



Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2020 – 10:28 pm BST

PDB ID : 2WLK
Title : STRUCTURE OF THE ATP-SENSITIVE INWARD RECTIFIER POTASSIUM CHANNEL FROM MAGNETOSPIRILLUM MAGNETOTACTICUM
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Deposited on : 2009-06-24
Resolution : 2.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

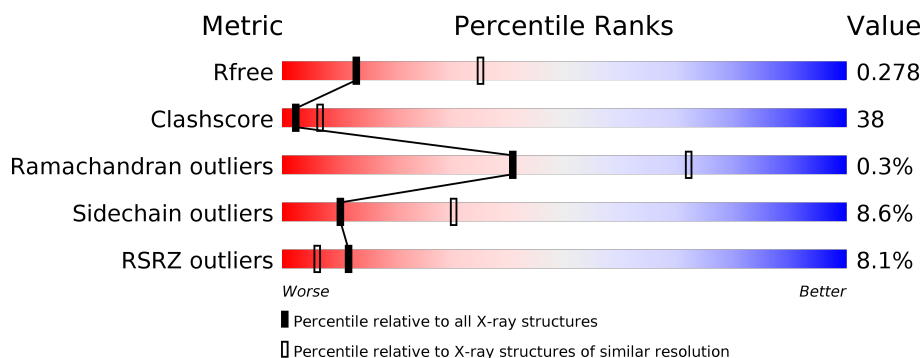
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 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	301	<div> <div>8%</div> <div>46%</div> <div>44%</div> <div>5% . .</div> </div>
1	B	301	<div> <div>8%</div> <div>45%</div> <div>44%</div> <div>6% . .</div> </div>

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
4	SPM	B	1302	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6100 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 ATP-SENSITIVE INWARD RECTIFIER POTASSIUM CHANNEL 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	20	103	0
			3021	1957	512	538	14			
1	B	291	Total	C	N	O	S	20	103	0
			3026	1960	514	538	14			

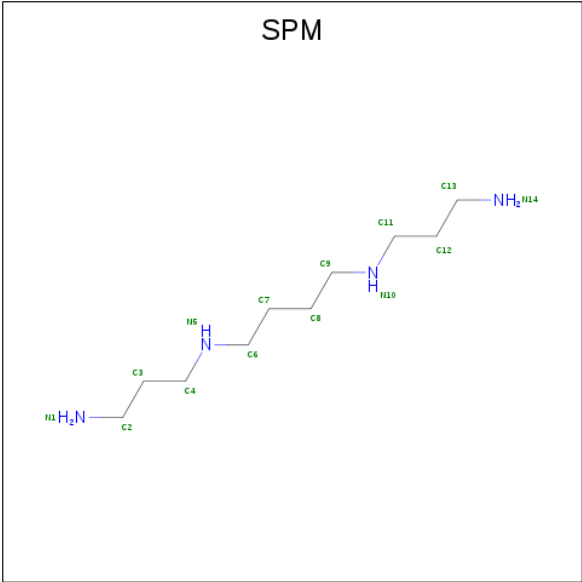
- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	K	0	0
			5	5		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	0
			1	1		

- Molecule 4 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			14	10	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	14	Total	O	0	0
			14	14		
5	B	19	Total	O	0	0
			19	19		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	105.76Å 107.53Å 89.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.76 – 2.80 28.17 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (28.76-2.80) 94.6 (28.17-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.247 , 0.280 0.248 , 0.278	Depositor DCC
R_{free} test set	1308 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	61.1	Xtriage
Anisotropy	0.463	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.357 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6100	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: K, SPM, CL

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	11.04	10/3122 (0.3%)	1.70	22/4253 (0.5%)
1	B	11.04	10/3128 (0.3%)	1.70	21/4261 (0.5%)
All	All	11.04	20/6250 (0.3%)	1.70	43/8514 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
All	All	0	8

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	37[A]	HIS	CB-CG	314.06	7.15	1.50
1	A	37[B]	HIS	CB-CG	314.06	7.15	1.50
1	B	37[A]	HIS	CB-CG	313.84	7.14	1.50
1	B	37[B]	HIS	CB-CG	313.84	7.14	1.50
1	B	40[A]	ASP	CB-CG	223.80	6.21	1.51
1	B	40[B]	ASP	CB-CG	223.80	6.21	1.51
1	A	40[A]	ASP	CB-CG	223.43	6.21	1.51
1	A	40[B]	ASP	CB-CG	223.43	6.21	1.51
1	B	39[A]	HIS	CB-CG	202.82	5.15	1.50
1	B	39[B]	HIS	CB-CG	202.82	5.15	1.50
1	A	39[A]	HIS	CB-CG	202.14	5.13	1.50
1	A	39[B]	HIS	CB-CG	202.14	5.13	1.50
1	A	136[B]	THR	C-N	-19.83	0.88	1.34
1	B	136[B]	THR	C-N	-19.65	0.88	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	31	ARG	C-N	13.56	1.57	1.33
1	A	31	ARG	C-N	10.79	1.52	1.33
1	A	262	CYS	CB-SG	-6.68	1.70	1.82
1	B	262	CYS	CB-SG	-5.73	1.72	1.81
1	A	29	GLU	C-N	-5.63	1.21	1.34
1	B	29	GLU	C-N	-5.37	1.21	1.34

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	136[B]	THR	O-C-N	-54.71	35.17	122.70
1	A	136[B]	THR	O-C-N	-53.71	36.76	122.70
1	B	40[A]	ASP	CB-CG-OD1	-37.71	84.36	118.30
1	B	40[B]	ASP	CB-CG-OD1	-37.71	84.36	118.30
1	A	40[A]	ASP	CB-CG-OD1	-37.66	84.41	118.30
1	A	40[B]	ASP	CB-CG-OD1	-37.66	84.41	118.30
1	B	29	GLU	O-C-N	-32.82	70.19	122.70
1	A	29	GLU	O-C-N	-32.24	71.11	122.70
1	B	39[A]	HIS	CB-CG-ND1	-19.30	74.95	123.20
1	B	39[B]	HIS	CB-CG-ND1	-19.30	74.95	123.20
1	A	39[A]	HIS	CB-CG-ND1	-19.21	75.17	123.20
1	A	39[B]	HIS	CB-CG-ND1	-19.21	75.17	123.20
1	A	39[A]	HIS	CB-CG-CD2	-19.10	71.59	130.80
1	A	39[B]	HIS	CB-CG-CD2	-19.10	71.59	130.80
1	B	39[A]	HIS	CB-CG-CD2	-19.03	71.81	130.80
1	B	39[B]	HIS	CB-CG-CD2	-19.03	71.81	130.80
1	B	40[A]	ASP	CB-CG-OD2	16.53	133.17	118.30
1	B	40[B]	ASP	CB-CG-OD2	16.53	133.17	118.30
1	A	40[A]	ASP	CB-CG-OD2	16.48	133.13	118.30
1	A	40[B]	ASP	CB-CG-OD2	16.48	133.13	118.30
1	B	29	GLU	CA-C-N	16.12	152.66	117.20
1	A	29	GLU	CA-C-N	15.76	151.87	117.20
1	B	37[A]	HIS	CB-CG-CD2	-14.57	85.62	130.80
1	B	37[B]	HIS	CB-CG-CD2	-14.57	85.62	130.80
1	A	37[A]	HIS	CB-CG-CD2	-14.49	85.89	130.80
1	A	37[B]	HIS	CB-CG-CD2	-14.49	85.89	130.80
1	B	136[B]	THR	CA-C-N	11.82	143.20	117.20
1	A	136[B]	THR	CA-C-N	11.18	141.80	117.20
1	A	30	LYS	N-CA-CB	-9.35	93.78	110.60
1	B	30	LYS	N-CA-CB	-9.33	93.80	110.60
1	B	29	GLU	C-N-CA	9.18	144.66	121.70
1	A	29	GLU	C-N-CA	8.95	144.07	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	136[B]	THR	C-N-CA	7.58	140.64	121.70
1	A	202	ARG	N-CA-CB	-6.71	98.53	110.60
1	B	136[B]	THR	C-N-CA	6.60	138.21	121.70
1	A	59[A]	VAL	CB-CA-C	6.33	123.43	111.40
1	A	59[B]	VAL	CB-CA-C	6.33	123.43	111.40
1	A	39[A]	HIS	CA-CB-CG	5.96	123.74	113.60
1	A	39[B]	HIS	CA-CB-CG	5.96	123.74	113.60
1	B	39[A]	HIS	CA-CB-CG	5.82	123.49	113.60
1	B	39[B]	HIS	CA-CB-CG	5.82	123.49	113.60
1	B	44[A]	VAL	CB-CA-C	-5.17	101.59	111.40
1	B	44[B]	VAL	CB-CA-C	-5.17	101.59	111.40

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136[B]	THR	Mainchain,Peptide
1	A	29	GLU	Mainchain,Peptide
1	B	136[B]	THR	Mainchain,Peptide
1	B	29	GLU	Mainchain,Peptide

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	3021	0	2981	240	0
1	B	3026	0	2987	242	0
2	A	5	0	0	0	0
3	A	1	0	0	0	0
4	B	14	0	26	5	1
5	A	14	0	0	2	0
5	B	19	0	0	6	1
All	All	6100	0	5994	453	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (453) 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:B:76[B]:GLU:O	1:B:102[B]:LEU:CD2	1.64	1.43
1:B:38[A]:TYR:CD1	1:B:42[A]:LEU:HD12	1.52	1.41
1:A:38[A]:TYR:CD1	1:A:42[A]:LEU:HD12	1.53	1.40
1:A:139:THR:HG22	1:A:167:ARG:NH2	1.49	1.27
1:A:139:THR:CG2	1:A:167:ARG:HH22	1.49	1.22
1:B:139:THR:HG22	1:B:167:ARG:NH2	1.56	1.20
1:A:44[B]:VAL:O	1:A:134[B]:ARG:NH2	1.75	1.19
1:B:44[B]:VAL:O	1:B:134[B]:ARG:NH2	1.77	1.17
1:A:278:LEU:HG	1:A:279:PRO:CD	1.74	1.17
1:B:139:THR:CG2	1:B:167:ARG:HH22	1.61	1.11
1:B:36[B]:ASP:CB	1:B:40[B]:ASP:OD2	1.98	1.11
1:A:278:LEU:CG	1:A:279:PRO:HD2	1.79	1.11
1:B:127[B]:ALA:O	1:B:131[B]:ILE:HD12	1.51	1.10
1:B:49[A]:PHE:CZ	1:B:53[A]:ILE:HD11	1.86	1.10
1:B:206:PRO:HD2	5:B:2011:HOH:O	1.51	1.09
1:A:127[B]:ALA:O	1:A:131[B]:ILE:HD12	1.53	1.09
1:A:36[B]:ASP:CB	1:A:40[B]:ASP:OD2	2.01	1.08
1:A:278:LEU:HG	1:A:279:PRO:HD2	1.09	1.07
1:B:76[B]:GLU:O	1:B:102[B]:LEU:HD23	0.91	1.06
1:A:114[B]:THR:HG22	1:B:91[B]:VAL:HG11	1.35	1.06
1:B:77[B]:ASN:C	1:B:102[B]:LEU:HD21	1.76	1.05
1:A:38[A]:TYR:CD1	1:A:42[A]:LEU:CD1	2.39	1.05
1:B:38[A]:TYR:CD1	1:B:42[A]:LEU:CD1	2.38	1.05
1:A:49[A]:PHE:CZ	1:A:53[A]:ILE:HD11	1.92	1.04
1:B:278:LEU:HB3	1:B:279:PRO:HD2	1.39	1.04
1:A:77[B]:ASN:C	1:A:102[B]:LEU:HD21	1.77	1.03
1:A:139:THR:CG2	1:A:167:ARG:NH2	2.15	0.99
1:A:127[B]:ALA:O	1:A:131[B]:ILE:CD1	2.12	0.97
1:A:33:TRP:O	1:A:38[B]:TYR:N	1.98	0.97
1:B:139:THR:HG22	1:B:167:ARG:HH22	0.81	0.97
1:B:139:THR:CG2	1:B:167:ARG:NH2	2.24	0.97
1:B:127[B]:ALA:O	1:B:131[B]:ILE:CD1	2.12	0.96
1:A:61[B]:ASN:ND2	1:A:90[B]:SER:OG	1.99	0.95
1:B:33:TRP:O	1:B:38[B]:TYR:N	2.00	0.93
1:A:114[A]:THR:HG22	1:B:91[A]:VAL:HG11	1.48	0.93
1:B:33:TRP:O	1:B:37[B]:HIS:N	2.02	0.92
1:B:38[A]:TYR:HD1	1:B:42[A]:LEU:HD12	1.14	0.92
1:A:33:TRP:O	1:A:37[B]:HIS:N	2.03	0.92
1:A:134[B]:ARG:HG2	1:A:134[B]:ARG:HH11	1.34	0.91
1:B:134[B]:ARG:HG2	1:B:134[B]:ARG:HH11	1.33	0.91
1:A:163:LEU:CD1	1:A:208:PHE:CZ	2.54	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61[B]:ASN:ND2	1:B:90[B]:SER:OG	2.03	0.91
1:A:138:PRO:HG3	1:A:252:GLN:OE1	1.71	0.90
1:A:38[A]:TYR:HD1	1:A:42[A]:LEU:HD12	1.14	0.90
1:B:161:MET:HE2	1:B:214:VAL:HB	1.52	0.89
1:B:161:MET:CE	1:B:214:VAL:HB	2.04	0.88
1:A:37[B]:HIS:O	1:A:41[B]:LEU:HD12	1.73	0.88
1:A:146:SER:H	1:A:291:HIS:HD2	1.16	0.87
1:B:38[A]:TYR:CE1	1:B:42[A]:LEU:CD1	2.58	0.87
1:A:38[A]:TYR:CE1	1:A:42[A]:LEU:CD1	2.59	0.86
1:B:146:SER:H	1:B:291:HIS:HD2	1.19	0.86
1:B:49[A]:PHE:CZ	1:B:53[A]:ILE:CD1	2.60	0.85
1:A:38[A]:TYR:CE1	1:A:42[A]:LEU:HD12	2.10	0.85
1:B:37[B]:HIS:O	1:B:41[B]:LEU:HD12	1.76	0.85
1:B:38[A]:TYR:CE1	1:B:42[A]:LEU:HD12	2.10	0.85
1:B:138:PRO:HG3	1:B:252:GLN:OE1	1.76	0.84
1:A:161:MET:HE2	1:A:214:VAL:HB	1.58	0.84
1:A:182:ARG:HA	1:A:193:ARG:NH1	1.95	0.82
1:B:59[A]:VAL:O	1:B:63[A]:LEU:HG	1.79	0.81
1:A:139:THR:HG22	1:A:167:ARG:HH22	0.67	0.81
1:A:121[B]:MET:SD	1:B:124[B]:LEU:HD12	2.21	0.81
1:B:140:ALA:HB2	1:B:254:VAL:HB	1.60	0.81
1:A:79[B]:ARG:HG3	1:A:85[B]:ASP:OD2	1.81	0.81
1:A:161:MET:CE	1:A:214:VAL:HB	2.11	0.80
1:B:182:ARG:HA	1:B:193:ARG:NH1	1.96	0.80
1:B:76[B]:GLU:O	1:B:102[B]:LEU:HD22	1.79	0.79
1:B:163:LEU:CD1	1:B:208:PHE:CZ	2.65	0.79
1:B:49[A]:PHE:CE2	1:B:53[A]:ILE:CD1	2.65	0.79
1:A:49[A]:PHE:CZ	1:A:53[A]:ILE:CD1	2.64	0.79
4:B:1302:SPM:H121	5:B:2019:HOH:O	1.82	0.79
1:B:169:GLU:HG2	1:B:249:ALA:HB2	1.65	0.78
1:A:169:GLU:HG2	1:A:249:ALA:HB2	1.66	0.77
1:A:134[B]:ARG:HG2	1:A:134[B]:ARG:NH1	1.96	0.77
1:A:146:SER:H	1:A:291:HIS:CD2	2.01	0.77
1:A:100[A]:GLY:O	1:A:103[A]:ILE:HG23	1.83	0.77
1:B:79[B]:ARG:HG3	1:B:85[B]:ASP:OD2	1.86	0.76
1:B:169:GLU:OE2	1:B:169:GLU:N	2.18	0.76
1:A:140:ALA:HB2	1:A:254:VAL:HB	1.67	0.75
1:A:210:LEU:HB3	1:A:285:LEU:CD1	2.17	0.74
1:A:38[B]:TYR:CZ	1:A:42[B]:LEU:HD11	2.22	0.74
1:B:103[A]:ILE:HG23	1:B:104[A]:PRO:HD2	1.69	0.74
1:A:49[A]:PHE:CE2	1:A:53[A]:ILE:CD1	2.71	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76[B]:GLU:C	1:B:102[B]:LEU:CD2	2.54	0.73
1:B:13:ARG:HD3	1:B:15:LEU:O	1.88	0.73
1:A:255:HIS:NE2	5:A:2009:HOH:O	2.21	0.73
1:A:13:ARG:HD3	1:A:15:LEU:O	1.89	0.73
1:A:169:GLU:OE2	1:A:169:GLU:N	2.22	0.72
1:A:255:HIS:CE1	1:B:246:HIS:CE1	2.77	0.72
1:A:42[A]:LEU:HD21	1:A:130[A]:LEU:HD22	1.69	0.72
1:B:76[B]:GLU:C	1:B:102[B]:LEU:HD23	2.02	0.72
1:B:77[B]:ASN:HB2	1:B:102[B]:LEU:HD23	1.72	0.72
1:B:77[B]:ASN:C	1:B:102[B]:LEU:CD2	2.57	0.72
1:A:104[B]:PRO:HG3	1:A:113[B]:VAL:HG21	1.70	0.72
1:A:163:LEU:HD12	1:A:208:PHE:CZ	2.23	0.72
1:B:100[A]:GLY:O	1:B:103[A]:ILE:HG13	1.89	0.72
1:A:285:LEU:HD21	1:A:287:LEU:CD2	2.20	0.71
1:B:68[A]:TYR:O	1:B:71[A]:CYS:HB2	1.88	0.71
1:A:207:ILE:HG22	1:A:207:ILE:O	1.88	0.70
1:B:146:SER:H	1:B:291:HIS:CD2	2.07	0.70
1:A:34[B]:LEU:C	1:A:36[B]:ASP:H	1.92	0.70
1:B:74[A]:VAL:O	1:B:105[A]:ILE:HB	1.91	0.70
1:A:278:LEU:HG	1:A:279:PRO:HD3	1.73	0.70
1:B:207:ILE:HG22	1:B:207:ILE:O	1.91	0.70
1:B:34[B]:LEU:C	1:B:36[B]:ASP:H	1.94	0.70
1:A:104[A]:PRO:O	1:A:105[A]:ILE:HD13	1.92	0.69
1:B:104[B]:PRO:HG3	1:B:113[B]:VAL:HG21	1.74	0.69
1:A:68[A]:TYR:O	1:A:71[A]:CYS:HB2	1.91	0.69
1:B:74[A]:VAL:HG22	1:B:74[A]:VAL:O	1.91	0.69
1:B:118[B]:LEU:O	1:B:121[B]:MET:HB3	1.92	0.69
1:A:255:HIS:HE1	1:B:246:HIS:CE1	2.11	0.69
1:A:74[A]:VAL:O	1:A:105[A]:ILE:HB	1.93	0.69
1:B:163:LEU:HD12	1:B:208:PHE:CZ	2.28	0.69
1:A:186:SER:OG	1:A:190:MET:HG3	1.93	0.68
1:B:42[A]:LEU:HD21	1:B:130[A]:LEU:HD22	1.73	0.68
1:B:182:ARG:HA	1:B:193:ARG:HH12	1.58	0.68
1:A:124[A]:LEU:HD12	1:A:124[A]:LEU:O	1.93	0.68
1:A:77[B]:ASN:C	1:A:102[B]:LEU:CD2	2.59	0.68
1:B:104[A]:PRO:O	1:B:105[A]:ILE:HD13	1.94	0.68
1:B:49[A]:PHE:CE2	1:B:53[A]:ILE:HD12	2.29	0.68
1:A:285:LEU:HD21	1:A:287:LEU:HD21	1.76	0.68
1:A:49[A]:PHE:CE2	1:A:53[A]:ILE:HD12	2.29	0.68
1:A:74[A]:VAL:HG22	1:A:74[A]:VAL:O	1.94	0.68
1:A:255:HIS:CD2	5:A:2009:HOH:O	2.47	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:SER:OG	1:B:190:MET:HG3	1.95	0.67
1:A:182:ARG:HA	1:A:193:ARG:HH12	1.57	0.67
1:B:134[B]:ARG:CG	1:B:134[B]:ARG:HH11	2.08	0.67
1:B:210:LEU:HB3	1:B:285:LEU:CD1	2.25	0.67
1:B:280:ASP:C	1:B:280:ASP:OD1	2.34	0.67
1:A:280:ASP:OD1	1:A:280:ASP:C	2.33	0.66
1:B:134[B]:ARG:HG2	1:B:134[B]:ARG:NH1	1.96	0.66
1:A:38[B]:TYR:HE2	1:B:138:PRO:HB3	1.60	0.66
1:B:278:LEU:HB3	1:B:279:PRO:CD	2.21	0.66
1:A:118[B]:LEU:O	1:A:121[B]:MET:HB3	1.96	0.66
1:B:38[B]:TYR:CZ	1:B:42[B]:LEU:HD11	2.31	0.66
1:A:77[B]:ASN:HB2	1:A:102[B]:LEU:HD23	1.78	0.65
1:B:124[A]:LEU:O	1:B:124[A]:LEU:HD12	1.96	0.65
1:A:32:GLY:CA	1:B:167:ARG:HE	2.09	0.65
1:B:186:SER:OG	1:B:190:MET:CG	2.45	0.65
1:B:110[B]:ASN:O	1:B:114[B]:THR:HG23	1.97	0.65
1:A:170:GLN:HG2	1:A:209:SER:HB3	1.79	0.65
1:B:37[A]:HIS:O	1:B:41[A]:LEU:CB	2.45	0.65
1:A:37[A]:HIS:O	1:A:41[A]:LEU:CB	2.46	0.64
1:A:42[B]:LEU:HD12	1:B:250:PHE:HD2	1.63	0.63
1:A:118[B]:LEU:HD13	1:B:57[B]:TYR:CD1	2.33	0.63
1:A:110[B]:ASN:O	1:A:114[B]:THR:HG23	1.99	0.62
1:A:278:LEU:CB	1:A:279:PRO:HD2	2.29	0.62
1:A:296:HIS:HE1	1:A:298:HIS:CD2	2.17	0.62
1:A:114[B]:THR:HG22	1:B:91[B]:VAL:CG1	2.23	0.62
1:A:198:LEU:HB3	1:A:216:HIS:ND1	2.15	0.62
1:A:107[B]:PRO:O	1:A:111[B]:THR:N	2.33	0.61
1:B:285:LEU:HD21	1:B:287:LEU:CD2	2.31	0.61
1:A:186:SER:OG	1:A:190:MET:CG	2.47	0.61
1:B:40[B]:ASP:O	1:B:44[B]:VAL:HG13	2.00	0.61
1:B:62[A]:ALA:O	1:B:65[A]:ALA:HB3	2.01	0.61
1:A:118[B]:LEU:HD13	1:B:57[B]:TYR:CE1	2.35	0.61
1:A:75[B]:ILE:HG22	1:A:102[B]:LEU:HD22	1.83	0.60
1:B:76[B]:GLU:O	1:B:77[B]:ASN:HB2	2.00	0.60
1:B:18:ASP:HB2	5:B:2002:HOH:O	2.00	0.60
1:B:75[B]:ILE:CG2	1:B:102[B]:LEU:HB3	2.31	0.60
1:A:127[B]:ALA:C	1:A:131[B]:ILE:CD1	2.70	0.59
1:A:40[B]:ASP:O	1:A:44[B]:VAL:HG13	2.02	0.59
1:A:95[A]:ALA:O	1:A:96[A]:THR:OG1	2.19	0.59
1:A:233:ARG:HH12	1:A:263:ASP:HB3	1.67	0.59
1:A:75[B]:ILE:CG2	1:A:102[B]:LEU:HB3	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:TRP:C	1:B:38[B]:TYR:H	2.06	0.59
1:B:161:MET:HE1	1:B:214:VAL:HB	1.83	0.59
1:B:75[B]:ILE:HG22	1:B:102[B]:LEU:HD22	1.85	0.58
1:B:93[B]:THR:O	1:B:96[B]:THR:N	2.35	0.58
1:B:42[A]:LEU:HD13	1:B:133[A]:ALA:HB3	1.85	0.58
1:B:285:LEU:HD21	1:B:287:LEU:HD21	1.86	0.58
1:B:127[B]:ALA:O	1:B:131[B]:ILE:HD13	2.03	0.58
1:B:127[B]:ALA:C	1:B:131[B]:ILE:CD1	2.72	0.58
1:B:296:HIS:HE1	1:B:298:HIS:CD2	2.21	0.58
1:B:74[B]:VAL:CG2	1:B:105[B]:ILE:O	2.52	0.58
1:B:37[B]:HIS:CG	1:B:38[B]:TYR:N	2.72	0.58
1:B:77[B]:ASN:CA	1:B:102[B]:LEU:HD21	2.33	0.58
1:B:107[B]:PRO:O	1:B:111[B]:THR:N	2.33	0.57
1:A:37[B]:HIS:CG	1:A:38[B]:TYR:N	2.72	0.57
1:A:78[B]:ALA:N	1:A:102[B]:LEU:CD2	2.67	0.57
1:B:239:PHE:CE1	1:B:265:ILE:HD11	2.40	0.57
1:B:45[A]:SER:OG	1:B:48[A]:VAL:HG23	2.04	0.57
1:B:34[B]:LEU:C	1:B:36[B]:ASP:N	2.58	0.57
1:B:89[A]:PHE:CE1	1:B:102[A]:LEU:O	2.58	0.57
1:B:34[B]:LEU:HB3	1:B:36[B]:ASP:H	1.69	0.57
1:A:127[B]:ALA:C	1:A:131[B]:ILE:HD13	2.25	0.57
1:A:74[B]:VAL:CG2	1:A:105[B]:ILE:O	2.52	0.57
1:B:77[B]:ASN:HB2	1:B:102[B]:LEU:CD2	2.34	0.57
1:A:34[B]:LEU:C	1:A:36[B]:ASP:N	2.57	0.56
1:A:127[B]:ALA:O	1:A:131[B]:ILE:HD13	1.99	0.56
1:B:37[A]:HIS:O	1:B:41[A]:LEU:HB3	2.05	0.56
1:B:198:LEU:HB3	1:B:216:HIS:ND1	2.20	0.56
1:A:45[A]:SER:OG	1:A:48[A]:VAL:HG23	2.06	0.56
1:A:134[B]:ARG:CG	1:A:134[B]:ARG:HH11	2.07	0.56
1:A:32:GLY:O	1:A:36[B]:ASP:HA	2.05	0.56
1:A:78[B]:ALA:N	1:A:102[B]:LEU:HD21	2.20	0.56
1:A:38[A]:TYR:CE1	1:A:42[A]:LEU:HD11	2.38	0.56
1:A:38[B]:TYR:OH	1:B:136[B]:THR:HG22	2.06	0.56
1:B:78[B]:ALA:N	1:B:102[B]:LEU:CD2	2.68	0.56
1:B:48[B]:VAL:O	1:B:52[B]:LEU:HG	2.06	0.55
1:B:38[A]:TYR:CE1	1:B:42[A]:LEU:HD11	2.38	0.55
1:A:33:TRP:C	1:A:38[B]:TYR:H	2.05	0.55
1:A:95[A]:ALA:HB3	1:A:97[A]:ILE:HG13	1.88	0.55
1:B:77[B]:ASN:CB	1:B:102[B]:LEU:CD2	2.84	0.55
1:A:34[B]:LEU:HB3	1:A:36[B]:ASP:H	1.71	0.55
1:B:169:GLU:HG2	1:B:249:ALA:CB	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108[A]:LEU:O	1:A:111[A]:THR:HG22	2.07	0.55
1:A:42[A]:LEU:O	1:A:137:ARG:NH1	2.40	0.55
1:A:48[B]:VAL:O	1:A:52[B]:LEU:HG	2.06	0.55
1:B:77[B]:ASN:CB	1:B:102[B]:LEU:HD21	2.37	0.55
1:A:32:GLY:HA3	1:B:167:ARG:HE	1.71	0.55
1:A:33:TRP:O	1:A:37[B]:HIS:ND1	2.40	0.55
1:B:170:GLN:HG2	1:B:209:SER:HB3	1.90	0.54
1:A:37[A]:HIS:O	1:A:41[A]:LEU:HB3	2.06	0.54
1:A:128[B]:ALA:HA	1:A:131[B]:ILE:HD13	1.90	0.54
1:A:110[B]:ASN:HB3	1:B:88[B]:PHE:CD2	2.42	0.54
1:A:89[A]:PHE:CE1	1:A:102[A]:LEU:O	2.61	0.54
1:A:200:LEU:O	1:A:201:THR:C	2.44	0.54
1:B:95[A]:ALA:HB3	1:B:97[A]:ILE:HG13	1.90	0.54
1:A:73[B]:ASP:OD2	1:A:80[B]:PRO:HB3	2.08	0.53
1:B:32:GLY:O	1:B:36[B]:ASP:HA	2.07	0.53
1:A:77[B]:ASN:CA	1:A:102[B]:LEU:HD21	2.38	0.53
1:B:276:THR:HG22	1:B:277:THR:N	2.24	0.53
1:A:93[B]:THR:O	1:A:96[B]:THR:N	2.37	0.53
1:B:33:TRP:O	1:B:37[B]:HIS:CA	2.57	0.53
1:A:161:MET:O	1:A:161:MET:HE2	2.09	0.53
1:A:161:MET:HE1	1:A:214:VAL:HB	1.90	0.53
1:B:108[A]:LEU:O	1:B:111[A]:THR:HG22	2.09	0.53
1:A:42[A]:LEU:HD13	1:A:133[A]:ALA:HB3	1.90	0.53
1:B:61[A]:ASN:HD21	1:B:94[A]:MET:HE2	1.74	0.53
1:A:172:ILE:O	1:A:173:GLU:HB2	2.07	0.52
1:B:76[B]:GLU:O	1:B:102[B]:LEU:HA	2.09	0.52
1:A:207:ILE:CG2	1:A:207:ILE:O	2.56	0.52
1:B:73[B]:ASP:CG	1:B:80[B]:PRO:HB3	2.29	0.52
1:A:110[A]:ASN:HB3	1:B:88[A]:PHE:CE2	2.44	0.52
1:A:121[B]:MET:HE1	1:B:127[B]:ALA:CB	2.39	0.52
1:A:139:THR:HG21	1:A:167:ARG:NH2	2.16	0.52
1:B:148:MET:HE1	1:B:239:PHE:HB2	1.90	0.52
1:A:251:ALA:O	1:A:252:GLN:HG3	2.10	0.52
1:B:33:TRP:O	1:B:37[B]:HIS:ND1	2.41	0.52
1:A:76[B]:GLU:O	1:A:77[B]:ASN:HB2	2.09	0.52
1:B:132[A]:TYR:CD2	4:B:1302:SPM:H82	2.44	0.52
1:A:110[A]:ASN:HB3	1:B:88[A]:PHE:CZ	2.45	0.52
1:B:127[B]:ALA:C	1:B:131[B]:ILE:HD13	2.30	0.52
1:A:33:TRP:O	1:A:37[B]:HIS:CA	2.57	0.52
1:B:42[A]:LEU:O	1:B:137:ARG:NH1	2.43	0.52
1:B:65[B]:ALA:O	1:B:68[B]:TYR:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:ALA:O	1:B:252:GLN:HG3	2.09	0.51
1:A:276:THR:HG22	1:A:277:THR:N	2.25	0.51
1:B:78[B]:ALA:N	1:B:102[B]:LEU:HD21	2.23	0.51
1:A:239:PHE:CE1	1:A:265:ILE:HD11	2.46	0.51
1:B:207:ILE:CG2	1:B:207:ILE:O	2.58	0.51
1:B:49[A]:PHE:CE1	1:B:53[A]:ILE:HD11	2.40	0.51
1:A:169:GLU:HG2	1:A:249:ALA:CB	2.38	0.51
1:A:192:PHE:CD2	1:A:192:PHE:N	2.78	0.51
1:B:39[B]:HIS:O	1:B:43[B]:THR:OG1	2.19	0.51
1:B:176:VAL:HG12	1:B:212:TRP:CH2	2.46	0.51
1:B:192:PHE:N	1:B:192:PHE:CD2	2.78	0.51
1:A:285:LEU:CD2	1:A:287:LEU:CD2	2.89	0.51
1:B:13:ARG:CG	5:B:2001:HOH:O	2.59	0.51
1:A:74[A]:VAL:CG2	1:A:105[A]:ILE:O	2.59	0.50
1:A:73[B]:ASP:CG	1:A:80[B]:PRO:HB3	2.31	0.50
1:A:209:SER:O	1:A:210:LEU:HD23	2.11	0.50
1:B:162:ARG:CZ	1:B:271:PHE:HB3	2.41	0.50
1:A:77[B]:ASN:HB2	1:A:102[B]:LEU:CD2	2.42	0.50
1:A:23:ILE:HG13	1:B:210:LEU:CD1	2.42	0.50
1:B:163:LEU:HD12	1:B:163:LEU:C	2.32	0.50
1:B:73[B]:ASP:OD1	1:B:80[B]:PRO:HA	2.11	0.50
1:A:92[B]:GLN:NE2	1:A:99[B]:TYR:HD1	2.10	0.50
1:A:61[B]:ASN:HB3	1:A:87[B]:PHE:CE1	2.47	0.50
1:B:128[B]:ALA:HA	1:B:131[B]:ILE:HD13	1.93	0.50
1:A:25:ARG:HD3	1:B:168:ILE:HD13	1.92	0.50
1:A:163:LEU:HD11	1:A:208:PHE:CZ	2.43	0.50
1:B:77[A]:ASN:HD22	1:B:101[A]:LYS:HD2	1.77	0.50
1:B:186:SER:OG	1:B:190:MET:HG2	2.11	0.50
1:A:27:GLY:O	1:A:28:LEU:HG	2.12	0.50
1:A:296:HIS:CE1	1:A:298:HIS:CD2	2.98	0.50
1:A:278:LEU:CG	1:A:279:PRO:CD	2.59	0.49
1:A:77[B]:ASN:CB	1:A:102[B]:LEU:CD2	2.91	0.49
1:B:37[A]:HIS:O	1:B:41[A]:LEU:HB2	2.12	0.49
1:A:163:LEU:C	1:A:163:LEU:HD12	2.32	0.49
1:A:76[B]:GLU:O	1:A:102[B]:LEU:HA	2.12	0.49
1:A:285:LEU:HD21	1:A:287:LEU:HD23	1.92	0.49
1:B:56[B]:LEU:O	1:B:60[B]:THR:OG1	2.30	0.49
1:A:279:PRO:HG2	1:A:280:ASP:H	1.77	0.49
1:A:103[B]:ILE:HG22	1:B:99[B]:TYR:CD2	2.48	0.49
1:B:77[B]:ASN:CA	1:B:102[B]:LEU:CD2	2.91	0.48
1:B:73[B]:ASP:OD2	1:B:80[B]:PRO:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37[A]:HIS:O	1:A:41[A]:LEU:HB2	2.12	0.48
1:A:62[A]:ALA:HB1	1:A:83[A]:PHE:HZ	1.79	0.48
1:B:169:GLU:CG	1:B:249:ALA:HB2	2.39	0.48
1:A:38[B]:TYR:CE2	1:B:138:PRO:HB3	2.45	0.48
1:B:69[A]:LEU:C	1:B:71[A]:CYS:H	2.17	0.48
1:A:110[A]:ASN:CB	1:B:88[A]:PHE:CE2	2.97	0.48
1:B:103[A]:ILE:HG23	1:B:104[A]:PRO:CD	2.43	0.48
1:B:103[A]:ILE:CG2	1:B:104[A]:PRO:HD2	2.43	0.48
1:B:210:LEU:HD22	1:B:285:LEU:HD13	1.94	0.48
1:A:278:LEU:CD2	1:A:279:PRO:HD2	2.43	0.48
1:B:172:ILE:O	1:B:173:GLU:HB2	2.13	0.48
1:B:299:HIS:N	1:B:299:HIS:ND1	2.62	0.48
1:A:104[B]:PRO:CG	1:A:113[B]:VAL:HG21	2.41	0.48
1:A:38[B]:TYR:CE1	1:B:136[B]:THR:HG22	2.48	0.48
1:B:296:HIS:CE1	1:B:298:HIS:CD2	3.02	0.48
1:A:122[A]:LEU:O	1:A:123[A]:GLY:C	2.51	0.48
1:A:69[A]:LEU:C	1:A:71[A]:CYS:H	2.18	0.47
1:B:163:LEU:HA	1:B:290:PHE:HZ	1.77	0.47
1:A:32:GLY:HA2	1:B:167:ARG:HH21	1.79	0.47
1:B:282:ARG:HB3	1:B:283:ARG:H	1.39	0.47
1:B:74[A]:VAL:CG2	1:B:105[A]:ILE:O	2.62	0.47
1:A:77[B]:ASN:O	1:A:102[B]:LEU:HD21	2.13	0.47
1:B:77[B]:ASN:O	1:B:102[B]:LEU:HD21	2.11	0.47
1:A:73[B]:ASP:OD1	1:A:80[B]:PRO:HA	2.13	0.47
1:B:233:ARG:HH12	1:B:263:ASP:HB3	1.79	0.47
1:B:89[A]:PHE:CD1	1:B:102[A]:LEU:O	2.68	0.47
1:A:33:TRP:O	1:A:37[B]:HIS:C	2.53	0.47
1:A:76[A]:GLU:HB2	1:A:105[A]:ILE:HD11	1.97	0.47
1:A:121[B]:MET:CE	1:B:127[B]:ALA:CB	2.92	0.47
1:A:74[B]:VAL:HG22	1:A:105[B]:ILE:O	2.15	0.47
1:B:74[B]:VAL:HG22	1:B:105[B]:ILE:O	2.14	0.47
1:B:76[A]:GLU:HB2	1:B:105[A]:ILE:HD11	1.97	0.47
1:A:148:MET:HE3	1:A:265:ILE:HG12	1.97	0.47
1:B:77[A]:ASN:ND2	1:B:101[A]:LYS:HD2	2.30	0.47
1:B:146:SER:N	1:B:291:HIS:HD2	2.00	0.47
1:A:162:ARG:CZ	1:A:271:PHE:HB3	2.46	0.46
1:A:146:SER:N	1:A:291:HIS:HD2	1.97	0.46
1:A:114[A]:THR:CG2	1:B:91[A]:VAL:HG11	2.32	0.46
4:B:1302:SPM:C13	5:B:2018:HOH:O	2.62	0.46
1:B:243:PHE:C	1:B:243:PHE:CD2	2.89	0.46
1:A:163:LEU:HD12	1:A:208:PHE:HZ	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PHE:CD2	1:A:243:PHE:C	2.89	0.46
1:B:27:GLY:O	1:B:28:LEU:HG	2.15	0.46
1:A:299:HIS:ND1	1:A:299:HIS:N	2.63	0.46
1:A:77[B]:ASN:CB	1:A:102[B]:LEU:HD21	2.45	0.46
1:B:139:THR:HG21	1:B:167:ARG:NH2	2.21	0.46
1:A:169:GLU:CG	1:A:249:ALA:HB2	2.42	0.46
1:B:191:VAL:HG13	1:B:191:VAL:O	2.16	0.46
1:B:33:TRP:O	1:B:37[B]:HIS:C	2.54	0.46
1:B:13:ARG:CD	1:B:15:LEU:O	2.60	0.46
1:A:95[B]:ALA:HB3	1:A:97[B]:ILE:HG13	1.97	0.45
1:B:124[A]:LEU:HD12	1:B:124[A]:LEU:C	2.37	0.45
1:A:74[A]:VAL:O	1:A:74[A]:VAL:CG2	2.63	0.45
1:B:182:ARG:CA	1:B:193:ARG:NH1	2.75	0.45
1:B:62[A]:ALA:HB1	1:B:83[A]:PHE:HZ	1.80	0.45
1:A:169:GLU:HB2	1:A:247:HIS:HE1	1.81	0.45
1:B:117[A]:ALA:O	1:B:118[A]:LEU:C	2.54	0.45
1:B:130[A]:LEU:O	1:B:131[A]:ILE:C	2.55	0.45
1:B:163:LEU:HD12	1:B:208:PHE:HZ	1.75	0.45
1:B:13:ARG:HG2	1:B:15:LEU:O	2.17	0.45
1:A:77[A]:ASN:HD22	1:A:101[A]:LYS:HD2	1.82	0.45
1:A:77[B]:ASN:CA	1:A:102[B]:LEU:CD2	2.95	0.45
1:A:191:VAL:O	1:A:191:VAL:HG13	2.16	0.45
1:A:138:PRO:CG	1:A:252:GLN:OE1	2.54	0.45
1:A:118[B]:LEU:HD22	1:B:57[B]:TYR:CE2	2.52	0.45
1:A:278:LEU:CB	1:A:279:PRO:CD	2.94	0.44
1:B:75[B]:ILE:HG23	1:B:102[B]:LEU:HB3	1.98	0.44
1:B:250:PHE:O	1:B:252:GLN:HG3	2.18	0.44
1:B:57[B]:TYR:C	1:B:57[B]:TYR:CD2	2.90	0.44
1:A:198:LEU:HB3	1:A:216:HIS:CE1	2.52	0.44
1:B:103[A]:ILE:HA	1:B:104[A]:PRO:HD3	1.86	0.44
1:B:139:THR:HG22	1:B:167:ARG:CZ	2.40	0.44
1:A:136[B]:THR:C	1:A:137:ARG:HG3	2.37	0.44
1:A:186:SER:OG	1:A:190:MET:HG2	2.17	0.44
1:B:61[B]:ASN:HB3	1:B:87[B]:PHE:CE1	2.52	0.44
1:A:178:LEU:HD13	1:A:241:VAL:HG22	1.99	0.44
1:A:65[B]:ALA:O	1:A:68[B]:TYR:N	2.48	0.44
1:B:92[B]:GLN:NE2	1:B:99[B]:TYR:HD1	2.15	0.44
1:A:168:ILE:O	1:A:168:ILE:CG2	2.65	0.44
1:A:89[A]:PHE:HZ	1:A:104[A]:PRO:HG3	1.83	0.43
1:A:117[A]:ALA:O	1:A:118[A]:LEU:C	2.56	0.43
1:A:38[B]:TYR:CZ	1:B:136[B]:THR:HG22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:MET:HE3	1:B:162:ARG:HA	1.99	0.43
1:B:178:LEU:HD13	1:B:241:VAL:HG22	2.00	0.43
1:A:124[A]:LEU:C	1:A:124[A]:LEU:HD12	2.38	0.43
1:B:108[B]:LEU:O	1:B:112[B]:LEU:HG	2.18	0.43
1:B:69[A]:LEU:C	1:B:71[A]:CYS:N	2.71	0.43
1:B:78[B]:ALA:N	1:B:102[B]:LEU:HD22	2.33	0.43
1:A:161:MET:CE	1:A:161:MET:C	2.87	0.43
1:B:200:LEU:HD13	1:B:214:VAL:HG13	2.01	0.43
1:B:275:PHE:CE2	1:B:285:LEU:HD12	2.53	0.43
1:A:108[B]:LEU:O	1:A:112[B]:LEU:HG	2.19	0.43
1:B:89[A]:PHE:HZ	1:B:104[A]:PRO:HG3	1.84	0.43
1:A:200:LEU:HD13	1:A:214:VAL:HG13	1.99	0.43
1:B:73[B]:ASP:OD1	1:B:80[B]:PRO:HB3	2.17	0.43
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.81	0.43
1:A:49[A]:PHE:CE1	1:A:53[A]:ILE:HD11	2.49	0.43
1:A:32:GLY:HA2	1:B:167:ARG:HE	1.81	0.43
1:B:25:ARG:HE	1:B:25:ARG:HB3	1.52	0.43
1:A:130[A]:LEU:O	1:A:131[A]:ILE:C	2.56	0.43
1:A:61[A]:ASN:HD21	1:A:94[A]:MET:HE2	1.84	0.43
1:A:39[B]:HIS:CD2	1:B:250:PHE:CZ	3.07	0.42
1:B:169:GLU:HB2	1:B:247:HIS:HE1	1.83	0.42
1:A:89[A]:PHE:CD1	1:A:102[A]:LEU:O	2.72	0.42
1:B:74[B]:VAL:O	1:B:74[B]:VAL:HG22	2.19	0.42
1:B:87[A]:PHE:O	1:B:90[A]:SER:HB3	2.19	0.42
1:B:95[B]:ALA:HB3	1:B:97[B]:ILE:HG13	2.01	0.42
1:B:136[B]:THR:C	1:B:137:ARG:HG3	2.40	0.42
1:B:228:THR:OG1	1:B:231:THR:HG23	2.19	0.42
1:A:162:ARG:HG3	1:A:290:PHE:CZ	2.55	0.42
1:A:32:GLY:HA3	1:B:167:ARG:NE	2.33	0.42
1:A:37[B]:HIS:CG	1:A:38[B]:TYR:H	2.37	0.42
1:A:57[A]:TYR:CE1	1:A:94[A]:MET:CE	3.03	0.42
1:A:200:LEU:HD23	1:A:200:LEU:HA	1.72	0.42
1:A:74[B]:VAL:O	1:A:74[B]:VAL:HG22	2.19	0.42
1:B:132[A]:TYR:CE2	4:B:1302:SPM:N10	2.85	0.42
1:A:285:LEU:CD2	1:A:287:LEU:HD23	2.49	0.42
1:B:118[A]:LEU:HA	1:B:118[A]:LEU:HD12	1.77	0.42
1:B:182:ARG:HB2	1:B:235:SER:HB2	2.01	0.42
1:B:159:LEU:HB3	1:B:216:HIS:HB3	2.01	0.42
1:A:16:ASN:O	1:A:259:ALA:HB3	2.19	0.42
1:B:61[A]:ASN:HD21	1:B:94[A]:MET:CE	2.32	0.42
1:A:205:SER:HA	1:A:206:PRO:HD3	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103[A]:ILE:HA	1:A:104[A]:PRO:HD3	1.85	0.41
1:A:69[A]:LEU:C	1:A:71[A]:CYS:N	2.72	0.41
1:A:114[A]:THR:CG2	1:B:91[A]:VAL:HG21	2.50	0.41
1:A:89[B]:PHE:CE1	1:A:102[B]:LEU:O	2.73	0.41
1:B:37[B]:HIS:CG	1:B:38[B]:TYR:H	2.38	0.41
1:A:25:ARG:HB3	1:A:25:ARG:HE	1.53	0.41
1:A:77[A]:ASN:ND2	1:A:101[A]:LYS:HD2	2.34	0.41
1:A:202:ARG:NH2	1:A:206:PRO:HD3	2.35	0.41
1:A:146:SER:N	1:A:291:HIS:CD2	2.80	0.41
1:A:34[A]:LEU:HD21	1:A:38[A]:TYR:HE2	1.86	0.41
1:A:57[B]:TYR:CD2	1:A:57[B]:TYR:C	2.93	0.41
1:A:75[B]:ILE:HG23	1:A:102[B]:LEU:HB3	1.99	0.41
1:B:276:THR:CG2	1:B:277:THR:N	2.83	0.41
1:A:163:LEU:HA	1:A:290:PHE:HZ	1.85	0.41
1:A:182:ARG:CA	1:A:193:ARG:NH1	2.75	0.41
1:A:210:LEU:HB3	1:A:285:LEU:HD13	1.98	0.41
1:A:176:VAL:HG12	1:A:212:TRP:CH2	2.55	0.41
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.69	0.41
1:B:42[A]:LEU:HD13	1:B:133[A]:ALA:CB	2.50	0.41
1:B:52[B]:LEU:HD23	1:B:52[B]:LEU:HA	1.80	0.41
1:B:74[A]:VAL:CG2	1:B:74[A]:VAL:O	2.61	0.41
1:A:163:LEU:O	1:A:163:LEU:HD12	2.21	0.41
1:A:182:ARG:HB2	1:A:235:SER:HB2	2.02	0.41
1:B:103[A]:ILE:CG2	1:B:104[A]:PRO:CD	2.98	0.41
1:A:36[B]:ASP:O	1:A:40[B]:ASP:HB2	2.21	0.41
1:B:161:MET:O	1:B:161:MET:HE2	2.21	0.41
1:A:78[B]:ALA:N	1:A:102[B]:LEU:HD22	2.35	0.40
1:A:92[B]:GLN:NE2	1:A:99[B]:TYR:CD1	2.88	0.40
1:A:23:ILE:HG12	1:A:23:ILE:H	1.43	0.40
1:B:122[A]:LEU:O	1:B:123[A]:GLY:C	2.59	0.40
4:B:1302:SPM:H131	5:B:2018:HOH:O	2.20	0.40
1:B:162:ARG:HG3	1:B:290:PHE:CZ	2.56	0.40
1:B:23:ILE:H	1:B:23:ILE:HG12	1.45	0.40
1:B:43[A]:THR:HG22	1:B:44[A]:VAL:N	2.35	0.40
1:B:285:LEU:CD2	1:B:287:LEU:CD2	2.99	0.40
1:B:93[B]:THR:O	1:B:96[B]:THR:HA	2.22	0.40
1:B:95[A]:ALA:O	1:B:96[A]:THR:OG1	2.39	0.40
1:A:131[B]:ILE:HD12	1:A:131[B]:ILE:H	1.86	0.40
1:A:159:LEU:HB3	1:A:216:HIS:HB3	2.03	0.40
1:A:161:MET:HE3	1:A:162:ARG:HA	2.03	0.40
1:B:278:LEU:CB	1:B:279:PRO:HD2	2.25	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56[B]:LEU:O	1:A:60[B]:THR:OG1	2.34	0.40
1:A:87[A]:PHE:O	1:A:90[A]:SER:HB3	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:1302:SPM:C13	5:B:2019:HOH:O[2_645]	2.13	0.07

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	390/301 (130%)	355 (91%)	34 (9%)	1 (0%)	41 72
1	B	390/301 (130%)	354 (91%)	35 (9%)	1 (0%)	41 72
All	All	780/602 (130%)	709 (91%)	69 (9%)	2 (0%)	41 72

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ARG
1	B	137	ARG

5.3.2 Protein sidechains [i](#)

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	324/256 (127%)	296 (91%)	28 (9%)	10	30
1	B	325/256 (127%)	297 (91%)	28 (9%)	10	30
All	All	649/512 (127%)	593 (91%)	56 (9%)	10	30

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ILE
1	A	25	ARG
1	A	31	ARG
1	A	37[A]	HIS
1	A	37[B]	HIS
1	A	39[A]	HIS
1	A	39[B]	HIS
1	A	40[A]	ASP
1	A	40[B]	ASP
1	A	43[A]	THR
1	A	43[B]	THR
1	A	71[A]	CYS
1	A	71[B]	CYS
1	A	73[A]	ASP
1	A	73[B]	ASP
1	A	111[A]	THR
1	A	111[B]	THR
1	A	135[B]	PHE
1	A	139	THR
1	A	161	MET
1	A	207	ILE
1	A	209	SER
1	A	235	SER
1	A	257	ARG
1	A	274	VAL
1	A	280	ASP
1	A	282	ARG
1	A	299	HIS
1	B	23	ILE
1	B	25	ARG
1	B	31	ARG
1	B	37[A]	HIS
1	B	37[B]	HIS
1	B	39[A]	HIS
1	B	39[B]	HIS

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Mol	Chain	Res	Type
1	B	40[A]	ASP
1	B	40[B]	ASP
1	B	43[A]	THR
1	B	43[B]	THR
1	B	71[A]	CYS
1	B	71[B]	CYS
1	B	73[A]	ASP
1	B	73[B]	ASP
1	B	111[A]	THR
1	B	111[B]	THR
1	B	135[B]	PHE
1	B	139	THR
1	B	161	MET
1	B	207	ILE
1	B	209	SER
1	B	235	SER
1	B	257	ARG
1	B	277	THR
1	B	280	ASP
1	B	282	ARG
1	B	299	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	255	HIS
1	A	291	HIS
1	A	296	HIS
1	A	298	HIS
1	B	246	HIS
1	B	291	HIS
1	B	296	HIS
1	B	298	HIS

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SPM	B	1302	-	13,13,13	0.54	0	12,12,12	0.90	1 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SPM	B	1302	-	-	2/11/11/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	B	1302	SPM	C11-N10-C9	2.00	122.90	113.45

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1302	SPM	N5-C6-C7-C8
4	B	1302	SPM	N10-C11-C12-C13

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1302	SPM	5	1

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	33:TRP	C	34[B]:LEU	N	8.30
1	B	33:TRP	C	34[B]:LEU	N	8.29
1	A	136[B]:THR	C	137:ARG	N	0.88
1	B	136[B]:THR	C	137:ARG	N	0.88

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	289/301 (96%)	-0.01	23 (7%)	12 6	34, 65, 162, 282	8 (2%)
1	B	289/301 (96%)	0.17	24 (8%)	11 6	35, 69, 173, 260	8 (2%)
All	All	578/602 (96%)	0.08	47 (8%)	12 6	34, 68, 174, 282	16 (2%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	29	GLU	8.2
1	A	29	GLU	7.3
1	A	33	TRP	7.2
1	B	33	TRP	7.1
1	B	70[A]	ALA	5.8
1	A	32	GLY	5.7
1	B	32	GLY	4.5
1	B	71[A]	CYS	4.2
1	B	28	LEU	3.7
1	A	301	HIS	3.6
1	B	11	LYS	3.4
1	A	280	ASP	3.4
1	A	85[A]	ASP	3.3
1	A	71[A]	CYS	3.3
1	A	70[A]	ALA	3.3
1	B	301	HIS	3.0
1	A	34[A]	LEU	2.9
1	A	80[A]	PRO	2.9
1	B	136[B]	THR	2.9
1	B	81[A]	GLY	2.8
1	B	49[A]	PHE	2.8
1	B	85[A]	ASP	2.6
1	A	49[A]	PHE	2.6
1	B	190	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	38[A]	TYR	2.5
1	B	67[A]	ALA	2.5
1	B	34[A]	LEU	2.5
1	A	67[A]	ALA	2.4
1	B	111[A]	THR	2.4
1	B	72[A]	GLY	2.4
1	A	281	GLY	2.4
1	A	81[A]	GLY	2.4
1	A	37[A]	HIS	2.3
1	A	136[B]	THR	2.3
1	B	73[A]	ASP	2.3
1	B	298	HIS	2.3
1	A	36[A]	ASP	2.3
1	B	80[A]	PRO	2.3
1	A	53[A]	ILE	2.3
1	B	36[A]	ASP	2.2
1	A	47[A]	PRO	2.2
1	A	12	PRO	2.2
1	A	113[A]	VAL	2.2
1	A	38[A]	TYR	2.1
1	B	35[A]	ASP	2.1
1	A	28	LEU	2.0
1	B	66[A]	LEU	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. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	K	A	1307	1/1	0.37	0.15	68,68,68,68	1
4	SPM	B	1302	14/14	0.77	0.45	45,57,60,60	14
3	CL	A	1306	1/1	0.82	0.14	92,92,92,92	0
2	K	A	1305	1/1	0.84	0.20	64,64,64,64	1
2	K	A	1302	1/1	0.97	0.12	38,38,38,38	1
2	K	A	1304	1/1	0.99	0.07	45,45,45,45	1
2	K	A	1303	1/1	0.99	0.11	33,33,33,33	1

6.5 Other polymers [i](#)

There are no such residues in this entry.