C:3067:ILE:HG13	1:C:3140:GLN:O	2.08	0.54
1:C:3236:TYR:HA	1:C:3251:PHE:CZ	2.25	0.54
1:D:4077:GLY:HA2	1:D:4082:ILE:HD12	1.88	0.54
1:A:1165:ARG:HD3	1:A:1243:ILE:HD11	1.89	0.53
1:D:4255:TYR:O	1:D:4258:THR:HG22	2.08	0.53
1:A:1295:THR:HA	1:B:2294:LEU:HD13	1.90	0.53
1:A:1327:TYR:HB3	1:A:1328:PRO:HD3	1.89	0.53
1:B:2327:TYR:HB3	1:B:2328:PRO:HD3	1.89	0.53
1:B:2061:TRP:HB2	1:B:2169:LEU:HD21	1.90	0.53
1:C:3255:TYR:O	1:C:3258:THR:HG22	2.08	0.53
1:C:3203:PRO:HG2	1:C:3286:LYS:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1232:LEU:HB3	1:A:1255:TYR:HB2	1.90	0.53
1:A:1202:ARG:O	1:A:1204:GLU:N	2.42	0.53
1:C:3240:PRO:CB	1:C:3241:PRO:HD3	2.23	0.53
1:D:4039:PHE:CZ	1:D:4155:ARG:HA	2.43	0.53
1:A:1240:PRO:CB	1:A:1241:PRO:HD3	2.23	0.52
1:D:4202:ARG:O	1:D:4204:GLU:N	2.42	0.52
1:E:5067:ILE:HG13	1:E:5140:GLN:O	2.09	0.52
1:A:1087:LEU:HA	1:A:1090:ILE:HD12	1.91	0.52
1:E:5202:ARG:O	1:E:5204:GLU:N	2.42	0.52
1:A:1299:THR:HG23	1:B:2297:ILE:HD13	1.91	0.52
1:B:2202:ARG:O	1:B:2204:GLU:N	2.42	0.52
1:C:3202:ARG:O	1:C:3204:GLU:N	2.42	0.52
1:D:4240:PRO:CB	1:D:4241:PRO:HD3	2.23	0.52
1:B:2218:LEU:HB3	1:B:2269:ARG:HG3	1.91	0.52
1:D:4303:PRO:HA	1:E:5301:PHE:CE2	2.44	0.52
1:B:2303:PRO:HB3	1:C:3301:PHE:CE2	2.44	0.52
1:E:5236:TYR:CA	1:E:5251:PHE:HZ	2.15	0.51
1:C:3260:GLN:HG3	1:D:4096:ARG:HG2	1.92	0.51
1:C:3295:THR:HA	1:D:4294:LEU:HD13	1.91	0.51
1:B:2295:THR:OG1	1:C:3293:VAL:HG12	2.10	0.51
1:D:4134:ASN:HA	1:D:4166:ALA:CB	2.41	0.51
1:B:2203:PRO:HG2	1:B:2286:LYS:HE3	1.91	0.51
1:D:4232:LEU:CD2	1:D:4254:VAL:HG12	2.41	0.51
1:C:3134:ASN:HA	1:C:3166:ALA:CB	2.41	0.51
1:C:3299:THR:HG23	1:D:4297:ILE:HD13	1.93	0.51
1:B:2029:ILE:HG12	1:B:2064:ILE:HG23	1.94	0.50
1:C:3087:LEU:HA	1:C:3090:ILE:HD12	1.94	0.50
1:A:1029:ILE:HG12	1:A:1064:ILE:HG23	1.94	0.50
1:A:1302:MET:H	1:A:1303:PRO:CD	2.23	0.50
1:E:5087:LEU:HA	1:E:5090:ILE:HD12	1.93	0.50
1:E:5134:ASN:HA	1:E:5166:ALA:CB	2.41	0.50
1:D:4029:ILE:HG12	1:D:4064:ILE:HG23	1.93	0.50
1:D:4087:LEU:HA	1:D:4090:ILE:HD12	1.93	0.50
1:A:1134:ASN:HA	1:A:1166:ALA:CB	2.41	0.50
1:A:1327:TYR:HA	1:E:5315:PHE:CZ	2.47	0.50
1:B:2134:ASN:HA	1:B:2166:ALA:CB	2.41	0.50
1:D:4067:ILE:HG13	1:D:4140:GLN:O	2.10	0.50
1:A:1290:VAL:HG12	1:E:5291:MET:CE	2.42	0.50
1:D:4240:PRO:CB	1:D:4241:PRO:CD	2.88	0.50
1:B:2009:LYS:HG3	1:B:2010:LYS:H	1.77	0.50
1:E:5009:LYS:HG3	1:E:5010:LYS:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5029:ILE:HG12	1:E:5064:ILE:HG23	1.94	0.50
1:D:4009:LYS:HG3	1:D:4010:LYS:H	1.77	0.49
1:E:5302:MET:H	1:E:5303:PRO:CD	2.23	0.49
1:A:1225:ILE:CG2	1:A:1262:ALA:HB2	2.42	0.49
1:C:3229:ARG:HE	1:C:3259:ILE:HG12	1.77	0.49
1:C:3029:ILE:HG12	1:C:3064:ILE:HG23	1.93	0.49
1:D:4236:TYR:CA	1:D:4251:PHE:HZ	2.15	0.49
1:A:1297:ILE:HG22	1:A:1297:ILE:O	2.13	0.49
1:A:1009:LYS:HG3	1:A:1010:LYS:H	1.77	0.49
1:D:4302:MET:H	1:D:4303:PRO:CD	2.23	0.49
1:A:1218:LEU:HB3	1:A:1269:ARG:HG3	1.94	0.49
1:B:2292:LYS:HD3	1:B:2348:LYS:HG2	1.95	0.49
1:C:3291:MET:CE	1:D:4290:VAL:HG12	2.43	0.49
1:A:1278:VAL:HA	1:B:2276:LEU:HD21	1.94	0.48
1:D:4239:VAL:HB	1:D:4242:LEU:HD23	1.96	0.48
1:D:4292:LYS:HD3	1:D:4348:LYS:HG2	1.95	0.48
1:A:1292:LYS:HD3	1:A:1348:LYS:HG2	1.95	0.48
1:E:5297:ILE:HG22	1:E:5297:ILE:O	2.13	0.48
1:B:2297:ILE:HG22	1:B:2297:ILE:O	2.13	0.48
1:C:3218:LEU:HB3	1:C:3269:ARG:HG3	1.94	0.48
1:C:3239:VAL:HB	1:C:3242:LEU:HD23	1.95	0.48
1:D:4182:PHE:HD2	1:E:5010:LYS:HD2	1.79	0.48
1:D:4225:ILE:HG21	1:D:4261:ILE:HG22	1.96	0.48
1:E:5292:LYS:HD3	1:E:5348:LYS:HG2	1.95	0.48
1:C:3297:ILE:HG22	1:C:3297:ILE:O	2.13	0.48
1:D:4064:ILE:HD12	1:D:4139:PHE:CE1	2.48	0.48
1:C:3009:LYS:HG3	1:C:3010:LYS:H	1.77	0.48
1:C:3292:LYS:HD3	1:C:3348:LYS:HG2	1.95	0.48
1:D:4339:VAL:HA	1:D:4342:VAL:HG12	1.95	0.48
1:A:1239:VAL:HB	1:A:1242:LEU:HD23	1.95	0.47
1:C:3236:TYR:CA	1:C:3251:PHE:HZ	2.15	0.47
1:D:4296:ILE:HA	1:D:4345:PHE:HE2	1.79	0.47
1:A:1337:ILE:C	1:A:1339:VAL:H	2.22	0.47
1:A:1339:VAL:HA	1:A:1342:VAL:HG12	1.96	0.47
1:B:2337:ILE:C	1:B:2339:VAL:H	2.22	0.47
1:B:2339:VAL:HA	1:B:2342:VAL:HG12	1.95	0.47
1:A:1296:ILE:HA	1:A:1345:PHE:HE2	1.80	0.47
1:D:4297:ILE:HG22	1:D:4297:ILE:O	2.13	0.47
1:E:5064:ILE:HD12	1:E:5139:PHE:CE1	2.49	0.47
1:B:2056:SER:C	1:B:2058:THR:H	2.22	0.47
1:A:1290:VAL:HG12	1:E:5291:MET:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3337:ILE:C	1:C:3339:VAL:H	2.22	0.47
1:A:1056:SER:C	1:A:1058:THR:H	2.22	0.47
1:B:2239:VAL:HB	1:B:2242:LEU:HD23	1.95	0.47
1:B:2306:PHE:CZ	1:C:3304:LEU:HD23	2.50	0.47
1:C:3056:SER:C	1:C:3058:THR:H	2.22	0.47
1:B:2291:MET:HE3	1:C:3290:VAL:HG12	1.97	0.47
1:C:3296:ILE:HA	1:C:3345:PHE:HE2	1.79	0.47
1:C:3339:VAL:HA	1:C:3342:VAL:HG12	1.95	0.47
1:D:4229:ARG:HE	1:D:4259:ILE:HG12	1.80	0.47
1:D:4337:ILE:C	1:D:4339:VAL:H	2.22	0.47
1:E:5337:ILE:C	1:E:5339:VAL:H	2.22	0.47
1:E:5339:VAL:HA	1:E:5342:VAL:HG12	1.95	0.47
1:A:1236:TYR:CA	1:A:1251:PHE:HZ	2.15	0.47
1:E:5239:VAL:HB	1:E:5242:LEU:HD23	1.95	0.47
1:B:2171:TYR:CD1	1:B:2247:THR:HG22	2.50	0.47
1:E:5194:VAL:C	1:E:5196:GLU:H	2.23	0.47
1:A:1110:LEU:HD13	1:A:1177:LEU:HD22	1.96	0.46
1:E:5171:TYR:CD1	1:E:5247:THR:HG22	2.50	0.46
1:E:5240:PRO:CB	1:E:5241:PRO:HD3	2.23	0.46
1:A:1064:ILE:HD12	1:A:1139:PHE:CE1	2.51	0.46
1:A:1096:ARG:HG2	1:E:5260:GLN:HG3	1.97	0.46
1:A:1203:PRO:HG2	1:A:1286:LYS:HE3	1.98	0.46
1:E:5296:ILE:HA	1:E:5345:PHE:HE2	1.80	0.46
1:A:1171:TYR:CD1	1:A:1247:THR:HG22	2.50	0.46
1:B:2061:TRP:CZ3	1:B:2151:ARG:HB3	2.50	0.46
1:A:1194:VAL:C	1:A:1196:GLU:H	2.23	0.46
1:A:1229:ARG:HE	1:A:1259:ILE:HG12	1.80	0.46
1:A:1291:MET:CE	1:B:2290:VAL:HG12	2.45	0.46
1:B:2211:THR:HG21	1:B:2276:LEU:HD13	1.96	0.46
1:D:4171:TYR:CD1	1:D:4247:THR:HG22	2.50	0.46
1:B:2296:ILE:HA	1:B:2345:PHE:HE2	1.80	0.46
1:B:2225:ILE:CG2	1:B:2262:ALA:HB2	2.44	0.46
1:B:2313:MET:SD	1:C:3311:TYR:HB2	2.56	0.46
1:D:4110:LEU:HD13	1:D:4177:LEU:HD22	1.98	0.46
1:E:5056:SER:C	1:E:5058:THR:H	2.22	0.46
1:D:4056:SER:C	1:D:4058:THR:H	2.22	0.46
1:C:3291:MET:HE3	1:D:4290:VAL:HG12	1.98	0.46
1:B:2110:LEU:HD13	1:B:2177:LEU:HD22	1.97	0.46
1:B:2291:MET:CE	1:C:3290:VAL:HG12	2.46	0.46
1:C:3110:LEU:HD13	1:C:3177:LEU:HD22	1.97	0.46
1:C:3299:THR:HG22	1:C:3299:THR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4194:VAL:C	1:D:4196:GLU:H	2.24	0.46
1:B:2229:ARG:HE	1:B:2259:ILE:HG12	1.81	0.45
1:B:2299:THR:HG22	1:B:2299:THR:O	2.16	0.45
1:E:5299:THR:HG22	1:E:5299:THR:O	2.16	0.45
1:C:3287:THR:O	1:C:3287:THR:CG2	2.65	0.45
1:A:1299:THR:HG22	1:A:1299:THR:O	2.16	0.45
1:B:2064:ILE:HD12	1:B:2139:PHE:CE1	2.51	0.45
1:C:3171:TYR:CD1	1:C:3247:THR:HG22	2.50	0.45
1:D:4064:ILE:HD11	1:D:4137:LEU:HD21	1.99	0.45
1:B:2295:THR:OG1	1:C:3294:LEU:HB2	2.17	0.45
1:E:5218:LEU:HB3	1:E:5269:ARG:HG3	1.99	0.45
1:A:1287:THR:O	1:A:1287:THR:CG2	2.65	0.45
1:E:5229:ARG:HE	1:E:5259:ILE:HG12	1.82	0.45
1:A:1291:MET:HE3	1:B:2290:VAL:HG12	1.99	0.45
1:B:2232:LEU:HB3	1:B:2255:TYR:HB2	1.98	0.45
1:C:3194:VAL:C	1:C:3196:GLU:H	2.23	0.45
1:D:4299:THR:HG22	1:D:4299:THR:O	2.16	0.45
1:A:1286:LYS:C	1:A:1288:ASN:H	2.25	0.45
1:B:2039:PHE:CE1	1:B:2155:ARG:HA	2.51	0.45
1:C:3064:ILE:HD12	1:C:3139:PHE:CE1	2.52	0.45
1:E:5064:ILE:HD11	1:E:5137:LEU:HD21	1.99	0.45
1:A:1238:ASP:HB3	1:A:1239:VAL:H	1.57	0.45
1:A:1311:TYR:HB2	1:E:5313:MET:SD	2.57	0.45
1:B:2250:TYR:O	1:B:2253:ASP:HB3	2.16	0.45
1:B:2194:VAL:C	1:B:2196:GLU:H	2.24	0.44
1:B:2238:ASP:HB3	1:B:2239:VAL:H	1.57	0.44
1:D:4287:THR:O	1:D:4287:THR:CG2	2.65	0.44
1:E:5110:LEU:HD13	1:E:5177:LEU:HD22	1.97	0.44
1:A:1153:ARG:NE	1:B:2014:PRO:HB3	2.32	0.44
1:C:3235:LEU:O	1:C:3251:PHE:CZ	2.71	0.44
1:D:4202:ARG:H	1:D:4203:PRO:CD	2.28	0.44
1:D:4286:LYS:C	1:D:4288:ASN:H	2.26	0.44
1:D:4291:MET:CE	1:E:5290:VAL:HG12	2.47	0.44
1:E:5240:PRO:CB	1:E:5241:PRO:CD	2.89	0.44
1:A:1202:ARG:H	1:A:1203:PRO:CD	2.28	0.44
1:C:3206:GLU:HB2	1:C:3209:GLN:HG2	2.00	0.44
1:C:3228:LEU:HD23	1:C:3258:THR:OG1	2.18	0.44
1:C:3185:LEU:HD13	1:C:3264:THR:HG21	1.99	0.44
1:D:4202:ARG:N	1:D:4203:PRO:CD	2.81	0.44
1:D:4206:GLU:HB2	1:D:4209:GLN:HG2	2.00	0.44
1:A:1293:VAL:HG12	1:E:5295:THR:OG1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1196:GLU:OE1	1:B:2216:ARG:NH2	2.51	0.44
1:A:1235:LEU:O	1:A:1251:PHE:CZ	2.71	0.44
1:B:2296:ILE:HG12	1:B:2345:PHE:CE2	2.53	0.44
1:B:2286:LYS:C	1:B:2288:ASN:H	2.26	0.44
1:D:4232:LEU:HB3	1:D:4255:TYR:HB2	1.99	0.44
1:A:1297:ILE:HD13	1:E:5299:THR:CG2	2.48	0.43
1:B:2064:ILE:HD11	1:B:2137:LEU:HD21	2.00	0.43
1:D:4235:LEU:O	1:D:4251:PHE:CZ	2.71	0.43
1:A:1206:GLU:HB2	1:A:1209:GLN:HG2	1.99	0.43
1:E:5286:LYS:C	1:E:5288:ASN:H	2.25	0.43
1:A:1099:VAL:HG23	1:A:1108:ILE:HG12	2.00	0.43
1:B:2235:LEU:O	1:B:2251:PHE:CZ	2.71	0.43
1:D:4232:LEU:HD21	1:D:4254:VAL:HG12	1.98	0.43
1:B:2303:PRO:CA	1:C:3301:PHE:CE2	2.98	0.43
1:D:4313:MET:SD	1:E:5311:TYR:HB2	2.59	0.43
1:B:2206:GLU:HB2	1:B:2209:GLN:HG2	1.99	0.43
1:C:3148:ASP:N	1:C:3149:PRO:HD2	2.34	0.43
1:C:3296:ILE:HG12	1:C:3345:PHE:CE2	2.53	0.43
1:A:1148:ASP:N	1:A:1149:PRO:HD2	2.34	0.43
1:A:1149:PRO:O	1:A:1153:ARG:HG3	2.18	0.43
1:A:1304:LEU:HB3	1:E:5306:PHE:HE1	1.77	0.43
1:D:4149:PRO:O	1:D:4153:ARG:HG3	2.19	0.43
1:E:5148:ASP:N	1:E:5149:PRO:HD2	2.33	0.43
1:E:5156:TYR:O	1:E:5157:ASN:C	2.61	0.43
1:E:5206:GLU:HB2	1:E:5209:GLN:HG2	2.00	0.43
1:E:5235:LEU:O	1:E:5251:PHE:CZ	2.71	0.43
1:B:2287:THR:O	1:B:2287:THR:CG2	2.65	0.43
1:D:4295:THR:OG1	1:E:5294:LEU:HB2	2.19	0.43
1:B:2303:PRO:CA	1:C:3301:PHE:HD2	2.15	0.43
1:C:3149:PRO:O	1:C:3153:ARG:HG3	2.19	0.43
1:C:3202:ARG:H	1:C:3203:PRO:CD	2.28	0.43
1:A:1061:TRP:CZ3	1:A:1151:ARG:HB3	2.54	0.43
1:C:3099:VAL:HG23	1:C:3108:ILE:HG12	2.01	0.43
1:C:3224:THR:O	1:C:3224:THR:CG2	2.67	0.43
1:D:4099:VAL:HG23	1:D:4108:ILE:HG12	2.00	0.43
1:E:5149:PRO:O	1:E:5153:ARG:HG3	2.19	0.43
1:E:5203:PRO:HG2	1:E:5286:LYS:HE3	2.00	0.43
1:B:2148:ASP:N	1:B:2149:PRO:HD2	2.33	0.42
1:B:2202:ARG:N	1:B:2203:PRO:CD	2.81	0.42
1:D:4148:ASP:N	1:D:4149:PRO:HD2	2.34	0.42
1:D:4156:TYR:O	1:D:4157:ASN:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4185:LEU:HD13	1:D:4264:THR:HG21	2.00	0.42
1:D:4211:THR:HG21	1:D:4276:LEU:HD13	2.00	0.42
1:D:4296:ILE:HG12	1:D:4345:PHE:CE2	2.54	0.42
1:A:1296:ILE:HG12	1:A:1345:PHE:CE2	2.54	0.42
1:E:5099:VAL:HG23	1:E:5108:ILE:HG12	2.00	0.42
1:E:5202:ARG:N	1:E:5203:PRO:CD	2.81	0.42
1:E:5296:ILE:HG12	1:E:5345:PHE:CE2	2.54	0.42
1:A:1156:TYR:O	1:A:1157:ASN:C	2.61	0.42
1:A:1224:THR:O	1:A:1224:THR:CG2	2.67	0.42
1:B:2099:VAL:HG23	1:B:2108:ILE:HG12	2.00	0.42
1:B:2224:THR:CG2	1:B:2224:THR:O	2.67	0.42
1:C:3240:PRO:CB	1:C:3241:PRO:CD	2.89	0.42
1:C:3286:LYS:C	1:C:3288:ASN:H	2.26	0.42
1:E:5287:THR:O	1:E:5287:THR:CG2	2.65	0.42
1:A:1202:ARG:N	1:A:1203:PRO:CD	2.81	0.42
1:B:2156:TYR:O	1:B:2157:ASN:C	2.61	0.42
1:C:3039:PHE:CE1	1:C:3155:ARG:HA	2.54	0.42
1:C:3156:TYR:O	1:C:3157:ASN:C	2.61	0.42
1:D:4242:LEU:O	1:D:4247:THR:HB	2.20	0.42
1:E:5238:ASP:HB3	1:E:5239:VAL:H	1.56	0.42
1:B:2149:PRO:O	1:B:2153:ARG:HG3	2.19	0.42
1:E:5242:LEU:O	1:E:5247:THR:HB	2.19	0.42
1:B:2242:LEU:O	1:B:2247:THR:HB	2.20	0.42
1:C:3064:ILE:HD11	1:C:3137:LEU:HD21	2.00	0.42
1:D:4238:ASP:HB3	1:D:4239:VAL:H	1.56	0.42
1:E:5232:LEU:HB3	1:E:5255:TYR:HB2	2.01	0.42
1:A:1064:ILE:HD11	1:A:1137:LEU:HD21	2.01	0.42
1:A:1301:PHE:CD2	1:E:5303:PRO:CA	2.93	0.42
1:D:4224:THR:O	1:D:4224:THR:CG2	2.67	0.42
1:D:4291:MET:HE3	1:E:5290:VAL:HG12	2.01	0.42
1:C:3346:LYS:HD2	1:C:3346:LYS:HA	1.91	0.41
1:E:5224:THR:O	1:E:5224:THR:CG2	2.67	0.41
1:B:2040:ARG:CZ	1:B:2040:ARG:HB2	2.47	0.41
1:C:3238:ASP:HB3	1:C:3239:VAL:H	1.56	0.41
1:C:3243:ILE:O	1:C:3244:GLU:C	2.63	0.41
1:D:4251:PHE:HA	1:D:4254:VAL:HG23	2.02	0.41
1:D:4303:PRO:CA	1:E:5301:PHE:CD2	2.95	0.41
1:B:2013:PRO:CB	1:B:2014:PRO:CD	2.98	0.41
1:D:4160:ILE:HG23	1:D:4163:LYS:HD2	2.03	0.41
1:C:3242:LEU:O	1:C:3247:THR:HB	2.20	0.41
1:D:4201:GLU:O	1:D:4202:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5202:ARG:H	1:E:5203:PRO:CD	2.28	0.41
1:A:1160:ILE:HG23	1:A:1163:LYS:HD2	2.03	0.41
1:A:1307:ILE:C	1:A:1309:GLY:H	2.29	0.41
1:B:2063:ASN:HA	1:B:2138:MET:HB3	2.02	0.41
1:B:2238:ASP:C	1:B:2239:VAL:HG23	2.46	0.41
1:B:2243:ILE:O	1:B:2244:GLU:C	2.64	0.41
1:B:2296:ILE:C	1:B:2298:ALA:H	2.29	0.41
1:C:3302:MET:H	1:C:3303:PRO:CD	2.23	0.41
1:C:3303:PRO:HA	1:D:4301:PHE:CE2	2.54	0.41
1:D:4061:TRP:CZ3	1:D:4151:ARG:HB3	2.56	0.41
1:D:4063:ASN:HA	1:D:4138:MET:HB3	2.03	0.41
1:A:1242:LEU:O	1:A:1247:THR:HB	2.20	0.41
1:B:2307:ILE:C	1:B:2309:GLY:H	2.29	0.41
1:E:5307:ILE:C	1:E:5309:GLY:H	2.29	0.41
1:C:3160:ILE:HG23	1:C:3163:LYS:HD2	2.02	0.41
1:C:3238:ASP:C	1:C:3239:VAL:HG23	2.46	0.41
1:D:4238:ASP:C	1:D:4239:VAL:HG23	2.46	0.41
1:A:1296:ILE:C	1:A:1298:ALA:H	2.29	0.41
1:B:2221:LEU:O	1:B:2225:ILE:HD12	2.21	0.41
1:D:4182:PHE:CD2	1:E:5010:LYS:HD2	2.56	0.41
1:E:5201:GLU:O	1:E:5202:ARG:HB2	2.21	0.41
1:A:1013:PRO:CB	1:A:1014:PRO:CD	2.98	0.41
1:A:1165:ARG:HB3	1:A:1166:ALA:H	1.74	0.41
1:A:1240:PRO:CB	1:A:1241:PRO:CD	2.89	0.41
1:A:1243:ILE:O	1:A:1244:GLU:C	2.63	0.41
1:A:1294:LEU:HB2	1:E:5295:THR:OG1	2.20	0.41
1:C:3063:ASN:HA	1:C:3138:MET:HB3	2.03	0.41
1:C:3296:ILE:C	1:C:3298:ALA:H	2.28	0.41
1:D:4013:PRO:CB	1:D:4014:PRO:CD	2.98	0.41
1:D:4243:ILE:O	1:D:4244:GLU:C	2.63	0.41
1:D:4296:ILE:C	1:D:4298:ALA:H	2.28	0.41
1:E:5243:ILE:O	1:E:5244:GLU:C	2.64	0.41
1:E:5296:ILE:C	1:E:5298:ALA:H	2.28	0.41
1:B:2310:ILE:HG21	1:C:3331:LEU:HD11	2.03	0.41
1:C:3013:PRO:CB	1:C:3014:PRO:CD	2.98	0.41
1:C:3221:LEU:O	1:C:3225:ILE:HD12	2.21	0.41
1:E:5221:LEU:O	1:E:5225:ILE:HD12	2.21	0.41
1:E:5232:LEU:CD2	1:E:5254:VAL:HG12	2.51	0.41
1:A:1211:THR:HG21	1:A:1276:LEU:HD13	2.04	0.40
1:A:1295:THR:OG1	1:B:2294:LEU:HB2	2.20	0.40
1:B:2225:ILE:HG21	1:B:2261:ILE:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4224:THR:O	1:D:4224:THR:HG22	2.21	0.40
1:D:4299:THR:CG2	1:E:5297:ILE:HD13	2.49	0.40
1:A:1200:LEU:HG	1:B:2209:GLN:HB2	2.02	0.40
1:B:2182:PHE:HD2	1:C:3010:LYS:HD2	1.87	0.40
1:B:2291:MET:HE2	1:C:3291:MET:HG2	2.03	0.40
1:D:4131:LEU:HD22	1:D:4170:LEU:HD22	2.03	0.40
1:D:4225:ILE:CG2	1:D:4262:ALA:HB2	2.50	0.40
1:E:5063:ASN:HA	1:E:5138:MET:HB3	2.02	0.40
1:A:1268:PHE:C	1:A:1270:ASP:H	2.29	0.40
1:B:2160:ILE:HG23	1:B:2163:LYS:HD2	2.03	0.40
1:D:4268:PHE:C	1:D:4270:ASP:H	2.29	0.40
1:D:4295:THR:OG1	1:E:5293:VAL:HG12	2.22	0.40
1:D:4307:ILE:C	1:D:4309:GLY:H	2.29	0.40
1:B:2061:TRP:HZ3	1:B:2151:ARG:HB3	1.86	0.40
1:B:2268:PHE:C	1:B:2270:ASP:H	2.30	0.40
1:E:5013:PRO:CB	1:E:5014:PRO:CD	2.99	0.40
1:E:5160:ILE:HG23	1:E:5163:LYS:HD2	2.03	0.40
1:B:2291:MET:HE1	1:C:3291:MET:HA	2.03	0.40
1:C:3315:PHE:CZ	1:D:4327:TYR:HA	2.56	0.40

All (3) 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:B:2038:GLU:OE2	1:E:5119:LEU:CD1[1_545]	2.07	0.13
1:C:3037:GLU:OE2	1:C:3162:ARG:NH2[2_556]	2.07	0.13
1:A:1045:THR:OG1	1:A:1116:ASP:OD1[2_555]	2.19	0.01

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	2	19
1	B	327/354 (92%)	258 (79%)	55 (17%)	14 (4%)	2	19
1	C	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	2	19
1	D	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	2	19
1	E	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	2	19
All	All	1635/1770 (92%)	1282 (78%)	283 (17%)	70 (4%)	2	19

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1202	ARG
1	A	1244	GLU
1	B	2202	ARG
1	B	2244	GLU
1	C	3202	ARG
1	C	3244	GLU
1	D	4202	ARG
1	D	4244	GLU
1	E	5202	ARG
1	E	5244	GLU
1	A	1120	HIS
1	A	1240	PRO
1	A	1298	ALA
1	B	2120	HIS
1	B	2240	PRO
1	B	2298	ALA
1	C	3120	HIS
1	C	3240	PRO
1	C	3298	ALA
1	D	4120	HIS
1	D	4240	PRO
1	D	4298	ALA
1	E	5120	HIS
1	E	5240	PRO
1	E	5298	ALA
1	A	1012	LEU
1	A	1016	THR
1	A	1157	ASN
1	A	1239	VAL
1	B	2012	LEU
1	B	2016	THR

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Mol	Chain	Res	Type
1	B	2157	ASN
1	B	2239	VAL
1	C	3012	LEU
1	C	3016	THR
1	C	3157	ASN
1	C	3239	VAL
1	D	4012	LEU
1	D	4016	THR
1	D	4157	ASN
1	D	4239	VAL
1	D	4297	ILE
1	E	5012	LEU
1	E	5016	THR
1	E	5157	ASN
1	E	5239	VAL
1	A	1118	ASN
1	A	1203	PRO
1	A	1297	ILE
1	B	2118	ASN
1	B	2203	PRO
1	B	2297	ILE
1	C	3118	ASN
1	C	3203	PRO
1	C	3297	ILE
1	D	4118	ASN
1	D	4203	PRO
1	E	5118	ASN
1	E	5203	PRO
1	E	5297	ILE
1	A	1015	GLY
1	A	1243	ILE
1	B	2015	GLY
1	C	3015	GLY
1	C	3243	ILE
1	D	4015	GLY
1	E	5015	GLY
1	E	5243	ILE
1	B	2243	ILE
1	D	4243	ILE

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	311/332 (94%)	273 (88%)	38 (12%)	5	22
1	B	311/332 (94%)	274 (88%)	37 (12%)	5	23
1	C	311/332 (94%)	273 (88%)	38 (12%)	5	22
1	D	311/332 (94%)	273 (88%)	38 (12%)	5	22
1	E	311/332 (94%)	273 (88%)	38 (12%)	5	22
All	All	1555/1660 (94%)	1366 (88%)	189 (12%)	5	22

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1038	GLU
1	A	1040	ARG
1	A	1047	VAL
1	A	1086	VAL
1	A	1109	VAL
1	A	1123	GLU
1	A	1137	LEU
1	A	1160	ILE
1	A	1162	ARG
1	A	1164	LYS
1	A	1184	LEU
1	A	1198	GLU
1	A	1200	LEU
1	A	1201	GLU
1	A	1202	ARG
1	A	1205	LYS
1	A	1207	THR
1	A	1209	GLN
1	A	1211	THR
1	A	1218	LEU
1	A	1220	GLU
1	A	1234	SER
1	A	1238	ASP

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Mol	Chain	Res	Type
1	A	1239	VAL
1	A	1242	LEU
1	A	1258	THR
1	A	1267	THR
1	A	1269	ARG
1	A	1271	ILE
1	A	1281	SER
1	A	1283	VAL
1	A	1293	VAL
1	A	1295	THR
1	A	1315	PHE
1	A	1330	VAL
1	A	1331	LEU
1	A	1333	VAL
1	A	1341	MET
1	B	2040	ARG
1	B	2047	VAL
1	B	2086	VAL
1	B	2109	VAL
1	B	2123	GLU
1	B	2137	LEU
1	B	2160	ILE
1	B	2162	ARG
1	B	2164	LYS
1	B	2184	LEU
1	B	2198	GLU
1	B	2200	LEU
1	B	2201	GLU
1	B	2202	ARG
1	B	2205	LYS
1	B	2207	THR
1	B	2209	GLN
1	B	2211	THR
1	B	2218	LEU
1	B	2220	GLU
1	B	2234	SER
1	B	2238	ASP
1	B	2239	VAL
1	B	2242	LEU
1	B	2258	THR
1	B	2267	THR
1	B	2269	ARG

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Mol	Chain	Res	Type
1	B	2271	ILE
1	B	2281	SER
1	B	2283	VAL
1	B	2293	VAL
1	B	2295	THR
1	B	2315	PHE
1	B	2330	VAL
1	B	2331	LEU
1	B	2333	VAL
1	B	2341	MET
1	C	3038	GLU
1	C	3040	ARG
1	C	3047	VAL
1	C	3086	VAL
1	C	3109	VAL
1	C	3123	GLU
1	C	3137	LEU
1	C	3160	ILE
1	C	3162	ARG
1	C	3164	LYS
1	C	3184	LEU
1	C	3198	GLU
1	C	3200	LEU
1	C	3201	GLU
1	C	3202	ARG
1	C	3205	LYS
1	C	3207	THR
1	C	3209	GLN
1	C	3211	THR
1	C	3218	LEU
1	C	3220	GLU
1	C	3234	SER
1	C	3238	ASP
1	C	3239	VAL
1	C	3242	LEU
1	C	3258	THR
1	C	3267	THR
1	C	3269	ARG
1	C	3271	ILE
1	C	3281	SER
1	C	3283	VAL
1	C	3293	VAL

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Mol	Chain	Res	Type
1	C	3295	THR
1	C	3315	PHE
1	C	3330	VAL
1	C	3331	LEU
1	C	3333	VAL
1	C	3341	MET
1	D	4038	GLU
1	D	4040	ARG
1	D	4047	VAL
1	D	4086	VAL
1	D	4109	VAL
1	D	4123	GLU
1	D	4137	LEU
1	D	4160	ILE
1	D	4162	ARG
1	D	4164	LYS
1	D	4184	LEU
1	D	4198	GLU
1	D	4200	LEU
1	D	4201	GLU
1	D	4202	ARG
1	D	4205	LYS
1	D	4207	THR
1	D	4209	GLN
1	D	4211	THR
1	D	4218	LEU
1	D	4220	GLU
1	D	4234	SER
1	D	4238	ASP
1	D	4239	VAL
1	D	4242	LEU
1	D	4258	THR
1	D	4267	THR
1	D	4269	ARG
1	D	4271	ILE
1	D	4281	SER
1	D	4283	VAL
1	D	4293	VAL
1	D	4295	THR
1	D	4315	PHE
1	D	4330	VAL
1	D	4331	LEU

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Mol	Chain	Res	Type
1	D	4333	VAL
1	D	4341	MET
1	E	5038	GLU
1	E	5040	ARG
1	E	5047	VAL
1	E	5086	VAL
1	E	5109	VAL
1	E	5123	GLU
1	E	5137	LEU
1	E	5160	ILE
1	E	5162	ARG
1	E	5164	LYS
1	E	5184	LEU
1	E	5198	GLU
1	E	5200	LEU
1	E	5201	GLU
1	E	5202	ARG
1	E	5205	LYS
1	E	5207	THR
1	E	5209	GLN
1	E	5211	THR
1	E	5218	LEU
1	E	5220	GLU
1	E	5234	SER
1	E	5238	ASP
1	E	5239	VAL
1	E	5242	LEU
1	E	5258	THR
1	E	5267	THR
1	E	5269	ARG
1	E	5271	ILE
1	E	5281	SER
1	E	5283	VAL
1	E	5293	VAL
1	E	5295	THR
1	E	5315	PHE
1	E	5330	VAL
1	E	5331	LEU
1	E	5333	VAL
1	E	5341	MET

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

Mol	Chain	Res	Type
1	A	1033	ASN
1	A	1095	GLN
1	A	1126	GLN
1	A	1217	ASN
1	B	2033	ASN
1	B	2126	GLN
1	B	2140	GLN
1	B	2217	ASN
1	B	2314	ASN
1	C	3033	ASN
1	C	3126	GLN
1	C	3217	ASN
1	D	4033	ASN
1	D	4095	GLN
1	D	4126	GLN
1	D	4217	ASN
1	D	4314	ASN
1	E	5033	ASN
1	E	5095	GLN
1	E	5126	GLN
1	E	5217	ASN
1	E	5314	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 13 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	331/354 (93%)	0.13	3 (0%) 81 58	37, 137, 197, 200	0
1	B	331/354 (93%)	0.06	6 (1%) 67 42	37, 120, 183, 200	0
1	C	331/354 (93%)	0.20	7 (2%) 63 40	45, 132, 195, 200	0
1	D	331/354 (93%)	0.09	5 (1%) 72 46	49, 143, 197, 200	0
1	E	331/354 (93%)	0.11	3 (0%) 81 58	54, 151, 199, 200	0
All	All	1655/1770 (93%)	0.12	24 (1%) 72 46	37, 137, 197, 200	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3203	PRO	4.1
1	C	3025	GLU	3.8
1	D	4244	GLU	2.9
1	B	2307	ILE	2.8
1	C	3118	ASN	2.7
1	A	1205	LYS	2.6
1	E	5229	ARG	2.5
1	D	4195	LEU	2.4
1	B	2205	LYS	2.4
1	B	2245	LYS	2.4
1	C	3014	PRO	2.4
1	A	1308	ALA	2.4
1	B	2203	PRO	2.3
1	D	4313	MET	2.3
1	D	4314	ASN	2.3
1	E	5075	ARG	2.2
1	B	2238	ASP	2.1
1	D	4248	VAL	2.1
1	B	2038	GLU	2.1
1	A	1018	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	3037	GLU	2.1
1	C	3161	ILE	2.1
1	C	3117	LYS	2.0
1	E	5209	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	D	6214	1/1	0.86	0.13	125,125,125,125	0
2	CA	A	6101	1/1	0.88	0.41	157,157,157,157	0
2	CA	B	6102	1/1	0.91	0.14	114,114,114,114	0
2	CA	C	6213	1/1	0.92	0.06	125,125,125,125	0
2	CA	A	6211	1/1	0.93	0.05	125,125,125,125	0
2	CA	E	6215	1/1	0.93	0.13	125,125,125,125	0
2	CA	B	6201	1/1	0.94	0.16	133,133,133,133	0
2	CA	C	6202	1/1	0.96	0.13	133,133,133,133	0
2	CA	A	6301	1/1	0.97	0.07	97,97,97,97	1
2	CA	D	6203	1/1	0.97	0.10	133,133,133,133	0
2	CA	D	6204	1/1	0.97	0.07	133,133,133,133	0
2	CA	B	6212	1/1	0.97	0.05	125,125,125,125	0
2	CA	A	6205	1/1	0.97	0.05	133,133,133,133	0

6.5 Other polymers [i](#)

There are no such residues in this entry.