



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 02:40 PM 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 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/ValidationPDFNotes.html>

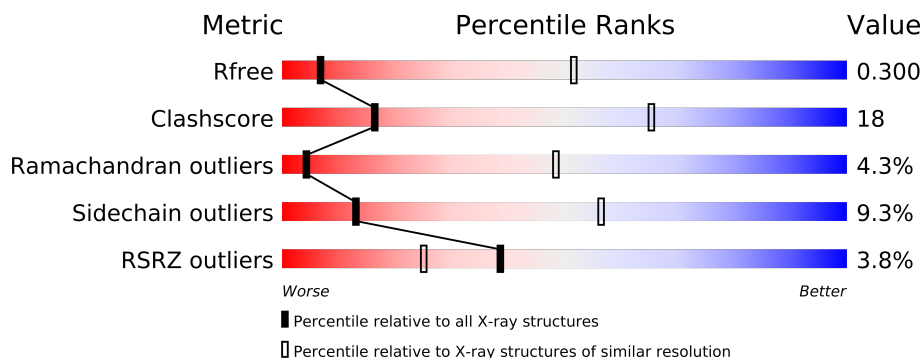
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **FAILED**
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1098 (4.00-3.40)
Clashscore	79885	1009 (3.94-3.46)
Ramachandran outliers	78287	1016 (3.98-3.42)
Sidechain outliers	78261	1014 (3.98-3.42)
RSRZ outliers	66119	1099 (4.00-3.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	354	
1	B	354	
1	C	354	
1	D	354	
1	E	354	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	A	6211	-	X
2	CA	B	6102	-	X
2	CA	B	6201	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	CA	B	6212	-	X
2	CA	D	6214	-	X
2	CA	E	6215	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13698 atoms, of which 0 are hydrogen and 0 are deuterium.

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).

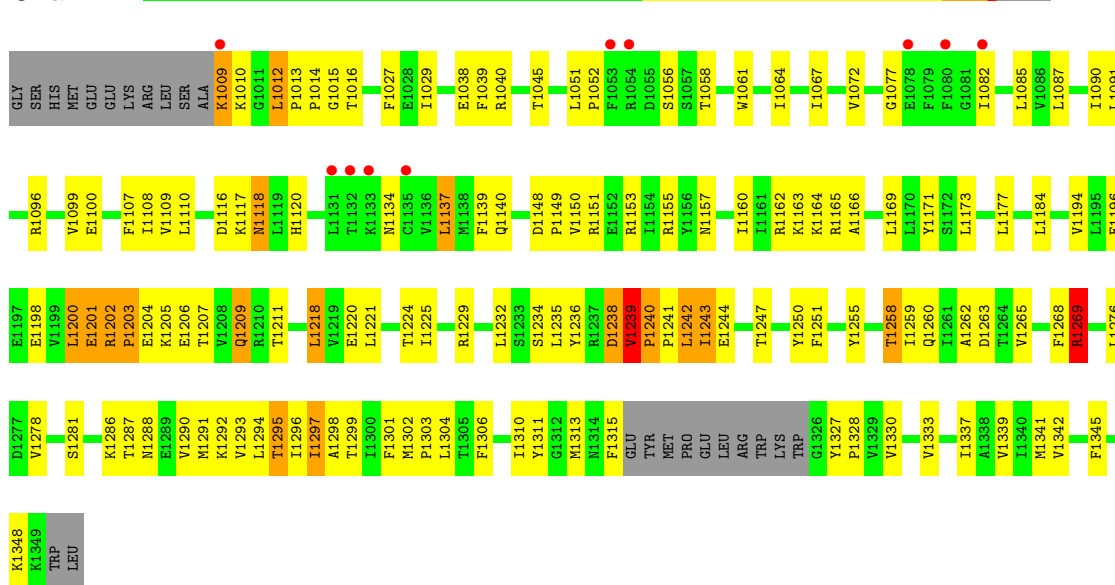
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Ca 3	0	0
2	A	4	Total 4	Ca 4	0	0
2	D	3	Total 3	Ca 3	0	0
2	C	2	Total 2	Ca 2	0	0
2	E	1	Total 1	Ca 1	0	0

3 Residue-property plots

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.

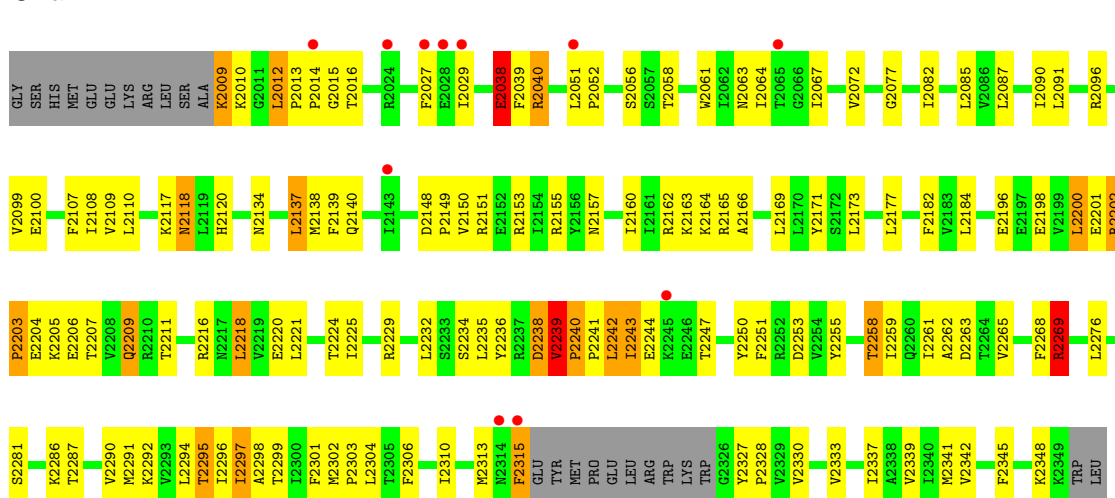
• Molecule 1: Magnesium transport protein corA

Chain A:



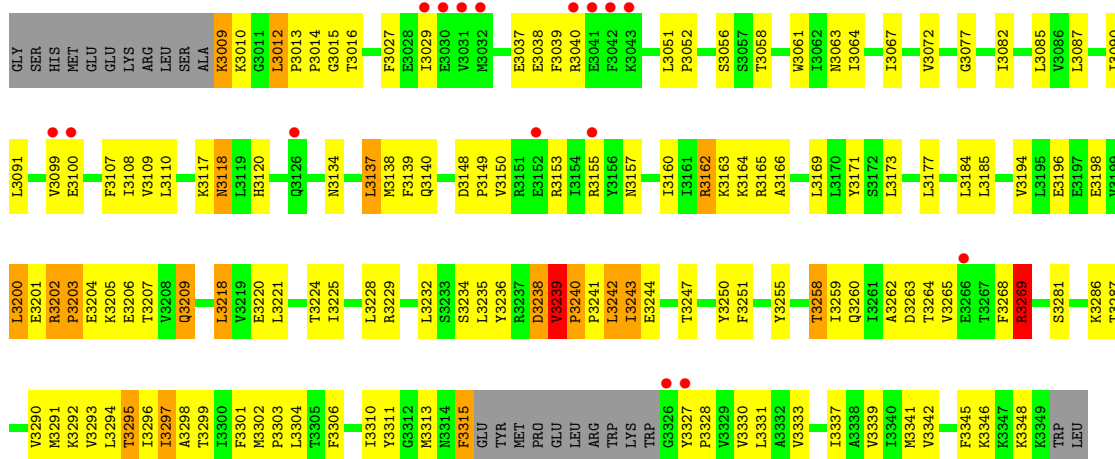
• Molecule 1: Magnesium transport protein corA

Chain B:



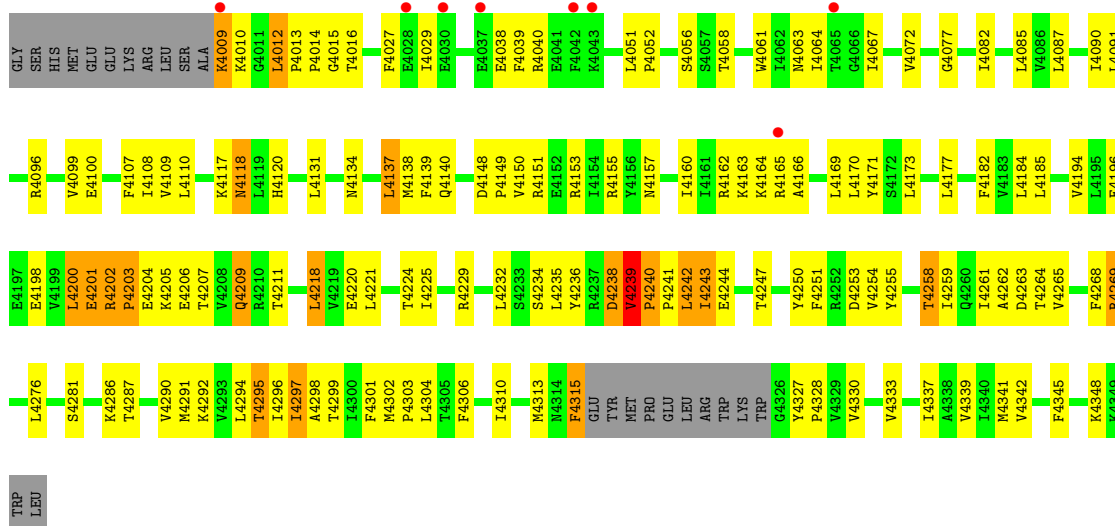
• Molecule 1: Magnesium transport protein corA

Chain C:



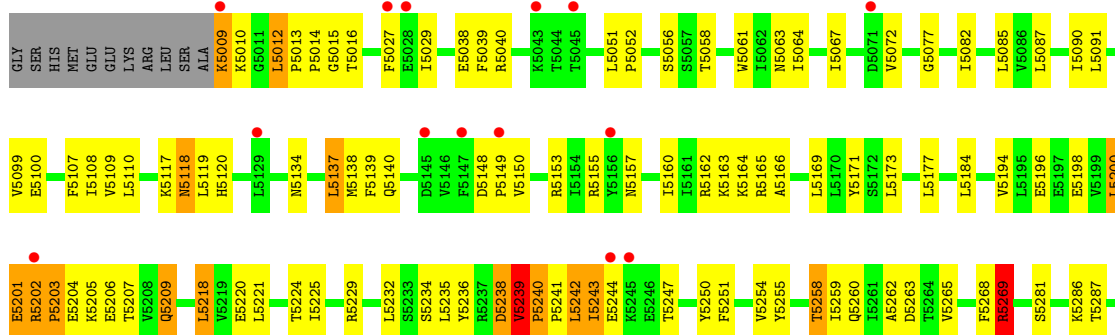
- Molecule 1: Magnesium transport protein corA

Chain D:



- Molecule 1: Magnesium transport protein corA

Chain E:



V5290	M5291	K5292	V5293	L5294	T5295	I5296	I5297	A5298	T5299	I5300	F5301	M5302	F5303	L5304	T5305	F5306	I5310	Y5311	G5312	M5313	M5314	F5315	GLI	TYR	NET	PRO	GLU	LEU	ARG	TRP	LYS	TRP	G5326	Y5327	P5328	V5329	V5330	V5333	I5337	A5338	V5339	I5340	M5341	V5342	V5343	Y5344	F5345	K5348	F5349	TRP	LEU
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4 Data and refinement statistics

Xtriage (Phenix) failed to run properly - this section will therefore be incomplete.

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
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
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 74.6	EDS
Estimated twinning fraction	No twinning to report.	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

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(°)	Ideal(°)
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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (499) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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	Distance(Å)	Clash(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%)	4	48
1	B	327/354 (92%)	258 (79%)	55 (17%)	14 (4%)	4	48
1	C	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	4	48
1	D	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	4	48
1	E	327/354 (92%)	256 (78%)	57 (17%)	14 (4%)	4	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1635/1770 (92%)	1282 (78%)	283 (17%)	70 (4%)	4 48

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
1	B	2157	ASN
1	B	2239	VAL
1	C	3012	LEU
1	C	3016	THR
1	C	3157	ASN
1	C	3239	VAL

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Mol	Chain	Res	Type
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%)	282 (91%)	29 (9%)	13	56
1	B	311/332 (94%)	282 (91%)	29 (9%)	13	56
1	C	311/332 (94%)	282 (91%)	29 (9%)	13	56
1	D	311/332 (94%)	282 (91%)	29 (9%)	13	56
1	E	311/332 (94%)	282 (91%)	29 (9%)	13	56
All	All	1555/1660 (94%)	1410 (91%)	145 (9%)	13	56

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 chains 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.

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%)	0.25	10 (3%) 48 29	37, 137, 197, 200	0
1	B	331/354 (93%)	0.19	11 (3%) 44 28	37, 120, 183, 200	0
1	C	331/354 (93%)	0.41	16 (4%) 29 19	45, 132, 195, 200	0
1	D	331/354 (93%)	0.13	8 (2%) 56 35	49, 143, 197, 200	0
1	E	331/354 (93%)	0.29	15 (4%) 32 21	54, 151, 199, 200	0
All	All	1655/1770 (93%)	0.25	60 (3%) 38 26	37, 137, 197, 200	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2315	PHE	6.3
1	C	3032	MET	4.2
1	C	3041	GLU	4.2
1	C	3042	PHE	3.7
1	E	5245	LYS	3.6
1	D	4043	LYS	3.6
1	A	1133	LYS	3.4
1	D	4030	GLU	3.3
1	C	3155	ARG	3.3
1	A	1132	THR	3.3
1	C	3100	GLU	3.3
1	D	4165	ARG	3.3
1	E	5027	PHE	3.2
1	C	3043	LYS	3.2
1	A	1135	CYS	3.1
1	C	3040	ARG	3.1
1	E	5202	ARG	3.1
1	A	1131	LEU	3.0
1	C	3030	GLU	3.0
1	A	1009	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	2245	LYS	2.8
1	B	2065	THR	2.7
1	A	1080	PHE	2.7
1	E	5145	ASP	2.7
1	B	2027	PHE	2.7
1	C	3327	TYR	2.7
1	D	4009	LYS	2.6
1	D	4037	GLU	2.6
1	E	5344	TYR	2.6
1	E	5009	LYS	2.6
1	D	4042	PHE	2.6
1	C	3029	ILE	2.6
1	B	2028	GLU	2.5
1	E	5244	GLU	2.5
1	E	5045	THR	2.5
1	E	5129	LEU	2.5
1	A	1054	ARG	2.5
1	A	1078	GLU	2.4
1	E	5028	GLU	2.4
1	E	5043	LYS	2.4
1	E	5156	TYR	2.4
1	D	4065	THR	2.4
1	C	3031	VAL	2.3
1	E	5147	PHE	2.3
1	C	3126	GLN	2.3
1	C	3152	GLU	2.3
1	E	5071	ASP	2.3
1	E	5149	PRO	2.3
1	D	4028	GLU	2.2
1	B	2314	ASN	2.2
1	B	2029	ILE	2.2
1	B	2051	LEU	2.2
1	C	3266	GLU	2.1
1	B	2024	ARG	2.1
1	A	1053	PHE	2.1
1	C	3099	VAL	2.1
1	B	2014	PRO	2.1
1	B	2143	ILE	2.0
1	C	3326	GLY	2.0
1	A	1082	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CA	B	6102	1/1	0.83	15.54	114,114,114,114	0
2	CA	A	6211	1/1	0.69	6.33	125,125,125,125	0
2	CA	B	6212	1/1	0.42	5.86	125,125,125,125	0
2	CA	E	6215	1/1	0.29	3.41	125,125,125,125	0
2	CA	D	6214	1/1	0.34	3.36	125,125,125,125	0
2	CA	B	6201	1/1	0.43	2.09	133,133,133,133	0
2	CA	C	6213	1/1	0.22	0.26	125,125,125,125	0
2	CA	C	6202	1/1	0.21	-0.34	133,133,133,133	0
2	CA	D	6204	1/1	0.17	-1.14	133,133,133,133	0
2	CA	D	6203	1/1	0.14	-1.15	133,133,133,133	0
2	CA	A	6205	1/1	0.07	-2.74	133,133,133,133	0
2	CA	A	6301	1/1	0.13	-3.06	97,97,97,97	1
2	CA	A	6101	1/1	0.74	-	157,157,157,157	0

6.5 Other polymers ⓘ

There are no such residues in this entry.