



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:32 AM UTC

PDB ID : 4MFV / pdb_00004mfv
Title : Crystal structure of human CTNNBL1(residues 33 563)
Authors : Ahn, J.W.; Kim, S.; Kim, K.J.
Deposited on : 2013-08-28
Resolution : 2.92 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

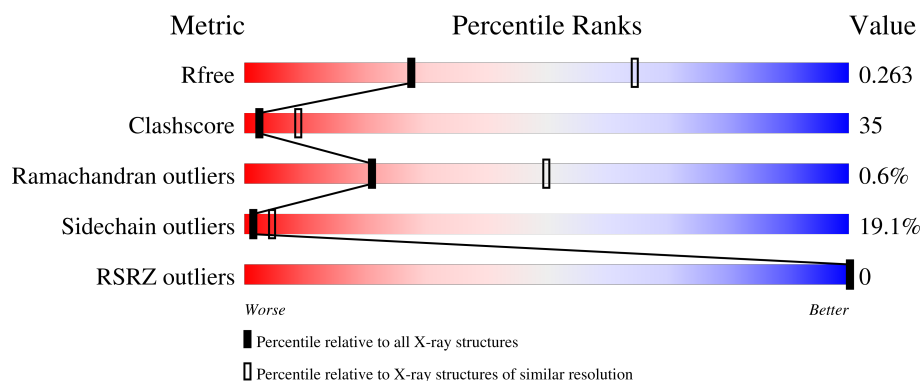
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	534	
1	B	534	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7866 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 Beta-catenin-like protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3933	2466	686	754	27			
1	B	489	Total	C	N	O	S	0	0	0
			3933	2466	686	754	27			

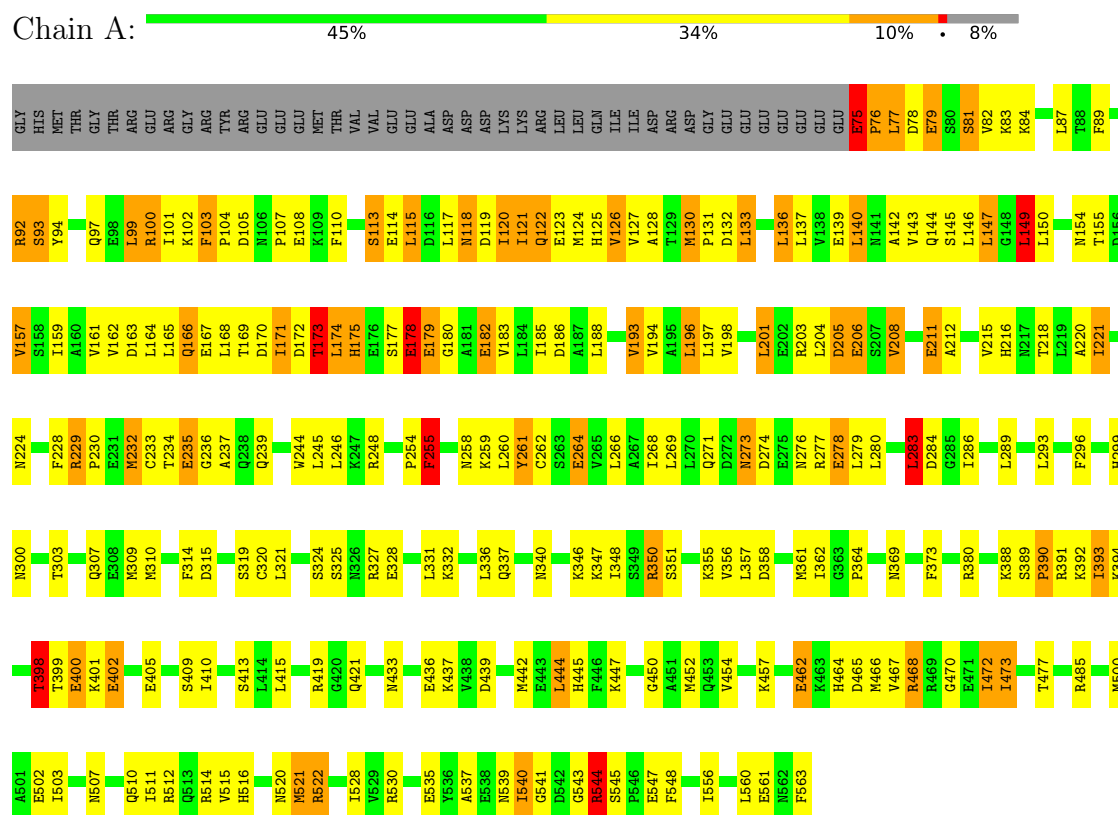
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	expression tag	UNP Q8WYA6
A	31	HIS	-	expression tag	UNP Q8WYA6
A	32	MET	-	expression tag	UNP Q8WYA6
B	30	GLY	-	expression tag	UNP Q8WYA6
B	31	HIS	-	expression tag	UNP Q8WYA6
B	32	MET	-	expression tag	UNP Q8WYA6

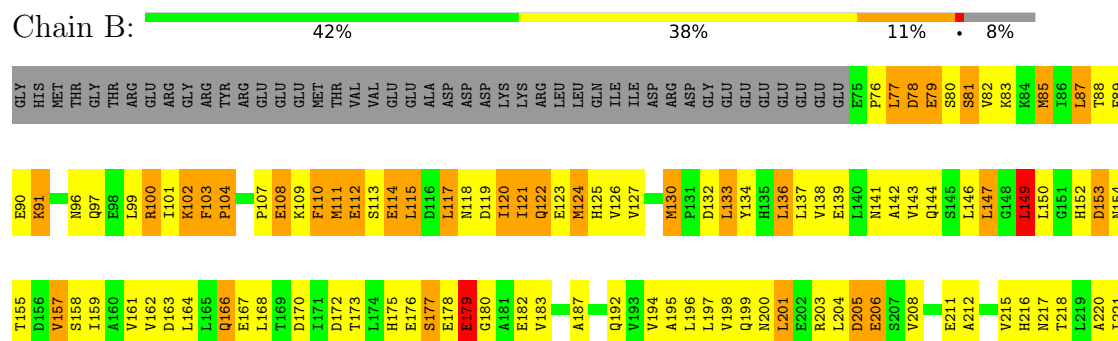
3 Residue-property plots

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: Beta-catenin-like protein 1



• Molecule 1: Beta-catenin-like protein 1



V492	T398	S302	N224
I499	T399	T303	
M500	E400	A304	F228
A501	K401	E305	R229
E502	E402	M310	P230
I503	H403		E231
G504	E404	F314	M232
N505	E405	D315	C233
A506			T234
N507	S409	S319	E235
	I410	G320	G236
Q510		L321	A237
I511	S413		Q238
R512	L414	S324	Q239
Q513	L415	S325	
R514	R416	N326	W244
V515	N417	R327	L245
H516	I418	R328	
Q517	R419	R329	R248
I518	G420	F330	
L519	Q421	L331	M253
N520		K332	P254
M521	T424	G333	F255
R522			D256
	K429	L336	A257
I528	K437	Q337	
E535		L338	L260
Y536	M442	M339	
A537	E443	N340	E264
E538	L444		V265
N539	H445	K347	L266
I540	F446	I348	A267
G541	K447	S349	I268
D542	Y448	R350	L269
G543		S351	
R544	M452	S352	N273
S545			D274
P546	K457	K355	E275
E547			N276
F548	E462	D358	R277
R549	K463		E278
E550	H464	M361	L279
N551	D465	I362	L280
E552	M466	G363	G281
	V467	P364	E282
I556	R468	E365	L283
L557	R469	F373	D284
G558	G470		G285
L559	E471	R380	I286
L560	I472	T381	D287
E561	I473		V288
N562	T477	S389	L289
F563		P390	
	E480	R391	L293
	R485	K392	
		I393	F296
		K394	
		K395	N300
			P301

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	90.04Å 90.04Å 175.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.84 – 2.92 46.84 – 2.92	Depositor EDS
% Data completeness (in resolution range)	94.1 (46.84-2.92) 94.1 (46.84-2.92)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.233 , 0.305 (Not available) , 0.263	Depositor DCC
R_{free} test set	1635 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l 0.480 for h,-h-k,-l 0.054 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7866	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.77	3/3985 (0.1%)	1.10	24/5358 (0.4%)
1	B	0.77	3/3985 (0.1%)	1.12	22/5358 (0.4%)
All	All	0.77	6/7970 (0.1%)	1.11	46/10716 (0.4%)

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	3
1	B	0	4
All	All	0	7

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	300	ASN	C-N	6.04	1.40	1.33
1	B	545	SER	C-N	5.40	1.40	1.33
1	B	104	PRO	N-CD	5.34	1.55	1.47
1	B	546	PRO	N-CD	5.23	1.55	1.47
1	A	76	PRO	N-CD	5.16	1.54	1.47
1	A	75	GLU	C-N	5.15	1.41	1.34

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	ARG	N-CA-C	8.81	120.66	111.14
1	A	175	HIS	N-CA-C	7.85	119.84	111.28
1	B	179	GLU	CA-C-N	-7.84	110.46	120.34
1	B	179	GLU	C-N-CA	-7.84	110.46	120.34
1	A	81	SER	N-CA-C	-7.78	102.80	111.28
1	B	347	LYS	N-CA-C	-7.64	97.09	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	333	GLY	N-CA-C	-7.62	102.31	112.14
1	B	178	GLU	N-CA-C	-6.74	103.96	111.71
1	B	112	GLU	N-CA-C	-6.69	103.99	111.28
1	A	300	ASN	CA-C-N	-6.65	112.92	119.90
1	A	300	ASN	C-N-CA	-6.65	112.92	119.90
1	A	221	ILE	CB-CA-C	-6.53	103.52	111.88
1	B	363	GLY	CA-C-N	6.31	125.80	119.24
1	B	363	GLY	C-N-CA	6.31	125.80	119.24
1	B	255	PHE	N-CA-C	6.23	117.32	108.54
1	A	208	VAL	N-CA-C	-6.20	101.58	109.58
1	A	178	GLU	N-CA-C	-6.09	104.55	111.07
1	A	149	LEU	N-CA-C	-6.00	104.74	111.28
1	A	171	ILE	CA-C-N	5.77	128.81	120.38
1	A	171	ILE	C-N-CA	5.77	128.81	120.38
1	B	103	PHE	CA-C-N	-5.71	112.72	119.05
1	B	103	PHE	C-N-CA	-5.71	112.72	119.05
1	A	206	GLU	N-CA-C	5.66	119.88	112.92
1	A	173	THR	N-CA-C	-5.62	105.25	111.71
1	B	469	ARG	N-CA-C	-5.56	105.22	111.28
1	B	545	SER	CA-C-N	-5.55	113.17	119.28
1	B	545	SER	C-N-CA	-5.55	113.17	119.28
1	A	75	GLU	CA-C-N	-5.54	112.90	119.05
1	A	75	GLU	C-N-CA	-5.54	112.90	119.05
1	A	278	GLU	N-CA-C	-5.51	105.28	111.28
1	B	149	LEU	N-CA-C	-5.42	105.38	111.28
1	A	229	ARG	CA-C-N	5.37	125.04	119.56
1	A	229	ARG	C-N-CA	5.37	125.04	119.56
1	A	283	LEU	N-CA-C	5.22	118.47	112.57
1	A	100	ARG	N-CA-C	-5.20	106.78	113.23
1	A	264	GLU	N-CA-C	-5.18	105.71	111.36
1	A	347	LYS	N-CA-C	-5.15	100.69	108.52
1	B	102	LYS	N-CA-C	5.14	116.69	111.14
1	B	405	GLU	N-CA-C	-5.12	105.69	111.28
1	B	206	GLU	N-CA-C	5.12	118.56	112.72
1	A	255	PHE	N-CA-C	5.11	116.92	108.49
1	B	81	SER	N-CA-C	-5.11	105.84	111.71
1	B	221	ILE	CB-CA-C	-5.10	102.93	111.29
1	A	147	LEU	N-CA-C	5.09	116.83	111.28
1	B	544	ARG	N-CA-C	-5.09	101.97	109.86
1	B	147	LEU	N-CA-C	5.02	116.75	111.28

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	HIS	Peptide
1	A	254	PRO	Peptide
1	A	398	THR	Peptide
1	B	254	PRO	Peptide
1	B	256	ASP	Peptide
1	B	347	LYS	Peptide
1	B	398	THR	Peptide

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	3933	0	3972	278	0
1	B	3933	0	3972	277	0
All	All	7866	0	7944	551	0

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 35.

All (551) 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:393:ILE:CG2	1:A:399:THR:HG21	1.35	1.53
1:B:201:LEU:HD23	1:B:244:TRP:CE2	1.48	1.48
1:B:201:LEU:HD21	1:B:244:TRP:CH2	1.64	1.31
1:B:124:MET:O	1:B:127:VAL:HG23	1.34	1.27
1:B:201:LEU:HD23	1:B:244:TRP:CZ2	1.72	1.25
1:B:208:VAL:HB	1:B:211:GLU:CG	1.67	1.24
1:B:201:LEU:CD2	1:B:244:TRP:CE2	2.20	1.23
1:B:201:LEU:HD21	1:B:244:TRP:CZ3	1.73	1.22
1:B:201:LEU:CD2	1:B:244:TRP:CZ2	2.26	1.18
1:B:464:HIS:O	1:B:467:VAL:HG22	1.37	1.17
1:A:393:ILE:HG23	1:A:399:THR:HG21	1.23	1.16
1:A:204:LEU:HD23	1:A:211:GLU:HG3	1.27	1.14
1:B:111:MET:HA	1:B:114:GLU:HG3	1.30	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:HG21	1:A:248:ARG:NH2	1.64	1.10
1:A:393:ILE:CG2	1:A:399:THR:CG2	2.28	1.10
1:A:92:ARG:HB3	1:A:117:LEU:HD13	1.24	1.09
1:B:201:LEU:CD2	1:B:244:TRP:CD2	2.37	1.06
1:B:208:VAL:CB	1:B:211:GLU:HG3	1.85	1.06
1:A:208:VAL:HB	1:A:211:GLU:HB2	1.36	1.04
1:A:215:VAL:CG2	1:A:248:ARG:HH22	1.70	1.04
1:A:393:ILE:HG22	1:A:399:THR:HG21	1.40	1.04
1:B:248:ARG:HH21	1:B:253:MET:HE1	1.21	1.03
1:B:201:LEU:CD2	1:B:244:TRP:CH2	2.40	1.03
1:A:204:LEU:CD2	1:A:211:GLU:HG3	1.88	1.03
1:B:100:ARG:O	1:B:104:PRO:HG3	1.58	1.02
1:B:279:LEU:O	1:B:283:LEU:HD12	1.62	0.99
1:B:208:VAL:HB	1:B:211:GLU:HG3	1.01	0.99
1:B:109:LYS:HE3	1:B:109:LYS:HA	1.44	0.97
1:A:215:VAL:HG21	1:A:248:ARG:HH22	0.82	0.97
1:A:237:ALA:HB2	1:A:276:ASN:OD1	1.64	0.97
1:B:237:ALA:HB2	1:B:276:ASN:OD1	1.65	0.96
1:B:537:ALA:O	1:B:540:ILE:HB	1.67	0.94
1:A:520:ASN:O	1:A:522:ARG:HA	1.69	0.92
1:B:248:ARG:NH2	1:B:253:MET:HE1	1.85	0.92
1:A:393:ILE:HG21	1:A:399:THR:HG21	1.51	0.92
1:A:171:ILE:O	1:A:174:LEU:HD13	1.68	0.92
1:B:201:LEU:CD2	1:B:244:TRP:CZ3	2.53	0.91
1:B:201:LEU:CD2	1:B:244:TRP:CE3	2.54	0.91
1:B:399:THR:CB	1:B:400:GLU:HG2	2.00	0.91
1:B:472:ILE:HD13	1:B:472:ILE:H	1.35	0.90
1:B:117:LEU:O	1:B:120:ILE:HG22	1.71	0.90
1:B:114:GLU:HA	1:B:117:LEU:HD23	1.53	0.90
1:B:232:MET:CE	1:B:233:CYS:HA	2.02	0.90
1:A:128:ALA:HB1	1:A:171:ILE:HG13	1.55	0.89
1:A:393:ILE:HG23	1:A:399:THR:CG2	1.99	0.89
1:A:117:LEU:O	1:A:120:ILE:HG22	1.73	0.88
1:A:544:ARG:HB2	1:A:544:ARG:HH11	1.36	0.88
1:A:390:PRO:HB2	1:A:391:ARG:HG3	1.54	0.87
1:A:540:ILE:HG13	1:A:541:GLY:H	1.38	0.87
1:B:164:LEU:O	1:B:168:LEU:HD12	1.73	0.86
1:A:232:MET:HE2	1:A:233:CYS:HA	1.57	0.86
1:A:117:LEU:O	1:A:121:ILE:HD13	1.76	0.86
1:A:163:ASP:O	1:A:166:GLN:HG2	1.77	0.85
1:B:520:ASN:O	1:B:522:ARG:HA	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLN:HG3	1:A:167:GLU:N	1.91	0.85
1:B:115:LEU:HD22	1:B:115:LEU:O	1.77	0.85
1:B:232:MET:HE3	1:B:232:MET:O	1.77	0.84
1:A:169:THR:O	1:A:172:ASP:HB3	1.78	0.84
1:A:92:ARG:HB3	1:A:117:LEU:CD1	2.07	0.84
1:A:94:TYR:OH	1:B:91:LYS:HD2	1.77	0.84
1:B:540:ILE:HG13	1:B:541:GLY:H	1.41	0.84
1:B:401:LYS:O	1:B:405:GLU:HG3	1.78	0.83
1:B:149:LEU:HB3	1:B:161:VAL:HG21	1.58	0.83
1:A:398:THR:O	1:A:402:GLU:HB3	1.78	0.83
1:A:212:ALA:O	1:A:215:VAL:HG22	1.78	0.82
1:A:204:LEU:HD23	1:A:211:GLU:CG	2.07	0.82
1:A:279:LEU:O	1:A:283:LEU:HD12	1.78	0.82
1:B:212:ALA:O	1:B:215:VAL:HG22	1.79	0.82
1:A:237:ALA:CB	1:A:276:ASN:OD1	2.27	0.82
1:A:125:HIS:HA	1:A:164:LEU:HD12	1.62	0.82
1:B:120:ILE:HD13	1:B:120:ILE:O	1.80	0.82
1:B:201:LEU:HD22	1:B:244:TRP:CD2	2.12	0.81
1:B:464:HIS:O	1:B:467:VAL:CG2	2.26	0.81
1:B:398:THR:O	1:B:402:GLU:HB3	1.79	0.81
1:B:78:ASP:HB3	1:B:81:SER:HB3	1.63	0.80
1:A:228:PHE:O	1:A:230:PRO:HD3	1.82	0.80
1:A:537:ALA:O	1:A:540:ILE:HB	1.81	0.80
1:A:78:ASP:HB2	1:A:130:MET:HE1	1.64	0.80
1:B:467:VAL:HG23	1:B:468:ARG:N	1.97	0.80
1:A:232:MET:HE3	1:A:232:MET:O	1.82	0.80
1:A:146:LEU:HD22	1:A:161:VAL:HG13	1.62	0.79
1:B:237:ALA:CB	1:B:276:ASN:OD1	2.30	0.79
1:A:78:ASP:HB2	1:A:130:MET:SD	2.22	0.79
1:A:102:LYS:C	1:A:104:PRO:HD3	2.06	0.79
1:A:544:ARG:HH11	1:A:544:ARG:CB	1.94	0.79
1:A:540:ILE:HD13	1:A:556:ILE:CD1	2.13	0.79
1:A:124:MET:O	1:A:127:VAL:HG23	1.83	0.78
1:A:163:ASP:O	1:A:166:GLN:CG	2.31	0.78
1:A:228:PHE:C	1:A:230:PRO:HD3	2.08	0.78
1:A:401:LYS:O	1:A:405:GLU:HG3	1.84	0.78
1:A:120:ILE:HD13	1:A:120:ILE:O	1.84	0.77
1:A:393:ILE:HG22	1:A:399:THR:CG2	2.07	0.77
1:B:78:ASP:CB	1:B:81:SER:HB3	2.14	0.77
1:B:399:THR:OG1	1:B:400:GLU:HG2	1.84	0.77
1:A:78:ASP:HB2	1:A:130:MET:CE	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:MET:HE3	1:B:232:MET:C	2.09	0.77
1:A:399:THR:CB	1:A:400:GLU:HG2	2.15	0.76
1:B:180:GLY:HA2	1:B:183:VAL:HG22	1.67	0.76
1:B:78:ASP:HB3	1:B:81:SER:CB	2.16	0.76
1:A:115:LEU:O	1:A:115:LEU:HD22	1.85	0.76
1:B:117:LEU:O	1:B:121:ILE:HD13	1.85	0.76
1:B:109:LYS:HA	1:B:109:LYS:CE	2.16	0.76
1:A:171:ILE:O	1:A:174:LEU:CD1	2.33	0.75
1:B:147:LEU:O	1:B:150:LEU:HB2	1.86	0.75
1:B:110:PHE:O	1:B:113:SER:HB3	1.86	0.75
1:B:158:SER:HB3	1:B:200:ASN:HD21	1.51	0.75
1:A:155:THR:HG22	1:A:203:ARG:HD2	1.69	0.75
1:A:235:GLU:O	1:A:239:GLN:HG2	1.87	0.75
1:B:121:ILE:HG23	1:B:164:LEU:HD13	1.69	0.75
1:A:166:GLN:HG3	1:A:167:GLU:H	1.49	0.74
1:B:111:MET:HA	1:B:114:GLU:CG	2.14	0.74
1:B:170:ASP:O	1:B:173:THR:HG22	1.88	0.74
1:A:390:PRO:HB2	1:A:391:ARG:CG	2.17	0.73
1:B:123:GLU:O	1:B:126:VAL:HG22	1.88	0.73
1:A:149:LEU:HB3	1:A:161:VAL:HG21	1.69	0.73
1:B:472:ILE:HD13	1:B:472:ILE:N	2.03	0.73
1:B:327:ARG:NH2	1:B:362:ILE:O	2.22	0.73
1:B:235:GLU:O	1:B:239:GLN:HG2	1.88	0.72
1:B:232:MET:HE3	1:B:233:CYS:HA	1.69	0.72
1:B:503:ILE:HB	1:B:511:ILE:HD12	1.71	0.72
1:B:399:THR:HB	1:B:400:GLU:HG2	1.69	0.72
1:B:201:LEU:HD21	1:B:244:TRP:CE3	2.19	0.72
1:A:452:MET:HE1	1:A:485:ARG:HG2	1.70	0.72
1:A:122:GLN:O	1:A:125:HIS:HB2	1.89	0.72
1:A:208:VAL:CG2	1:A:211:GLU:OE1	2.37	0.72
1:A:544:ARG:HB2	1:A:544:ARG:NH1	2.03	0.72
1:B:132:ASP:O	1:B:177:SER:HB3	1.89	0.72
1:A:150:LEU:CD1	1:A:161:VAL:HG11	2.20	0.71
1:B:399:THR:HB	1:B:400:GLU:OE2	1.89	0.71
1:B:232:MET:HE2	1:B:233:CYS:HA	1.72	0.71
1:A:327:ARG:NH2	1:A:362:ILE:O	2.22	0.71
1:B:134:TYR:HB2	1:B:180:GLY:HA3	1.71	0.71
1:B:201:LEU:HD12	1:B:218:THR:HG21	1.72	0.71
1:A:165:LEU:HA	1:A:168:LEU:HD12	1.71	0.71
1:A:125:HIS:NE2	1:A:167:GLU:HG3	2.04	0.70
1:A:503:ILE:HB	1:A:511:ILE:HD12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:LYS:N	1:A:393:ILE:HA	2.06	0.70
1:A:155:THR:HG22	1:A:203:ARG:CD	2.22	0.70
1:A:442:MET:HE1	1:A:500:MET:HG3	1.74	0.70
1:A:150:LEU:CD1	1:A:161:VAL:CG1	2.70	0.70
1:A:521:MET:HA	1:A:522:ARG:HD3	1.73	0.69
1:B:149:LEU:HD22	1:B:161:VAL:CG2	2.23	0.69
1:B:205:ASP:HB3	1:B:206:GLU:CD	2.17	0.69
1:B:164:LEU:HD23	1:B:168:LEU:HD13	1.74	0.69
1:A:173:THR:HG22	1:A:174:LEU:HD12	1.75	0.69
1:A:521:MET:HA	1:A:522:ARG:CD	2.23	0.69
1:A:544:ARG:HH11	1:A:544:ARG:CG	2.05	0.68
1:B:399:THR:HB	1:B:400:GLU:CD	2.17	0.68
1:B:540:ILE:HG23	1:B:541:GLY:N	2.08	0.68
1:A:540:ILE:HG23	1:A:541:GLY:N	2.08	0.68
1:A:466:MET:HE1	1:A:477:THR:HG21	1.76	0.68
1:A:179:GLU:O	1:A:183:VAL:HG22	1.93	0.68
1:B:149:LEU:CD2	1:B:161:VAL:CG2	2.72	0.68
1:A:147:LEU:O	1:A:150:LEU:HB2	1.95	0.67
1:B:201:LEU:HD22	1:B:244:TRP:CE3	2.28	0.67
1:A:125:HIS:CA	1:A:164:LEU:HD12	2.24	0.67
1:A:174:LEU:HD12	1:A:174:LEU:H	1.60	0.67
1:B:337:GLN:N	1:B:337:GLN:OE1	2.27	0.67
1:B:399:THR:C	1:B:400:GLU:HG2	2.19	0.67
1:A:79:GLU:O	1:A:79:GLU:HG3	1.94	0.67
1:B:164:LEU:HD23	1:B:168:LEU:CD1	2.25	0.67
1:A:77:LEU:H	1:A:77:LEU:HD23	1.60	0.67
1:B:324:SER:O	1:B:327:ARG:HB2	1.95	0.66
1:A:540:ILE:HG13	1:A:541:GLY:N	2.09	0.66
1:B:547:GLU:O	1:B:551:ASN:HB2	1.94	0.66
1:A:399:THR:HB	1:A:400:GLU:HG2	1.77	0.66
1:B:229:ARG:O	1:B:232:MET:HG2	1.95	0.66
1:A:167:GLU:O	1:A:171:ILE:HG12	1.95	0.66
1:A:174:LEU:HD12	1:A:174:LEU:N	2.11	0.66
1:B:155:THR:HG22	1:B:203:ARG:HD2	1.76	0.66
1:A:540:ILE:CD1	1:A:556:ILE:CD1	2.74	0.66
1:B:540:ILE:HD13	1:B:556:ILE:CD1	2.26	0.65
1:B:109:LYS:O	1:B:109:LYS:HD3	1.96	0.65
1:B:115:LEU:HD22	1:B:115:LEU:C	2.21	0.65
1:B:164:LEU:CD2	1:B:168:LEU:HD11	2.26	0.65
1:B:119:ASP:O	1:B:123:GLU:HG2	1.97	0.64
1:A:464:HIS:O	1:A:467:VAL:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:CD1	1:B:218:THR:HG21	2.28	0.64
1:B:78:ASP:OD1	1:B:78:ASP:N	2.30	0.64
1:A:232:MET:HE3	1:A:232:MET:C	2.22	0.64
1:B:150:LEU:CD1	1:B:161:VAL:HG11	2.28	0.64
1:B:399:THR:HB	1:B:400:GLU:CG	2.27	0.64
1:A:125:HIS:HA	1:A:164:LEU:CD1	2.28	0.63
1:A:232:MET:CE	1:A:233:CYS:HA	2.29	0.63
1:B:164:LEU:CD2	1:B:168:LEU:CD1	2.76	0.63
1:B:122:GLN:O	1:B:125:HIS:HB2	1.99	0.63
1:B:176:GLU:CD	1:B:177:SER:N	2.57	0.62
1:B:442:MET:HE1	1:B:500:MET:HG3	1.79	0.62
1:B:466:MET:HE1	1:B:477:THR:HG21	1.81	0.62
1:A:415:LEU:HB3	1:A:502:GLU:HG2	1.81	0.62
1:A:93:SER:HA	1:A:117:LEU:HD22	1.82	0.62
1:B:85:MET:HE1	1:B:123:GLU:C	2.25	0.62
1:A:75:GLU:HG3	1:A:76:PRO:HD3	1.82	0.61
1:A:115:LEU:HD22	1:A:115:LEU:C	2.25	0.61
1:B:195:ALA:O	1:B:199:GLN:HG3	2.00	0.61
1:A:83:LYS:O	1:A:87:LEU:HD12	2.01	0.61
1:B:279:LEU:O	1:B:283:LEU:CD1	2.43	0.61
1:B:540:ILE:HG13	1:B:541:GLY:N	2.13	0.61
1:A:164:LEU:HG	1:A:168:LEU:HD11	1.82	0.61
1:B:452:MET:HE1	1:B:485:ARG:HG2	1.82	0.61
1:B:205:ASP:HB3	1:B:206:GLU:OE2	2.00	0.60
1:B:503:ILE:O	1:B:511:ILE:HD11	2.01	0.60
1:A:147:LEU:HB3	1:A:196:LEU:HD12	1.84	0.60
1:A:472:ILE:HD13	1:A:472:ILE:H	1.65	0.60
1:B:103:PHE:CE2	1:B:107:PRO:O	2.54	0.60
1:B:392:LYS:N	1:B:393:ILE:HA	2.17	0.60
1:A:194:VAL:O	1:A:198:VAL:HG23	2.02	0.59
1:A:206:GLU:OE1	1:A:206:GLU:HA	2.01	0.59
1:A:539:ASN:C	1:A:540:ILE:HG22	2.27	0.59
1:B:108:GLU:HB2	1:B:110:PHE:HE1	1.67	0.59
1:B:331:LEU:O	1:B:333:GLY:O	2.21	0.59
1:A:465:ASP:HA	1:A:468:ARG:HH22	1.67	0.59
1:A:130:MET:HE2	1:A:131:PRO:HD2	1.85	0.59
1:B:279:LEU:HD12	1:B:283:LEU:HD11	1.84	0.59
1:B:152:HIS:ND1	1:B:157:VAL:HG11	2.18	0.58
1:B:398:THR:O	1:B:402:GLU:CB	2.50	0.58
1:B:467:VAL:HG23	1:B:468:ARG:H	1.68	0.58
1:B:176:GLU:OE1	1:B:177:SER:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:ARG:NH1	1:A:258:ASN:HB3	2.18	0.58
1:A:164:LEU:O	1:A:168:LEU:HD12	2.03	0.58
1:B:467:VAL:CG2	1:B:468:ARG:N	2.66	0.58
1:A:77:LEU:H	1:A:77:LEU:CD2	2.17	0.58
1:A:260:LEU:O	1:A:260:LEU:HD12	2.04	0.58
1:A:159:ILE:HA	1:A:162:VAL:HG12	1.85	0.58
1:B:232:MET:HE3	1:B:233:CYS:CA	2.34	0.58
1:B:405:GLU:HG2	1:B:492:VAL:HB	1.86	0.58
1:B:415:LEU:HB3	1:B:502:GLU:HG2	1.86	0.57
1:B:289:LEU:O	1:B:293:LEU:HD12	2.04	0.57
1:A:84:LYS:HA	1:A:87:LEU:HD12	1.86	0.57
1:A:103:PHE:N	1:A:104:PRO:HD3	2.18	0.57
1:A:125:HIS:CD2	1:A:167:GLU:HG3	2.39	0.57
1:B:539:ASN:C	1:B:540:ILE:HG22	2.30	0.57
1:A:196:LEU:N	1:A:196:LEU:HD23	2.18	0.57
1:A:77:LEU:HD23	1:A:77:LEU:O	2.04	0.57
1:B:208:VAL:CG2	1:B:211:GLU:HG3	2.34	0.57
1:B:296:PHE:HB3	1:B:310:MET:CE	2.35	0.57
1:B:114:GLU:HA	1:B:117:LEU:CD2	2.31	0.56
1:A:280:LEU:HD23	1:A:280:LEU:C	2.31	0.56
1:A:399:THR:OG1	1:A:400:GLU:HG2	2.06	0.56
1:B:101:ILE:O	1:B:104:PRO:HD3	2.05	0.56
1:A:157:VAL:O	1:A:161:VAL:HG23	2.06	0.56
1:A:170:ASP:O	1:A:173:THR:HB	2.05	0.56
1:B:220:ALA:O	1:B:224:ASN:OD1	2.24	0.56
1:A:331:LEU:HD23	1:A:331:LEU:O	2.06	0.56
1:B:117:LEU:HG	1:B:118:ASN:N	2.20	0.56
1:B:146:LEU:HD22	1:B:161:VAL:HG13	1.88	0.56
1:B:361:MET:HE1	1:B:373:PHE:CG	2.41	0.56
1:A:229:ARG:O	1:A:232:MET:HG2	2.06	0.56
1:A:89:PHE:CD1	1:A:121:ILE:HD11	2.40	0.55
1:B:336:LEU:O	1:B:340:ASN:HB2	2.07	0.55
1:A:137:LEU:HD23	1:A:142:ALA:CB	2.36	0.55
1:B:521:MET:HA	1:B:522:ARG:CD	2.36	0.55
1:A:185:ILE:O	1:A:186:ASP:C	2.50	0.55
1:B:296:PHE:CB	1:B:310:MET:CE	2.85	0.55
1:B:274:ASP:HA	1:B:277:ARG:HD2	1.89	0.55
1:A:540:ILE:CD1	1:A:556:ILE:HD11	2.37	0.55
1:A:125:HIS:N	1:A:164:LEU:CD1	2.70	0.55
1:A:399:THR:C	1:A:400:GLU:HG2	2.31	0.55
1:A:124:MET:O	1:A:127:VAL:N	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ASN:O	1:B:157:VAL:HG12	2.07	0.54
1:A:163:ASP:O	1:A:166:GLN:HG3	2.05	0.54
1:A:274:ASP:HA	1:A:277:ARG:HD2	1.89	0.54
1:A:324:SER:O	1:A:327:ARG:HB2	2.08	0.54
1:B:82:VAL:CG2	1:B:136:LEU:HD23	2.36	0.54
1:A:201:LEU:HD22	1:A:218:THR:HG21	1.89	0.54
1:B:358:ASP:OD1	1:B:409:SER:OG	2.26	0.54
1:A:146:LEU:CD2	1:A:161:VAL:HG13	2.37	0.54
1:A:125:HIS:CA	1:A:164:LEU:CD1	2.85	0.54
1:B:143:VAL:HG13	1:B:144:GLN:N	2.24	0.54
1:A:545:SER:O	1:A:547:GLU:N	2.41	0.53
1:B:146:LEU:O	1:B:149:LEU:HB2	2.08	0.53
1:B:150:LEU:CD1	1:B:161:VAL:CG1	2.86	0.53
1:B:362:ILE:HA	1:B:413:SER:OG	2.09	0.53
1:A:147:LEU:HB3	1:A:196:LEU:CD1	2.39	0.53
1:B:520:ASN:C	1:B:522:ARG:HA	2.33	0.53
1:B:108:GLU:HB2	1:B:110:PHE:CE1	2.43	0.53
1:B:365:GLU:OE1	1:B:365:GLU:N	2.35	0.53
1:B:204:LEU:HD23	1:B:211:GLU:O	2.08	0.53
1:A:163:ASP:OD1	1:A:166:GLN:OE1	2.27	0.53
1:A:540:ILE:HD11	1:A:556:ILE:HD11	1.89	0.53
1:A:296:PHE:HB3	1:A:310:MET:CE	2.39	0.53
1:B:150:LEU:HD11	1:B:161:VAL:CG1	2.39	0.53
1:B:153:ASP:OD1	1:B:153:ASP:N	2.42	0.53
1:B:208:VAL:HB	1:B:211:GLU:HG2	1.79	0.53
1:A:143:VAL:HG13	1:A:144:GLN:N	2.24	0.53
1:A:180:GLY:O	1:A:183:VAL:HG23	2.08	0.53
1:A:155:THR:CG2	1:A:203:ARG:HD2	2.37	0.53
1:A:133:LEU:H	1:A:133:LEU:HD12	1.73	0.52
1:B:540:ILE:HG23	1:B:541:GLY:H	1.73	0.52
1:A:188:LEU:O	1:A:193:VAL:HG12	2.08	0.52
1:A:336:LEU:O	1:A:340:ASN:HB2	2.09	0.52
1:B:155:THR:HG22	1:B:203:ARG:CD	2.38	0.52
1:B:279:LEU:CD1	1:B:283:LEU:HD11	2.38	0.52
1:A:514:ARG:O	1:A:515:VAL:C	2.52	0.52
1:A:540:ILE:HD13	1:A:556:ILE:HD12	1.89	0.52
1:B:521:MET:HA	1:B:522:ARG:HD3	1.90	0.52
1:A:220:ALA:O	1:A:224:ASN:OD1	2.27	0.52
1:A:236:GLY:HA2	1:A:239:GLN:HG3	1.90	0.52
1:A:362:ILE:HA	1:A:413:SER:OG	2.10	0.52
1:A:132:ASP:HB2	1:A:177:SER:HB3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:PHE:CB	1:A:310:MET:CE	2.88	0.52
1:A:361:MET:HE1	1:A:373:PHE:CG	2.45	0.52
1:B:206:GLU:OE1	1:B:206:GLU:HA	2.10	0.52
1:B:514:ARG:O	1:B:515:VAL:C	2.51	0.52
1:A:208:VAL:O	1:A:211:GLU:N	2.43	0.52
1:B:546:PRO:HA	1:B:549:ARG:HB2	1.92	0.52
1:A:337:GLN:OE1	1:A:337:GLN:N	2.39	0.52
1:A:520:ASN:C	1:A:522:ARG:HA	2.32	0.52
1:B:78:ASP:HB2	1:B:81:SER:HB3	1.90	0.52
1:B:149:LEU:HD23	1:B:161:VAL:CG2	2.40	0.52
1:B:248:ARG:HH21	1:B:253:MET:CE	2.07	0.52
1:B:88:THR:HG22	1:B:120:ILE:HG13	1.91	0.51
1:B:208:VAL:CB	1:B:211:GLU:CG	2.60	0.51
1:A:299:HIS:HD1	1:A:299:HIS:N	2.09	0.51
1:B:229:ARG:O	1:B:232:MET:CG	2.57	0.51
1:B:469:ARG:HD2	1:B:471:GLU:OE2	2.09	0.51
1:A:390:PRO:HB2	1:A:391:ARG:CA	2.40	0.51
1:B:120:ILE:HD13	1:B:120:ILE:C	2.35	0.51
1:B:467:VAL:O	1:B:470:GLY:N	2.44	0.51
1:A:540:ILE:CG1	1:A:541:GLY:N	2.73	0.51
1:B:121:ILE:N	1:B:121:ILE:CD1	2.73	0.51
1:A:244:TRP:CH2	1:A:248:ARG:HG3	2.46	0.51
1:A:544:ARG:HH11	1:A:544:ARG:HG3	1.76	0.51
1:A:204:LEU:HD22	1:A:211:GLU:HG3	1.86	0.51
1:B:416:ARG:NH2	1:B:417:ASN:OD1	2.44	0.51
1:A:174:LEU:CD1	1:A:174:LEU:H	2.23	0.51
1:A:545:SER:O	1:A:548:PHE:N	2.44	0.51
1:B:236:GLY:HA2	1:B:239:GLN:HG3	1.91	0.51
1:B:149:LEU:HD22	1:B:161:VAL:HG22	1.91	0.50
1:B:149:LEU:CD2	1:B:161:VAL:HG21	2.40	0.50
1:A:82:VAL:CG2	1:A:136:LEU:HD23	2.42	0.50
1:A:544:ARG:NH1	1:A:544:ARG:CG	2.72	0.50
1:B:180:GLY:CA	1:B:183:VAL:HG22	2.40	0.50
1:A:234:THR:HA	1:A:276:ASN:HD21	1.77	0.50
1:B:228:PHE:C	1:B:230:PRO:HD3	2.37	0.50
1:B:166:GLN:CG	1:B:167:GLU:N	2.75	0.50
1:A:465:ASP:HA	1:A:468:ARG:NH2	2.26	0.50
1:B:110:PHE:CD1	1:B:110:PHE:N	2.77	0.50
1:A:150:LEU:HD12	1:A:161:VAL:CG1	2.41	0.50
1:B:78:ASP:HB3	1:B:81:SER:HB2	1.92	0.50
1:B:147:LEU:N	1:B:147:LEU:HD23	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:GLU:O	1:B:80:SER:HB2	2.11	0.49
1:B:147:LEU:O	1:B:150:LEU:N	2.45	0.49
1:B:286:ILE:HD12	1:B:287:ASP:H	1.76	0.49
1:A:299:HIS:N	1:A:299:HIS:ND1	2.60	0.49
1:B:137:LEU:HD23	1:B:142:ALA:CB	2.43	0.49
1:B:558:GLY:O	1:B:561:GLU:HG2	2.13	0.49
1:A:208:VAL:HG21	1:A:211:GLU:OE1	2.11	0.49
1:B:303:THR:OG1	1:B:305:GLU:HG2	2.13	0.49
1:A:540:ILE:HG23	1:A:541:GLY:H	1.77	0.49
1:B:82:VAL:HA	1:B:85:MET:HB2	1.95	0.49
1:B:462:GLU:O	1:B:466:MET:HG3	2.13	0.49
1:A:539:ASN:O	1:A:540:ILE:HG22	2.13	0.49
1:B:159:ILE:HA	1:B:162:VAL:HG12	1.94	0.49
1:A:171:ILE:C	1:A:174:LEU:HD13	2.37	0.48
1:B:89:PHE:CE1	1:B:121:ILE:HD11	2.48	0.48
1:B:175:HIS:CD2	1:B:175:HIS:H	2.32	0.48
1:A:279:LEU:O	1:A:283:LEU:CD1	2.56	0.48
1:B:192:GLN:O	1:B:196:LEU:HG	2.13	0.48
1:A:146:LEU:O	1:A:149:LEU:HB2	2.12	0.48
1:A:232:MET:C	1:A:232:MET:CE	2.85	0.48
1:A:244:TRP:HH2	1:A:248:ARG:NE	2.11	0.48
1:A:215:VAL:HG23	1:A:216:HIS:N	2.27	0.48
1:A:143:VAL:HG13	1:A:144:GLN:H	1.79	0.48
1:A:99:LEU:HD13	1:A:113:SER:OG	2.13	0.48
1:B:118:ASN:OD1	1:B:119:ASP:N	2.46	0.48
1:B:149:LEU:HD23	1:B:157:VAL:CG2	2.44	0.48
1:B:399:THR:CB	1:B:400:GLU:CG	2.82	0.48
1:B:544:ARG:HB3	1:B:548:PHE:CD1	2.49	0.48
1:A:331:LEU:HD12	1:A:369:ASN:OD1	2.14	0.47
1:B:296:PHE:CB	1:B:310:MET:HE2	2.44	0.47
1:B:157:VAL:O	1:B:161:VAL:HG23	2.14	0.47
1:A:165:LEU:HB3	1:A:221:ILE:CD1	2.44	0.47
1:A:280:LEU:HD13	1:A:320:CYS:SG	2.54	0.47
1:A:358:ASP:OD1	1:A:409:SER:OG	2.30	0.47
1:B:102:LYS:C	1:B:104:PRO:HD3	2.38	0.47
1:A:97:GLN:OE1	1:B:141:ASN:HB2	2.14	0.47
1:A:462:GLU:O	1:A:466:MET:HG3	2.15	0.47
1:A:530:ARG:NH2	1:A:563:PHE:O	2.47	0.47
1:B:103:PHE:CE2	1:B:107:PRO:C	2.93	0.47
1:B:109:LYS:HE3	1:B:109:LYS:CA	2.16	0.47
1:B:399:THR:O	1:B:402:GLU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:VAL:HG23	1:A:211:GLU:OE1	2.14	0.47
1:B:78:ASP:O	1:B:130:MET:HE1	2.15	0.47
1:B:147:LEU:HB3	1:B:196:LEU:CD1	2.45	0.46
1:B:215:VAL:HG23	1:B:216:HIS:N	2.30	0.46
1:A:450:GLY:O	1:A:454:VAL:HG23	2.16	0.46
1:A:244:TRP:CH2	1:A:248:ARG:NE	2.83	0.46
1:A:391:ARG:HD2	1:A:394:LYS:HE2	1.97	0.46
1:B:89:PHE:CD1	1:B:121:ILE:HD11	2.50	0.46
1:B:164:LEU:HG	1:B:168:LEU:HD11	1.96	0.46
1:A:150:LEU:HD12	1:A:161:VAL:HG11	1.96	0.46
1:A:255:PHE:HB3	1:A:259:LYS:HD3	1.98	0.46
1:A:289:LEU:O	1:A:293:LEU:HD12	2.14	0.46
1:B:109:LYS:CE	1:B:109:LYS:CA	2.85	0.46
1:B:176:GLU:CD	1:B:177:SER:H	2.22	0.46
1:B:280:LEU:C	1:B:280:LEU:HD23	2.41	0.46
1:B:264:GLU:O	1:B:268:ILE:HG12	2.16	0.46
1:A:178:GLU:O	1:A:182:GLU:HB2	2.15	0.46
1:A:232:MET:HE2	1:A:233:CYS:CA	2.38	0.46
1:A:541:GLY:C	1:A:543:GLY:HA2	2.41	0.46
1:B:429:LYS:O	1:B:437:LYS:CD	2.64	0.46
1:B:472:ILE:HG12	1:B:472:ILE:O	2.16	0.46
1:A:548:PHE:CD1	1:A:548:PHE:C	2.94	0.46
1:A:467:VAL:O	1:A:470:GLY:N	2.49	0.45
1:B:506:ALA:O	1:B:507:ASN:HB3	2.16	0.45
1:A:164:LEU:CD2	1:A:168:LEU:HD11	2.46	0.45
1:A:123:GLU:O	1:A:126:VAL:HG22	2.15	0.45
1:B:404:GLU:OE1	1:B:448:TYR:OH	2.30	0.45
1:B:544:ARG:CZ	1:B:545:SER:OG	2.64	0.45
1:A:102:LYS:C	1:A:104:PRO:CD	2.86	0.45
1:A:248:ARG:HD2	1:A:262:CYS:SG	2.55	0.45
1:A:350:ARG:HH22	1:A:390:PRO:HG3	1.81	0.45
1:A:521:MET:HA	1:A:522:ARG:HD2	1.98	0.45
1:B:164:LEU:O	1:B:168:LEU:CD1	2.56	0.45
1:B:539:ASN:O	1:B:540:ILE:HG22	2.15	0.45
1:B:103:PHE:O	1:B:103:PHE:CD2	2.70	0.45
1:B:180:GLY:O	1:B:183:VAL:HG22	2.16	0.45
1:B:358:ASP:HA	1:B:410:ILE:HG12	1.98	0.45
1:B:540:ILE:CD1	1:B:556:ILE:HD11	2.47	0.45
1:A:77:LEU:CD2	1:A:77:LEU:N	2.79	0.44
1:A:278:GLU:OE2	1:B:278:GLU:OE1	2.35	0.44
1:B:393:ILE:HG22	1:B:394:LYS:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:MET:O	1:A:125:HIS:C	2.60	0.44
1:B:296:PHE:HB2	1:B:310:MET:HE2	1.99	0.44
1:B:472:ILE:N	1:B:472:ILE:CD1	2.73	0.44
1:A:165:LEU:CA	1:A:168:LEU:HD12	2.43	0.44
1:B:512:ARG:O	1:B:516:HIS:HD2	2.00	0.44
1:A:103:PHE:N	1:A:104:PRO:CD	2.79	0.44
1:B:194:VAL:O	1:B:198:VAL:HG23	2.17	0.44
1:A:97:GLN:O	1:A:101:ILE:HG13	2.18	0.44
1:A:125:HIS:N	1:A:164:LEU:HD11	2.32	0.44
1:A:140:LEU:N	1:A:140:LEU:HD12	2.33	0.44
1:A:165:LEU:O	1:A:169:THR:HG23	2.17	0.44
1:A:174:LEU:CD1	1:A:174:LEU:N	2.80	0.44
1:A:358:ASP:HA	1:A:410:ILE:HG12	1.98	0.44
1:B:330:PHE:O	1:B:333:GLY:O	2.35	0.44
1:B:350:ARG:O	1:B:351:SER:C	2.61	0.44
1:B:540:ILE:CD1	1:B:556:ILE:CD1	2.95	0.44
1:A:150:LEU:HD11	1:A:161:VAL:HG12	1.99	0.43
1:A:260:LEU:HD12	1:A:260:LEU:C	2.43	0.43
1:A:390:PRO:HB2	1:A:391:ARG:CB	2.47	0.43
1:B:77:LEU:O	1:B:77:LEU:HG	2.17	0.43
1:A:401:LYS:HE3	1:A:401:LYS:HB3	1.78	0.43
1:A:468:ARG:NH2	1:A:468:ARG:HB3	2.34	0.43
1:B:120:ILE:HG23	1:B:121:ILE:HD12	2.00	0.43
1:A:154:ASN:O	1:A:157:VAL:HG12	2.18	0.43
1:A:436:GLU:O	1:A:439:ASP:HB2	2.18	0.43
1:A:465:ASP:CA	1:A:468:ARG:HH22	2.32	0.43
1:B:516:HIS:O	1:B:519:LEU:N	2.52	0.43
1:A:178:GLU:H	1:A:178:GLU:HG3	1.52	0.43
1:A:351:SER:HB2	1:A:398:THR:HG21	1.99	0.43
1:B:166:GLN:NE2	1:B:217:ASN:OD1	2.52	0.43
1:B:177:SER:C	1:B:179:GLU:N	2.70	0.43
1:B:278:GLU:OE2	1:B:282:GLU:OE2	2.36	0.43
1:B:467:VAL:CG2	1:B:468:ARG:H	2.30	0.43
1:B:548:PHE:CZ	1:B:552:GLU:OE2	2.71	0.43
1:A:466:MET:CE	1:A:477:THR:HG21	2.47	0.43
1:B:103:PHE:HE2	1:B:107:PRO:C	2.25	0.43
1:B:180:GLY:HA2	1:B:183:VAL:CG2	2.44	0.43
1:B:511:ILE:HG13	1:B:512:ARG:N	2.33	0.43
1:A:122:GLN:O	1:A:125:HIS:CB	2.63	0.43
1:A:264:GLU:O	1:A:268:ILE:HG12	2.17	0.43
1:B:96:ASN:HD22	1:B:117:LEU:CD2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:SER:HB3	1:B:403:HIS:ND1	2.34	0.43
1:B:286:ILE:HD12	1:B:287:ASP:N	2.34	0.43
1:B:400:GLU:HB2	1:B:401:LYS:H	1.56	0.43
1:B:415:LEU:CD1	1:B:499:ILE:HG23	2.49	0.43
1:A:229:ARG:O	1:A:232:MET:CG	2.67	0.43
1:B:103:PHE:O	1:B:103:PHE:CG	2.70	0.43
1:B:150:LEU:HD11	1:B:161:VAL:HG12	1.99	0.43
1:A:93:SER:HA	1:A:117:LEU:CD2	2.46	0.43
1:A:140:LEU:N	1:A:140:LEU:CD1	2.82	0.43
1:B:138:VAL:CG2	1:B:187:ALA:HB2	2.49	0.43
1:B:166:GLN:HG2	1:B:167:GLU:N	2.33	0.43
1:B:257:ALA:O	1:B:260:LEU:HB3	2.19	0.43
1:B:279:LEU:O	1:B:280:LEU:C	2.61	0.43
1:B:540:ILE:CG1	1:B:541:GLY:N	2.73	0.43
1:B:179:GLU:H	1:B:179:GLU:HG2	1.47	0.42
1:A:92:ARG:CG	1:A:117:LEU:HA	2.49	0.42
1:A:150:LEU:HD13	1:A:161:VAL:HG11	2.00	0.42
1:B:111:MET:O	1:B:114:GLU:N	2.52	0.42
1:B:505:ASN:OD1	1:B:562:ASN:HB2	2.19	0.42
1:A:120:ILE:HD13	1:A:120:ILE:C	2.40	0.42
1:A:215:VAL:CG2	1:A:216:HIS:N	2.82	0.42
1:A:356:VAL:O	1:A:357:LEU:C	2.61	0.42
1:A:545:SER:C	1:A:547:GLU:N	2.78	0.42
1:A:205:ASP:HB3	1:A:206:GLU:OE2	2.19	0.42
1:A:208:VAL:O	1:A:212:ALA:N	2.41	0.42
1:A:314:PHE:O	1:A:315:ASP:C	2.61	0.42
1:B:133:LEU:HD12	1:B:133:LEU:H	1.84	0.42
1:B:232:MET:CE	1:B:232:MET:C	2.88	0.42
1:B:232:MET:CE	1:B:233:CYS:CA	2.86	0.42
1:A:351:SER:OG	1:A:398:THR:HB	2.19	0.42
1:A:507:ASN:CG	1:A:507:ASN:O	2.62	0.42
1:A:208:VAL:HB	1:A:211:GLU:OE1	2.19	0.42
1:A:273:ASN:ND2	1:A:276:ASN:HD22	2.17	0.42
1:B:176:GLU:HG3	1:B:177:SER:OG	2.20	0.42
1:A:278:GLU:OE1	1:B:278:GLU:OE2	2.37	0.41
1:A:392:LYS:C	1:A:393:ILE:HG13	2.43	0.41
1:B:134:TYR:HD1	1:B:137:LEU:HD12	1.85	0.41
1:A:197:LEU:HD22	1:A:218:THR:HG23	2.01	0.41
1:B:104:PRO:HA	1:B:110:PHE:HE2	1.84	0.41
1:B:516:HIS:O	1:B:517:GLN:C	2.63	0.41
1:A:89:PHE:HD1	1:A:121:ILE:HD11	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:LEU:O	1:A:358:ASP:C	2.63	0.41
1:A:364:PRO:HG2	1:A:548:PHE:HE2	1.84	0.41
1:B:154:ASN:O	1:B:157:VAL:CG1	2.68	0.41
1:B:164:LEU:CD2	1:B:168:LEU:HD13	2.45	0.41
1:A:130:MET:O	1:A:131:PRO:C	2.63	0.41
1:A:145:SER:O	1:A:146:LEU:C	2.59	0.41
1:A:228:PHE:O	1:A:230:PRO:CD	2.60	0.41
1:A:115:LEU:C	1:A:115:LEU:CD2	2.91	0.41
1:A:124:MET:HA	1:A:127:VAL:HG23	2.02	0.41
1:A:390:PRO:CB	1:A:391:ARG:HA	2.50	0.41
1:B:103:PHE:N	1:B:104:PRO:HD3	2.35	0.41
1:A:163:ASP:O	1:A:164:LEU:C	2.62	0.41
1:A:166:GLN:CG	1:A:167:GLU:N	2.73	0.41
1:A:260:LEU:HD13	1:A:309:MET:HB2	2.01	0.41
1:A:121:ILE:N	1:A:121:ILE:CD1	2.84	0.41
1:A:147:LEU:N	1:A:147:LEU:HD23	2.35	0.41
1:A:193:VAL:HG22	1:A:197:LEU:HD12	2.03	0.41
1:A:261:TYR:HD1	1:A:261:TYR:HA	1.77	0.41
1:A:444:LEU:O	1:A:445:HIS:C	2.63	0.41
1:B:286:ILE:HG12	1:B:329:ARG:HB3	2.02	0.41
1:A:473:ILE:C	1:A:473:ILE:HD12	2.46	0.41
1:A:511:ILE:HG13	1:A:512:ARG:N	2.35	0.41
1:B:83:LYS:O	1:B:87:LEU:HD22	2.20	0.41
1:B:134:TYR:HB2	1:B:180:GLY:CA	2.44	0.41
1:B:538:GLU:O	1:B:540:ILE:HG22	2.20	0.41
1:B:541:GLY:O	1:B:549:ARG:CG	2.68	0.41
1:B:147:LEU:HB3	1:B:196:LEU:HD13	2.03	0.41
1:B:273:ASN:C	1:B:273:ASN:HD22	2.28	0.41
1:A:118:ASN:OD1	1:A:119:ASP:N	2.54	0.40
1:A:155:THR:CG2	1:A:203:ARG:CD	2.97	0.40
1:A:246:LEU:HD23	1:A:246:LEU:HA	1.84	0.40
1:B:208:VAL:O	1:B:211:GLU:N	2.54	0.40
1:A:124:MET:CA	1:A:127:VAL:HG23	2.51	0.40
1:A:503:ILE:O	1:A:511:ILE:HD11	2.21	0.40
1:B:300:ASN:HB3	1:B:301:PRO:CD	2.51	0.40
1:A:105:ASP:O	1:A:107:PRO:O	2.38	0.40
1:B:163:ASP:O	1:B:164:LEU:C	2.64	0.40
1:B:314:PHE:O	1:B:315:ASP:C	2.63	0.40
1:B:444:LEU:O	1:B:445:HIS:C	2.65	0.40
1:B:500:MET:O	1:B:503:ILE:HG12	2.21	0.40
1:A:164:LEU:CG	1:A:168:LEU:HD11	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLY:HA2	1:A:183:VAL:CG2	2.50	0.40
1:A:516:HIS:O	1:A:520:ASN:ND2	2.54	0.40
1:B:472:ILE:H	1:B:472:ILE:CD1	2.12	0.40
1:A:472:ILE:HG12	1:A:472:ILE:O	2.21	0.40
1:B:197:LEU:HA	1:B:197:LEU:HD23	1.87	0.40

There are no symmetry-related clashes.

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	487/534 (91%)	452 (93%)	32 (7%)	3 (1%)	21	50
1	B	487/534 (91%)	444 (91%)	40 (8%)	3 (1%)	21	50
All	All	974/1068 (91%)	896 (92%)	72 (7%)	6 (1%)	21	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	540	ILE
1	B	540	ILE
1	B	76	PRO
1	B	390	PRO
1	A	103	PHE
1	A	390	PRO

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	442/482 (92%)	357 (81%)	85 (19%)	1	4
1	B	442/482 (92%)	358 (81%)	84 (19%)	1	5
All	All	884/964 (92%)	715 (81%)	169 (19%)	1	4

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	GLU
1	A	77	LEU
1	A	79	GLU
1	A	81	SER
1	A	92	ARG
1	A	93	SER
1	A	99	LEU
1	A	100	ARG
1	A	108	GLU
1	A	110	PHE
1	A	113	SER
1	A	114	GLU
1	A	115	LEU
1	A	118	ASN
1	A	120	ILE
1	A	121	ILE
1	A	122	GLN
1	A	126	VAL
1	A	130	MET
1	A	133	LEU
1	A	136	LEU
1	A	139	GLU
1	A	140	LEU
1	A	149	LEU
1	A	157	VAL
1	A	166	GLN
1	A	173	THR
1	A	174	LEU
1	A	178	GLU
1	A	179	GLU
1	A	182	GLU
1	A	193	VAL
1	A	196	LEU

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Mol	Chain	Res	Type
1	A	201	LEU
1	A	205	ASP
1	A	211	GLU
1	A	232	MET
1	A	235	GLU
1	A	245	LEU
1	A	255	PHE
1	A	261	TYR
1	A	266	LEU
1	A	269	LEU
1	A	271	GLN
1	A	273	ASN
1	A	283	LEU
1	A	284	ASP
1	A	286	ILE
1	A	303	THR
1	A	307	GLN
1	A	319	SER
1	A	321	LEU
1	A	325	SER
1	A	328	GLU
1	A	332	LYS
1	A	346	LYS
1	A	348	ILE
1	A	350	ARG
1	A	355	LYS
1	A	380	ARG
1	A	388	LYS
1	A	389	SER
1	A	393	ILE
1	A	398	THR
1	A	400	GLU
1	A	402	GLU
1	A	419	ARG
1	A	421	GLN
1	A	433	ASN
1	A	437	LYS
1	A	444	LEU
1	A	447	LYS
1	A	457	LYS
1	A	462	GLU
1	A	468	ARG

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Mol	Chain	Res	Type
1	A	472	ILE
1	A	473	ILE
1	A	510	GLN
1	A	521	MET
1	A	522	ARG
1	A	528	ILE
1	A	535	GLU
1	A	544	ARG
1	A	560	LEU
1	A	561	GLU
1	B	77	LEU
1	B	78	ASP
1	B	79	GLU
1	B	85	MET
1	B	87	LEU
1	B	90	GLU
1	B	91	LYS
1	B	97	GLN
1	B	99	LEU
1	B	100	ARG
1	B	108	GLU
1	B	110	PHE
1	B	111	MET
1	B	112	GLU
1	B	114	GLU
1	B	115	LEU
1	B	117	LEU
1	B	120	ILE
1	B	121	ILE
1	B	122	GLN
1	B	124	MET
1	B	130	MET
1	B	133	LEU
1	B	136	LEU
1	B	139	GLU
1	B	149	LEU
1	B	153	ASP
1	B	157	VAL
1	B	166	GLN
1	B	172	ASP
1	B	177	SER
1	B	179	GLU

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Mol	Chain	Res	Type
1	B	182	GLU
1	B	201	LEU
1	B	205	ASP
1	B	232	MET
1	B	235	GLU
1	B	245	LEU
1	B	255	PHE
1	B	266	LEU
1	B	269	LEU
1	B	273	ASN
1	B	284	ASP
1	B	286	ILE
1	B	303	THR
1	B	319	SER
1	B	321	LEU
1	B	325	SER
1	B	328	GLU
1	B	332	LYS
1	B	338	LEU
1	B	348	ILE
1	B	350	ARG
1	B	352	SER
1	B	355	LYS
1	B	380	ARG
1	B	381	THR
1	B	389	SER
1	B	395	LYS
1	B	400	GLU
1	B	402	GLU
1	B	409	SER
1	B	419	ARG
1	B	421	GLN
1	B	424	THR
1	B	437	LYS
1	B	444	LEU
1	B	447	LYS
1	B	457	LYS
1	B	472	ILE
1	B	473	ILE
1	B	480	GLU
1	B	510	GLN
1	B	514	ARG

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Mol	Chain	Res	Type
1	B	521	MET
1	B	522	ARG
1	B	528	ILE
1	B	535	GLU
1	B	542	ASP
1	B	544	ARG
1	B	545	SER
1	B	547	GLU
1	B	560	LEU
1	B	561	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	ASN
1	A	122	GLN
1	A	166	GLN
1	A	276	ASN
1	A	326	ASN
1	A	510	GLN
1	A	531	HIS
1	A	562	ASN
1	B	122	GLN
1	B	166	GLN
1	B	175	HIS
1	B	312	ASN
1	B	359	HIS
1	B	433	ASN
1	B	510	GLN
1	B	513	GLN
1	B	531	HIS
1	B	539	ASN
1	B	562	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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	489/534 (91%)	-0.93	0 100 100	24, 85, 128, 157	0
1	B	489/534 (91%)	-0.90	0 100 100	24, 87, 130, 158	0
All	All	978/1068 (91%)	-0.92	0 100 100	24, 86, 130, 158	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.