



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 08:25 PM UTC

PDB ID : 1P7B / pdb_00001p7b
Title : Crystal structure of an inward rectifier potassium channel
Authors : Kuo, A.; Gulbis, J.M.; Antcliff, J.F.; Rahman, T.; Lowe, E.D.; Zimmer, J.;
Cuthbertson, J.; Ashcroft, F.M.; Ezaki, T.; Doyle, D.A.
Deposited on : 2003-05-01
Resolution : 3.65 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

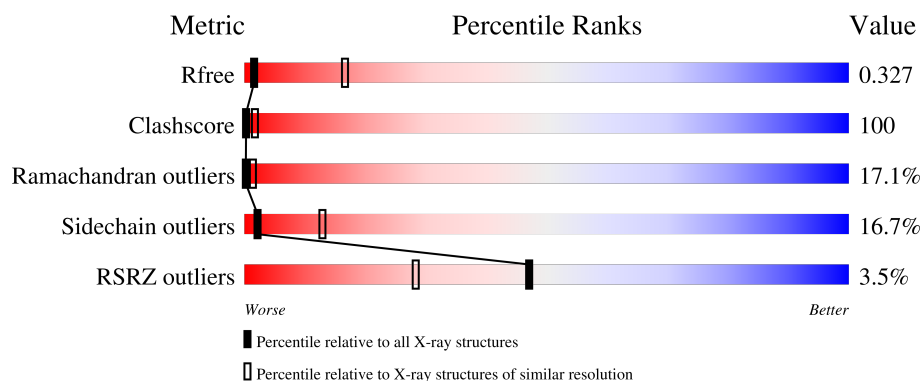
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
Ramachandran outliers	187476	1054 (3.78-3.54)
Sidechain outliers	187428	1052 (3.78-3.54)
RSRZ outliers	180081	1061 (3.78-3.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	333	
1	B	333	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4059 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 integral membrane channel and cytosolic domains.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2024	1313	349	348	14			
1	B	258	Total	C	N	O	S	0	0	0
			2024	1313	349	348	14			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	K	0	0
			3	3		
2	B	1	Total	K	0	0
			1	1		

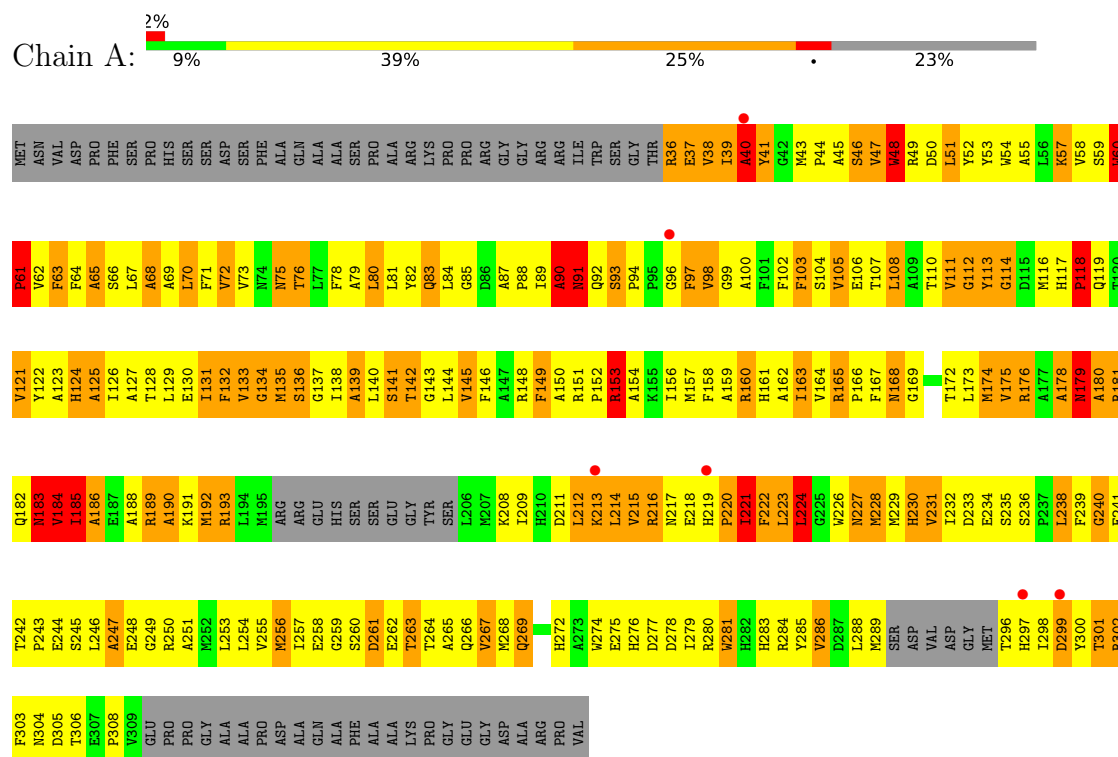
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	3	Total	O	0	0
			3	3		

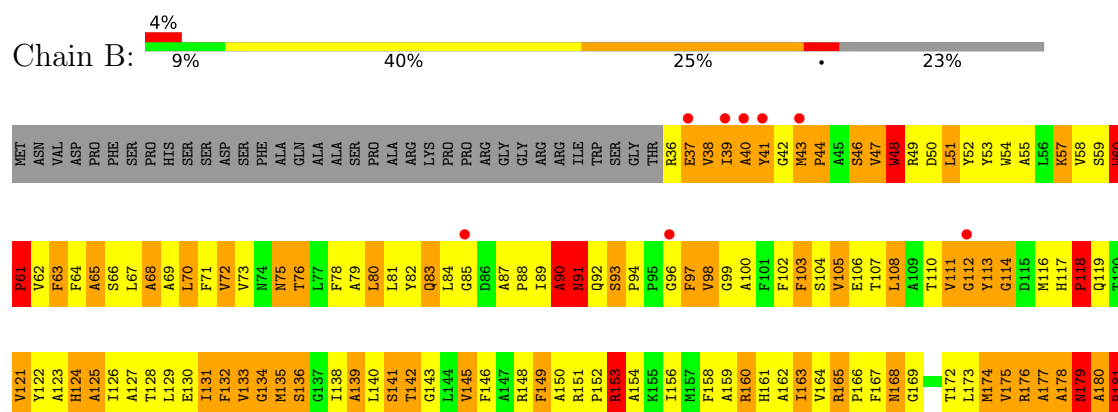
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: integral membrane channel and cytosolic domains



- Molecule 1: integral membrane channel and cytosolic domains



R302	T242	Q182
F303	T243	M183
N304	T244	V184
D305	T245	L185
T306	T246	A186
E307	T247	F187
P308	T248	A188
V309	T249	R189
GLU	T250	A190
PRO	T251	K191
PRO	T252	M192
GLY	T253	R193
ALA	T254	L194
ALA	T255	
PRO	T256	
PRO	T257	
ASP	T258	ARG
ALA	T259	GLU
GLN	T260	His
ALA	T261	SER
PHE	T262	GLY
ALA	T263	GLY
LYS	T264	THR
PRO	T265	TVR
GLY	T266	
GLU	T267	T206
GLY	T268	M207
ASP	T269	I208
ALA	T270	I209
ASP	T271	H210
ARG	T272	D211
PRO	T273	L212
VAL	T274	K213
	T275	L214
	T276	V215
	T277	R216
	T278	N217
	T279	E218
	T280	H219
	T281	P220
	T282	I221
	T283	F222
	T284	L223
	T285	I224
	T286	G225
	T287	V226
	T288	N227
	T289	N228
	SER	N229
	ASP	H230
	GLY	V231
	GLY	L232
	GLY	D233
	MET	E234
	T296	S235
	T297	T236
	T298	P237
	T299	L238
	T300	F239
	T301	G240
		E241

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	92.84Å 105.62Å 258.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.50 – 3.65 7.50 – 3.65	Depositor EDS
% Data completeness (in resolution range)	100.0 (7.50-3.65) 87.6 (7.50-3.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.02 (at 3.62Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.295 , 0.329 0.295 , 0.327	Depositor DCC
R_{free} test set	725 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	127.3	Xtriage
Anisotropy	0.507	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 137.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4059	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.30	18/2079 (0.9%)	1.65	48/2827 (1.7%)
1	B	1.35	20/2079 (1.0%)	1.63	45/2827 (1.6%)
All	All	1.33	38/4158 (0.9%)	1.64	93/5654 (1.6%)

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	1
1	B	0	1
All	All	0	2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	38	VAL	C-N	-15.90	1.12	1.33
1	A	38	VAL	C-N	-15.85	1.12	1.33
1	B	41	TYR	C-N	-13.15	1.14	1.33
1	B	42	GLY	C-N	12.93	1.60	1.33
1	A	184	VAL	CA-C	7.87	1.62	1.52
1	B	184	VAL	CA-C	7.86	1.62	1.52
1	A	229	MET	SD-CE	7.07	1.97	1.79
1	B	222	PHE	CA-C	6.93	1.62	1.52
1	A	40	ALA	C-N	6.87	1.43	1.33
1	B	40	ALA	C-N	6.84	1.43	1.33
1	A	222	PHE	CA-C	6.66	1.61	1.52
1	B	229	MET	SD-CE	6.50	1.95	1.79
1	A	296	THR	C-N	-6.45	1.24	1.33
1	B	296	THR	C-N	-6.44	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	THR	C-N	-6.24	1.25	1.33
1	B	190	ALA	CA-CB	-5.91	1.44	1.53
1	A	178	ALA	CA-CB	-5.77	1.44	1.53
1	A	190	ALA	CA-CB	-5.75	1.44	1.53
1	A	174	MET	CG-SD	5.71	1.95	1.80
1	A	228	MET	CG-SD	-5.70	1.66	1.80
1	A	185	ILE	CA-C	5.69	1.59	1.52
1	B	44	PRO	C-N	5.68	1.41	1.33
1	B	178	ALA	CA-CB	-5.59	1.44	1.53
1	B	180	ALA	N-CA	-5.55	1.42	1.47
1	A	221	ILE	CA-CB	5.54	1.61	1.54
1	B	174	MET	CG-SD	5.50	1.94	1.80
1	A	231	VAL	CA-CB	-5.44	1.48	1.54
1	B	268	MET	SD-CE	5.41	1.93	1.79
1	B	44	PRO	N-CD	5.41	1.55	1.47
1	B	177	ALA	CA-CB	-5.38	1.45	1.53
1	A	180	ALA	N-CA	-5.32	1.42	1.47
1	B	181	ARG	CA-C	5.30	1.59	1.52
1	B	297	HIS	C-O	-5.30	1.17	1.23
1	A	157	MET	CG-SD	5.28	1.94	1.80
1	A	297	HIS	C-O	-5.23	1.17	1.23
1	A	300	TYR	CB-CG	5.17	1.63	1.51
1	B	221	ILE	CA-CB	5.09	1.61	1.54
1	B	207	MET	CG-SD	5.06	1.93	1.80

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	VAL	CA-C-O	-21.67	98.07	122.13
1	A	38	VAL	CA-C-O	-21.66	98.09	122.13
1	B	38	VAL	CA-C-N	18.32	154.95	121.97
1	B	38	VAL	C-N-CA	18.32	154.95	121.97
1	A	38	VAL	CA-C-N	18.31	154.93	121.97
1	A	38	VAL	C-N-CA	18.31	154.93	121.97
1	B	38	VAL	O-C-N	-17.87	104.13	122.54
1	A	38	VAL	O-C-N	-17.87	104.13	122.54
1	A	37	GLU	CA-C-N	10.98	137.69	120.34
1	A	37	GLU	C-N-CA	10.98	137.69	120.34
1	B	37	GLU	CA-C-N	10.98	137.69	120.34
1	B	37	GLU	C-N-CA	10.98	137.69	120.34
1	B	297	HIS	O-C-N	10.78	135.77	123.27
1	A	297	HIS	O-C-N	10.73	135.72	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	PHE	N-CA-C	-9.17	99.41	111.24
1	B	103	PHE	N-CA-C	-9.17	99.41	111.24
1	A	149	PHE	N-CA-C	-9.09	101.06	110.97
1	B	149	PHE	N-CA-C	-9.06	101.10	110.97
1	A	299	ASP	O-C-N	-8.66	113.07	123.29
1	A	65	ALA	N-CA-C	-8.31	101.91	110.97
1	B	65	ALA	N-CA-C	-8.16	102.07	110.97
1	B	186	ALA	N-CA-C	8.05	121.54	109.95
1	A	186	ALA	N-CA-C	7.87	121.28	109.95
1	B	142	THR	N-CA-C	-7.74	101.84	111.75
1	A	142	THR	N-CA-C	-7.74	101.85	111.75
1	B	281	TRP	N-CA-C	7.72	120.72	110.53
1	A	281	TRP	N-CA-C	7.68	120.67	110.53
1	B	60	TRP	CA-C-N	-6.89	111.23	119.84
1	B	60	TRP	C-N-CA	-6.89	111.23	119.84
1	B	119	GLN	N-CA-C	6.74	119.20	111.11
1	A	119	GLN	N-CA-C	6.74	119.20	111.11
1	A	60	TRP	CA-C-N	-6.68	111.49	119.84
1	A	60	TRP	C-N-CA	-6.68	111.49	119.84
1	B	209	ILE	N-CA-C	6.34	117.23	109.30
1	A	40	ALA	N-CA-C	6.23	124.07	110.80
1	B	193	ARG	N-CA-C	6.23	119.05	108.90
1	B	40	ALA	N-CA-C	6.22	124.06	110.80
1	A	193	ARG	N-CA-C	6.20	119.01	108.90
1	A	108	LEU	N-CA-C	-6.18	103.69	111.11
1	A	209	ILE	N-CA-C	6.16	117.00	109.30
1	B	108	LEU	N-CA-C	-6.01	103.89	111.11
1	B	41	TYR	CB-CA-C	-5.97	97.96	109.37
1	A	61	PRO	N-CA-C	-5.96	100.19	112.47
1	A	41	TYR	CB-CA-C	-5.96	97.99	109.37
1	B	61	PRO	N-CA-C	-5.95	100.21	112.47
1	A	301	THR	CA-C-N	5.94	132.51	122.65
1	A	301	THR	C-N-CA	5.94	132.51	122.65
1	A	236	SER	CA-C-N	5.85	126.36	120.04
1	A	236	SER	C-N-CA	5.85	126.36	120.04
1	B	189	ARG	N-CA-C	-5.81	100.82	110.17
1	B	236	SER	CA-C-N	5.80	126.31	120.04
1	B	236	SER	C-N-CA	5.80	126.31	120.04
1	A	153	ARG	N-CA-C	5.79	122.16	114.12
1	A	304	ASN	N-CA-C	5.78	119.51	112.23
1	B	230	HIS	N-CA-C	5.74	118.81	108.48
1	A	36	ARG	CA-C-N	5.72	131.75	122.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	ARG	C-N-CA	5.72	131.75	122.53
1	A	189	ARG	N-CA-C	-5.72	100.96	110.17
1	B	36	ARG	CA-C-N	5.72	131.74	122.53
1	B	36	ARG	C-N-CA	5.72	131.74	122.53
1	B	153	ARG	N-CA-C	5.71	122.06	114.12
1	A	230	HIS	N-CA-C	5.70	118.74	108.48
1	A	90	ALA	N-CA-C	5.65	122.84	110.80
1	B	304	ASN	N-CA-C	5.65	119.35	112.23
1	A	301	THR	O-C-N	-5.63	116.27	122.07
1	B	90	ALA	N-CA-C	5.63	122.78	110.80
1	B	297	HIS	CA-C-O	-5.53	114.65	121.06
1	B	236	SER	N-CA-C	5.52	116.84	109.83
1	A	297	HIS	CA-C-O	-5.50	114.68	121.06
1	B	183	ASN	N-CA-C	5.48	122.48	110.80
1	A	236	SER	N-CA-C	5.48	116.79	109.83
1	B	135	MET	N-CA-C	-5.45	105.24	111.07
1	A	135	MET	N-CA-C	-5.44	105.25	111.07
1	B	224	LEU	N-CA-C	-5.37	99.36	110.80
1	A	224	LEU	N-CA-C	-5.36	99.38	110.80
1	A	183	ASN	N-CA-C	5.34	122.17	110.80
1	B	41	TYR	N-CA-C	5.32	118.08	109.40
1	A	41	TYR	N-CA-C	5.30	118.04	109.40
1	B	43	MET	O-C-N	5.25	127.35	121.32
1	A	238	LEU	N-CA-C	-5.23	106.75	112.72
1	A	300	TYR	N-CA-C	5.15	119.66	113.17
1	B	238	LEU	N-CA-C	-5.13	106.87	112.72
1	B	111	VAL	N-CA-C	-5.12	108.52	113.53
1	A	118	PRO	N-CA-C	-5.07	102.03	112.47
1	A	111	VAL	N-CA-C	-5.05	108.58	113.53
1	A	223	LEU	CA-C-N	5.04	131.17	121.54
1	A	223	LEU	C-N-CA	5.04	131.17	121.54
1	A	229	MET	N-CA-C	5.04	116.73	109.07
1	B	118	PRO	N-CA-C	-5.03	102.12	112.47
1	B	223	LEU	CA-C-N	5.02	131.13	121.54
1	B	223	LEU	C-N-CA	5.02	131.13	121.54
1	B	259	GLY	CA-C-N	-5.01	115.19	122.65
1	B	259	GLY	C-N-CA	-5.01	115.19	122.65

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	38	VAL	Mainchain
1	B	38	VAL	Mainchain

5.2 Too-close contacts [i](#)

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	2024	0	1974	428	2
1	B	2024	0	1974	425	2
2	A	3	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	3	0	0	2	0
All	All	4059	0	3948	804	2

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 100.

All (804) 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:A:190:ALA:CB	1:A:214:LEU:H	1.60	1.15
1:A:190:ALA:HB3	1:A:214:LEU:H	1.00	1.13
1:A:213:LYS:HB3	1:A:215:VAL:HG22	1.30	1.12
1:B:190:ALA:HB3	1:B:214:LEU:H	0.98	1.11
1:B:213:LYS:HB3	1:B:215:VAL:HG22	1.31	1.10
1:B:190:ALA:CB	1:B:214:LEU:H	1.64	1.08
1:A:190:ALA:HB1	1:A:214:LEU:HD13	1.36	1.08
1:B:213:LYS:O	1:B:216:ARG:N	1.88	1.05
1:B:190:ALA:HB1	1:B:214:LEU:HD13	1.34	1.05
1:A:214:LEU:O	1:A:228:MET:HB3	1.58	1.03
1:A:213:LYS:O	1:A:216:ARG:N	1.88	1.03
1:B:106:GLU:CD	1:B:113:TYR:HB2	1.85	1.01
1:B:214:LEU:O	1:B:228:MET:HB3	1.58	1.01
1:B:213:LYS:C	1:B:215:VAL:H	1.69	1.01
1:B:165:ARG:CZ	1:B:284:ARG:HB2	1.89	1.01
1:B:179:ASN:ND2	1:B:183:ASN:HA	1.75	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:CD	1:A:113:TYR:HB2	1.85	1.00
1:A:41:TYR:O	1:A:41:TYR:CD1	2.14	1.00
1:B:41:TYR:O	1:B:41:TYR:CD1	2.14	1.00
1:A:208:LYS:NZ	1:B:222:PHE:HB3	1.76	1.00
1:A:179:ASN:ND2	1:A:183:ASN:HA	1.77	0.99
1:A:185:ILE:HD13	1:A:185:ILE:O	1.63	0.99
1:A:190:ALA:HB3	1:A:214:LEU:N	1.79	0.98
1:A:189:ARG:HA	1:A:213:LYS:HG2	1.40	0.98
1:A:43:MET:HB2	1:A:44:PRO:HD2	1.46	0.98
1:B:213:LYS:O	1:B:215:VAL:N	1.97	0.97
1:A:128:THR:HG23	1:B:105:VAL:HG11	1.44	0.97
1:A:154:ALA:HB3	1:A:268:MET:SD	2.04	0.97
1:A:213:LYS:O	1:A:215:VAL:N	1.97	0.97
1:B:185:ILE:HD13	1:B:185:ILE:O	1.63	0.96
1:B:190:ALA:HB3	1:B:214:LEU:N	1.80	0.96
1:B:148:ARG:O	1:B:151:ARG:HG3	1.66	0.95
1:A:41:TYR:O	1:A:41:TYR:HD1	1.49	0.95
1:A:148:ARG:O	1:A:151:ARG:HG3	1.67	0.95
1:B:189:ARG:HA	1:B:213:LYS:HG2	1.48	0.94
1:B:213:LYS:CB	1:B:215:VAL:HG22	1.98	0.93
1:A:213:LYS:CB	1:A:215:VAL:HG22	1.98	0.93
1:A:213:LYS:C	1:A:215:VAL:H	1.68	0.93
1:B:215:VAL:CG2	1:B:219:HIS:HA	1.99	0.93
1:A:215:VAL:CG2	1:A:219:HIS:HA	2.00	0.92
1:B:41:TYR:O	1:B:41:TYR:HD1	1.49	0.91
1:A:173:LEU:HD12	1:A:174:MET:H	1.33	0.91
1:B:89:ILE:HG23	1:B:117:HIS:CD2	2.06	0.91
1:A:165:ARG:CZ	1:A:284:ARG:HB2	2.02	0.90
1:B:173:LEU:HD12	1:B:174:MET:H	1.33	0.90
1:A:89:ILE:HG23	1:A:117:HIS:CD2	2.07	0.90
1:B:289:MET:HG2	1:B:298:ILE:HG12	1.54	0.89
1:A:126:ILE:HG23	1:A:127:ALA:N	1.88	0.89
1:A:223:LEU:O	1:A:224:LEU:HG	1.73	0.89
1:B:223:LEU:O	1:B:224:LEU:HG	1.74	0.88
1:A:213:LYS:HB3	1:A:215:VAL:CG2	2.03	0.87
1:B:126:ILE:HG23	1:B:127:ALA:N	1.88	0.87
1:B:93:SER:OG	1:B:94:PRO:HD3	1.75	0.87
1:A:93:SER:OG	1:A:94:PRO:HD3	1.75	0.86
1:B:213:LYS:HB3	1:B:215:VAL:CG2	2.04	0.86
1:B:299:ASP:OD1	1:B:301:THR:HG23	1.74	0.86
1:B:92:GLN:HG2	1:B:93:SER:N	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ASP:O	1:A:213:LYS:N	2.09	0.86
1:A:92:GLN:HG2	1:A:93:SER:H	1.41	0.85
1:A:92:GLN:HG2	1:A:93:SER:N	1.90	0.85
1:B:180:ALA:O	1:B:181:ARG:CG	2.24	0.85
1:A:208:LYS:HZ1	1:B:222:PHE:HB3	1.42	0.85
1:B:106:GLU:OE1	1:B:113:TYR:HB2	1.76	0.85
1:B:211:ASP:O	1:B:213:LYS:N	2.09	0.85
1:A:269:GLN:HE22	1:B:185:ILE:HG21	1.42	0.84
1:B:91:ASN:OD1	1:B:91:ASN:O	1.96	0.84
1:A:39:ILE:HD12	1:B:296:THR:N	1.93	0.84
1:A:180:ALA:O	1:A:181:ARG:CG	2.26	0.84
1:B:92:GLN:HG2	1:B:93:SER:H	1.41	0.83
1:B:188:ALA:O	1:B:215:VAL:HG11	1.79	0.83
1:A:91:ASN:OD1	1:A:91:ASN:O	1.96	0.83
1:A:106:GLU:OE1	1:A:113:TYR:HB2	1.76	0.83
1:B:215:VAL:O	1:B:218:GLU:N	2.12	0.83
1:A:215:VAL:O	1:A:218:GLU:N	2.12	0.82
1:A:188:ALA:O	1:A:215:VAL:HG11	1.78	0.82
1:A:256:MET:HE2	1:B:185:ILE:HD12	1.62	0.82
1:A:215:VAL:O	1:A:217:ASN:N	2.13	0.82
1:A:134:GLY:O	1:A:138:ILE:HG13	1.79	0.82
1:B:154:ALA:HB3	1:B:268:MET:SD	2.20	0.81
1:A:153:ARG:HG2	1:A:153:ARG:HH11	1.45	0.81
1:A:89:ILE:HA	1:A:117:HIS:NE2	1.95	0.81
1:A:299:ASP:OD1	1:A:299:ASP:O	1.98	0.81
1:A:39:ILE:CD1	1:B:296:THR:O	2.29	0.81
1:B:153:ARG:HH11	1:B:153:ARG:HG2	1.45	0.81
1:B:215:VAL:O	1:B:217:ASN:N	2.13	0.81
1:B:134:GLY:O	1:B:138:ILE:HG13	1.80	0.80
1:A:124:HIS:HB3	1:B:102:PHE:CE2	2.17	0.80
1:A:49:ARG:NE	1:B:181:ARG:HH21	1.78	0.80
1:B:89:ILE:HA	1:B:117:HIS:NE2	1.96	0.80
1:B:193:ARG:O	1:B:251:ALA:HA	1.82	0.80
1:A:153:ARG:HG2	1:A:153:ARG:NH1	1.98	0.79
1:B:58:VAL:HG12	1:B:59:SER:N	1.98	0.79
1:B:116:MET:C	1:B:118:PRO:HD3	2.08	0.79
1:B:186:ALA:HB1	1:B:258:GLU:O	1.83	0.78
1:A:37:GLU:OE2	1:B:224:LEU:CD2	2.31	0.78
1:A:156:ILE:HG21	1:A:257:ILE:HD12	1.66	0.78
1:A:58:VAL:HG12	1:A:59:SER:N	1.98	0.78
1:A:186:ALA:HB1	1:A:258:GLU:O	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:MET:C	1:A:118:PRO:HD3	2.08	0.77
1:B:153:ARG:HG2	1:B:153:ARG:NH1	1.98	0.77
1:B:243:PRO:HG3	1:B:281:TRP:NE1	2.00	0.76
1:A:180:ALA:O	1:A:181:ARG:HG2	1.84	0.75
1:A:243:PRO:HG3	1:A:281:TRP:NE1	2.01	0.75
1:B:43:MET:HB2	1:B:44:PRO:CD	2.16	0.75
1:B:165:ARG:NH2	1:B:284:ARG:HB2	2.01	0.75
1:A:231:VAL:HG12	1:A:233:ASP:H	1.52	0.75
1:B:89:ILE:HD13	1:B:117:HIS:NE2	2.02	0.75
1:B:215:VAL:HG21	1:B:219:HIS:HA	1.69	0.75
1:B:180:ALA:O	1:B:181:ARG:HG2	1.83	0.74
1:B:159:ALA:O	1:B:161:HIS:N	2.20	0.74
1:A:213:LYS:C	1:A:215:VAL:N	2.37	0.74
1:B:231:VAL:HG12	1:B:233:ASP:H	1.52	0.74
1:A:193:ARG:HG3	1:A:208:LYS:HG2	1.70	0.74
1:A:54:TRP:O	1:A:58:VAL:HG23	1.87	0.74
1:A:89:ILE:HD13	1:A:117:HIS:NE2	2.02	0.73
1:A:144:LEU:HD23	1:B:149:PHE:HE2	1.52	0.73
1:B:190:ALA:CB	1:B:214:LEU:HD13	2.16	0.73
1:A:215:VAL:HG21	1:A:219:HIS:HA	1.70	0.73
1:A:289:MET:HG2	1:A:298:ILE:HG12	1.69	0.73
1:A:104:SER:C	1:A:106:GLU:H	1.96	0.73
1:B:104:SER:C	1:B:106:GLU:H	1.95	0.73
1:A:39:ILE:HD12	1:B:296:THR:O	1.87	0.72
1:A:159:ALA:O	1:A:161:HIS:N	2.21	0.72
1:B:84:LEU:HG	1:B:85:GLY:H	1.54	0.72
1:A:49:ARG:NE	1:B:181:ARG:NH2	2.36	0.72
1:A:84:LEU:HG	1:A:85:GLY:H	1.54	0.72
1:A:100:ALA:O	1:A:103:PHE:HB3	1.90	0.72
1:B:54:TRP:O	1:B:58:VAL:HG23	1.88	0.72
1:B:165:ARG:HG3	1:B:166:PRO:CD	2.20	0.72
1:A:43:MET:CB	1:A:44:PRO:HD2	2.18	0.72
1:B:286:VAL:HG11	1:B:305:ASP:HB2	1.70	0.71
1:A:189:ARG:HH12	1:B:220:PRO:CG	2.02	0.71
1:A:208:LYS:HZ1	1:B:222:PHE:CB	2.03	0.71
1:A:124:HIS:CE1	1:B:102:PHE:HB3	2.24	0.71
1:A:165:ARG:NH2	1:A:284:ARG:HB2	2.06	0.70
1:A:176:ARG:HD2	1:A:285:TYR:CD2	2.26	0.70
1:A:126:ILE:HG23	1:A:127:ALA:H	1.56	0.70
1:B:100:ALA:O	1:B:103:PHE:HB3	1.90	0.70
1:B:180:ALA:O	1:B:181:ARG:HG3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:O	1:A:228:MET:CB	2.39	0.70
1:A:39:ILE:HG13	1:A:39:ILE:O	1.92	0.70
1:B:133:VAL:O	1:B:136:SER:N	2.24	0.70
1:A:40:ALA:HB3	1:B:297:HIS:CB	2.22	0.69
1:A:153:ARG:HH11	1:A:153:ARG:CG	2.05	0.69
1:A:165:ARG:HG3	1:A:166:PRO:CD	2.21	0.69
1:A:193:ARG:O	1:A:251:ALA:HA	1.92	0.69
1:B:176:ARG:HD2	1:B:285:TYR:CD2	2.26	0.69
1:B:126:ILE:HG23	1:B:127:ALA:H	1.57	0.69
1:A:173:LEU:HD21	1:A:253:LEU:CD1	2.22	0.69
1:B:173:LEU:HD12	1:B:174:MET:N	2.07	0.69
1:A:133:VAL:O	1:A:136:SER:N	2.26	0.69
1:A:104:SER:O	1:A:106:GLU:N	2.26	0.69
1:B:104:SER:O	1:B:106:GLU:N	2.26	0.69
1:B:175:VAL:HG11	1:B:274:TRP:CZ3	2.27	0.69
1:A:179:ASN:HD21	1:A:183:ASN:HA	1.56	0.68
1:B:153:ARG:HH11	1:B:153:ARG:CG	2.06	0.68
1:B:179:ASN:HD21	1:B:183:ASN:HA	1.54	0.68
1:B:141:SER:O	1:B:145:VAL:HG23	1.93	0.68
1:B:39:ILE:HG13	1:B:39:ILE:O	1.92	0.68
1:B:156:ILE:HG21	1:B:257:ILE:HD12	1.75	0.68
1:A:242:THR:H	1:A:245:SER:HB2	1.57	0.68
1:B:106:GLU:HA	1:B:111:VAL:HG12	1.76	0.68
1:B:118:PRO:HB2	1:B:124:HIS:NE2	2.08	0.68
1:B:126:ILE:CG2	1:B:127:ALA:N	2.56	0.68
1:A:173:LEU:HD12	1:A:174:MET:N	2.07	0.68
1:A:118:PRO:HB2	1:A:124:HIS:NE2	2.08	0.67
1:A:141:SER:O	1:A:145:VAL:HG23	1.93	0.67
1:A:180:ALA:O	1:A:181:ARG:HG3	1.93	0.67
1:A:103:PHE:O	1:A:106:GLU:HB3	1.94	0.67
1:A:239:PHE:O	1:A:240:GLY:C	2.38	0.67
1:B:232:ILE:HG22	1:B:232:ILE:O	1.93	0.67
1:A:106:GLU:HA	1:A:111:VAL:HG12	1.76	0.67
1:A:126:ILE:CG2	1:A:127:ALA:N	2.56	0.67
1:A:60:TRP:CD1	1:A:148:ARG:NH2	2.63	0.67
1:B:103:PHE:O	1:B:106:GLU:HB3	1.93	0.67
1:A:173:LEU:HD21	1:A:253:LEU:HD11	1.76	0.67
1:A:173:LEU:O	1:A:174:MET:HG2	1.95	0.67
1:A:179:ASN:CG	1:A:183:ASN:HA	2.20	0.67
1:B:242:THR:H	1:B:245:SER:HB2	1.57	0.67
1:A:58:VAL:CG1	1:A:62:VAL:HB	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:VAL:HG11	1:A:274:TRP:CZ3	2.30	0.67
1:B:67:LEU:O	1:B:68:ALA:C	2.38	0.67
1:A:208:LYS:HZ3	1:B:222:PHE:HB3	1.57	0.66
1:B:180:ALA:C	1:B:181:ARG:HG3	2.20	0.66
1:B:179:ASN:CG	1:B:183:ASN:HA	2.20	0.66
1:A:43:MET:HB2	1:A:44:PRO:CD	2.23	0.66
1:B:159:ALA:O	1:B:160:ARG:C	2.38	0.66
1:A:90:ALA:C	1:A:92:GLN:H	2.04	0.66
1:B:60:TRP:CD1	1:B:148:ARG:NH2	2.64	0.66
1:B:90:ALA:C	1:B:92:GLN:H	2.04	0.66
1:B:58:VAL:CG1	1:B:62:VAL:HB	2.26	0.66
1:A:232:ILE:O	1:A:232:ILE:HG22	1.94	0.66
1:A:59:SER:OG	1:A:62:VAL:HG23	1.96	0.66
1:B:193:ARG:HG3	1:B:208:LYS:HG2	1.77	0.66
1:A:242:THR:H	1:A:245:SER:CB	2.09	0.66
1:B:176:ARG:HD2	1:B:285:TYR:CE2	2.31	0.66
1:A:162:ALA:HB3	1:A:279:ILE:HA	1.78	0.66
1:A:180:ALA:C	1:A:181:ARG:HG3	2.21	0.66
1:B:162:ALA:HB3	1:B:279:ILE:HA	1.75	0.66
1:B:214:LEU:O	1:B:228:MET:CB	2.38	0.66
1:A:226:TRP:HD1	1:A:227:ASN:H	1.44	0.65
1:A:256:MET:HE2	1:B:185:ILE:CD1	2.26	0.65
1:B:82:TYR:CE2	1:B:126:ILE:HG21	2.31	0.65
1:B:165:ARG:HG3	1:B:166:PRO:HD2	1.78	0.65
1:B:253:LEU:HD23	1:B:274:TRP:CE3	2.31	0.65
1:A:60:TRP:NE1	1:A:148:ARG:HE	1.93	0.65
1:A:159:ALA:O	1:A:160:ARG:C	2.37	0.65
1:A:176:ARG:HD2	1:A:285:TYR:CE2	2.32	0.65
1:B:239:PHE:O	1:B:240:GLY:C	2.39	0.65
1:A:190:ALA:CB	1:A:214:LEU:HD13	2.20	0.65
1:B:261:ASP:OD2	1:B:264:THR:HB	1.96	0.65
1:A:75:ASN:ND2	1:A:105:VAL:HG22	2.11	0.65
1:A:253:LEU:HD23	1:A:274:TRP:CE3	2.32	0.65
1:B:213:LYS:C	1:B:215:VAL:N	2.37	0.65
1:B:173:LEU:O	1:B:174:MET:HG2	1.96	0.65
1:B:284:ARG:O	1:B:306:THR:HB	1.96	0.65
1:A:190:ALA:CB	1:A:214:LEU:N	2.46	0.65
1:A:60:TRP:HE1	1:A:148:ARG:HE	1.44	0.65
1:A:261:ASP:OD2	1:A:264:THR:HB	1.96	0.65
1:B:173:LEU:HD21	1:B:253:LEU:CD1	2.25	0.65
1:A:37:GLU:OE2	1:B:224:LEU:HD21	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:SER:OG	1:B:62:VAL:HG23	1.97	0.65
1:B:75:ASN:ND2	1:B:105:VAL:HG22	2.11	0.64
1:B:253:LEU:HB3	1:B:274:TRP:HB2	1.78	0.64
1:A:67:LEU:O	1:A:68:ALA:C	2.38	0.64
1:A:253:LEU:HB3	1:A:274:TRP:HB2	1.78	0.64
1:B:226:TRP:HD1	1:B:227:ASN:H	1.45	0.64
1:B:242:THR:H	1:B:245:SER:CB	2.10	0.64
1:A:82:TYR:CE2	1:A:126:ILE:HG21	2.31	0.64
1:B:60:TRP:NE1	1:B:148:ARG:HE	1.95	0.64
1:B:159:ALA:C	1:B:161:HIS:N	2.53	0.64
1:B:84:LEU:CG	1:B:85:GLY:H	2.11	0.64
1:B:299:ASP:OD1	1:B:301:THR:CG2	2.44	0.64
1:A:106:GLU:HG3	1:A:111:VAL:HG13	1.80	0.64
1:B:185:ILE:O	1:B:185:ILE:CD1	2.43	0.64
1:A:212:LEU:O	1:A:216:ARG:CB	2.46	0.64
1:B:212:LEU:O	1:B:216:ARG:CB	2.46	0.63
1:A:84:LEU:CG	1:A:85:GLY:H	2.11	0.63
1:A:185:ILE:O	1:A:185:ILE:CD1	2.43	0.63
1:A:269:GLN:HE22	1:B:185:ILE:CG2	2.11	0.63
1:A:94:PRO:HB2	1:A:99:GLY:CA	2.29	0.63
1:B:192:MET:HE2	1:B:238:LEU:HD21	1.80	0.63
1:B:94:PRO:HB2	1:B:99:GLY:CA	2.29	0.63
1:B:226:TRP:HD1	1:B:227:ASN:N	1.97	0.63
1:A:89:ILE:HA	1:A:117:HIS:CE1	2.33	0.63
1:A:165:ARG:HG3	1:A:166:PRO:HD2	1.79	0.63
1:A:140:LEU:HD23	1:A:140:LEU:N	2.13	0.63
1:B:91:ASN:O	1:B:91:ASN:CG	2.41	0.63
1:B:106:GLU:HG3	1:B:111:VAL:HG13	1.80	0.63
1:B:173:LEU:HD21	1:B:253:LEU:HD11	1.80	0.63
1:A:226:TRP:HD1	1:A:227:ASN:N	1.96	0.62
1:A:151:ARG:O	1:A:152:PRO:C	2.41	0.62
1:A:58:VAL:HG12	1:A:62:VAL:HB	1.81	0.62
1:A:299:ASP:O	1:A:299:ASP:CG	2.43	0.62
1:B:89:ILE:HA	1:B:117:HIS:CE1	2.34	0.62
1:B:140:LEU:N	1:B:140:LEU:HD23	2.12	0.62
1:B:190:ALA:HB2	1:B:214:LEU:HB2	1.82	0.62
1:B:226:TRP:CD1	1:B:227:ASN:N	2.68	0.62
1:A:280:ARG:NH2	1:A:306:THR:OG1	2.33	0.62
1:A:91:ASN:O	1:A:91:ASN:CG	2.42	0.62
1:A:123:ALA:O	1:A:126:ILE:HG22	2.00	0.62
1:B:60:TRP:HE1	1:B:148:ARG:HE	1.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:ILE:HG13	1:B:296:THR:O	2.00	0.62
1:A:159:ALA:C	1:A:161:HIS:N	2.54	0.62
1:B:215:VAL:HG23	1:B:219:HIS:HA	1.81	0.62
1:A:226:TRP:CD1	1:A:227:ASN:N	2.68	0.61
1:B:192:MET:CE	1:B:238:LEU:HD21	2.29	0.61
1:B:281:TRP:O	1:B:283:HIS:CD2	2.53	0.61
1:B:43:MET:HB2	1:B:44:PRO:HD2	1.81	0.61
1:B:246:LEU:O	1:B:249:GLY:N	2.29	0.61
1:B:302:ARG:HG3	1:B:305:ASP:OD2	2.00	0.61
1:B:81:LEU:HD23	1:B:126:ILE:CD1	2.31	0.61
1:A:165:ARG:HG3	1:A:166:PRO:N	2.15	0.61
1:A:281:TRP:O	1:A:283:HIS:CD2	2.53	0.61
1:B:123:ALA:O	1:B:126:ILE:HG22	2.00	0.61
1:B:165:ARG:HG3	1:B:166:PRO:N	2.14	0.61
1:B:87:ALA:HB1	1:B:88:PRO:HD2	1.83	0.61
1:A:133:VAL:HG12	1:A:134:GLY:N	2.15	0.60
1:A:302:ARG:HG3	1:A:305:ASP:OD2	2.01	0.60
1:A:136:SER:HG	1:B:64:PHE:HE2	1.47	0.60
1:A:172:THR:HG22	1:A:231:VAL:HA	1.81	0.60
1:A:246:LEU:O	1:A:249:GLY:N	2.30	0.60
1:B:133:VAL:HG12	1:B:134:GLY:N	2.15	0.60
1:A:221:ILE:HG12	1:A:222:PHE:N	2.16	0.60
1:A:126:ILE:CG2	1:A:127:ALA:H	2.15	0.60
1:B:151:ARG:O	1:B:152:PRO:C	2.41	0.60
1:A:87:ALA:HB1	1:A:88:PRO:HD2	1.84	0.60
1:A:221:ILE:HG12	1:A:222:PHE:H	1.67	0.60
1:A:81:LEU:HD23	1:A:126:ILE:CD1	2.31	0.60
1:A:264:THR:HB	1:A:266:GLN:HG3	1.83	0.60
1:B:58:VAL:HG12	1:B:62:VAL:HB	1.82	0.60
1:B:82:TYR:C	1:B:84:LEU:H	2.10	0.60
1:B:221:ILE:HG12	1:B:222:PHE:N	2.17	0.60
1:A:184:VAL:CG2	1:A:223:LEU:HD22	2.32	0.60
1:B:83:GLN:NE2	1:B:97:PHE:N	2.50	0.60
1:B:126:ILE:CG2	1:B:127:ALA:H	2.15	0.60
1:A:124:HIS:HB3	1:B:102:PHE:CD2	2.37	0.59
1:A:219:HIS:N	1:A:220:PRO:HD3	2.16	0.59
1:B:58:VAL:CG1	1:B:59:SER:N	2.65	0.59
1:B:96:GLY:O	1:B:99:GLY:N	2.33	0.59
1:A:82:TYR:C	1:A:84:LEU:H	2.10	0.59
1:A:192:MET:SD	1:A:192:MET:C	2.84	0.59
1:B:265:ALA:HA	3:B:404:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:HE	1:A:208:LYS:NZ	2.00	0.59
1:B:105:VAL:HG12	1:B:105:VAL:O	2.01	0.59
1:A:83:GLN:NE2	1:A:97:PHE:N	2.49	0.59
1:A:105:VAL:HG12	1:A:105:VAL:O	2.02	0.59
1:B:180:ALA:C	1:B:181:ARG:CG	2.76	0.59
1:B:190:ALA:CB	1:B:214:LEU:N	2.50	0.59
1:B:212:LEU:O	1:B:216:ARG:CA	2.51	0.59
1:A:58:VAL:CG1	1:A:59:SER:N	2.65	0.59
1:A:215:VAL:HG23	1:A:219:HIS:HA	1.81	0.59
1:A:39:ILE:CG1	1:B:296:THR:O	2.51	0.59
1:A:89:ILE:HG23	1:A:117:HIS:HD2	1.64	0.59
1:A:192:MET:SD	1:A:193:ARG:N	2.75	0.59
1:A:212:LEU:O	1:A:216:ARG:CA	2.51	0.58
1:A:261:ASP:O	1:A:265:ALA:N	2.36	0.58
1:B:63:PHE:O	1:B:66:SER:N	2.36	0.58
1:B:192:MET:SD	1:B:193:ARG:N	2.76	0.58
1:B:219:HIS:N	1:B:220:PRO:HD3	2.16	0.58
1:A:52:TYR:O	1:A:53:TYR:C	2.47	0.58
1:A:67:LEU:O	1:A:70:LEU:N	2.36	0.58
1:A:189:ARG:NH1	1:B:220:PRO:HG2	2.18	0.58
1:B:88:PRO:O	1:B:89:ILE:HD13	2.03	0.58
1:B:219:HIS:N	1:B:220:PRO:CD	2.66	0.58
1:A:88:PRO:O	1:A:89:ILE:HD13	2.03	0.58
1:B:148:ARG:HB3	1:B:151:ARG:NH1	2.19	0.58
1:B:192:MET:SD	1:B:192:MET:C	2.86	0.58
1:B:288:LEU:HD21	1:B:303:PHE:HA	1.84	0.58
1:B:121:VAL:O	1:B:122:TYR:C	2.46	0.58
1:A:43:MET:HE3	1:B:300:TYR:CD1	2.39	0.58
1:B:67:LEU:O	1:B:70:LEU:N	2.37	0.58
1:A:43:MET:CB	1:A:44:PRO:CD	2.80	0.58
1:A:219:HIS:N	1:A:220:PRO:CD	2.66	0.58
1:A:211:ASP:C	1:A:211:ASP:OD1	2.44	0.57
1:A:275:GLU:O	1:A:278:ASP:N	2.32	0.57
1:A:96:GLY:O	1:A:99:GLY:N	2.33	0.57
1:A:100:ALA:O	1:A:104:SER:N	2.26	0.57
1:A:139:ALA:O	1:A:143:GLY:N	2.30	0.57
1:B:221:ILE:HG12	1:B:222:PHE:H	1.68	0.57
1:B:264:THR:HB	1:B:266:GLN:HG3	1.85	0.57
1:A:60:TRP:HE1	1:A:148:ARG:NE	2.02	0.57
1:A:61:PRO:O	1:A:62:VAL:C	2.46	0.57
1:A:63:PHE:O	1:A:66:SER:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:PRO:O	1:B:62:VAL:C	2.46	0.57
1:A:36:ARG:NH2	1:A:45:ALA:CB	2.67	0.57
1:A:215:VAL:HB	1:A:218:GLU:O	2.05	0.57
1:B:52:TYR:O	1:B:53:TYR:C	2.47	0.57
1:B:261:ASP:O	1:B:265:ALA:N	2.37	0.57
1:A:125:ALA:O	1:A:128:THR:N	2.37	0.56
1:A:302:ARG:CG	1:A:305:ASP:OD2	2.52	0.56
1:B:43:MET:CB	1:B:44:PRO:CD	2.78	0.56
1:B:302:ARG:CG	1:B:305:ASP:OD2	2.52	0.56
1:A:79:ALA:C	1:A:81:LEU:H	2.13	0.56
1:B:190:ALA:CB	1:B:214:LEU:HB2	2.35	0.56
1:B:215:VAL:HB	1:B:218:GLU:O	2.04	0.56
1:A:148:ARG:HB3	1:A:151:ARG:NH1	2.19	0.56
1:B:275:GLU:O	1:B:278:ASP:HB2	2.05	0.56
1:A:60:TRP:NE1	1:A:148:ARG:NE	2.54	0.56
1:A:97:PHE:C	1:A:99:GLY:H	2.13	0.56
1:B:79:ALA:C	1:B:81:LEU:H	2.14	0.56
1:B:163:ILE:C	1:B:163:ILE:HD12	2.30	0.56
1:A:190:ALA:HB2	1:A:214:LEU:HB2	1.87	0.56
1:B:60:TRP:HE1	1:B:148:ARG:NE	2.03	0.56
1:A:154:ALA:CB	1:A:268:MET:SD	2.86	0.56
1:A:184:VAL:HG22	1:A:223:LEU:HD22	1.87	0.56
1:A:275:GLU:O	1:A:278:ASP:HB2	2.06	0.56
1:A:118:PRO:HB2	1:A:124:HIS:HE2	1.68	0.56
1:B:61:PRO:C	1:B:63:PHE:N	2.62	0.56
1:B:182:GLN:O	1:B:183:ASN:O	2.24	0.56
1:B:211:ASP:OD1	1:B:211:ASP:C	2.46	0.56
1:A:121:VAL:O	1:A:124:HIS:N	2.38	0.55
1:A:231:VAL:HG12	1:A:233:ASP:OD2	2.06	0.55
1:B:184:VAL:CG2	1:B:223:LEU:HD22	2.37	0.55
1:A:40:ALA:CB	1:B:297:HIS:CB	2.84	0.55
1:A:219:HIS:HB2	1:A:220:PRO:HD3	1.88	0.55
1:A:256:MET:CE	1:B:185:ILE:CD1	2.85	0.55
1:B:97:PHE:C	1:B:99:GLY:H	2.13	0.55
1:B:190:ALA:HB1	1:B:214:LEU:CD1	2.23	0.55
1:A:121:VAL:O	1:A:122:TYR:C	2.46	0.55
1:A:192:MET:HE2	1:A:238:LEU:HD21	1.88	0.55
1:B:219:HIS:HB2	1:B:220:PRO:HD3	1.88	0.55
1:B:220:PRO:O	1:B:221:ILE:HB	2.07	0.55
1:A:163:ILE:HD12	1:A:163:ILE:C	2.31	0.55
1:B:51:LEU:O	1:B:52:TYR:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:CE2	1:A:126:ILE:CG2	2.90	0.55
1:A:182:GLN:O	1:A:183:ASN:O	2.24	0.55
1:B:59:SER:OG	1:B:61:PRO:HD2	2.07	0.55
1:B:192:MET:HE2	1:B:238:LEU:CD2	2.36	0.55
1:B:82:TYR:CE2	1:B:126:ILE:CG2	2.90	0.55
1:B:172:THR:HG22	1:B:231:VAL:HA	1.87	0.55
1:B:60:TRP:NE1	1:B:148:ARG:NE	2.55	0.55
1:B:125:ALA:O	1:B:128:THR:N	2.38	0.55
1:A:36:ARG:CZ	1:A:45:ALA:CB	2.86	0.54
1:B:63:PHE:O	1:B:66:SER:HB3	2.07	0.54
1:B:121:VAL:O	1:B:124:HIS:N	2.38	0.54
1:B:163:ILE:HD12	1:B:164:VAL:N	2.23	0.54
1:A:153:ARG:H	1:A:268:MET:HE1	1.73	0.54
1:A:189:ARG:NH1	1:B:220:PRO:CG	2.69	0.54
1:B:116:MET:C	1:B:118:PRO:CD	2.80	0.54
1:B:208:LYS:HZ2	1:B:254:LEU:CD1	2.20	0.54
1:B:241:GLU:HG3	1:B:245:SER:HB3	1.90	0.54
1:B:275:GLU:O	1:B:278:ASP:N	2.32	0.54
1:B:231:VAL:HG12	1:B:233:ASP:OD2	2.08	0.54
1:A:72:VAL:HG12	1:A:73:VAL:N	2.22	0.54
1:A:162:ALA:O	1:A:163:ILE:HG22	2.08	0.54
1:B:133:VAL:O	1:B:134:GLY:C	2.51	0.54
1:A:65:ALA:O	1:A:66:SER:C	2.51	0.54
1:A:154:ALA:N	1:A:268:MET:SD	2.80	0.54
1:A:184:VAL:HG23	1:A:185:ILE:H	1.73	0.54
1:A:220:PRO:O	1:A:221:ILE:HB	2.08	0.54
1:B:72:VAL:HG12	1:B:73:VAL:N	2.22	0.54
1:B:104:SER:C	1:B:106:GLU:N	2.61	0.53
1:B:149:PHE:O	1:B:151:ARG:N	2.40	0.53
1:A:163:ILE:HD12	1:A:164:VAL:N	2.24	0.53
1:A:228:MET:HE1	1:A:257:ILE:HD11	1.90	0.53
1:B:107:THR:O	1:B:108:LEU:C	2.51	0.53
1:A:116:MET:C	1:A:118:PRO:CD	2.81	0.53
1:A:116:MET:HB2	1:A:118:PRO:HD3	1.90	0.53
1:A:154:ALA:H	1:A:268:MET:CE	2.21	0.53
1:B:162:ALA:O	1:B:163:ILE:HG22	2.09	0.53
1:A:51:LEU:O	1:A:52:TYR:C	2.50	0.53
1:A:63:PHE:O	1:A:66:SER:HB3	2.08	0.53
1:A:98:VAL:HG12	1:A:98:VAL:O	2.08	0.53
1:B:75:ASN:CG	1:B:105:VAL:HG22	2.33	0.53
1:B:116:MET:HB2	1:B:118:PRO:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:HA	1:A:111:VAL:CG1	2.39	0.53
1:B:89:ILE:HG23	1:B:117:HIS:HD2	1.64	0.53
1:B:106:GLU:HA	1:B:111:VAL:CG1	2.39	0.53
1:B:139:ALA:O	1:B:143:GLY:N	2.31	0.53
1:A:283:HIS:CD2	1:A:308:PRO:HA	2.44	0.53
1:B:167:PHE:O	1:B:169:GLY:N	2.41	0.53
1:A:59:SER:OG	1:A:61:PRO:HD2	2.09	0.53
1:A:190:ALA:HB1	1:A:214:LEU:CD1	2.24	0.53
1:B:89:ILE:CD1	1:B:117:HIS:NE2	2.71	0.53
1:B:98:VAL:O	1:B:98:VAL:HG12	2.07	0.53
1:B:58:VAL:HG12	1:B:59:SER:H	1.72	0.53
1:B:100:ALA:O	1:B:104:SER:N	2.27	0.53
1:B:215:VAL:HG23	1:B:219:HIS:ND1	2.24	0.53
1:B:215:VAL:C	1:B:217:ASN:N	2.64	0.53
1:A:75:ASN:CG	1:A:105:VAL:HG22	2.33	0.53
1:A:269:GLN:HE21	1:B:262:GLU:HG2	1.74	0.53
1:B:92:GLN:HG2	1:B:93:SER:OG	2.09	0.53
1:A:49:ARG:HE	1:B:181:ARG:HH21	1.57	0.52
1:A:215:VAL:HG23	1:A:219:HIS:ND1	2.24	0.52
1:B:193:ARG:HE	1:B:208:LYS:NZ	2.07	0.52
1:A:68:ALA:O	1:A:71:PHE:N	2.43	0.52
1:A:133:VAL:O	1:A:134:GLY:C	2.53	0.52
1:A:215:VAL:C	1:A:217:ASN:N	2.64	0.52
1:B:65:ALA:O	1:B:66:SER:C	2.52	0.52
1:B:107:THR:O	1:B:110:THR:N	2.42	0.52
1:B:175:VAL:HG11	1:B:274:TRP:CH2	2.44	0.52
1:B:228:MET:HE1	1:B:257:ILE:HD11	1.90	0.52
1:A:89:ILE:CD1	1:A:117:HIS:NE2	2.71	0.52
1:A:192:MET:CE	1:A:238:LEU:HD21	2.39	0.52
1:A:48:TRP:HA	1:A:48:TRP:CE3	2.44	0.52
1:A:167:PHE:O	1:A:169:GLY:N	2.42	0.52
1:B:130:GLU:O	1:B:131:ILE:C	2.53	0.52
1:B:186:ALA:HB2	1:B:259:GLY:HA3	1.92	0.52
1:A:97:PHE:C	1:A:99:GLY:N	2.67	0.52
1:B:189:ARG:HH11	1:B:191:LYS:HZ1	1.58	0.52
1:A:241:GLU:HG3	1:A:245:SER:HB3	1.91	0.52
1:B:68:ALA:O	1:B:71:PHE:N	2.42	0.52
1:B:107:THR:C	1:B:110:THR:H	2.18	0.52
1:B:141:SER:O	1:B:142:THR:C	2.52	0.52
1:A:184:VAL:C	1:A:185:ILE:HG22	2.35	0.52
1:A:52:TYR:O	1:A:55:ALA:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ARG:CG	1:B:166:PRO:N	2.72	0.52
1:B:184:VAL:C	1:B:185:ILE:HG22	2.35	0.52
1:A:84:LEU:HG	1:A:85:GLY:N	2.24	0.51
1:A:85:GLY:HA3	1:A:122:TYR:CE2	2.45	0.51
1:A:149:PHE:O	1:A:151:ARG:N	2.43	0.51
1:A:180:ALA:C	1:A:181:ARG:CG	2.77	0.51
1:B:85:GLY:HA3	1:B:122:TYR:CE2	2.45	0.51
1:B:159:ALA:C	1:B:161:HIS:H	2.18	0.51
1:A:61:PRO:C	1:A:63:PHE:N	2.62	0.51
1:A:165:ARG:CG	1:A:166:PRO:N	2.73	0.51
1:B:48:TRP:HA	1:B:48:TRP:CE3	2.44	0.51
1:A:154:ALA:H	1:A:268:MET:HE1	1.74	0.51
1:B:48:TRP:HA	1:B:48:TRP:HE3	1.75	0.51
1:B:221:ILE:CG1	1:B:222:PHE:H	2.24	0.51
1:B:261:ASP:O	1:B:261:ASP:CG	2.53	0.51
1:B:52:TYR:O	1:B:55:ALA:HB3	2.10	0.51
1:B:176:ARG:HG2	1:B:303:PHE:CE1	2.45	0.51
1:A:58:VAL:HG12	1:A:59:SER:H	1.72	0.51
1:A:110:THR:O	1:A:110:THR:OG1	2.28	0.51
1:A:221:ILE:CG1	1:A:222:PHE:H	2.23	0.51
1:A:107:THR:C	1:A:110:THR:H	2.18	0.51
1:A:124:HIS:O	1:A:125:ALA:C	2.53	0.51
1:A:193:ARG:HE	1:A:208:LYS:HZ2	1.57	0.51
1:A:92:GLN:HG2	1:A:93:SER:OG	2.10	0.51
1:A:107:THR:O	1:A:110:THR:N	2.43	0.51
1:A:256:MET:CE	1:B:185:ILE:HD11	2.41	0.51
1:B:241:GLU:HG3	1:B:245:SER:CB	2.41	0.51
1:B:242:THR:O	1:B:245:SER:N	2.44	0.51
1:A:41:TYR:CD1	1:A:41:TYR:C	2.89	0.51
1:A:212:LEU:O	1:A:213:LYS:O	2.29	0.51
1:B:212:LEU:O	1:B:213:LYS:O	2.29	0.51
1:B:289:MET:HA	1:B:297:HIS:O	2.09	0.51
1:A:46:SER:O	1:A:47:VAL:C	2.54	0.51
1:A:141:SER:O	1:A:142:THR:C	2.52	0.51
1:A:58:VAL:HG11	1:A:62:VAL:CG1	2.41	0.50
1:A:124:HIS:NE2	1:B:92:GLN:OE1	2.30	0.50
1:A:107:THR:O	1:A:108:LEU:C	2.51	0.50
1:B:233:ASP:OD2	1:B:233:ASP:N	2.44	0.50
1:A:132:PHE:O	1:A:133:VAL:C	2.55	0.50
1:B:124:HIS:O	1:B:125:ALA:C	2.54	0.50
1:B:208:LYS:NZ	1:B:254:LEU:HD13	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ALA:CA	3:B:404:HOH:O	2.59	0.50
1:A:176:ARG:CZ	1:A:285:TYR:HB3	2.42	0.50
1:A:189:ARG:HH12	1:B:220:PRO:HG3	1.76	0.50
1:A:215:VAL:C	1:A:217:ASN:H	2.19	0.50
1:A:239:PHE:O	1:A:241:GLU:N	2.44	0.50
1:B:153:ARG:H	1:B:268:MET:HE1	1.75	0.50
1:B:215:VAL:C	1:B:217:ASN:H	2.19	0.50
1:A:144:LEU:CD2	1:B:149:PHE:HE2	2.23	0.50
1:A:124:HIS:CG	1:B:102:PHE:CD2	3.00	0.50
1:A:130:GLU:O	1:A:131:ILE:C	2.53	0.50
1:A:241:GLU:HG3	1:A:245:SER:CB	2.41	0.50
1:B:212:LEU:O	1:B:216:ARG:HA	2.11	0.50
1:B:239:PHE:O	1:B:241:GLU:N	2.44	0.50
1:B:300:TYR:O	1:B:301:THR:C	2.53	0.50
1:A:212:LEU:O	1:A:216:ARG:HA	2.12	0.50
1:A:261:ASP:O	1:A:261:ASP:CG	2.55	0.50
1:A:288:LEU:O	1:A:299:ASP:OD1	2.30	0.50
1:B:165:ARG:HB2	1:B:283:HIS:O	2.12	0.50
1:A:48:TRP:HA	1:A:48:TRP:HE3	1.75	0.49
1:A:107:THR:CG2	1:A:131:ILE:HG13	2.42	0.49
1:A:189:ARG:HH11	1:A:191:LYS:HZ1	1.58	0.49
1:B:58:VAL:HG11	1:B:62:VAL:CG1	2.42	0.49
1:B:97:PHE:C	1:B:99:GLY:N	2.67	0.49
1:B:84:LEU:HG	1:B:85:GLY:N	2.24	0.49
1:A:108:LEU:HD12	1:A:134:GLY:CA	2.42	0.49
1:A:242:THR:O	1:A:245:SER:N	2.45	0.49
1:A:190:ALA:CB	1:A:214:LEU:HB2	2.42	0.49
1:A:272:HIS:HD2	1:A:274:TRP:CZ2	2.31	0.49
1:B:108:LEU:HD12	1:B:134:GLY:CA	2.42	0.49
1:B:132:PHE:O	1:B:133:VAL:C	2.54	0.49
1:A:96:GLY:O	1:A:97:PHE:C	2.55	0.49
1:B:47:VAL:O	1:B:50:ASP:HB2	2.12	0.49
1:B:96:GLY:O	1:B:97:PHE:C	2.56	0.49
1:B:107:THR:CG2	1:B:131:ILE:HG13	2.43	0.49
1:B:184:VAL:HG23	1:B:185:ILE:H	1.77	0.49
1:A:208:LYS:HZ1	1:A:254:LEU:HD13	1.78	0.49
1:A:173:LEU:HD21	1:A:253:LEU:HD13	1.92	0.49
1:B:261:ASP:OD2	1:B:264:THR:CB	2.61	0.49
1:A:208:LYS:NZ	1:A:254:LEU:HD13	2.28	0.48
1:A:151:ARG:C	1:A:152:PRO:O	2.56	0.48
1:A:184:VAL:HG23	1:A:185:ILE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:ALA:O	1:B:126:ILE:C	2.56	0.48
1:B:215:VAL:CG2	1:B:219:HIS:ND1	2.76	0.48
1:A:261:ASP:OD2	1:A:264:THR:CB	2.61	0.48
1:A:263:THR:O	1:A:263:THR:CG2	2.58	0.48
1:B:83:GLN:NE2	1:B:97:PHE:H	2.12	0.48
1:A:83:GLN:NE2	1:A:97:PHE:H	2.11	0.48
1:A:175:VAL:CG2	1:A:214:LEU:HD23	2.43	0.48
1:B:90:ALA:C	1:B:92:GLN:N	2.71	0.48
1:B:110:THR:O	1:B:110:THR:OG1	2.30	0.48
1:A:215:VAL:CG2	1:A:219:HIS:ND1	2.76	0.48
1:A:233:ASP:OD2	1:A:233:ASP:N	2.44	0.48
1:B:46:SER:O	1:B:47:VAL:C	2.55	0.48
1:A:159:ALA:C	1:A:161:HIS:H	2.20	0.48
1:A:163:ILE:HG13	1:A:174:MET:HB2	1.95	0.48
1:A:192:MET:HE2	1:A:238:LEU:CD2	2.44	0.48
1:A:302:ARG:NH1	1:A:302:ARG:HB2	2.28	0.48
1:A:175:VAL:HG23	1:A:228:MET:HB2	1.95	0.48
1:B:234:GLU:O	1:B:235:SER:C	2.57	0.48
1:B:272:HIS:HD2	1:B:274:TRP:CZ2	2.31	0.48
1:B:302:ARG:HB2	1:B:302:ARG:NH1	2.28	0.48
1:A:246:LEU:O	1:A:248:GLU:N	2.46	0.48
1:A:246:LEU:HB3	1:A:251:ALA:HB3	1.94	0.48
1:A:141:SER:C	1:A:143:GLY:N	2.68	0.48
1:A:234:GLU:O	1:A:235:SER:C	2.56	0.48
1:B:276:HIS:CG	1:B:277:ASP:N	2.82	0.48
1:A:83:GLN:HE22	1:A:97:PHE:N	2.11	0.48
1:A:190:ALA:HB2	1:A:214:LEU:H	1.66	0.48
1:A:221:ILE:CG1	1:A:222:PHE:N	2.77	0.48
1:A:186:ALA:CB	1:A:258:GLU:O	2.60	0.47
1:B:83:GLN:HE22	1:B:97:PHE:N	2.11	0.47
1:A:264:THR:HG22	1:A:264:THR:O	2.14	0.47
1:B:84:LEU:CG	1:B:85:GLY:N	2.78	0.47
1:B:106:GLU:CA	1:B:111:VAL:HG12	2.44	0.47
1:A:47:VAL:O	1:A:48:TRP:C	2.57	0.47
1:A:60:TRP:CD1	1:A:148:ARG:CZ	2.97	0.47
1:A:76:THR:O	1:A:79:ALA:N	2.47	0.47
1:B:123:ALA:O	1:B:126:ILE:CG2	2.62	0.47
1:B:163:ILE:HG13	1:B:174:MET:HB2	1.95	0.47
1:B:246:LEU:HB3	1:B:251:ALA:HB3	1.95	0.47
1:A:54:TRP:O	1:A:55:ALA:C	2.57	0.47
1:A:84:LEU:CG	1:A:85:GLY:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PRO:HB2	1:A:99:GLY:HA2	1.97	0.47
1:A:123:ALA:O	1:A:126:ILE:CG2	2.62	0.47
1:B:249:GLY:C	1:B:251:ALA:N	2.71	0.47
1:A:106:GLU:CA	1:A:111:VAL:HG12	2.45	0.47
1:B:208:LYS:NZ	1:B:254:LEU:CD1	2.78	0.47
1:A:98:VAL:O	1:A:102:PHE:HD1	1.98	0.47
1:A:175:VAL:HG11	1:A:274:TRP:CH2	2.49	0.47
1:A:208:LYS:HZ2	1:A:254:LEU:CD1	2.28	0.47
1:A:241:GLU:HG3	1:A:245:SER:OG	2.14	0.47
1:A:301:THR:HG23	1:A:302:ARG:N	2.29	0.47
1:B:54:TRP:O	1:B:55:ALA:C	2.57	0.47
1:B:92:GLN:O	1:B:93:SER:C	2.58	0.47
1:B:186:ALA:CB	1:B:258:GLU:O	2.58	0.47
1:B:246:LEU:O	1:B:248:GLU:N	2.48	0.47
1:B:263:THR:O	1:B:263:THR:CG2	2.59	0.47
1:B:50:ASP:O	1:B:53:TYR:HB3	2.15	0.47
1:A:112:GLY:HA3	1:B:111:VAL:O	2.15	0.47
1:A:186:ALA:HB2	1:A:259:GLY:HA3	1.97	0.47
1:A:276:HIS:CG	1:A:277:ASP:N	2.82	0.47
1:B:47:VAL:O	1:B:48:TRP:C	2.58	0.47
1:B:179:ASN:OD1	1:B:184:VAL:HG22	2.15	0.47
1:B:277:ASP:C	1:B:277:ASP:OD2	2.57	0.47
1:A:79:ALA:C	1:A:81:LEU:N	2.73	0.47
1:A:163:ILE:HG13	1:A:163:ILE:O	2.15	0.47
1:B:98:VAL:O	1:B:98:VAL:CG1	2.63	0.47
1:B:117:HIS:N	1:B:118:PRO:HD3	2.29	0.47
1:B:176:ARG:NH2	1:B:288:LEU:HD11	2.29	0.47
1:A:50:ASP:O	1:A:53:TYR:HB3	2.15	0.46
1:B:112:GLY:O	1:B:113:TYR:C	2.58	0.46
1:B:221:ILE:CG1	1:B:222:PHE:N	2.77	0.46
1:A:162:ALA:C	1:A:163:ILE:CG2	2.88	0.46
1:A:277:ASP:OD2	1:A:277:ASP:C	2.58	0.46
1:B:65:ALA:O	1:B:68:ALA:HB3	2.15	0.46
1:B:76:THR:O	1:B:79:ALA:N	2.48	0.46
1:B:141:SER:C	1:B:143:GLY:N	2.68	0.46
1:B:158:PHE:CD1	1:B:158:PHE:N	2.83	0.46
1:B:173:LEU:HD21	1:B:253:LEU:HD13	1.95	0.46
1:A:103:PHE:O	1:A:106:GLU:N	2.48	0.46
1:B:243:PRO:HG3	1:B:281:TRP:CD1	2.51	0.46
1:A:92:GLN:O	1:A:93:SER:C	2.58	0.46
1:A:167:PHE:C	1:A:169:GLY:N	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:LEU:HD23	1:B:126:ILE:HD12	1.98	0.46
1:B:98:VAL:O	1:B:102:PHE:HD1	1.99	0.46
1:B:241:GLU:HG3	1:B:245:SER:OG	2.15	0.46
1:A:125:ALA:O	1:A:126:ILE:C	2.56	0.46
1:B:128:THR:O	1:B:129:LEU:C	2.58	0.46
1:B:162:ALA:C	1:B:163:ILE:CG2	2.88	0.46
1:B:167:PHE:C	1:B:169:GLY:N	2.69	0.46
1:A:90:ALA:O	1:A:92:GLN:N	2.49	0.46
1:A:158:PHE:N	1:A:158:PHE:CD1	2.83	0.46
1:B:60:TRP:CD1	1:B:148:ARG:CZ	2.98	0.46
1:A:98:VAL:O	1:A:98:VAL:CG1	2.63	0.46
1:A:176:ARG:NH1	1:A:285:TYR:HB3	2.30	0.46
1:A:176:ARG:HG2	1:A:303:PHE:CE1	2.51	0.46
1:B:264:THR:O	1:B:264:THR:HG22	2.16	0.46
1:A:63:PHE:O	1:A:64:PHE:C	2.59	0.45
1:A:112:GLY:O	1:A:113:TYR:C	2.59	0.45
1:A:269:GLN:HE21	1:B:262:GLU:CG	2.29	0.45
1:B:151:ARG:O	1:B:152:PRO:O	2.34	0.45
1:A:117:HIS:N	1:A:118:PRO:HD3	2.30	0.45
1:A:128:THR:O	1:A:129:LEU:C	2.59	0.45
1:B:97:PHE:O	1:B:99:GLY:N	2.49	0.45
1:B:176:ARG:NH1	1:B:285:TYR:HB3	2.31	0.45
1:A:97:PHE:O	1:A:99:GLY:N	2.49	0.45
1:A:146:PHE:CD2	1:B:146:PHE:CZ	3.05	0.45
1:A:176:ARG:NH1	1:A:285:TYR:CB	2.80	0.45
1:B:63:PHE:O	1:B:64:PHE:C	2.59	0.45
1:A:144:LEU:HD23	1:B:149:PHE:CE2	2.43	0.45
1:A:151:ARG:O	1:A:152:PRO:O	2.33	0.45
1:A:178:ALA:O	1:A:179:ASN:O	2.34	0.45
1:A:193:ARG:CG	1:A:208:LYS:HG2	2.45	0.45
1:B:94:PRO:HB2	1:B:99:GLY:HA2	1.97	0.45
1:B:90:ALA:O	1:B:92:GLN:N	2.49	0.45
1:B:220:PRO:O	1:B:221:ILE:CB	2.65	0.45
1:B:261:ASP:OD1	1:B:263:THR:HB	2.17	0.45
1:B:57:LYS:HA	1:B:57:LYS:HD3	1.81	0.45
1:B:103:PHE:O	1:B:106:GLU:N	2.49	0.45
1:B:178:ALA:O	1:B:179:ASN:O	2.34	0.45
1:B:184:VAL:HG23	1:B:185:ILE:N	2.31	0.45
1:A:118:PRO:HB2	1:B:92:GLN:OE1	2.17	0.45
1:B:108:LEU:HD12	1:B:134:GLY:HA3	1.97	0.45
1:A:243:PRO:HG3	1:A:281:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ASP:OD1	1:A:263:THR:HB	2.17	0.45
1:A:108:LEU:HD12	1:A:134:GLY:HA3	1.98	0.45
1:B:81:LEU:HB3	1:B:126:ILE:HD11	1.99	0.45
1:B:194:LEU:O	1:B:195:MET:CB	2.63	0.45
1:A:208:LYS:NZ	1:A:254:LEU:CD1	2.80	0.44
1:B:60:TRP:CD1	1:B:148:ARG:HH21	2.34	0.44
1:A:128:THR:HG23	1:B:105:VAL:CG1	2.32	0.44
1:A:163:ILE:C	1:A:163:ILE:CD1	2.90	0.44
1:A:249:GLY:C	1:A:251:ALA:N	2.72	0.44
1:B:79:ALA:C	1:B:81:LEU:N	2.73	0.44
1:B:80:LEU:CD2	1:B:97:PHE:CE1	3.00	0.44
1:B:184:VAL:HG22	1:B:223:LEU:HD22	1.98	0.44
1:A:36:ARG:CZ	1:A:45:ALA:HB2	2.47	0.44
1:A:80:LEU:CD2	1:A:97:PHE:CE1	3.00	0.44
1:A:220:PRO:O	1:A:221:ILE:CB	2.65	0.44
1:B:163:ILE:HG13	1:B:163:ILE:O	2.16	0.44
1:A:58:VAL:CG1	1:A:59:SER:H	2.29	0.44
1:A:103:PHE:O	1:A:106:GLU:CB	2.65	0.44
1:B:236:SER:HA	1:B:237:PRO:HD3	1.71	0.44
1:A:49:ARG:HD3	1:B:181:ARG:HE	1.82	0.44
1:A:64:PHE:O	1:A:65:ALA:C	2.61	0.44
1:B:78:PHE:CZ	1:B:130:GLU:HA	2.53	0.44
1:B:94:PRO:HB2	1:B:99:GLY:N	2.33	0.44
1:A:60:TRP:CD1	1:A:148:ARG:HH21	2.34	0.44
1:A:94:PRO:HB2	1:A:99:GLY:N	2.33	0.44
1:B:208:LYS:HZ1	1:B:254:LEU:HD13	1.82	0.44
1:A:49:ARG:C	1:A:51:LEU:N	2.74	0.43
1:A:61:PRO:O	1:A:63:PHE:N	2.51	0.43
1:B:58:VAL:CG1	1:B:59:SER:H	2.29	0.43
1:B:175:VAL:HG23	1:B:228:MET:HB2	1.99	0.43
1:A:90:ALA:C	1:A:92:GLN:N	2.71	0.43
1:A:246:LEU:O	1:A:247:ALA:C	2.61	0.43
1:A:243:PRO:HG3	1:A:281:TRP:CE2	2.54	0.43
1:B:47:VAL:HB	1:B:48:TRP:H	1.63	0.43
1:B:163:ILE:HA	1:B:280:ARG:O	2.18	0.43
1:A:288:LEU:HD21	1:A:303:PHE:HA	2.00	0.43
1:A:81:LEU:HB3	1:A:126:ILE:HD11	1.99	0.43
1:A:65:ALA:O	1:A:68:ALA:HB3	2.17	0.43
1:A:81:LEU:HD23	1:A:126:ILE:HD12	1.98	0.43
1:A:82:TYR:HB3	1:A:89:ILE:HG13	2.01	0.43
1:B:285:TYR:O	1:B:286:VAL:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:O	1:A:73:VAL:C	2.61	0.43
1:B:41:TYR:CD1	1:B:41:TYR:C	2.89	0.43
1:B:48:TRP:O	1:B:51:LEU:N	2.49	0.43
1:B:49:ARG:C	1:B:51:LEU:N	2.75	0.43
1:B:112:GLY:O	1:B:114:GLY:N	2.52	0.43
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.74	0.43
1:B:61:PRO:O	1:B:63:PHE:N	2.51	0.43
1:B:151:ARG:C	1:B:152:PRO:O	2.57	0.43
1:B:176:ARG:HG2	1:B:303:PHE:HE1	1.83	0.43
1:A:59:SER:HG	1:A:62:VAL:HG23	1.83	0.43
1:A:212:LEU:HD23	1:A:216:ARG:CB	2.49	0.42
1:A:175:VAL:HG21	1:A:214:LEU:HD23	2.01	0.42
1:B:41:TYR:O	1:B:41:TYR:CG	2.65	0.42
1:B:64:PHE:O	1:B:65:ALA:C	2.59	0.42
1:B:118:PRO:CB	1:B:124:HIS:NE2	2.81	0.42
1:A:49:ARG:O	1:A:50:ASP:C	2.62	0.42
1:A:176:ARG:CD	1:A:285:TYR:CD2	2.98	0.42
1:B:103:PHE:O	1:B:106:GLU:CB	2.64	0.42
1:B:283:HIS:HA	1:B:308:PRO:HA	2.00	0.42
1:A:112:GLY:O	1:A:114:GLY:N	2.52	0.42
1:B:132:PHE:HA	1:B:135:MET:HE3	2.01	0.42
1:A:78:PHE:CZ	1:A:130:GLU:HA	2.53	0.42
1:A:176:ARG:HG2	1:A:303:PHE:HE1	1.84	0.42
1:A:213:LYS:HB2	1:A:215:VAL:HG22	1.96	0.42
1:A:179:ASN:OD1	1:A:184:VAL:HG22	2.19	0.42
1:B:78:PHE:CD2	1:B:130:GLU:OE1	2.73	0.42
1:B:133:VAL:O	1:B:135:MET:N	2.53	0.42
1:B:163:ILE:C	1:B:163:ILE:CD1	2.89	0.42
1:B:175:VAL:CG2	1:B:214:LEU:HD23	2.50	0.42
1:A:57:LYS:HA	1:A:57:LYS:HD3	1.82	0.42
1:B:215:VAL:O	1:B:216:ARG:C	2.62	0.42
1:B:246:LEU:O	1:B:247:ALA:C	2.63	0.42
1:B:267:VAL:O	1:B:267:VAL:HG13	2.19	0.42
1:A:145:VAL:O	1:A:146:PHE:C	2.63	0.42
1:B:82:TYR:HB3	1:B:89:ILE:HG13	2.01	0.42
1:B:152:PRO:HA	1:B:266:GLN:OE1	2.19	0.42
1:B:167:PHE:O	1:B:168:ASN:C	2.63	0.42
1:B:213:LYS:HB2	1:B:215:VAL:HG22	1.96	0.42
1:A:118:PRO:CB	1:A:124:HIS:NE2	2.81	0.42
1:A:190:ALA:HB3	1:A:213:LYS:HA	2.00	0.42
1:A:242:THR:C	1:A:244:GLU:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:LEU:HD23	1:B:216:ARG:CB	2.49	0.42
1:B:242:THR:C	1:B:244:GLU:N	2.77	0.42
1:A:68:ALA:O	1:A:69:ALA:C	2.63	0.41
1:B:177:ALA:HA	1:B:303:PHE:HZ	1.84	0.41
1:A:132:PHE:CE1	1:B:68:ALA:HA	2.54	0.41
1:A:132:PHE:HA	1:A:135:MET:HE3	2.01	0.41
1:B:94:PRO:HB3	1:B:98:VAL:HG12	2.02	0.41
1:B:243:PRO:HG3	1:B:281:TRP:CE2	2.55	0.41
1:B:286:VAL:HG12	1:B:305:ASP:C	2.45	0.41
1:A:219:HIS:CB	1:A:220:PRO:HD3	2.47	0.41
1:B:68:ALA:O	1:B:69:ALA:C	2.63	0.41
1:B:176:ARG:CZ	1:B:285:TYR:HB3	2.51	0.41
1:B:193:ARG:HE	1:B:208:LYS:HZ2	1.68	0.41
1:A:163:ILE:HA	1:A:280:ARG:O	2.21	0.41
1:B:49:ARG:O	1:B:50:ASP:C	2.62	0.41
1:A:137:GLY:O	1:A:138:ILE:C	2.61	0.41
1:A:267:VAL:O	1:A:267:VAL:HG13	2.21	0.41
1:A:302:ARG:HG2	1:A:305:ASP:OD2	2.20	0.41
1:B:192:MET:O	1:B:192:MET:HG3	2.20	0.41
1:A:78:PHE:CD2	1:A:130:GLU:OE1	2.74	0.41
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.74	0.41
1:B:186:ALA:HB1	1:B:258:GLU:C	2.44	0.41
1:B:286:VAL:CG1	1:B:305:ASP:O	2.69	0.41
1:B:145:VAL:O	1:B:146:PHE:C	2.63	0.41
1:A:49:ARG:CZ	1:B:181:ARG:CZ	2.99	0.41
1:A:82:TYR:C	1:A:84:LEU:N	2.77	0.41
1:A:133:VAL:O	1:A:135:MET:N	2.54	0.41
1:A:190:ALA:CB	1:A:214:LEU:CD1	2.94	0.41
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.87	0.41
1:B:71:PHE:CE1	1:B:108:LEU:HD23	2.56	0.41
1:B:72:VAL:O	1:B:73:VAL:C	2.61	0.41
1:B:268:MET:O	1:B:268:MET:HG3	2.21	0.41
1:A:94:PRO:HB3	1:A:98:VAL:HG12	2.02	0.40
1:B:176:ARG:CD	1:B:285:TYR:CD2	3.01	0.40
1:A:79:ALA:O	1:A:81:LEU:N	2.54	0.40
1:A:142:THR:O	1:A:145:VAL:HB	2.21	0.40
1:A:146:PHE:HD2	1:B:146:PHE:CZ	2.38	0.40
1:A:215:VAL:O	1:A:216:ARG:C	2.62	0.40
1:A:250:ARG:O	1:A:251:ALA:C	2.64	0.40
1:A:289:MET:CG	1:A:298:ILE:HG12	2.46	0.40
1:B:176:ARG:HH22	1:B:288:LEU:HG	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:SER:OG	1:B:64:PHE:HE2	2.04	0.40
1:A:80:LEU:HD23	1:A:97:PHE:CE1	2.57	0.40
1:A:208:LYS:O	1:B:218:GLU:OE1	2.39	0.40
1:A:285:TYR:O	1:A:286:VAL:C	2.62	0.40
1:B:249:GLY:C	1:B:251:ALA:H	2.28	0.40
1:A:167:PHE:O	1:A:168:ASN:C	2.64	0.40
1:A:283:HIS:CE1	1:A:308:PRO:HD3	2.56	0.40
1:B:79:ALA:O	1:B:81:LEU:N	2.54	0.40
1:B:176:ARG:NH2	1:B:288:LEU:HG	2.37	0.40

All (2) 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:A:224:LEU:CD2	1:B:37:GLU:OE2[2_665]	1.99	0.21
1:A:262:GLU:OE2	1:B:271:ARG:NE[2_665]	2.10	0.10

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	252/333 (76%)	154 (61%)	55 (22%)	43 (17%)	0	1
1	B	252/333 (76%)	153 (61%)	56 (22%)	43 (17%)	0	1
All	All	504/666 (76%)	307 (61%)	111 (22%)	86 (17%)	0	1

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ALA
1	A	47	VAL
1	A	90	ALA

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Mol	Chain	Res	Type
1	A	97	PHE
1	A	105	VAL
1	A	113	TYR
1	A	133	VAL
1	A	179	ASN
1	A	183	ASN
1	A	185	ILE
1	A	212	LEU
1	A	213	LYS
1	A	214	LEU
1	A	216	ARG
1	A	220	PRO
1	A	221	ILE
1	A	240	GLY
1	A	247	ALA
1	B	40	ALA
1	B	47	VAL
1	B	90	ALA
1	B	97	PHE
1	B	105	VAL
1	B	113	TYR
1	B	133	VAL
1	B	179	ASN
1	B	183	ASN
1	B	185	ILE
1	B	212	LEU
1	B	213	LYS
1	B	214	LEU
1	B	216	ARG
1	B	220	PRO
1	B	221	ILE
1	B	240	GLY
1	B	247	ALA
1	A	48	TRP
1	A	63	PHE
1	A	80	LEU
1	A	150	ALA
1	A	160	ARG
1	A	168	ASN
1	A	181	ARG
1	A	184	VAL
1	A	224	LEU

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Mol	Chain	Res	Type
1	B	48	TRP
1	B	63	PHE
1	B	80	LEU
1	B	150	ALA
1	B	160	ARG
1	B	168	ASN
1	B	181	ARG
1	B	224	LEU
1	A	61	PRO
1	A	91	ASN
1	A	131	ILE
1	A	132	PHE
1	B	61	PRO
1	B	91	ASN
1	B	131	ILE
1	B	132	PHE
1	B	184	VAL
1	A	83	GLN
1	A	98	VAL
1	B	83	GLN
1	B	98	VAL
1	A	68	ALA
1	A	112	GLY
1	A	134	GLY
1	A	139	ALA
1	B	68	ALA
1	B	134	GLY
1	A	114	GLY
1	A	125	ALA
1	B	112	GLY
1	B	114	GLY
1	B	125	ALA
1	B	139	ALA
1	A	39	ILE
1	A	121	VAL
1	B	39	ILE
1	B	121	VAL
1	A	118	PRO
1	B	118	PRO
1	A	145	VAL
1	B	145	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	204/269 (76%)	170 (83%)	34 (17%)	2	13
1	B	204/269 (76%)	170 (83%)	34 (17%)	2	13
All	All	408/538 (76%)	340 (83%)	68 (17%)	2	13

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	A	48	TRP
1	A	51	LEU
1	A	57	LYS
1	A	60	TRP
1	A	70	LEU
1	A	72	VAL
1	A	75	ASN
1	A	76	THR
1	A	91	ASN
1	A	93	SER
1	A	124	HIS
1	A	136	SER
1	A	141	SER
1	A	153	ARG
1	A	163	ILE
1	A	165	ARG
1	A	175	VAL
1	A	176	ARG
1	A	179	ASN
1	A	185	ILE
1	A	192	MET
1	A	215	VAL
1	A	227	ASN
1	A	230	HIS
1	A	255	VAL
1	A	256	MET

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Mol	Chain	Res	Type
1	A	260	SER
1	A	261	ASP
1	A	263	THR
1	A	267	VAL
1	A	269	GLN
1	A	286	VAL
1	A	302	ARG
1	B	46	SER
1	B	48	TRP
1	B	51	LEU
1	B	57	LYS
1	B	60	TRP
1	B	70	LEU
1	B	72	VAL
1	B	75	ASN
1	B	76	THR
1	B	91	ASN
1	B	93	SER
1	B	124	HIS
1	B	136	SER
1	B	141	SER
1	B	153	ARG
1	B	163	ILE
1	B	165	ARG
1	B	175	VAL
1	B	176	ARG
1	B	179	ASN
1	B	185	ILE
1	B	192	MET
1	B	215	VAL
1	B	227	ASN
1	B	230	HIS
1	B	255	VAL
1	B	256	MET
1	B	260	SER
1	B	261	ASP
1	B	263	THR
1	B	267	VAL
1	B	269	GLN
1	B	286	VAL
1	B	302	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	A	269	GLN
1	A	272	HIS
1	B	168	ASN
1	B	272	HIS
1	B	283	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	2
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	41:TYR	C	42:GLY	N	1.14
1	A	38:VAL	C	39:ILE	N	1.12
1	B	38:VAL	C	39:ILE	N	1.12

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	258/333 (77%)	0.06	6 (2%) 61 36	45, 89, 138, 159	0
1	B	258/333 (77%)	0.06	12 (4%) 36 22	43, 89, 137, 157	0
All	All	516/666 (77%)	0.06	18 (3%) 47 28	43, 89, 138, 159	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	HIS	7.2
1	A	299	ASP	3.9
1	B	43	MET	3.1
1	B	40	ALA	2.9
1	B	39	ILE	2.7
1	B	112	GLY	2.7
1	B	297	HIS	2.6
1	A	219	HIS	2.6
1	B	85	GLY	2.6
1	B	96	GLY	2.5
1	A	96	GLY	2.4
1	B	213	LYS	2.4
1	B	296	THR	2.3
1	B	37	GLU	2.2
1	B	41	TYR	2.2
1	A	40	ALA	2.1
1	A	213	LYS	2.0
1	B	219	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	K	B	401	1/1	0.47	0.25	22,22,22,22	1
2	K	A	403	1/1	0.83	0.19	5,5,5,5	1
2	K	A	404	1/1	0.84	0.29	56,56,56,56	1
2	K	A	402	1/1	0.90	0.36	57,57,57,57	1

6.5 Other polymers [i](#)

There are no such residues in this entry.