Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:33 AM GMT

PDB ID	:	2HN2
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

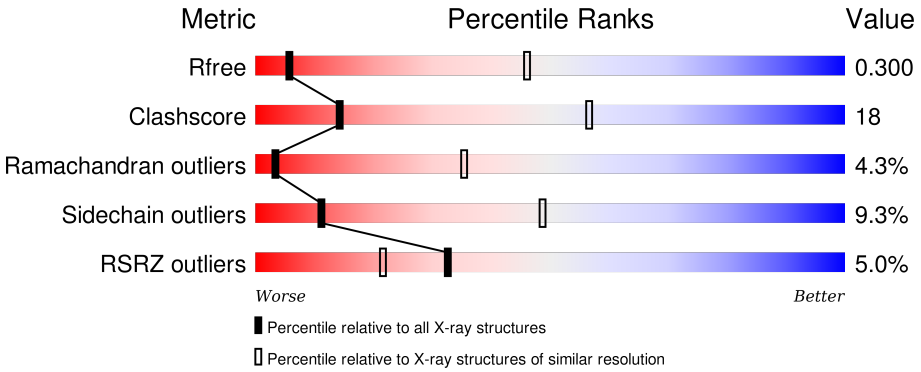
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	1101 (3.90-3.50)
Clashscore	102246	1224 (3.90-3.50)
Ramachandran outliers	100387	1172 (3.90-3.50)
Sidechain outliers	100360	1170 (3.90-3.50)
RSRZ outliers	91569	1108 (3.90-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	2% 55% 33% 5% • 6%
1	B	354	4% 55% 32% 5% • 6%
1	C	354	6% 55% 33% 5% • 6%
1	D	354	5% 54% 34% 5% 6%
1	E	354	7% 56% 32% 5% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CA	B	6201	-	-	-	X
2	CA	B	6212	-	-	-	X

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 (three-letter code: CA) (formula: Ca).

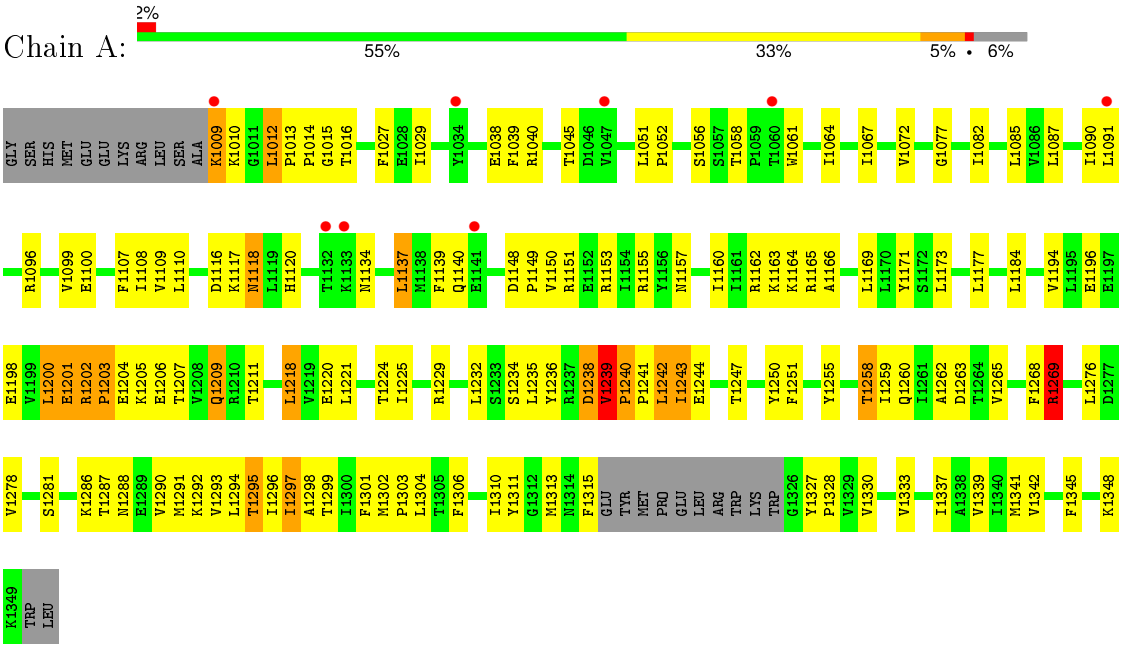
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Ca 3 3	0	0
2	A	4	Total Ca 4 4	0	0
2	D	3	Total Ca 3 3	0	0
2	C	2	Total Ca 2 2	0	0
2	E	1	Total Ca 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

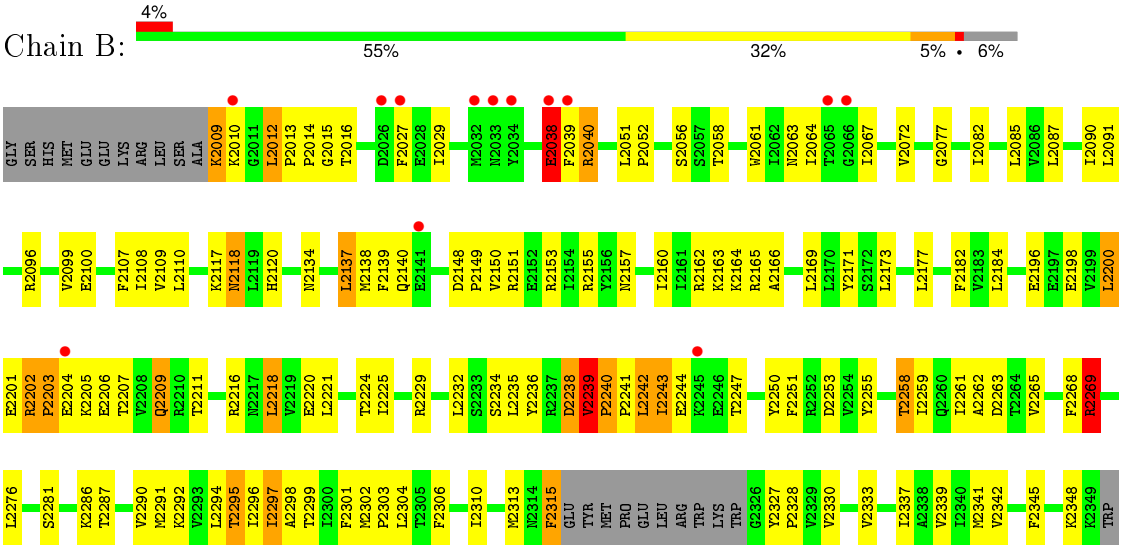
• Molecule 1: Magnesium transport protein corA

Chain A:



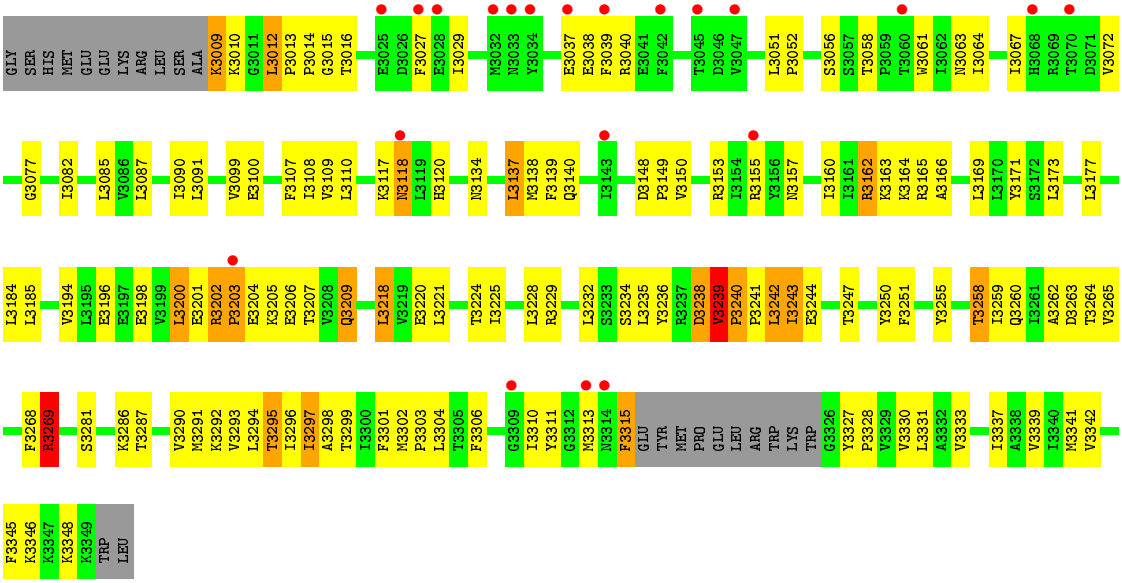
• Molecule 1: Magnesium transport protein corA

Chain B:



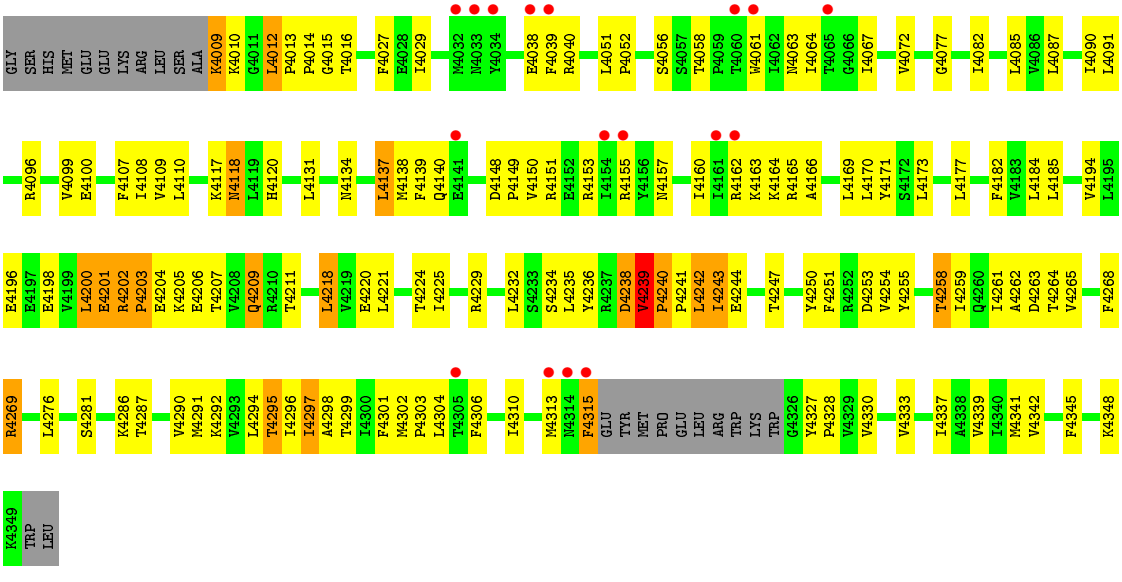
• Molecule 1: Magnesium transport protein corA

Chain C:



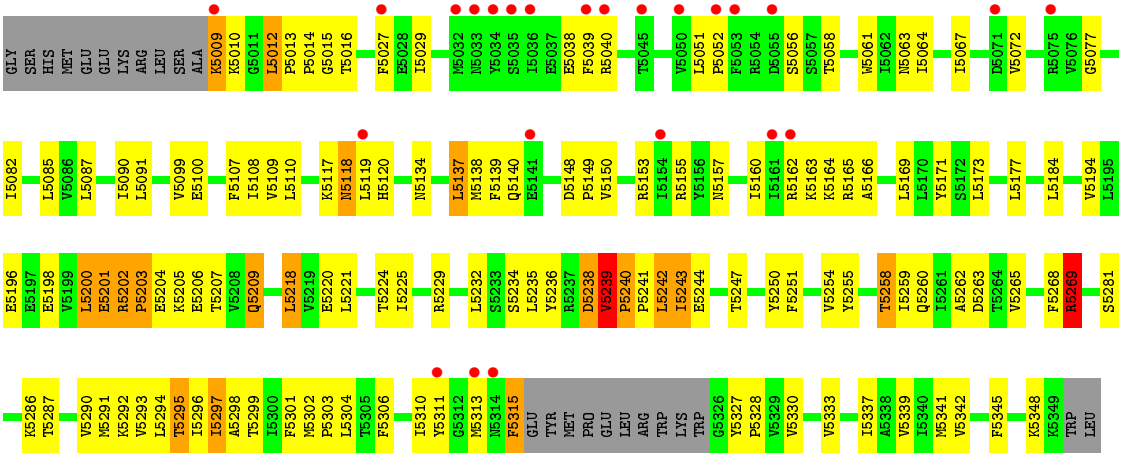
• Molecule 1: Magnesium transport protein corA

Chain D:



• Molecule 1: Magnesium transport protein corA

Chain E:


GLY SER HIS MET GLU GLU LYS ARG LEU SER ALA K5009 K5010 G5011 L5012 P5013 P5014 G5015 T5016 F5027 E5028 I5029 M5032 N5033 Y5034 S5035 I5036 E5037 E5038 F5039 R5040 T5045 V5050 L5051 P5052 F5053 R5054 D5055 S5056 S5057 T5058 W5061 I5062 N5063 I5064 I5067 D5071 V5072 R5075 V5076 G5077
I5082 L5085 V5086 L5087 I5090 L5091 V5099 E5100 F5107 I5108 V5109 L5110 K5117 N5118 L5119 H5120 N5134 L5137 M5138 F5139 Q5140 E5141 D5148 P5149 V5150 R5153 I5154 R5155 Y5156 N5157 I5160 I5161 R5162 K5163 K5164 R5165 A5166 L5169 L5170 Y5171 S5172 L5173 L5177 L5184 V5194 L5195
E5196 E5197 E5198 V5199 L5200 E5201 R5202 P5203 E5204 K5205 E5206 T5207 V5208 Q5209 L5218 V5219 E5220 L5221 T5224 I5225 R5229 L5232 S5233 S5234 L5235 Y5236 R5237 D5238 V5239 P5240 P5241 L5242 I5243 E5244 T5247 Y5250 F5251 V5254 Y5255 T5258 I5259 Q5260 I5261 A5262 D5263 T5264 V5265 F5268 R5269 S5281
K5286 T5287 V5290 M5291 K5292 V5293 L5294 T5295 I5296 I5297 A5298 T5299 I5300 F5301 M5302 P5303 L5304 T5305 F5306 I5310 Y5311 G5312 M5313 N5314 F5315 GLU TYR MET PRO GLU LEU ARG TRP LYS TRP G5326 Y5327 P5328 V5329 V5330 V5333 I5337 A5338 V5339 I5340 M5341 V5342 F5345 K5348 K5349 TRP LEU

4 Data and refinement statistics (i)

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 49.58 – 3.66	Depositor EDS
% Data completeness (in resolution range)	92.0 (20.00-3.70) 90.5 (49.58-3.66)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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	1521 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	120.5	Xtriage
Anisotropy	0.320	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 117.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 31060 reflections	Xtriage
F_o,F_c correlation	0.85	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.34	0/2794	0.55	1/3785 (0.0%)
1	B	0.34	0/2794	0.55	3/3785 (0.1%)
1	C	0.35	0/2794	0.55	1/3785 (0.0%)
1	D	0.35	0/2794	0.68	3/3785 (0.1%)
1	E	0.34	0/2794	0.55	1/3785 (0.0%)
All	All	0.34	0/13970	0.58	9/18925 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	4269	ARG	NE-CZ-NH2	-17.72	111.44	120.30
1	D	4269	ARG	NE-CZ-NH1	17.20	128.90	120.30
1	D	4269	ARG	CD-NE-CZ	8.40	135.36	123.60
1	B	2269	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	C	3269	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	1269	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	B	2269	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	B	2038	GLU	CA-CB-CG	5.06	124.52	113.40
1	E	5269	ARG	NE-CZ-NH1	-5.04	117.78	120.30

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	113	1
1	B	2737	0	2790	116	1
1	C	2737	0	2790	114	1
1	D	2737	0	2790	116	0
1	E	2737	0	2790	115	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	499	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 18.

All (499) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:5240:PRO:HB2	1:E:5241:PRO:CD	2.12	0.77
1:D:4240:PRO:HB2	1:D:4241: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: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:A:1302:MET:H	1:A:1303:PRO:HD2	1.50	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:E:5012:LEU:H	1:E:5013:PRO:CD	1.97	0.74
1:D:4202:ARG:H	1:D:4203:PRO:HD3	1.53	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:2302:MET:N	1:B:2303:PRO:HD2	2.05	0.72
1:B:2202:ARG:H	1:B:2203:PRO:HD3	1.53	0.72
1:E:5302:MET:N	1:E:5303:PRO:HD2	2.05	0.71
1:A:1303:PRO:HA	1:B:2301:PHE:HD2	1.54	0.71
1:C:3012:LEU:N	1:C:3013:PRO:HD3	1.99	0.71
1:A:1302:MET:N	1:A:1303:PRO:HD2	2.06	0.71
1:C:3225:ILE:HG22	1:C:3262:ALA:HB2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:4202:ARG:N	1:D:4203:PRO:HD3	2.11	0.65
1:A:1202:ARG:N	1:A:1203: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:E:5202:ARG:N	1:E:5203:PRO:HD3	2.11	0.64
1:B:2202:ARG:N	1:B:2203:PRO:HD3	2.11	0.64
1:A:1225:ILE:HG22	1:A:1262:ALA:HB2	1.79	0.64
1:C:3225:ILE:HD13	1:C:3265:VAL:HG21	1.80	0.64
1:D:4221:LEU:HG	1:D:4225:ILE:HD11	1.80	0.63
1:B:2225:ILE:HG22	1:B:2262:ALA:HB2	1.80	0.63
1:C:3287:THR:O	1:C:3287:THR:HG22	1.98	0.63
1:A:1287:THR:HG22	1:A:1287: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:O	1:D:4287:THR:HG22	1.98	0.63
1:B:2039:PHE:CZ	1:B:2155:ARG:HA	2.34	0.62
1:D:4085:LEU:HD23	1:D:4085:LEU:H	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:C:3085:LEU:HD23	1:C:3085:LEU:H	1.64	0.62
1:D:4171:TYR:OH	1:D:4235:LEU:HG	1.99	0.62
1:A:1221:LEU:HG	1:A:1225:ILE:HD11	1.80	0.62
1:C:3171:TYR:O	1:C:3250:TYR:CE2	2.53	0.62
1:C:3171:TYR:OH	1:C:3235:LEU:HG	2.00	0.62
1:B:2287:THR:HG22	1:B:2287:THR:O	1.99	0.62
1:B:2303:PRO:CA	1:C:3301:PHE:CD2	2.80	0.62
1:B:2171:TYR:OH	1:B:2235:LEU:HG	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:LEU:HD21	1:A:1268:PHE:HB3	1.82	0.62
1:A:1085:LEU:H	1:A:1085:LEU:HD23	1.64	0.62
1:C:3218:LEU:HD21	1:C:3268:PHE:HB3	1.82	0.62
1:D:4236:TYR:HA	1:D:4251:PHE:CZ	2.25	0.61
1:D:4067:ILE:HG22	1:D:4091:LEU:HD23	1.81	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:E:5171:TYR:CD1	1:E:5251:PHE:HB3	2.36	0.61
1:D:4171:TYR:CD1	1:D:4251:PHE:HB3	2.35	0.61
1:E:5171:TYR:O	1:E:5250:TYR:CE2	2.53	0.61
1:D:4295:THR:HA	1:E:5294:LEU:HD13	1.80	0.61
1:C:3232:LEU:HB3	1:C:3255:TYR:HB2	1.82	0.61
1:E:5085:LEU:HD23	1:E:5085:LEU:H	1.65	0.61
1:B:2171:TYR:CD1	1:B:2251:PHE:HB3	2.35	0.60
1:A:1171:TYR:OH	1:A:1235:LEU:HG	2.00	0.60
1:E:5067:ILE:HG22	1:E:5091:LEU:HD23	1.83	0.60
1:A:1297:ILE:HD13	1:E:5299:THR:HG23	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:B:2171:TYR:O	1:B:2250:TYR:CE2	2.53	0.60
1:A:1171:TYR:CD1	1:A:1251:PHE:HB3	2.36	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:E:5117:LYS:O	1:E:5118:ASN:HB2	2.00	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:B:2236:TYR:HA	1:B:2251:PHE:CZ	2.25	0.59
1:A:1225:ILE:HD13	1:A:1265:VAL:HG21	1.84	0.59
1:E:5051:LEU:N	1:E:5052:PRO:HD2	2.18	0.59
1:C:3067:ILE:HG22	1:C:3091:LEU:HD23	1.84	0.59
1:D:4218:LEU:HD21	1:D:4268:PHE:HB3	1.84	0.59
1:C:3061:TRP:HB2	1:C:3169:LEU:HD21	1.83	0.59
1:B:2067:ILE:HG22	1:B:2091:LEU:HD23	1.85	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:B:2051:LEU:N	1:B:2052:PRO:HD2	2.17	0.58
1:A:1067:ILE:HG22	1:A:1091:LEU:HD23	1.85	0.58
1:C:3051:LEU:N	1:C:3052:PRO:HD2	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1150:VAL:HG11	1:A:1173:LEU:HD23	1.85	0.58
1:A:1051:LEU:N	1:A:1052:PRO:HD2	2.17	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:D:4150:VAL:HG11	1:D:4173:LEU:HD23	1.86	0.57
1:B:2218:LEU:HD21	1:B:2268:PHE:HB3	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:E:5150:VAL:HG11	1:E:5173:LEU:HD23	1.86	0.57
1:B:2117:LYS:O	1:B:2118:ASN:HB2	2.04	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:E:5236:TYR:HA	1:E:5251:PHE:CZ	2.25	0.56
1:C:3225:ILE:CG2	1:C:3262:ALA:HB2	2.35	0.56
1:E:5225:ILE:HG22	1:E:5262:ALA:HB2	1.87	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: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: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:D:4117:LYS:O	1:D:4118:ASN:HB2	2.05	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:B:2077:GLY:HA2	1:B:2082:ILE:HD12	1.88	0.56
1:A:1099:VAL:HG21	1:A:1235:LEU:HD13	1.88	0.55
1:C:3099:VAL:HG21	1:C:3235:LEU:HD13	1.88	0.55
1:E:5302:MET:N	1:E:5303:PRO:CD	2.69	0.55
1:C:3077:GLY:HA2	1:C:3082:ILE:HD12	1.88	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:D:4302:MET:N	1:D:4303:PRO:CD	2.69	0.55
1:C:3302:MET:N	1:C:3303:PRO:CD	2.69	0.55
1:D:4061:TRP:HB2	1:D:4169:LEU:HD21	1.87	0.55
1:B:2165:ARG:HD3	1:B:2243:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5099:VAL:HG21	1:E:5235:LEU:HD13	1.88	0.55
1:A:1302:MET:N	1:A:1303:PRO:CD	2.69	0.55
1:A:1077:GLY:HA2	1:A:1082:ILE:HD12	1.88	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:A:1255:TYR:O	1:A:1258:THR:HG22	2.07	0.55
1:A:1061:TRP:HB2	1:A:1169:LEU:HD21	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:C:3327:TYR:HB3	1:C:3328:PRO:HD3	1.89	0.55
1:B:2087:LEU:HA	1:B:2090:ILE:HD12	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:1100:GLU:HB2	1:A:1107:PHE:HB3	1.88	0.54
1:E:5255:TYR:O	1:E:5258:THR:HG22	2.07	0.54
1:E:5165:ARG:HD3	1:E:5243:ILE:HD11	1.89	0.54
1:A:1039:PHE:CZ	1:A:1155:ARG:HA	2.41	0.54
1:B:2099:VAL:HG21	1:B:2235:LEU:HD13	1.89	0.54
1:A:1301:PHE:CE2	1:E:5303:PRO:HA	2.42	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:3236:TYR:HA	1:C:3251:PHE:CZ	2.25	0.54
1:C:3067:ILE:HG13	1:C:3140:GLN:O	2.08	0.54
1:D:4077:GLY:HA2	1:D:4082:ILE:HD12	1.88	0.54
1:D:4255:TYR:O	1:D:4258:THR:HG22	2.08	0.53
1:A:1165:ARG:HD3	1:A:1243:ILE:HD11	1.89	0.53
1:A:1295:THR:HA	1:B:2294:LEU:HD13	1.90	0.53
1:B:2327:TYR:HB3	1:B:2328:PRO:HD3	1.89	0.53
1:A:1327:TYR:HB3	1:A:1328:PRO:HD3	1.89	0.53
1:C:3255:TYR:O	1:C:3258:THR:HG22	2.08	0.53
1:B:2061:TRP:HB2	1:B:2169:LEU:HD21	1.90	0.53
1:C:3203:PRO:HG2	1:C:3286:LYS:HE3	1.90	0.53
1:A:1232:LEU:HB3	1:A:1255:TYR:HB2	1.90	0.53
1:C:3240:PRO:CB	1:C:3241:PRO:HD3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1202:ARG:O	1:A:1204:GLU:N	2.42	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:C:3202:ARG:O	1:C:3204:GLU:N	2.42	0.52
1:B:2202:ARG:O	1:B:2204:GLU:N	2.42	0.52
1:A:1299:THR:HG23	1:B:2297:ILE:HD13	1.91	0.52
1:D:4240:PRO:CB	1:D:4241:PRO:HD3	2.23	0.52
1:D:4303:PRO:HA	1:E:5301:PHE:CE2	2.44	0.52
1:B:2218:LEU:HB3	1:B:2269:ARG:HG3	1.91	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:D:4232:LEU:CD2	1:D:4254:VAL:HG12	2.41	0.51
1:B:2203:PRO:HG2	1:B:2286:LYS:HE3	1.91	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:2291:MET:HE1	1:C:3291:MET:HA	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:1302:MET:H	1:A:1303:PRO:CD	2.23	0.50
1:E:5134:ASN:HA	1:E:5166:ALA:CB	2.41	0.50
1:E:5087:LEU:HA	1:E:5090:ILE:HD12	1.93	0.50
1:A:1029:ILE:HG12	1:A:1064:ILE:HG23	1.94	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:D:4067:ILE:HG13	1:D:4140:GLN:O	2.10	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: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
1:E:5029:ILE:HG12	1:E:5064:ILE:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:4236:TYR:CA	1:D:4251:PHE:HZ	2.15	0.49
1:C:3029:ILE:HG12	1:C:3064:ILE:HG23	1.93	0.49
1:A:1297:ILE:O	1:A:1297:ILE:HG22	2.13	0.49
1:D:4302:MET:H	1:D:4303:PRO:CD	2.23	0.49
1:A:1009:LYS:HG3	1:A:1010:LYS:H	1.77	0.49
1:A:1218:LEU:HB3	1:A:1269:ARG:HG3	1.94	0.49
1:C:3291:MET:CE	1:D:4290:VAL:HG12	2.43	0.49
1:B:2292:LYS:HD3	1:B:2348:LYS:HG2	1.95	0.49
1:D:4239:VAL:HB	1:D:4242:LEU:HD23	1.96	0.48
1:A:1278:VAL:HA	1:B:2276:LEU:HD21	1.94	0.48
1:D:4292:LYS:HD3	1:D:4348:LYS:HG2	1.95	0.48
1:E:5297:ILE:O	1:E:5297:ILE:HG22	2.13	0.48
1:A:1292:LYS:HD3	1:A:1348:LYS:HG2	1.95	0.48
1:C:3218:LEU:HB3	1:C:3269:ARG:HG3	1.94	0.48
1:B:2297:ILE:HG22	1:B:2297:ILE:O	2.13	0.48
1:D:4297:ILE:O	1:D:4297:ILE:HG22	2.13	0.48
1:C:3239:VAL:HB	1:C:3242:LEU:HD23	1.95	0.48
1:D:4225:ILE:HG21	1:D:4261:ILE:HG22	1.96	0.48
1:D:4182:PHE:HD2	1:E:5010:LYS:HD2	1.79	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:D:4339:VAL:HA	1:D:4342:VAL:HG12	1.95	0.48
1:C:3292:LYS:HD3	1:C:3348:LYS:HG2	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:B:2339:VAL:HA	1:B:2342:VAL:HG12	1.95	0.47
1:A:1339:VAL:HA	1:A:1342:VAL:HG12	1.96	0.47
1:E:5064:ILE:HD12	1:E:5139:PHE:CE1	2.49	0.47
1:A:1296:ILE:HA	1:A:1345:PHE:HE2	1.80	0.47
1:B:2306:PHE:CZ	1:C:3304:LEU:HD23	2.50	0.47
1:B:2239:VAL:HB	1:B:2242:LEU:HD23	1.95	0.47
1:C:3339:VAL:HA	1:C:3342:VAL:HG12	1.95	0.47
1:E:5339:VAL:HA	1:E:5342:VAL:HG12	1.95	0.47
1:C:3296:ILE:HA	1:C:3345:PHE:HE2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4229:ARG:HE	1:D:4259:ILE:HG12	1.80	0.47
1:E:5239:VAL:HB	1:E:5242:LEU:HD23	1.95	0.47
1:A:1236:TYR:CA	1:A:1251:PHE:HZ	2.15	0.47
1:B:2171:TYR:CD1	1:B:2247:THR:HG22	2.50	0.47
1:E:5240:PRO:CB	1:E:5241:PRO:HD3	2.23	0.46
1:E:5171:TYR:CD1	1:E:5247:THR:HG22	2.50	0.46
1:A:1110:LEU:HD13	1:A:1177:LEU:HD22	1.96	0.46
1:A:1203:PRO:HG2	1:A:1286:LYS:HE3	1.98	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: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:D:4171:TYR:CD1	1:D:4247:THR:HG22	2.50	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:A:1229:ARG:HE	1:A:1259:ILE:HG12	1.80	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:C:3299:THR:HG22	1:C:3299:THR:O	2.16	0.46
1:B:2291:MET:CE	1:C:3290:VAL:HG12	2.46	0.46
1:B:2110:LEU:HD13	1:B:2177:LEU:HD22	1.97	0.46
1:C:3110:LEU:HD13	1:C:3177:LEU:HD22	1.97	0.46
1:B:2299:THR:O	1:B:2299:THR:HG22	2.16	0.45
1:E:5299:THR:HG22	1:E:5299:THR:O	2.16	0.45
1:B:2229:ARG:HE	1:B:2259:ILE:HG12	1.81	0.45
1:C:3287:THR:O	1:C:3287:THR:CG2	2.65	0.45
1:A:1291:MET:HA	1:E:5291:MET:HE1	1.97	0.45
1:C:3171:TYR:CD1	1:C:3247:THR:HG22	2.50	0.45
1:A:1299:THR:O	1:A:1299:THR:HG22	2.16	0.45
1:B:2064:ILE:HD12	1:B:2139:PHE:CE1	2.51	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:D:4299:THR:O	1:D:4299:THR:HG22	2.16	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:B:2232:LEU:HB3	1:B:2255:TYR:HB2	1.98	0.45
1:B:2039:PHE:CE1	1:B:2155:ARG:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5064:ILE:HD11	1:E:5137:LEU:HD21	1.99	0.45
1:C:3064:ILE:HD12	1:C:3139:PHE:CE1	2.52	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:A:1238:ASP:HB3	1:A:1239:VAL:H	1.57	0.45
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:E:5240:PRO:CB	1:E:5241:PRO:CD	2.89	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:4291:MET:CE	1:E:5290:VAL:HG12	2.47	0.44
1:A:1202:ARG:H	1:A:1203:PRO:CD	2.28	0.44
1:C:3228:LEU:HD23	1:C:3258:THR:OG1	2.18	0.44
1:C:3206:GLU:HB2	1:C:3209:GLN:HG2	2.00	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:C:3185:LEU:HD13	1:C:3264:THR:HG21	1.99	0.44
1:A:1293:VAL:HG12	1:E:5295:THR:OG1	2.17	0.44
1:A:1235:LEU:O	1:A:1251:PHE:CZ	2.71	0.44
1:A:1196:GLU:OE1	1:B:2216:ARG:NH2	2.51	0.44
1:B:2296:ILE:HG12	1:B:2345:PHE:CE2	2.53	0.44
1:D:4232:LEU:HB3	1:D:4255:TYR:HB2	1.99	0.44
1:D:4235:LEU:O	1:D:4251:PHE:CZ	2.71	0.43
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:A:1206:GLU:HB2	1:A:1209:GLN:HG2	1.99	0.43
1:B:2235:LEU:O	1:B:2251:PHE:CZ	2.71	0.43
1:A:1099:VAL:HG23	1:A:1108:ILE:HG12	2.00	0.43
1:D:4232:LEU:HD21	1:D:4254:VAL:HG12	1.98	0.43
1:D:4313:MET:SD	1:E:5311:TYR:HB2	2.59	0.43
1:B:2303:PRO:CA	1:C:3301:PHE:CE2	2.98	0.43
1:B:2206:GLU:HB2	1:B:2209:GLN:HG2	1.99	0.43
1:C:3296:ILE:HG12	1:C:3345:PHE:CE2	2.53	0.43
1:C:3148:ASP:N	1:C:3149:PRO:HD2	2.34	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:E:5235:LEU:O	1:E:5251:PHE:CZ	2.71	0.43
1:A:1304:LEU:HB3	1:E:5306:PHE:HE1	1.77	0.43
1:E:5148:ASP:N	1:E:5149:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4149:PRO:O	1:D:4153:ARG:HG3	2.19	0.43
1:E:5206:GLU:HB2	1:E:5209:GLN:HG2	2.00	0.43
1:B:2287:THR:CG2	1:B:2287:THR:O	2.65	0.43
1:D:4295:THR:OG1	1:E:5294:LEU:HB2	2.19	0.43
1:C:3056:SER:C	1:C:3058:THR:H	2.22	0.43
1:B:2303:PRO:CA	1:C:3301:PHE:HD2	2.15	0.43
1:C:3202:ARG:H	1:C:3203:PRO:CD	2.28	0.43
1:B:2337:ILE:C	1:B:2339:VAL:H	2.22	0.43
1:A:1337:ILE:C	1:A:1339:VAL:H	2.22	0.43
1:C:3149:PRO:O	1:C:3153:ARG:HG3	2.19	0.43
1:C:3099:VAL:HG23	1:C:3108:ILE:HG12	2.01	0.43
1:D:4099:VAL:HG23	1:D:4108:ILE:HG12	2.00	0.43
1:E:5203:PRO:HG2	1:E:5286:LYS:HE3	2.00	0.43
1:A:1061:TRP:CZ3	1:A:1151:ARG:HB3	2.54	0.43
1:D:4291:MET:HE1	1:E:5291:MET:HA	2.01	0.43
1:E:5149:PRO:O	1:E:5153:ARG:HG3	2.19	0.43
1:C:3224:THR:CG2	1:C:3224:THR:O	2.67	0.43
1:B:2202:ARG:N	1:B:2203:PRO:CD	2.81	0.42
1:D:4337:ILE:C	1:D:4339:VAL:H	2.22	0.42
1:D:4296:ILE:HG12	1:D:4345:PHE:CE2	2.54	0.42
1:D:4148:ASP:N	1:D:4149:PRO:HD2	2.34	0.42
1:B:2148:ASP:N	1:B:2149:PRO:HD2	2.33	0.42
1:B:2056:SER:C	1:B:2058:THR:H	2.22	0.42
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: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:A:1296:ILE:HG12	1:A:1345:PHE:CE2	2.54	0.42
1:C:3337:ILE:C	1:C:3339:VAL:H	2.22	0.42
1:E:5296:ILE:HG12	1:E:5345:PHE:CE2	2.54	0.42
1:C:3240:PRO:CB	1:C:3241:PRO:CD	2.89	0.42
1:B:2099:VAL:HG23	1:B:2108:ILE:HG12	2.00	0.42
1:E:5287:THR:CG2	1:E:5287:THR:O	2.65	0.42
1:B:2224:THR:O	1:B:2224:THR:CG2	2.67	0.42
1:A:1224:THR:CG2	1:A:1224:THR:O	2.67	0.42
1:A:1056:SER:C	1:A:1058:THR:H	2.22	0.42
1:E:5238:ASP:HB3	1:E:5239:VAL:H	1.56	0.42
1:D:4242:LEU:O	1:D:4247:THR:HB	2.20	0.42
1:A:1202:ARG:N	1:A:1203:PRO:CD	2.81	0.42
1:C:3039:PHE:CE1	1:C:3155:ARG:HA	2.54	0.42
1:E:5337:ILE:C	1:E:5339:VAL:H	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5242:LEU:O	1:E:5247:THR:HB	2.19	0.42
1:A:1290:VAL:HG12	1:E:5291:MET:HE3	2.01	0.42
1:B:2149:PRO:O	1:B:2153:ARG:HG3	2.19	0.42
1:B:2242:LEU:O	1:B:2247:THR:HB	2.20	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:C:3064:ILE:HD11	1:C:3137:LEU:HD21	2.00	0.42
1:A:1301:PHE:CD2	1:E:5303:PRO:CA	2.93	0.42
1:A:1064:ILE:HD11	1:A:1137:LEU:HD21	2.01	0.42
1:D:4224:THR:O	1:D:4224:THR:CG2	2.67	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:C:3238:ASP:HB3	1:C:3239:VAL:H	1.56	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:A:1194:VAL:C	1:A:1196:GLU:H	2.23	0.41
1:B:2040:ARG:CZ	1:B:2040:ARG:HB2	2.47	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
1:E:5202:ARG:H	1:E:5203:PRO:CD	2.28	0.41
1:E:5194:VAL:C	1:E:5196:GLU:H	2.23	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:E:5056:SER:C	1:E:5058:THR:H	2.22	0.41
1:D:4063:ASN:HA	1:D:4138:MET:HB3	2.03	0.41
1:B:2063:ASN:HA	1:B:2138:MET:HB3	2.02	0.41
1:A:1160:ILE:HG23	1:A:1163:LYS:HD2	2.03	0.41
1:A:1242:LEU:O	1:A:1247:THR:HB	2.20	0.41
1:A:1201:GLU:O	1:A:1202:ARG:HB2	2.21	0.41
1:C:3160:ILE:HG23	1:C:3163:LYS:HD2	2.02	0.41
1:E:5201:GLU:O	1:E:5202:ARG:HB2	2.21	0.41
1:B:2221:LEU:O	1:B:2225:ILE:HD12	2.21	0.41
1:D:4194:VAL:C	1:D:4196:GLU:H	2.24	0.41
1:D:4182:PHE:CD2	1:E:5010:LYS:HD2	2.56	0.41
1:A:1240:PRO:CB	1:A:1241:PRO:CD	2.89	0.41
1:A:1013:PRO:CB	1:A:1014:PRO:CD	2.98	0.41
1:D:4013:PRO:CB	1:D:4014:PRO:CD	2.98	0.41
1:A:1294:LEU:HB2	1:E:5295:THR:OG1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1165:ARG:HB3	1:A:1166:ALA:H	1.74	0.41
1:C:3063:ASN:HA	1:C:3138:MET:HB3	2.03	0.41
1:D:4056:SER:C	1:D:4058:THR:H	2.22	0.41
1:C:3013:PRO:CB	1:C:3014:PRO:CD	2.98	0.41
1:B:2310:ILE:HG21	1:C:3331:LEU:HD11	2.03	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:B:2225:ILE:HG21	1:B:2261:ILE:HG22	2.02	0.40
1:D:4299:THR:CG2	1:E:5297:ILE:HD13	2.49	0.40
1:A:1295:THR:OG1	1:B:2294:LEU:HB2	2.20	0.40
1:D:4224:THR:O	1:D:4224:THR:HG22	2.21	0.40
1:A:1211:THR:HG21	1:A:1276:LEU:HD13	2.04	0.40
1:D:4225:ILE:CG2	1:D:4262:ALA:HB2	2.50	0.40
1:A:1200:LEU:HG	1:B:2209:GLN:HB2	2.02	0.40
1:C:3194:VAL:C	1:C:3196:GLU:H	2.23	0.40
1:B:2182:PHE:HD2	1:C:3010:LYS:HD2	1.87	0.40
1:E:5063:ASN:HA	1:E:5138:MET:HB3	2.02	0.40
1:D:4131:LEU:HD22	1:D:4170:LEU:HD22	2.03	0.40
1:D:4295:THR:OG1	1:E:5293:VAL:HG12	2.22	0.40
1:B:2160:ILE:HG23	1:B:2163:LYS:HD2	2.03	0.40
1:E:5013:PRO:CB	1:E:5014:PRO:CD	2.99	0.40
1:B:2061:TRP:HZ3	1:B:2151:ARG:HB3	1.86	0.40
1:E:5160:ILE:HG23	1:E:5163:LYS:HD2	2.03	0.40
1:A:1286:LYS:C	1:A:1288:ASN:H	2.25	0.40
1:C:3315:PHE:CZ	1:D:4327:TYR:HA	2.56	0.40
1:C:3291:MET:HE3	1:D:4290:VAL:HG12	2.03	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 (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	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	3	35
1	B	327/354 (92%)	258 (79%)	55 (17%)	14 (4%)	3	35
1	C	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	3	35
1	D	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	3	35
1	E	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	3	35
All	All	1635/1770 (92%)	1282 (78%)	283 (17%)	70 (4%)	3	35

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	282 (91%)	29 (9%)	11	49
1	B	311/332 (94%)	282 (91%)	29 (9%)	11	49
1	C	311/332 (94%)	282 (91%)	29 (9%)	11	49
1	D	311/332 (94%)	282 (91%)	29 (9%)	11	49
1	E	311/332 (94%)	282 (91%)	29 (9%)	11	49
All	All	1555/1660 (94%)	1410 (91%)	145 (9%)	11	49

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1009	LYS
1	A	1038	GLU
1	A	1040	ARG
1	A	1109	VAL
1	A	1137	LEU
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	1205	LYS

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Mol	Chain	Res	Type
1	A	1207	THR
1	A	1209	GLN
1	A	1218	LEU
1	A	1220	GLU
1	A	1234	SER
1	A	1238	ASP
1	A	1239	VAL
1	A	1242	LEU
1	A	1258	THR
1	A	1263	ASP
1	A	1269	ARG
1	A	1281	SER
1	A	1295	THR
1	A	1315	PHE
1	A	1330	VAL
1	A	1333	VAL
1	A	1341	MET
1	B	2009	LYS
1	B	2038	GLU
1	B	2040	ARG
1	B	2109	VAL
1	B	2137	LEU
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	2205	LYS
1	B	2207	THR
1	B	2209	GLN
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	2263	ASP
1	B	2269	ARG
1	B	2281	SER
1	B	2295	THR

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Mol	Chain	Res	Type
1	B	2315	PHE
1	B	2330	VAL
1	B	2333	VAL
1	B	2341	MET
1	C	3009	LYS
1	C	3038	GLU
1	C	3040	ARG
1	C	3109	VAL
1	C	3137	LEU
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	3205	LYS
1	C	3207	THR
1	C	3209	GLN
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	3263	ASP
1	C	3269	ARG
1	C	3281	SER
1	C	3295	THR
1	C	3315	PHE
1	C	3330	VAL
1	C	3333	VAL
1	C	3341	MET
1	D	4009	LYS
1	D	4038	GLU
1	D	4040	ARG
1	D	4109	VAL
1	D	4137	LEU
1	D	4162	ARG
1	D	4164	LYS
1	D	4184	LEU
1	D	4198	GLU

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Mol	Chain	Res	Type
1	D	4200	LEU
1	D	4201	GLU
1	D	4205	LYS
1	D	4207	THR
1	D	4209	GLN
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	4253	ASP
1	D	4258	THR
1	D	4263	ASP
1	D	4281	SER
1	D	4295	THR
1	D	4315	PHE
1	D	4330	VAL
1	D	4333	VAL
1	D	4341	MET
1	E	5009	LYS
1	E	5038	GLU
1	E	5040	ARG
1	E	5109	VAL
1	E	5137	LEU
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	5205	LYS
1	E	5207	THR
1	E	5209	GLN
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	5263	ASP

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Mol	Chain	Res	Type
1	E	5269	ARG
1	E	5281	SER
1	E	5295	THR
1	E	5315	PHE
1	E	5330	VAL
1	E	5333	VAL
1	E	5341	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1033	ASN
1	A	1095	GLN
1	A	1217	ASN
1	B	2033	ASN
1	B	2095	GLN
1	B	2217	ASN
1	B	2314	ASN
1	C	3033	ASN
1	C	3095	GLN
1	C	3217	ASN
1	D	4033	ASN
1	D	4095	GLN
1	D	4217	ASN
1	E	5033	ASN
1	E	5095	GLN
1	E	5217	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 carbohydrates in this entry.

5.6 Ligand geometry

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, 95^{th} 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%)	0.03	8 (2%)	62	46	37, 137, 197, 200	0
1	B	331/354 (93%)	-0.03	13 (3%)	43	29	37, 120, 183, 200	0
1	C	331/354 (93%)	0.27	21 (6%)	23	14	45, 132, 195, 200	0
1	D	331/354 (93%)	0.15	17 (5%)	32	21	49, 143, 197, 200	0
1	E	331/354 (93%)	0.25	24 (7%)	18	11	54, 151, 199, 200	0
All	All	1655/1770 (93%)	0.14	83 (5%)	32	21	37, 137, 197, 200	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2033	ASN	5.1
1	C	3032	MET	4.4
1	D	4154	ILE	4.1
1	C	3033	ASN	4.1
1	D	4065	THR	4.1
1	D	4314	ASN	3.7
1	D	4313	MET	3.6
1	B	2141	GLU	3.5
1	C	3314	ASN	3.3
1	C	3034	TYR	3.3
1	C	3118	ASN	3.2
1	D	4039	PHE	3.2
1	E	5313	MET	3.2
1	D	4032	MET	3.1
1	E	5027	PHE	3.1
1	B	2065	THR	3.1
1	C	3028	GLU	3.0
1	E	5154	ILE	3.0
1	A	1009	LYS	3.0
1	D	4033	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	5009	LYS	3.0
1	E	5034	TYR	2.9
1	E	5161	ILE	2.9
1	C	3060	THR	2.9
1	E	5311	TYR	2.9
1	C	3025	GLU	2.9
1	D	4034	TYR	2.8
1	E	5033	ASN	2.8
1	E	5075	ARG	2.8
1	D	4161	ILE	2.8
1	C	3039	PHE	2.7
1	D	4162	ARG	2.7
1	E	5071	ASP	2.7
1	C	3313	MET	2.7
1	E	5032	MET	2.6
1	E	5036	ILE	2.6
1	C	3155	ARG	2.6
1	A	1141	GLU	2.6
1	D	4060	THR	2.6
1	E	5119	LEU	2.6
1	B	2026	ASP	2.6
1	D	4038	GLU	2.6
1	A	1060	THR	2.6
1	E	5045	THR	2.6
1	B	2027	PHE	2.6
1	A	1034	TYR	2.5
1	C	3027	PHE	2.5
1	A	1091	LEU	2.5
1	B	2034	TYR	2.5
1	E	5050	VAL	2.5
1	D	4315	PHE	2.5
1	B	2204	GLU	2.5
1	C	3068	HIS	2.5
1	C	3143	ILE	2.4
1	A	1132	THR	2.4
1	C	3070	THR	2.4
1	B	2032	MET	2.4
1	E	5162	ARG	2.4
1	A	1133	LYS	2.3
1	D	4141	GLU	2.3
1	E	5040	ARG	2.3
1	E	5035	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	5055	ASP	2.3
1	D	4061	TRP	2.3
1	E	5141	GLU	2.3
1	B	2010	LYS	2.3
1	D	4305	THR	2.2
1	C	3203	PRO	2.2
1	C	3037	GLU	2.2
1	B	2039	PHE	2.2
1	B	2066	GLY	2.2
1	E	5039	PHE	2.2
1	E	5053	PHE	2.2
1	B	2038	GLU	2.2
1	B	2245	LYS	2.1
1	C	3047	VAL	2.1
1	E	5314	ASN	2.1
1	D	4155	ARG	2.1
1	C	3309	GLY	2.1
1	C	3045	THR	2.1
1	A	1047	VAL	2.1
1	C	3042	PHE	2.1
1	E	5052	PRO	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	CA	B	6201	1/1	0.92	0.36	4.93	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	CA	B	6212	1/1	0.90	0.34	2.83	125,125,125,125	0
2	CA	D	6214	1/1	0.74	0.33	1.68	125,125,125,125	0
2	CA	C	6202	1/1	0.85	0.19	-0.83	133,133,133,133	0
2	CA	D	6204	1/1	0.95	0.16	-1.16	133,133,133,133	0
2	CA	D	6203	1/1	0.97	0.12	-1.60	133,133,133,133	0
2	CA	A	6205	1/1	0.93	0.07	-3.22	133,133,133,133	0
2	CA	C	6213	1/1	0.96	0.18	-	125,125,125,125	0
2	CA	A	6301	1/1	0.94	0.14	-	97,97,97,97	1
2	CA	B	6102	1/1	0.95	0.96	-	114,114,114,114	0
2	CA	A	6101	1/1	0.82	0.66	-	157,157,157,157	0
2	CA	A	6211	1/1	0.97	0.63	-	125,125,125,125	0
2	CA	E	6215	1/1	0.85	0.33	-	125,125,125,125	0

6.5 Other polymers

There are no such residues in this entry.