



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:05 PM UTC

PDB ID : 3S4W / pdb_00003s4w
Title : Structure of the FANCI-FANCD2 complex
Authors : Pavletich, N.P.
Deposited on : 2011-05-20
Resolution : 3.41 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

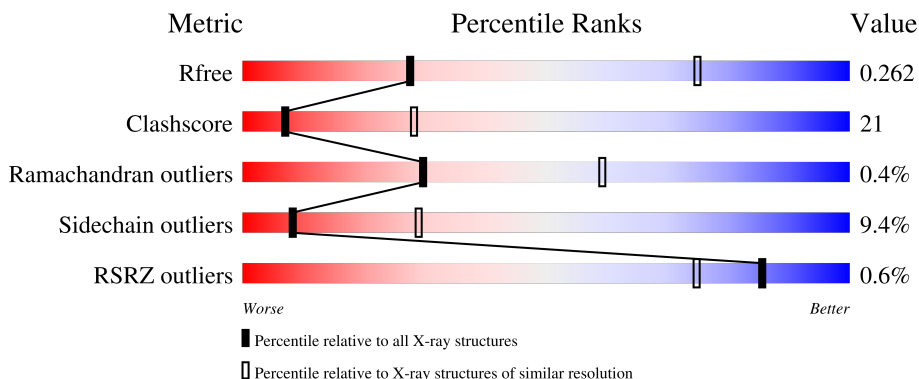
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.41 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	1308	
2	B	1323	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18671 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 Fanconi anemia group I protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1206	Total	C	N	O	S	0	0	0
			9506	6093	1579	1778	56			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1303	HIS	-	expression tag	UNP Q8K368
A	1304	HIS	-	expression tag	UNP Q8K368
A	1305	HIS	-	expression tag	UNP Q8K368
A	1306	HIS	-	expression tag	UNP Q8K368
A	1307	HIS	-	expression tag	UNP Q8K368
A	1308	HIS	-	expression tag	UNP Q8K368

- Molecule 2 is a protein called Fanconi anemia group D2 protein homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1146	Total	C	N	O	S	0	0	0
			9165	5905	1543	1664	53			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP Q80V62
B	?	-	SER	deletion	UNP Q80V62
B	?	-	SER	deletion	UNP Q80V62
B	?	-	ALA	deletion	UNP Q80V62
B	?	-	VAL	deletion	UNP Q80V62
B	?	-	ALA	deletion	UNP Q80V62
B	?	-	ALA	deletion	UNP Q80V62
B	?	-	LYS	deletion	UNP Q80V62
B	?	-	ASN	deletion	UNP Q80V62
B	?	-	ARG	deletion	UNP Q80V62

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASN	deletion	UNP Q80V62
B	?	-	LYS	deletion	UNP Q80V62
B	?	-	GLY	deletion	UNP Q80V62
B	?	-	LYS	deletion	UNP Q80V62
B	?	-	THR	deletion	UNP Q80V62
B	?	-	GLY	deletion	UNP Q80V62
B	?	-	GLY	deletion	UNP Q80V62
B	?	-	LYS	deletion	UNP Q80V62
B	?	-	LYS	deletion	UNP Q80V62
B	?	-	GLN	deletion	UNP Q80V62
B	?	-	LYS	deletion	UNP Q80V62
B	?	-	ALA	deletion	UNP Q80V62
B	?	-	ASP	deletion	UNP Q80V62
B	?	-	SER	deletion	UNP Q80V62
B	?	-	ASN	deletion	UNP Q80V62
B	?	-	LYS	deletion	UNP Q80V62
B	?	-	ALA	deletion	UNP Q80V62
B	?	-	SER	deletion	UNP Q80V62
B	?	-	CYS	deletion	UNP Q80V62
B	?	-	SER	deletion	UNP Q80V62
B	?	-	ASP	deletion	UNP Q80V62
B	?	-	THR	deletion	UNP Q80V62
B	?	-	LEU	deletion	UNP Q80V62
B	?	-	LEU	deletion	UNP Q80V62
B	?	-	THR	deletion	UNP Q80V62
B	?	-	GLU	deletion	UNP Q80V62
B	?	-	ASP	deletion	UNP Q80V62
B	?	-	THR	deletion	UNP Q80V62
B	?	-	SER	deletion	UNP Q80V62
B	?	-	GLU	deletion	UNP Q80V62
B	?	-	CYS	deletion	UNP Q80V62
B	?	-	ASP	deletion	UNP Q80V62
B	?	-	MET	deletion	UNP Q80V62
B	?	-	ALA	deletion	UNP Q80V62
B	?	-	PRO	deletion	UNP Q80V62
B	?	-	SER	deletion	UNP Q80V62
B	?	-	GLY	deletion	UNP Q80V62
B	?	-	ARG	deletion	UNP Q80V62
B	?	-	SER	deletion	UNP Q80V62
B	?	-	HIS	deletion	UNP Q80V62
B	?	-	VAL	deletion	UNP Q80V62
B	?	-	ASP	deletion	UNP Q80V62

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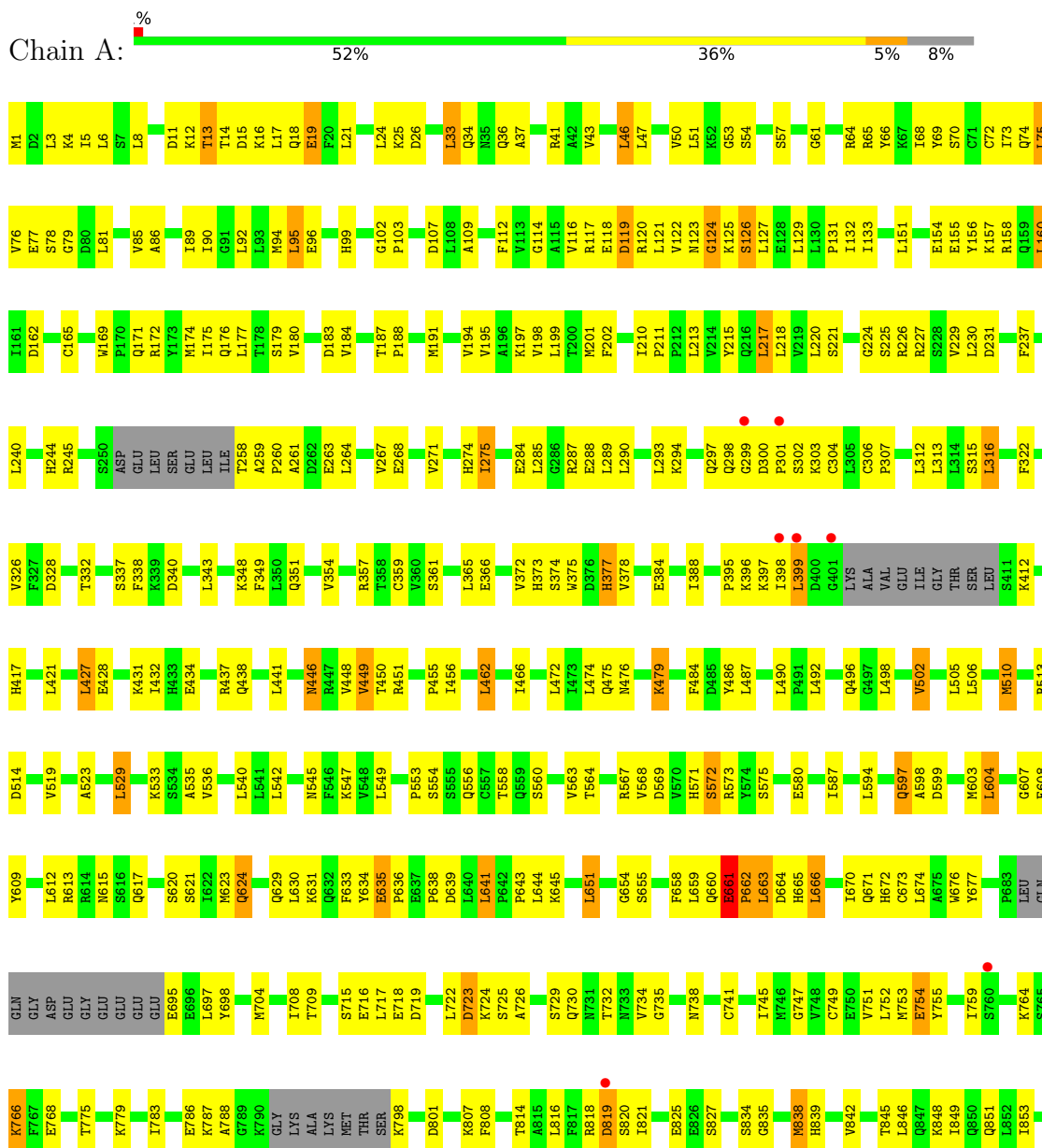
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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	LYS	deletion	UNP Q80V62
B	?	-	GLU	deletion	UNP Q80V62
B	?	-	SER	deletion	UNP Q80V62
B	?	-	THR	deletion	UNP Q80V62
B	?	-	GLY	deletion	UNP Q80V62
B	?	-	LYS	deletion	UNP Q80V62
B	?	-	GLU	deletion	UNP Q80V62
B	?	-	GLY	deletion	UNP Q80V62

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: Fanconi anemia group I protein homolog







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.80Å 110.40Å 350.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 3.41 19.86 – 3.41	Depositor EDS
% Data completeness (in resolution range)	90.0 (19.86-3.41) 88.3 (19.86-3.41)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.44Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.240 , 0.272 0.229 , 0.262	Depositor DCC
R_{free} test set	1738 reflections (4.05%)	wwPDB-VP
Wilson B-factor (Å ²)	90.3	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 72.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18671	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.35	0/9655	0.80	13/13038 (0.1%)
2	B	0.33	0/9336	0.81	26/12621 (0.2%)
All	All	0.34	0/18991	0.80	39/25659 (0.2%)

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
2	B	0	3
All	All	0	4

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1221	PHE	CA-C-N	12.45	135.40	119.84
2	B	1221	PHE	C-N-CA	12.45	135.40	119.84
2	B	693	ILE	N-CA-C	9.20	121.04	108.89
1	A	1037	SER	CA-C-N	9.15	128.78	119.82
1	A	1037	SER	C-N-CA	9.15	128.78	119.82
1	A	661	GLU	CA-C-N	7.92	129.74	119.84
1	A	661	GLU	C-N-CA	7.92	129.74	119.84
2	B	765	GLY	N-CA-C	-7.54	102.69	115.80
1	A	635	GLU	CA-C-N	6.97	126.58	119.19
1	A	635	GLU	C-N-CA	6.97	126.58	119.19
2	B	686	GLU	N-CA-C	-6.80	104.45	112.89
2	B	1286	TYR	CA-C-N	6.67	126.25	119.19
2	B	1286	TYR	C-N-CA	6.67	126.25	119.19
2	B	772	SER	N-CA-C	6.63	116.74	108.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1019	THR	CA-C-N	-6.35	113.33	121.91
2	B	1019	THR	C-N-CA	-6.35	113.33	121.91
2	B	291	THR	N-CA-C	-6.25	104.92	113.30
1	A	723	ASP	CB-CA-C	-6.17	109.47	116.63
2	B	663	VAL	N-CA-C	6.16	116.79	108.17
1	A	572	SER	N-CA-C	5.95	118.56	111.71
1	A	124	GLY	N-CA-C	-5.93	106.30	115.73
1	A	819	ASP	CB-CA-C	-5.82	108.19	116.34
2	B	1123	VAL	CA-C-N	5.81	125.18	118.85
2	B	1123	VAL	C-N-CA	5.81	125.18	118.85
2	B	682	TYR	N-CA-C	5.79	118.26	111.02
2	B	155	VAL	CB-CA-C	-5.62	108.39	114.35
2	B	802	SER	CA-C-N	5.57	125.10	119.19
2	B	802	SER	C-N-CA	5.57	125.10	119.19
2	B	1095	ARG	N-CA-C	-5.51	104.79	112.45
1	A	354	VAL	N-CA-C	5.33	113.74	107.77
1	A	938	THR	CB-CA-C	-5.28	108.94	116.34
2	B	289	ASP	CA-C-N	-5.23	115.03	122.77
2	B	289	ASP	C-N-CA	-5.23	115.03	122.77
2	B	662	PHE	N-CA-C	5.21	119.74	113.17
1	A	938	THR	N-CA-C	5.13	115.60	108.00
2	B	1103	GLN	CA-C-N	5.11	125.11	119.90
2	B	1103	GLN	C-N-CA	5.11	125.11	119.90
2	B	376	LYS	N-CA-C	5.08	117.38	109.60
2	B	683	GLY	N-CA-C	-5.08	104.23	112.31

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1062	ILE	Peptide
2	B	1094	ASN	Peptide
2	B	1284	ASP	Peptide
2	B	290	THR	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9506	0	9792	393	0
2	B	9165	0	9297	407	0
All	All	18671	0	19089	792	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 21.

All (792) 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)
2:B:698:LEU:HD22	2:B:760:PRO:HD3	1.38	1.04
1:A:764:LYS:HG2	1:A:827:SER:HB3	1.40	1.02
2:B:1123:VAL:HG13	2:B:1128:CYS:HB2	1.48	0.95
1:A:1071:VAL:HG13	1:A:1076:ALA:HB2	1.49	0.95
2:B:426:LEU:HD23	2:B:429:ILE:HD12	1.51	0.93
2:B:763:GLU:HB2	2:B:764:PRO:HD3	1.52	0.88
2:B:1195:LEU:HB2	2:B:1266:TRP:HZ3	1.37	0.88
2:B:836:PRO:HD3	2:B:914:VAL:HG23	1.55	0.88
2:B:916:LEU:O	2:B:919:TYR:HD2	1.59	0.85
1:A:1136:VAL:HG11	1:A:1194:THR:HG22	1.57	0.85
1:A:259:ALA:HB3	1:A:260:PRO:HD3	1.59	0.85
2:B:749:ILE:HG23	2:B:752:LEU:HD12	1.59	0.85
1:A:1077:ALA:HB3	1:A:1078:PRO:HD3	1.60	0.81
1:A:3:LEU:HD23	1:A:6:LEU:HD12	1.64	0.80
1:A:306:CYS:HB2	1:A:307:PRO:HD2	1.66	0.78
2:B:771:MET:O	2:B:776:ARG:NH1	2.16	0.78
1:A:877:THR:OG1	1:A:914:THR:HG21	1.83	0.78
1:A:399:LEU:HB2	1:A:455:PRO:HG3	1.64	0.78
2:B:1315:PHE:HA	2:B:1322:VAL:HG21	1.65	0.77
1:A:838:MET:HA	1:A:838:MET:HE2	1.66	0.77
2:B:411:GLN:HE22	2:B:1077:THR:HG21	1.50	0.77
1:A:34:GLN:O	1:A:37:ALA:N	2.18	0.76
2:B:763:GLU:HB2	2:B:764:PRO:CD	2.15	0.76
2:B:665:ASP:HA	2:B:692:GLY:O	1.84	0.76
2:B:1191:THR:HG22	2:B:1192:ASP:H	1.49	0.75
2:B:1277:LEU:HD13	2:B:1288:VAL:HG13	1.68	0.74
2:B:296:ILE:HD12	2:B:361:ALA:HB3	1.70	0.74
2:B:523:SER:HB2	2:B:524:PRO:HD2	1.69	0.74
2:B:776:ARG:HH21	2:B:779:MET:HG3	1.53	0.74
2:B:102:THR:HG23	2:B:108:LEU:HD13	1.70	0.73
1:A:1103:LYS:HG2	1:A:1180:TYR:HD1	1.51	0.73
2:B:697:LEU:HD23	2:B:759:LEU:HD21	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ILE:HG22	1:A:752:LEU:HD11	1.71	0.72
1:A:1142:LEU:HA	1:A:1145:PHE:HB3	1.71	0.72
2:B:735:ARG:HD2	2:B:796:ALA:HA	1.71	0.72
2:B:1223:THR:HG22	2:B:1228:THR:HG21	1.70	0.72
1:A:121:LEU:C	1:A:123:ASN:H	1.96	0.72
1:A:202:PHE:CE1	1:A:210:ILE:HG23	2.25	0.72
1:A:818:ARG:NH1	1:A:825:GLU:OE1	2.22	0.72
2:B:1206:VAL:N	2:B:1207:PRO:HD2	2.04	0.72
2:B:1277:LEU:HA	2:B:1280:MET:HB2	1.70	0.72
1:A:18:GLN:HG2	1:A:53:GLY:O	1.90	0.72
1:A:373:HIS:O	1:A:374:SER:OG	2.06	0.72
1:A:623:MET:HE1	1:A:673:CYS:HB3	1.70	0.72
2:B:765:GLY:O	2:B:769:GLU:HG3	1.90	0.71
2:B:104:ASP:HB3	2:B:107:SER:HB2	1.72	0.71
1:A:275:ILE:HD11	1:A:312:LEU:HD11	1.73	0.71
1:A:533:LYS:HA	1:A:603:MET:HE1	1.73	0.71
2:B:49:LEU:HD11	2:B:80:ALA:HB1	1.72	0.71
2:B:469:GLN:HA	2:B:508:ASN:ND2	2.06	0.71
1:A:361:SER:HA	1:A:421:LEU:HD11	1.73	0.71
1:A:1048:ASP:HB3	1:A:1071:VAL:HG11	1.73	0.70
2:B:581:GLY:HA2	2:B:636:LEU:HD13	1.73	0.70
1:A:1053:LEU:HD21	1:A:1077:ALA:HB2	1.70	0.70
1:A:448:VAL:HA	1:A:456:ILE:HG21	1.74	0.70
2:B:549:ILE:HG22	2:B:553:MET:HE2	1.73	0.70
1:A:1136:VAL:HG12	1:A:1198:LEU:HD12	1.74	0.70
2:B:1025:LEU:O	2:B:1029:HIS:HD2	1.75	0.70
1:A:1285:ASP:OD1	1:A:1286:PHE:N	2.21	0.70
1:A:338:PHE:CE2	1:A:417:HIS:HB3	2.27	0.69
2:B:800:GLN:HB3	2:B:805:MET:HG2	1.74	0.69
2:B:258:SER:HA	2:B:261:ARG:HH11	1.55	0.69
2:B:636:LEU:HD12	2:B:636:LEU:O	1.92	0.69
2:B:1233:PHE:CZ	2:B:1273:PHE:HB3	2.27	0.69
2:B:742:HIS:O	2:B:743:ASP:HB2	1.92	0.68
1:A:598:ALA:HB2	1:A:660:GLN:HA	1.75	0.68
1:A:641:LEU:HG	1:A:715:SER:HB3	1.75	0.68
1:A:662:PRO:HB2	1:A:665:HIS:HB2	1.75	0.68
1:A:959:GLN:HB2	1:A:1005:TRP:CZ2	2.29	0.68
2:B:1107:GLU:O	2:B:1111:GLN:HG2	1.94	0.68
2:B:1015:VAL:HG22	2:B:1070:LEU:HD11	1.76	0.68
1:A:449:VAL:HA	1:A:490:LEU:HD21	1.75	0.68
2:B:155:VAL:N	2:B:156:PRO:HD2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1053:LEU:HD11	1:A:1077:ALA:HA	1.76	0.67
2:B:352:ILE:HD11	2:B:385:ILE:HG22	1.74	0.67
2:B:1285:SER:CB	2:B:1288:VAL:HB	2.24	0.67
2:B:1116:LEU:HB2	2:B:1136:LEU:HD21	1.76	0.67
2:B:1195:LEU:HB2	2:B:1266:TRP:CZ3	2.27	0.67
2:B:210:ILE:HG22	2:B:246:VAL:HG21	1.77	0.67
2:B:1330:GLN:O	2:B:1334:ARG:HG3	1.94	0.67
1:A:558:THR:HB	1:A:563:VAL:HG23	1.75	0.67
1:A:174:MET:HE2	1:A:213:LEU:HD11	1.78	0.66
2:B:925:GLU:H	2:B:925:GLU:CD	2.03	0.66
2:B:1236:MET:HB3	2:B:1273:PHE:CE2	2.30	0.66
1:A:202:PHE:HE1	1:A:210:ILE:HG23	1.60	0.65
2:B:666:PHE:CG	2:B:666:PHE:O	2.49	0.65
1:A:85:VAL:O	1:A:89:ILE:HG13	1.96	0.65
1:A:349:PHE:CZ	1:A:1138:GLN:HG3	2.32	0.65
2:B:545:THR:HG22	2:B:546:SER:H	1.61	0.65
1:A:1270:SER:OG	1:A:1271:LYS:N	2.28	0.65
2:B:1061:GLN:HG3	2:B:1128:CYS:SG	2.37	0.65
1:A:258:THR:N	1:A:261:ALA:HB3	2.12	0.65
2:B:1090:GLU:HA	2:B:1093:SER:HB3	1.79	0.65
2:B:412:GLU:HG2	2:B:454:LEU:HD11	1.79	0.65
2:B:583:MET:HG3	2:B:608:VAL:HG22	1.77	0.65
2:B:784:PHE:HD1	2:B:823:LEU:HD11	1.62	0.65
2:B:826:TYR:O	2:B:830:ILE:HG22	1.96	0.65
2:B:45:VAL:HG21	2:B:93:GLU:HG2	1.80	0.64
2:B:178:LEU:HB3	2:B:216:ILE:HG23	1.78	0.64
2:B:1020:PRO:O	2:B:1021:MET:HE3	1.97	0.64
2:B:763:GLU:CB	2:B:764:PRO:HD3	2.25	0.64
1:A:1070:VAL:O	1:A:1071:VAL:HB	1.98	0.64
2:B:411:GLN:NE2	2:B:1077:THR:HG21	2.12	0.64
1:A:633:PHE:HB3	1:A:663:LEU:HD11	1.79	0.63
2:B:131:LYS:HG3	2:B:136:LEU:HD22	1.80	0.63
2:B:914:VAL:HG22	2:B:922:PHE:CE1	2.33	0.63
2:B:1326:LEU:HD11	2:B:1372:MET:HG2	1.81	0.63
2:B:1342:HIS:HE1	2:B:1344:LYS:HB2	1.64	0.63
1:A:127:LEU:HB3	1:A:180:VAL:HG21	1.79	0.63
2:B:454:LEU:O	2:B:458:TYR:HD1	1.82	0.63
2:B:830:ILE:HD13	2:B:834:VAL:HG22	1.81	0.63
2:B:735:ARG:HD2	2:B:796:ALA:CA	2.28	0.63
1:A:109:ALA:HB2	1:A:133:ILE:HG21	1.81	0.62
2:B:802:SER:OG	2:B:804:GLU:HG2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1245:LYS:HZ1	2:B:1298:ARG:HD2	1.64	0.62
2:B:1342:HIS:CE1	2:B:1344:LYS:HB2	2.33	0.62
2:B:203:VAL:HA	2:B:206:GLN:HG2	1.79	0.62
2:B:1285:SER:HB2	2:B:1288:VAL:HB	1.81	0.62
1:A:873:LEU:HD22	1:A:914:THR:HG23	1.81	0.62
1:A:1280:LEU:HD23	1:A:1280:LEU:H	1.64	0.62
2:B:528:ARG:HD2	2:B:632:GLU:OE1	1.99	0.62
1:A:21:LEU:O	1:A:64:ARG:NH2	2.33	0.62
1:A:174:MET:HE3	1:A:201:MET:HE3	1.82	0.62
2:B:55:LEU:CD2	2:B:133:LEU:HD13	2.29	0.62
2:B:528:ARG:HH22	2:B:1000:SER:HB2	1.65	0.62
1:A:946:THR:HG22	1:A:947:VAL:H	1.66	0.61
2:B:760:PRO:HG3	2:B:779:MET:HE1	1.81	0.61
2:B:1022:CYS:HA	2:B:1025:LEU:HB2	1.82	0.61
2:B:638:GLN:HB3	2:B:736:LEU:HD13	1.82	0.61
2:B:1326:LEU:CD1	2:B:1372:MET:HG2	2.30	0.61
1:A:33:LEU:HA	1:A:75:LEU:HD11	1.83	0.61
2:B:963:LEU:HD23	2:B:1059:CYS:SG	2.41	0.61
2:B:1085:LEU:HD11	2:B:1142:LYS:HE3	1.82	0.61
1:A:66:TYR:CE1	1:A:107:ASP:HB3	2.35	0.61
2:B:502:ALA:O	2:B:506:ARG:HG2	2.00	0.61
2:B:830:ILE:HG23	2:B:830:ILE:O	2.01	0.61
2:B:836:PRO:HD3	2:B:914:VAL:CG2	2.29	0.61
1:A:835:GLY:HA2	1:A:838:MET:HB2	1.82	0.60
1:A:1014:SER:HB2	1:A:1072:ASN:HD21	1.66	0.60
1:A:1198:LEU:HA	1:A:1201:LEU:HB2	1.81	0.60
1:A:199:LEU:HD23	1:A:202:PHE:HE2	1.66	0.60
2:B:1059:CYS:O	2:B:1063:LEU:HG	2.01	0.60
2:B:344:VAL:O	2:B:348:ILE:HG13	2.02	0.60
2:B:735:ARG:HD2	2:B:796:ALA:CB	2.32	0.60
1:A:395:PRO:HB3	1:A:398:ILE:HD12	1.83	0.60
1:A:816:LEU:HD13	1:A:838:MET:CE	2.32	0.60
2:B:779:MET:HB3	2:B:826:TYR:CZ	2.37	0.60
1:A:594:LEU:CD2	1:A:604:LEU:HD23	2.32	0.59
1:A:1265:GLN:O	1:A:1269:LYS:HB2	2.01	0.59
1:A:908:LEU:HD13	1:A:980:LEU:HD21	1.83	0.59
2:B:640:ARG:H	2:B:640:ARG:HD2	1.68	0.59
2:B:611:LEU:O	2:B:615:VAL:HG23	2.02	0.59
2:B:1017:LEU:O	2:B:1021:MET:HG3	2.01	0.59
1:A:226:ARG:HB2	1:A:288:GLU:HG2	1.84	0.59
2:B:430:CYS:HB3	2:B:431:PRO:HD3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:772:SER:HA	2:B:776:ARG:HD2	1.84	0.59
1:A:510:MET:HA	1:A:513:ARG:NH1	2.18	0.59
1:A:754:GLU:OE1	1:A:808:PHE:HB2	2.02	0.59
2:B:760:PRO:CG	2:B:779:MET:HE1	2.33	0.59
1:A:726:ALA:HB1	1:A:738:ASN:ND2	2.17	0.59
2:B:271:VAL:HG11	2:B:279:ILE:HD12	1.83	0.59
2:B:453:SER:HB2	2:B:493:VAL:HG21	1.84	0.59
2:B:831:PRO:O	2:B:833:TYR:N	2.36	0.59
1:A:498:LEU:O	1:A:502:VAL:HB	2.01	0.59
2:B:654:ILE:HD13	2:B:733:LEU:HG	1.85	0.59
1:A:660:GLN:O	1:A:661:GLU:HB2	2.01	0.59
2:B:694:VAL:HG22	2:B:756:PRO:HG2	1.85	0.59
1:A:66:TYR:HE1	1:A:107:ASP:HB3	1.68	0.58
1:A:1085:LEU:HD13	1:A:1162:THR:HG22	1.85	0.58
2:B:151:LEU:O	2:B:155:VAL:HG23	2.03	0.58
1:A:86:ALA:O	1:A:90:ILE:HG13	2.03	0.58
2:B:914:VAL:HG12	2:B:915:SER:N	2.18	0.58
1:A:434:GLU:HG2	1:A:437:ARG:HH21	1.68	0.58
1:A:853:ILE:HG12	1:A:917:VAL:CG2	2.34	0.58
1:A:594:LEU:HD21	1:A:604:LEU:HD23	1.85	0.58
2:B:1354:HIS:C	2:B:1356:PRO:HD2	2.29	0.58
2:B:398:GLU:O	2:B:402:ARG:HG3	2.04	0.58
1:A:123:ASN:HB3	1:A:125:LYS:HB2	1.86	0.58
1:A:211:PRO:HG3	1:A:267:VAL:HG13	1.85	0.58
1:A:1011:LYS:O	1:A:1069:ALA:HB2	2.04	0.58
1:A:375:TRP:CE3	1:A:378:VAL:HG21	2.39	0.57
2:B:111:CYS:HB3	2:B:134:ILE:HG13	1.86	0.57
1:A:563:VAL:HG23	1:A:563:VAL:O	2.04	0.57
1:A:814:THR:O	1:A:818:ARG:HB2	2.04	0.57
1:A:397:LYS:HE3	1:A:412:LYS:HE2	1.86	0.57
1:A:484:PHE:O	1:A:519:VAL:HG11	2.04	0.57
1:A:623:MET:HE3	1:A:677:TYR:HD1	1.67	0.57
2:B:654:ILE:HD12	2:B:737:CYS:SG	2.44	0.57
2:B:1025:LEU:O	2:B:1029:HIS:CD2	2.56	0.57
1:A:298:GLN:C	1:A:301:PRO:HD2	2.30	0.57
1:A:1136:VAL:CG1	1:A:1198:LEU:HD12	2.34	0.57
2:B:1289:LEU:HD22	2:B:1342:HIS:CE1	2.39	0.57
1:A:372:VAL:HG22	1:A:432:ILE:CG2	2.35	0.57
1:A:1095:VAL:HG13	1:A:1135:ILE:HG23	1.86	0.57
1:A:65:ARG:HA	1:A:68:ILE:HD12	1.85	0.57
2:B:1278:ASN:HA	2:B:1281:LYS:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LEU:HD22	1:A:533:LYS:HE3	1.87	0.56
1:A:723:ASP:OD2	1:A:724:LYS:HG3	2.04	0.56
1:A:838:MET:HA	1:A:838:MET:CE	2.33	0.56
1:A:881:LEU:HA	1:A:911:LEU:HD11	1.87	0.56
1:A:1061:GLU:C	1:A:1062:ILE:HG13	2.29	0.56
2:B:1271:ARG:HB3	2:B:1332:ASN:OD1	2.05	0.56
1:A:298:GLN:HB3	1:A:340:ASP:OD2	2.05	0.56
1:A:651:LEU:HD21	1:A:658:PHE:HB2	1.87	0.56
1:A:54:SER:HB2	1:A:61:GLY:O	2.04	0.56
1:A:191:MET:HE1	1:A:220:LEU:HD22	1.87	0.56
1:A:858:VAL:HG12	1:A:859:SER:N	2.21	0.56
1:A:908:LEU:HD13	1:A:980:LEU:CD2	2.36	0.56
1:A:937:GLY:O	1:A:941:GLU:HG3	2.04	0.56
2:B:1162:CYS:HA	2:B:1222:PRO:HD2	1.87	0.56
1:A:158:ARG:HD3	1:A:158:ARG:C	2.30	0.56
1:A:635:GLU:HG3	1:A:645:LYS:HE2	1.88	0.56
2:B:790:PHE:O	2:B:794:VAL:HG23	2.05	0.56
2:B:1245:LYS:NZ	2:B:1298:ARG:HD2	2.21	0.56
1:A:121:LEU:C	1:A:123:ASN:N	2.64	0.56
1:A:237:PHE:CD2	1:A:268:GLU:HG2	2.41	0.56
1:A:634:TYR:CG	1:A:704:MET:HE3	2.41	0.56
1:A:609:TYR:CZ	1:A:613:ARG:HD2	2.40	0.56
1:A:199:LEU:HD23	1:A:202:PHE:CE2	2.41	0.56
1:A:300:ASP:O	1:A:303:LYS:N	2.39	0.56
1:A:427:LEU:HD22	1:A:431:LYS:HD2	1.88	0.56
2:B:483:THR:O	2:B:487:VAL:HG23	2.06	0.56
2:B:523:SER:O	2:B:527:ILE:HG13	2.06	0.56
1:A:1071:VAL:HG13	1:A:1076:ALA:CB	2.32	0.56
2:B:664:VAL:HG12	2:B:665:ASP:N	2.19	0.56
2:B:1225:THR:HG22	2:B:1226:ARG:H	1.71	0.56
1:A:671:GLN:HG3	1:A:755:TYR:HB2	1.87	0.55
1:A:1214:ILE:HD11	1:A:1252:LEU:HD13	1.87	0.55
2:B:829:VAL:O	2:B:831:PRO:HD3	2.06	0.55
1:A:120:ARG:HG2	1:A:172:ARG:NH1	2.21	0.55
2:B:454:LEU:HD22	2:B:458:TYR:HE1	1.72	0.55
1:A:729:SER:O	1:A:735:GLY:HA3	2.07	0.55
2:B:1018:LEU:HG	2:B:1022:CYS:SG	2.47	0.55
2:B:1204:VAL:C	2:B:1207:PRO:HD2	2.31	0.55
2:B:781:SER:O	2:B:785:LEU:HD12	2.06	0.55
1:A:651:LEU:HD11	1:A:658:PHE:CD1	2.42	0.55
1:A:1156:SER:HB3	1:A:1220:LYS:HE2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:766:LYS:HB2	1:A:766:LYS:NZ	2.22	0.55
2:B:814:LYS:HG2	2:B:962:GLU:OE2	2.07	0.55
1:A:881:LEU:HG	1:A:911:LEU:HD21	1.89	0.55
2:B:1075:GLY:O	2:B:1081:LYS:HG3	2.07	0.54
1:A:732:THR:HG22	1:A:734:VAL:H	1.71	0.54
1:A:1105:SER:O	1:A:1106:ALA:C	2.50	0.54
2:B:812:ARG:O	2:B:816:LEU:HB2	2.07	0.54
1:A:64:ARG:O	1:A:68:ILE:HG13	2.07	0.54
1:A:479:LYS:HE3	1:A:479:LYS:HA	1.90	0.54
1:A:941:GLU:O	1:A:945:VAL:HG23	2.08	0.54
1:A:1059:ASP:O	1:A:1060:VAL:HG23	2.08	0.54
1:A:651:LEU:HD11	1:A:658:PHE:HD1	1.71	0.54
2:B:370:GLU:HB2	2:B:404:LYS:NZ	2.21	0.54
1:A:187:THR:HG22	1:A:188:PRO:HD2	1.89	0.54
1:A:299:GLY:O	1:A:302:SER:OG	2.26	0.54
1:A:580:GLU:HB2	2:B:129:TYR:CG	2.42	0.54
2:B:1247:LEU:HD11	2:B:1263:LEU:HG	1.90	0.54
1:A:572:SER:HA	1:A:575:SER:HB2	1.90	0.54
2:B:102:THR:CG2	2:B:108:LEU:HD13	2.38	0.54
1:A:24:LEU:C	1:A:26:ASP:H	2.16	0.54
2:B:698:LEU:HB3	2:B:699:PRO:HD3	1.89	0.54
2:B:1087:SER:O	2:B:1091:VAL:HG23	2.07	0.54
2:B:1139:LEU:O	2:B:1142:LYS:HB2	2.08	0.54
1:A:573:ARG:HB2	1:A:573:ARG:HH11	1.72	0.54
1:A:923:GLN:HB3	1:A:924:PRO:HD3	1.90	0.54
2:B:247:PHE:CD2	2:B:260:ILE:HD13	2.43	0.54
1:A:300:ASP:O	1:A:304:CYS:N	2.41	0.53
1:A:1056:ILE:HG23	1:A:1216:TYR:CD1	2.42	0.53
1:A:475:GLN:HG3	1:A:476:ASN:N	2.24	0.53
1:A:783:ILE:O	1:A:787:LYS:HG2	2.08	0.53
2:B:84:HIS:CD2	2:B:85:PRO:HD2	2.42	0.53
1:A:838:MET:O	1:A:842:VAL:HG23	2.08	0.53
2:B:172:ARG:HG3	2:B:205:LEU:HD11	1.90	0.53
2:B:1297:ARG:NH2	2:B:1354:HIS:HA	2.23	0.53
1:A:75:LEU:HD22	1:A:81:LEU:HD21	1.91	0.53
1:A:966:LEU:HD22	1:A:1015:GLN:OE1	2.07	0.53
1:A:21:LEU:HD13	1:A:64:ARG:HD3	1.89	0.53
2:B:469:GLN:HA	2:B:508:ASN:HD21	1.70	0.53
1:A:244:HIS:CD2	1:A:260:PRO:HB2	2.44	0.53
2:B:1353:LYS:HG3	2:B:1354:HIS:CE1	2.43	0.53
1:A:77:GLU:OE1	1:A:126:SER:OG	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:TYR:O	1:A:160:LEU:HB2	2.09	0.53
1:A:328:ASP:O	1:A:332:THR:HG22	2.09	0.53
1:A:1249:ILE:O	1:A:1253:VAL:HG23	2.08	0.53
2:B:375:HIS:CE1	2:B:409:CYS:SG	3.02	0.53
2:B:1011:VAL:O	2:B:1014:VAL:HG12	2.09	0.53
1:A:563:VAL:HG12	2:B:167:GLY:C	2.34	0.53
2:B:735:ARG:HD2	2:B:796:ALA:HB2	1.91	0.53
2:B:1315:PHE:CZ	2:B:1375:LEU:HD13	2.44	0.53
1:A:69:TYR:O	1:A:73:ILE:HG13	2.09	0.52
2:B:1007:VAL:O	2:B:1011:VAL:HG23	2.09	0.52
1:A:456:ILE:O	1:A:456:ILE:HG22	2.08	0.52
1:A:563:VAL:HG12	2:B:167:GLY:O	2.09	0.52
1:A:1070:VAL:HG12	1:A:1071:VAL:H	1.74	0.52
1:A:1207:THR:N	1:A:1208:PRO:HD2	2.24	0.52
2:B:1266:TRP:HA	2:B:1266:TRP:CE3	2.43	0.52
1:A:1026:ASN:OD1	1:A:1083:LEU:HD21	2.09	0.52
2:B:1308:MET:N	2:B:1309:PRO:HD2	2.24	0.52
1:A:865:ASN:OD1	1:A:868:LYS:HB2	2.09	0.52
2:B:814:LYS:HG2	2:B:962:GLU:CD	2.34	0.52
1:A:46:LEU:O	1:A:50:VAL:HG23	2.09	0.52
1:A:845:THR:O	1:A:849:ILE:HG13	2.09	0.52
2:B:293:LEU:O	2:B:293:LEU:HD23	2.10	0.52
2:B:787:PHE:CE1	2:B:820:GLN:HB2	2.44	0.52
2:B:1114:SER:O	2:B:1117:GLN:HG2	2.10	0.52
1:A:47:LEU:HD22	1:A:51:LEU:HD11	1.91	0.52
1:A:158:ARG:HD3	1:A:158:ARG:O	2.09	0.52
2:B:735:ARG:CD	2:B:796:ALA:HB2	2.40	0.52
1:A:545:ASN:HD22	1:A:549:LEU:HB2	1.75	0.52
2:B:252:LEU:HD23	2:B:252:LEU:H	1.74	0.52
2:B:926:LEU:O	2:B:973:LYS:NZ	2.30	0.52
2:B:1086:HIS:O	2:B:1090:GLU:HG3	2.10	0.52
2:B:106:GLU:HG2	2:B:109:ARG:NH1	2.25	0.52
2:B:1308:MET:HE1	2:B:1329:LEU:HD11	1.92	0.52
1:A:245:ARG:HD2	1:A:366:GLU:OE1	2.09	0.52
1:A:227:ARG:HG3	1:A:288:GLU:HG3	1.92	0.52
1:A:641:LEU:O	1:A:643:PRO:HD3	2.09	0.52
2:B:430:CYS:HG	2:B:467:CYS:HG	1.58	0.52
1:A:227:ARG:HG3	1:A:288:GLU:CG	2.40	0.51
1:A:1198:LEU:HD22	1:A:1201:LEU:HD12	1.91	0.51
2:B:647:LEU:HD23	2:B:741:GLN:HG2	1.92	0.51
2:B:925:GLU:CD	2:B:925:GLU:N	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:977:MET:HA	2:B:977:MET:HE2	1.92	0.51
2:B:1342:HIS:CD2	2:B:1343:SER:H	2.28	0.51
2:B:1345:ILE:HA	2:B:1351:LEU:HD12	1.92	0.51
2:B:1264:LEU:HG	2:B:1325:LEU:HG	1.92	0.51
1:A:553:PRO:HB2	1:A:558:THR:HG23	1.93	0.51
2:B:98:LEU:O	2:B:102:THR:OG1	2.22	0.51
2:B:206:GLN:O	2:B:210:ILE:HG13	2.10	0.51
2:B:931:PHE:HE1	2:B:973:LYS:HD2	1.75	0.51
1:A:227:ARG:O	1:A:231:ASP:HB2	2.11	0.51
1:A:1072:ASN:H	1:A:1075:THR:HB	1.74	0.51
2:B:1291:VAL:O	2:B:1295:TYR:HD1	1.94	0.51
1:A:372:VAL:HG22	1:A:432:ILE:HG21	1.92	0.51
1:A:662:PRO:O	1:A:665:HIS:N	2.40	0.51
1:A:848:LYS:HD3	1:A:858:VAL:HG13	1.92	0.51
1:A:1249:ILE:N	1:A:1250:PRO:HD2	2.25	0.51
2:B:149:LYS:HE3	2:B:153:GLU:OE2	2.11	0.51
2:B:1297:ARG:HH22	2:B:1354:HIS:CD2	2.28	0.51
1:A:348:LYS:HD2	1:A:351:GLN:OE1	2.10	0.51
1:A:977:GLU:O	1:A:981:LEU:HB2	2.11	0.51
2:B:674:PHE:O	2:B:676:PHE:N	2.39	0.51
1:A:102:GLY:N	1:A:103:PRO:HD2	2.25	0.50
1:A:462:LEU:O	1:A:466:ILE:HG13	2.11	0.50
1:A:540:LEU:HD13	1:A:607:GLY:HA3	1.93	0.50
1:A:938:THR:HG22	1:A:939:GLU:N	2.26	0.50
1:A:536:VAL:HB	1:A:603:MET:HE3	1.93	0.50
2:B:55:LEU:HD21	2:B:133:LEU:HD13	1.92	0.50
1:A:755:TYR:CZ	1:A:759:ILE:HD11	2.47	0.50
1:A:1:MET:O	1:A:5:ILE:HG13	2.11	0.50
1:A:523:ALA:HB3	1:A:535:ALA:HB2	1.92	0.50
1:A:722:LEU:O	1:A:725:SER:OG	2.29	0.50
1:A:1150:VAL:HG22	1:A:1167:LEU:HD11	1.93	0.50
1:A:129:LEU:O	1:A:133:ILE:HG13	2.12	0.50
1:A:617:GLN:HG2	2:B:128:PHE:N	2.27	0.50
1:A:671:GLN:CG	1:A:755:TYR:HB2	2.40	0.50
2:B:531:PHE:CE2	2:B:557:ILE:HD13	2.46	0.50
2:B:916:LEU:O	2:B:919:TYR:CD2	2.51	0.50
2:B:791:ARG:HH12	2:B:965:PHE:HZ	1.58	0.50
2:B:1149:LYS:O	2:B:1153:LEU:HG	2.12	0.50
1:A:927:GLN:HG2	1:A:947:VAL:HG22	1.93	0.50
1:A:1131:ILE:O	1:A:1135:ILE:HG13	2.10	0.50
1:A:1139:LEU:O	1:A:1143:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:HIS:CG	2:B:85:PRO:HD2	2.46	0.50
2:B:800:GLN:CB	2:B:805:MET:HG2	2.40	0.50
2:B:55:LEU:HD23	2:B:133:LEU:HD13	1.93	0.49
2:B:753:LEU:HD21	2:B:808:LYS:HB3	1.93	0.49
2:B:786:THR:HG22	2:B:819:LEU:HD11	1.93	0.49
2:B:974:LEU:HD11	2:B:1014:VAL:HG21	1.94	0.49
1:A:492:LEU:HD22	1:A:533:LYS:HG2	1.94	0.49
2:B:287:VAL:HG13	2:B:292:SER:HB3	1.93	0.49
2:B:503:SER:O	2:B:506:ARG:HG3	2.13	0.49
2:B:1100:GLU:HB2	2:B:1103:GLN:HG2	1.94	0.49
2:B:1286:TYR:N	2:B:1287:PRO:HD2	2.27	0.49
2:B:287:VAL:O	2:B:287:VAL:CG1	2.60	0.49
2:B:1123:VAL:CG1	2:B:1128:CYS:HB2	2.33	0.49
2:B:1220:THR:O	2:B:1221:PHE:HB3	2.12	0.49
1:A:43:VAL:HA	1:A:46:LEU:HB2	1.94	0.49
1:A:174:MET:CE	1:A:201:MET:HE3	2.42	0.49
1:A:709:THR:HA	1:A:752:LEU:HD13	1.94	0.49
1:A:919:LEU:O	1:A:923:GLN:HB2	2.11	0.49
2:B:87:TYR:O	2:B:90:VAL:HG12	2.11	0.49
1:A:927:GLN:HG2	1:A:947:VAL:CG2	2.42	0.49
1:A:547:LYS:HE3	1:A:615:ASN:HA	1.95	0.49
2:B:674:PHE:C	2:B:676:PHE:H	2.20	0.49
1:A:946:THR:HG22	1:A:947:VAL:N	2.27	0.49
1:A:1009:ILE:HG22	1:A:1024:LEU:HD11	1.94	0.49
2:B:738:VAL:HG13	2:B:742:HIS:ND1	2.28	0.49
1:A:848:LYS:NZ	1:A:859:SER:HB2	2.28	0.49
1:A:1156:SER:HB3	1:A:1220:LYS:CE	2.43	0.49
2:B:535:SER:OG	2:B:582:ILE:HD12	2.12	0.49
2:B:1062:LYS:O	2:B:1066:VAL:HG23	2.12	0.49
1:A:284:GLU:HG3	1:A:287:ARG:HH12	1.77	0.49
1:A:558:THR:HB	1:A:563:VAL:CG2	2.42	0.49
2:B:963:LEU:HD11	2:B:1025:LEU:HD13	1.94	0.49
1:A:70:SER:O	1:A:74:GLN:HG3	2.13	0.48
1:A:195:VAL:HG13	1:A:217:LEU:HD21	1.95	0.48
1:A:937:GLY:O	1:A:941:GLU:CG	2.61	0.48
2:B:402:ARG:NH2	2:B:443:SER:HB3	2.28	0.48
2:B:969:ASP:OD1	2:B:973:LYS:HE3	2.12	0.48
2:B:1149:LYS:N	2:B:1149:LYS:HD2	2.28	0.48
1:A:158:ARG:NH1	1:A:162:ASP:HB2	2.27	0.48
2:B:821:GLY:O	2:B:825:LYS:HG3	2.13	0.48
2:B:1022:CYS:O	2:B:1026:GLU:N	2.30	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1343:SER:O	2:B:1346:ARG:HB2	2.12	0.48
2:B:611:LEU:O	2:B:611:LEU:HD23	2.13	0.48
1:A:472:LEU:O	1:A:475:GLN:HG2	2.14	0.48
2:B:929:GLU:O	2:B:932:SER:OG	2.24	0.48
1:A:1156:SER:HB3	1:A:1220:LYS:NZ	2.29	0.48
2:B:222:HIS:ND1	2:B:250:LEU:HD22	2.29	0.48
2:B:684:LEU:C	2:B:686:GLU:H	2.20	0.48
2:B:1033:GLN:HB2	2:B:1122:SER:HB2	1.94	0.48
1:A:644:LEU:HD21	1:A:708:ILE:HD13	1.96	0.48
1:A:853:ILE:HG12	1:A:917:VAL:HG22	1.95	0.48
1:A:1103:LYS:CG	1:A:1180:TYR:HD1	2.21	0.48
2:B:150:MET:O	2:B:153:GLU:HB2	2.13	0.48
2:B:198:ILE:HD13	2:B:210:ILE:HG12	1.94	0.48
2:B:421:THR:HB	2:B:422:HIS:CD2	2.49	0.48
2:B:444:GLN:CD	2:B:444:GLN:H	2.20	0.48
2:B:1343:SER:HA	2:B:1346:ARG:HD3	1.96	0.48
1:A:199:LEU:HA	1:A:202:PHE:CD2	2.49	0.48
1:A:666:LEU:O	1:A:670:ILE:HG13	2.14	0.48
1:A:747:GLY:O	1:A:751:VAL:HG23	2.14	0.48
1:A:755:TYR:CE2	1:A:759:ILE:HD11	2.49	0.48
1:A:962:LEU:HB2	1:A:981:LEU:HD13	1.95	0.48
2:B:241:VAL:HB	2:B:242:PRO:HD3	1.95	0.48
2:B:257:LEU:HA	2:B:260:ILE:HD12	1.95	0.48
2:B:784:PHE:CD1	2:B:823:LEU:HD11	2.46	0.48
2:B:1029:HIS:ND1	2:B:1056:MET:HE2	2.29	0.48
2:B:1233:PHE:CD2	2:B:1277:LEU:HD11	2.48	0.48
2:B:1342:HIS:CD2	2:B:1343:SER:N	2.82	0.48
1:A:94:MET:HE3	1:A:132:ILE:HD11	1.96	0.48
1:A:1071:VAL:H	1:A:1075:THR:HG21	1.77	0.48
2:B:732:ARG:HD2	2:B:792:GLU:OE2	2.14	0.48
2:B:1158:LYS:HG3	2:B:1187:TYR:CE1	2.49	0.48
2:B:133:LEU:HD12	2:B:137:LEU:HD13	1.95	0.48
2:B:388:SER:OG	2:B:429:ILE:HG23	2.14	0.48
2:B:1019:THR:C	2:B:1021:MET:H	2.22	0.48
1:A:165:CYS:HB3	1:A:197:LYS:HG3	1.95	0.48
1:A:502:VAL:O	1:A:502:VAL:HG13	2.13	0.48
1:A:976:LYS:O	1:A:980:LEU:HD22	2.14	0.48
2:B:1277:LEU:HB3	2:B:1288:VAL:HG13	1.95	0.48
1:A:580:GLU:HB2	2:B:129:TYR:CD2	2.49	0.47
1:A:851:GLN:O	1:A:851:GLN:HG2	2.14	0.47
2:B:287:VAL:HG13	2:B:292:SER:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:362:TRP:CE2	2:B:382:MET:HG2	2.47	0.47
1:A:124:GLY:O	1:A:127:LEU:N	2.45	0.47
1:A:716:GLU:O	1:A:718:GLU:N	2.44	0.47
1:A:1075:THR:HG22	1:A:1080:VAL:HG23	1.95	0.47
2:B:138:LEU:HD12	2:B:138:LEU:HA	1.75	0.47
2:B:680:ALA:HB2	2:B:758:PHE:CE2	2.49	0.47
1:A:131:PRO:HB3	1:A:183:ASP:HB2	1.96	0.47
1:A:641:LEU:HG	1:A:715:SER:CB	2.44	0.47
2:B:1120:HIS:CG	2:B:1121:HIS:N	2.81	0.47
1:A:629:GLN:NE2	1:A:661:GLU:OE2	2.47	0.47
2:B:305:VAL:O	2:B:306:GLN:HG3	2.13	0.47
1:A:284:GLU:HG3	1:A:287:ARG:NH1	2.29	0.47
2:B:545:THR:HG22	2:B:546:SER:N	2.28	0.47
2:B:1149:LYS:HD2	2:B:1149:LYS:H	1.79	0.47
2:B:1263:LEU:HD13	2:B:1307:CYS:SG	2.54	0.47
2:B:1355:VAL:N	2:B:1356:PRO:HD2	2.30	0.47
1:A:1:MET:HE1	1:A:24:LEU:HD21	1.96	0.47
1:A:13:THR:HG23	1:A:14:THR:N	2.29	0.47
1:A:316:LEU:HD22	1:A:322:PHE:HB2	1.96	0.47
2:B:459:ALA:O	2:B:463:PHE:HB2	2.14	0.47
2:B:472:VAL:O	2:B:476:VAL:HG23	2.14	0.47
2:B:830:ILE:O	2:B:830:ILE:CG2	2.63	0.47
1:A:695:GLU:HA	1:A:698:TYR:HE2	1.78	0.47
1:A:1076:ALA:HA	1:A:1080:VAL:HB	1.96	0.47
1:A:1077:ALA:CB	1:A:1078:PRO:HD3	2.40	0.47
2:B:170:MET:O	2:B:174:ILE:HG13	2.15	0.47
2:B:433:ILE:HG23	2:B:455:LEU:HD22	1.96	0.47
2:B:1173:ASN:HB2	2:B:1174:PRO:HD2	1.96	0.47
2:B:1350:ARG:O	2:B:1353:LYS:HG2	2.14	0.47
1:A:218:LEU:HD11	1:A:275:ILE:HG22	1.96	0.47
1:A:377:HIS:HD2	1:A:378:VAL:HG23	1.80	0.47
2:B:189:ASP:O	2:B:193:GLN:HG3	2.15	0.47
2:B:1375:LEU:O	2:B:1376:ASN:C	2.58	0.47
1:A:24:LEU:O	1:A:26:ASP:N	2.47	0.47
1:A:215:TYR:HB2	1:A:274:HIS:ND1	2.30	0.47
1:A:337:SER:OG	1:A:359:CYS:HB2	2.15	0.47
1:A:580:GLU:HB2	2:B:129:TYR:CD1	2.50	0.47
1:A:641:LEU:HD23	1:A:719:ASP:OD2	2.14	0.47
1:A:486:TYR:CE1	2:B:354:TYR:HD1	2.32	0.46
1:A:959:GLN:HB2	1:A:1005:TRP:CH2	2.50	0.46
2:B:462:PHE:O	2:B:463:PHE:CD2	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:686:GLU:OE2	2:B:808:LYS:HE2	2.14	0.46
2:B:1105:LEU:O	2:B:1109:VAL:HG23	2.15	0.46
2:B:1184:LEU:HD13	2:B:1232:PHE:HA	1.98	0.46
2:B:1233:PHE:HZ	2:B:1273:PHE:HB3	1.73	0.46
1:A:217:LEU:HD22	1:A:229:VAL:HG13	1.98	0.46
1:A:558:THR:O	1:A:563:VAL:HG22	2.15	0.46
1:A:634:TYR:CD2	1:A:704:MET:HE3	2.50	0.46
1:A:814:THR:OG1	1:A:879:VAL:HG21	2.15	0.46
1:A:948:THR:HG23	1:A:992:LEU:HA	1.97	0.46
2:B:410:ILE:HG22	2:B:451:PHE:CE1	2.50	0.46
1:A:4:LYS:O	1:A:8:LEU:HG	2.14	0.46
1:A:131:PRO:HA	1:A:184:VAL:HG22	1.96	0.46
2:B:222:HIS:HB2	2:B:251:ARG:HG2	1.97	0.46
2:B:382:MET:O	2:B:386:ILE:HG13	2.16	0.46
1:A:154:GLU:O	1:A:157:LYS:HB3	2.16	0.46
2:B:1206:VAL:N	2:B:1207:PRO:CD	2.75	0.46
2:B:1257:GLN:O	2:B:1261:GLU:HG3	2.16	0.46
1:A:613:ARG:HG2	1:A:676:TRP:CE3	2.51	0.46
2:B:541:GLN:C	2:B:542:GLN:HG3	2.41	0.46
2:B:695:ILE:HB	2:B:757:LEU:CD2	2.45	0.46
1:A:597:GLN:H	1:A:597:GLN:HG2	1.34	0.46
1:A:835:GLY:CA	1:A:838:MET:HB2	2.46	0.46
1:A:1014:SER:HB2	1:A:1072:ASN:ND2	2.30	0.46
2:B:816:LEU:HD12	2:B:816:LEU:HA	1.81	0.46
2:B:1342:HIS:CG	2:B:1343:SER:N	2.83	0.46
1:A:275:ILE:CD1	1:A:312:LEU:HD11	2.42	0.46
1:A:448:VAL:O	1:A:456:ILE:HD13	2.16	0.46
2:B:752:LEU:HA	2:B:755:CYS:SG	2.56	0.46
1:A:41:ARG:HD3	1:A:41:ARG:N	2.31	0.46
2:B:375:HIS:NE2	2:B:409:CYS:SG	2.88	0.46
1:A:604:LEU:HG	1:A:608:PHE:CE1	2.51	0.46
1:A:1075:THR:HG22	1:A:1080:VAL:CG2	2.45	0.46
2:B:401:LEU:O	2:B:405:ILE:HG13	2.15	0.46
2:B:1277:LEU:HD13	2:B:1288:VAL:O	2.15	0.46
1:A:118:GLU:O	1:A:119:ASP:OD1	2.33	0.46
2:B:427:LYS:HA	2:B:463:PHE:CE1	2.51	0.46
2:B:1229:PHE:CZ	2:B:1280:MET:HG3	2.51	0.46
2:B:1350:ARG:HA	2:B:1353:LYS:HE2	1.97	0.46
1:A:112:PHE:O	1:A:116:VAL:HG23	2.16	0.45
1:A:764:LYS:HA	1:A:827:SER:HB2	1.97	0.45
2:B:666:PHE:O	2:B:667:CYS:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1326:LEU:HA	2:B:1329:LEU:HD12	1.97	0.45
1:A:754:GLU:OE1	1:A:808:PHE:CB	2.64	0.45
1:A:908:LEU:HD11	1:A:981:LEU:HG	1.99	0.45
2:B:581:GLY:CA	2:B:636:LEU:HD13	2.45	0.45
2:B:1324:SER:HB3	2:B:1385:GLY:HA2	1.97	0.45
1:A:78:SER:OG	1:A:79:GLY:N	2.48	0.45
1:A:114:GLY:HA2	1:A:117:ARG:NH1	2.31	0.45
1:A:271:VAL:O	1:A:275:ILE:HG23	2.17	0.45
1:A:322:PHE:O	1:A:326:VAL:HG23	2.17	0.45
1:A:545:ASN:O	1:A:549:LEU:HB3	2.16	0.45
2:B:695:ILE:HB	2:B:757:LEU:HD23	1.99	0.45
2:B:1265:TYR:HA	2:B:1268:MET:HB2	1.99	0.45
1:A:620:SER:O	1:A:624:GLN:HB2	2.16	0.45
1:A:1046:SER:HB3	1:A:1145:PHE:CD1	2.52	0.45
2:B:1240:LEU:O	2:B:1244:VAL:HG23	2.17	0.45
2:B:1236:MET:HB3	2:B:1273:PHE:CZ	2.51	0.45
2:B:1300:VAL:HG13	2:B:1365:LEU:HD12	1.99	0.45
1:A:819:ASP:HB3	1:A:820:SER:H	1.52	0.45
2:B:443:SER:O	2:B:449:ILE:HD11	2.17	0.45
2:B:541:GLN:O	2:B:542:GLN:HG3	2.17	0.45
2:B:976:ASN:OD1	2:B:1003:HIS:CE1	2.69	0.45
2:B:1277:LEU:CD1	2:B:1288:VAL:HG13	2.43	0.45
1:A:1146:PHE:O	1:A:1150:VAL:HG23	2.17	0.45
2:B:1281:LYS:HA	2:B:1284:ASP:O	2.17	0.45
2:B:1342:HIS:CE1	2:B:1344:LYS:H	2.35	0.45
2:B:1361:SER:HA	2:B:1364:LEU:HD12	1.99	0.45
1:A:1200:LYS:HB2	1:A:1277:HIS:HB3	1.98	0.45
2:B:605:ARG:HG2	2:B:646:THR:HG23	1.99	0.45
2:B:1192:ASP:O	2:B:1193:ASN:C	2.57	0.45
1:A:1078:PRO:O	1:A:1082:LEU:HG	2.17	0.45
2:B:1278:ASN:O	2:B:1281:LYS:HD3	2.17	0.45
1:A:1050:HIS:ND1	1:A:1148:GLU:OE1	2.50	0.44
1:A:1261:LYS:O	1:A:1264:ILE:HB	2.17	0.44
2:B:1285:SER:OG	2:B:1288:VAL:HB	2.18	0.44
1:A:8:LEU:HD13	1:A:17:LEU:HA	1.99	0.44
1:A:221:SER:HB3	1:A:229:VAL:HG21	1.98	0.44
1:A:290:LEU:O	1:A:294:LYS:HG2	2.17	0.44
1:A:1071:VAL:HG12	1:A:1071:VAL:O	2.16	0.44
2:B:252:LEU:HD11	2:B:257:LEU:HD13	1.99	0.44
2:B:565:VAL:HB	2:B:568:TYR:HD1	1.83	0.44
2:B:570:LEU:HD12	2:B:628:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:604:GLN:O	2:B:608:VAL:HG23	2.18	0.44
1:A:1021:CYS:SG	1:A:1075:THR:HG23	2.58	0.44
1:A:1059:ASP:O	1:A:1060:VAL:CG2	2.65	0.44
1:A:1140:GLY:HA3	1:A:1198:LEU:HD13	2.00	0.44
1:A:1154:LEU:CD1	1:A:1163:LEU:HD12	2.47	0.44
2:B:763:GLU:HA	2:B:822:ILE:HD13	2.00	0.44
1:A:428:GLU:HA	1:A:431:LYS:HD3	1.99	0.44
1:A:787:LYS:O	1:A:788:ALA:HB3	2.18	0.44
1:A:1084:VAL:CG1	1:A:1145:PHE:HE1	2.31	0.44
2:B:626:SER:OG	2:B:726:CYS:SG	2.75	0.44
2:B:820:GLN:HE22	2:B:920:ARG:HH12	1.65	0.44
2:B:341:ILE:HD11	2:B:422:HIS:CE1	2.53	0.44
2:B:967:LEU:HB3	2:B:1062:LYS:HB3	1.99	0.44
1:A:567:ARG:C	1:A:569:ASP:H	2.25	0.44
1:A:661:GLU:HA	1:A:662:PRO:HD3	1.68	0.44
1:A:670:ILE:O	1:A:674:LEU:HB2	2.18	0.44
1:A:1249:ILE:H	1:A:1249:ILE:HG13	1.47	0.44
2:B:1116:LEU:HA	2:B:1119:PHE:HD1	1.83	0.44
2:B:1266:TRP:HA	2:B:1266:TRP:HE3	1.80	0.44
2:B:1349:THR:O	2:B:1351:LEU:N	2.51	0.44
1:A:1:MET:HE1	1:A:24:LEU:CD2	2.47	0.44
1:A:858:VAL:CG1	1:A:859:SER:N	2.81	0.44
2:B:557:ILE:HD12	2:B:557:ILE:HA	1.85	0.44
2:B:1281:LYS:HE3	2:B:1342:HIS:HE2	1.83	0.44
2:B:1331:LEU:HD12	2:B:1334:ARG:HD2	2.00	0.44
1:A:466:ILE:HG22	1:A:474:LEU:HD11	1.99	0.44
1:A:834:SER:OG	1:A:835:GLY:N	2.47	0.44
2:B:370:GLU:HB2	2:B:404:LYS:HZ1	1.83	0.44
2:B:1277:LEU:HD22	2:B:1288:VAL:HG13	1.99	0.44
2:B:1323:LEU:O	2:B:1327:GLN:HG3	2.17	0.44
1:A:293:LEU:HD13	1:A:313:LEU:HD11	2.00	0.43
2:B:352:ILE:HG22	2:B:358:ILE:HG22	2.00	0.43
2:B:415:LEU:HD23	2:B:454:LEU:HB3	2.00	0.43
2:B:574:ILE:HA	2:B:632:GLU:HG2	2.00	0.43
1:A:90:ILE:CD1	1:A:125:LYS:HB3	2.48	0.43
1:A:275:ILE:HD11	1:A:312:LEU:HD21	2.00	0.43
1:A:798:LYS:N	1:A:801:ASP:OD1	2.51	0.43
1:A:973:PHE:CE2	1:A:1015:GLN:HG2	2.51	0.43
1:A:1164:LEU:HD22	1:A:1252:LEU:HD12	2.00	0.43
1:A:123:ASN:C	1:A:125:LYS:H	2.25	0.43
1:A:654:GLY:O	1:A:655:SER:OG	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:TYR:N	2:B:88:PRO:CD	2.81	0.43
2:B:258:SER:HA	2:B:261:ARG:NH1	2.30	0.43
2:B:1162:CYS:O	2:B:1222:PRO:HD2	2.18	0.43
1:A:297:GLN:O	1:A:301:PRO:HD3	2.18	0.43
2:B:257:LEU:HD12	2:B:260:ILE:HD12	1.99	0.43
2:B:931:PHE:CE1	2:B:973:LYS:HD2	2.53	0.43
2:B:1049:THR:HA	2:B:1052:GLU:HB2	2.00	0.43
2:B:1198:ILE:HG12	2:B:1236:MET:HE2	2.00	0.43
2:B:1359:LYS:O	2:B:1363:GLU:HG3	2.19	0.43
1:A:15:ASP:O	1:A:19:GLU:HB2	2.18	0.43
1:A:396:LYS:HB3	1:A:396:LYS:HE2	1.76	0.43
1:A:451:ARG:HB3	1:A:456:ILE:HD11	2.00	0.43
1:A:1139:LEU:HA	1:A:1142:LEU:CD2	2.49	0.43
2:B:366:ILE:HD13	2:B:383:LEU:HG	2.00	0.43
2:B:1101:GLN:H	2:B:1101:GLN:HG2	1.55	0.43
1:A:12:LYS:HB2	1:A:16:LYS:NZ	2.34	0.43
1:A:300:ASP:N	1:A:301:PRO:HD2	2.33	0.43
1:A:1070:VAL:O	1:A:1071:VAL:CB	2.62	0.43
2:B:155:VAL:N	2:B:156:PRO:CD	2.79	0.43
1:A:151:LEU:HB2	1:A:156:TYR:CE1	2.54	0.43
1:A:225:SER:O	1:A:229:VAL:HG23	2.19	0.43
2:B:476:VAL:O	2:B:479:VAL:HB	2.19	0.43
2:B:753:LEU:HD21	2:B:808:LYS:CB	2.49	0.43
1:A:285:LEU:HD23	1:A:285:LEU:O	2.18	0.43
1:A:941:GLU:O	1:A:945:VAL:N	2.51	0.43
1:A:1042:LEU:HD21	1:A:1087:GLN:HB3	2.01	0.43
2:B:252:LEU:HD23	2:B:252:LEU:N	2.34	0.43
2:B:665:ASP:CA	2:B:692:GLY:O	2.63	0.43
1:A:1048:ASP:CB	1:A:1071:VAL:HG11	2.44	0.43
2:B:573:ILE:O	2:B:577:VAL:HG23	2.19	0.43
2:B:701:PHE:HE2	2:B:778:LEU:HD23	1.84	0.43
2:B:974:LEU:HD12	2:B:1066:VAL:HG13	2.01	0.43
1:A:194:VAL:O	1:A:198:VAL:HG23	2.19	0.43
1:A:428:GLU:O	1:A:432:ILE:HG12	2.18	0.43
1:A:514:ASP:OD1	1:A:554:SER:HB2	2.19	0.43
1:A:620:SER:HB3	2:B:128:PHE:HE1	1.83	0.43
1:A:749:CYS:O	1:A:753:MET:HB2	2.19	0.43
1:A:1016:GLU:HB3	1:A:1074:ARG:HD3	2.00	0.43
1:A:1025:MET:HA	1:A:1025:MET:HE2	2.01	0.43
1:A:230:LEU:HD22	1:A:289:LEU:HD13	2.01	0.42
1:A:636:PRO:O	1:A:638:PRO:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:PRO:O	1:A:639:ASP:HB2	2.18	0.42
1:A:1103:LYS:HG2	1:A:1180:TYR:CD1	2.41	0.42
2:B:787:PHE:O	2:B:791:ARG:HB2	2.19	0.42
2:B:914:VAL:HG22	2:B:922:PHE:HE1	1.81	0.42
2:B:928:ILE:H	2:B:928:ILE:HG13	1.62	0.42
2:B:1277:LEU:HD12	2:B:1292:CYS:SG	2.59	0.42
1:A:487:LEU:HD12	1:A:498:LEU:HD23	2.01	0.42
1:A:884:TYR:CE1	1:A:908:LEU:HG	2.54	0.42
2:B:1286:TYR:HB2	2:B:1287:PRO:HD3	2.01	0.42
1:A:72:CYS:O	1:A:76:VAL:HG23	2.18	0.42
1:A:316:LEU:HD23	1:A:316:LEU:O	2.19	0.42
1:A:475:GLN:HA	1:A:505:LEU:HD22	2.01	0.42
2:B:296:ILE:HD12	2:B:361:ALA:CB	2.45	0.42
2:B:1000:SER:O	2:B:1004:GLN:HG2	2.20	0.42
2:B:1384:LEU:HD23	2:B:1384:LEU:O	2.20	0.42
1:A:187:THR:CG2	1:A:188:PRO:HD2	2.49	0.42
2:B:271:VAL:HG12	2:B:272:ARG:O	2.19	0.42
1:A:1156:SER:HB3	1:A:1220:LYS:HZ1	1.85	0.42
2:B:1345:ILE:O	2:B:1345:ILE:CG2	2.68	0.42
1:A:1007:SER:O	1:A:1011:LYS:HB2	2.20	0.42
2:B:513:LYS:HE2	2:B:513:LYS:HB3	1.74	0.42
2:B:749:ILE:O	2:B:749:ILE:HG22	2.18	0.42
1:A:176:GLN:HA	1:A:179:SER:OG	2.19	0.42
1:A:1150:VAL:CG1	1:A:1209:VAL:HG12	2.49	0.42
1:A:1248:PRO:HG2	1:A:1249:ILE:H	1.85	0.42
2:B:1228:THR:O	2:B:1232:PHE:HD1	2.02	0.42
1:A:1278:MET:HE2	1:A:1278:MET:HB3	1.98	0.42
2:B:633:PHE:HB3	2:B:733:LEU:HD13	2.01	0.42
2:B:742:HIS:O	2:B:743:ASP:CB	2.65	0.42
2:B:1345:ILE:O	2:B:1345:ILE:HG22	2.20	0.42
1:A:446:ASN:O	1:A:450:THR:HG22	2.20	0.42
2:B:213:LEU:HD22	2:B:217:LEU:HD11	2.01	0.42
2:B:664:VAL:HG12	2:B:665:ASP:H	1.84	0.42
1:A:1001:GLN:HE21	1:A:1001:GLN:HB3	1.60	0.41
2:B:762:LEU:HD13	2:B:783:THR:HA	2.01	0.41
2:B:831:PRO:C	2:B:833:TYR:H	2.27	0.41
2:B:1090:GLU:O	2:B:1093:SER:OG	2.27	0.41
1:A:34:GLN:C	1:A:36:GLN:N	2.78	0.41
1:A:372:VAL:HG12	1:A:372:VAL:O	2.20	0.41
1:A:919:LEU:HD11	1:A:991:LEU:HD21	2.01	0.41
2:B:638:GLN:HB3	2:B:736:LEU:CD1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:977:MET:HE1	2:B:1003:HIS:CD2	2.56	0.41
1:A:169:TRP:HB2	1:A:201:MET:HE1	2.02	0.41
1:A:623:MET:HE3	1:A:677:TYR:CD1	2.52	0.41
1:A:672:HIS:CD2	1:A:861:PRO:HG2	2.56	0.41
1:A:945:VAL:HG11	1:A:950:ARG:NE	2.35	0.41
2:B:149:LYS:O	2:B:153:GLU:HG3	2.20	0.41
2:B:547:ASN:O	2:B:548:HIS:C	2.63	0.41
2:B:1294:LYS:HG3	2:B:1354:HIS:CD2	2.55	0.41
1:A:816:LEU:HD13	1:A:838:MET:HE1	2.01	0.41
1:A:865:ASN:O	1:A:866:PRO:C	2.63	0.41
2:B:1014:VAL:HG22	2:B:1014:VAL:O	2.20	0.41
2:B:1374:VAL:O	2:B:1375:LEU:HG	2.21	0.41
1:A:573:ARG:HB2	1:A:573:ARG:NH1	2.35	0.41
1:A:1098:LEU:HD22	1:A:1131:ILE:CG2	2.50	0.41
2:B:429:ILE:O	2:B:433:ILE:HG13	2.21	0.41
2:B:791:ARG:NH1	2:B:965:PHE:HZ	2.18	0.41
2:B:1221:PHE:N	2:B:1222:PRO:HD3	2.35	0.41
1:A:1052:GLN:HG3	1:A:1071:VAL:HG12	2.01	0.41
2:B:1284:ASP:O	2:B:1285:SER:HB3	2.20	0.41
1:A:154:GLU:HG3	1:A:155:GLU:N	2.36	0.41
1:A:315:SER:OG	1:A:377:HIS:HB2	2.21	0.41
1:A:662:PRO:O	1:A:663:LEU:C	2.63	0.41
1:A:787:LYS:HA	1:A:787:LYS:HD3	1.76	0.41
1:A:1011:LYS:O	1:A:1069:ALA:CB	2.67	0.41
1:A:1144:THR:O	1:A:1148:GLU:HG2	2.21	0.41
2:B:968:GLU:O	2:B:972:GLN:HG3	2.20	0.41
2:B:1204:VAL:O	2:B:1207:PRO:CG	2.68	0.41
1:A:90:ILE:HD13	1:A:125:LYS:HB3	2.01	0.41
1:A:462:LEU:HD22	1:A:466:ILE:HD11	2.03	0.41
1:A:863:GLY:O	1:A:869:ILE:HD11	2.20	0.41
1:A:1200:LYS:HD3	1:A:1277:HIS:CE1	2.55	0.41
2:B:45:VAL:HG21	2:B:93:GLU:CG	2.50	0.41
2:B:88:PRO:HB2	2:B:89:LYS:HD2	2.03	0.41
2:B:112:LEU:HD23	2:B:134:ILE:HD12	2.03	0.41
2:B:287:VAL:O	2:B:289:ASP:O	2.39	0.41
2:B:469:GLN:HG3	2:B:508:ASN:HD21	1.86	0.41
2:B:532:CYS:HA	2:B:582:ILE:HD11	2.02	0.41
2:B:914:VAL:CG1	2:B:915:SER:N	2.82	0.41
1:A:92:LEU:HA	1:A:95:LEU:HB2	2.02	0.41
1:A:348:LYS:HD3	1:A:1034:LEU:O	2.20	0.41
1:A:608:PHE:HD2	1:A:608:PHE:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:818:ARG:O	1:A:819:ASP:HB2	2.21	0.41
2:B:117:ARG:HD2	2:B:117:ARG:HA	1.93	0.41
2:B:150:MET:HA	2:B:153:GLU:OE1	2.21	0.41
2:B:222:HIS:CD2	2:B:251:ARG:HG2	2.56	0.41
2:B:413:GLN:HG3	2:B:414:LEU:N	2.35	0.41
2:B:556:VAL:O	2:B:560:GLN:HG2	2.20	0.41
2:B:609:THR:O	2:B:613:GLN:HG2	2.20	0.41
2:B:787:PHE:HA	2:B:819:LEU:HD13	2.02	0.41
2:B:1123:VAL:HA	2:B:1124:PRO:HD3	1.76	0.41
2:B:1198:ILE:HG12	2:B:1236:MET:CE	2.51	0.41
2:B:1211:SER:OG	2:B:1212:ALA:N	2.53	0.41
2:B:1229:PHE:HE2	2:B:1277:LEU:HD21	1.86	0.41
2:B:1277:LEU:HD22	2:B:1288:VAL:CG1	2.51	0.41
1:A:651:LEU:CD2	1:A:658:PHE:HB2	2.49	0.41
1:A:741:CYS:O	1:A:745:ILE:HG13	2.20	0.41
1:A:923:GLN:HA	1:A:926:VAL:HG23	2.03	0.41
2:B:265:MET:HE2	2:B:283:LEU:HD13	2.02	0.41
2:B:296:ILE:HD11	2:B:358:ILE:HG23	2.02	0.41
2:B:401:LEU:HD12	2:B:401:LEU:HA	1.96	0.41
2:B:1155:SER:HA	2:B:1158:LYS:HB2	2.02	0.41
2:B:1306:GLN:O	2:B:1309:PRO:HG2	2.21	0.41
1:A:210:ILE:N	1:A:211:PRO:CD	2.84	0.40
1:A:221:SER:C	1:A:224:GLY:H	2.28	0.40
1:A:858:VAL:HG12	1:A:859:SER:H	1.85	0.40
1:A:1070:VAL:HG12	1:A:1071:VAL:N	2.34	0.40
2:B:144:GLN:HB3	2:B:145:PRO:HD3	2.02	0.40
2:B:207:HIS:CD2	2:B:242:PRO:HG3	2.56	0.40
2:B:237:THR:O	2:B:237:THR:HG22	2.22	0.40
2:B:539:PHE:CZ	2:B:583:MET:HE2	2.56	0.40
2:B:812:ARG:HD2	2:B:812:ARG:HA	1.69	0.40
2:B:1323:LEU:HG	2:B:1381:ALA:HB1	2.04	0.40
1:A:506:LEU:O	1:A:513:ARG:NH2	2.48	0.40
1:A:779:LYS:O	1:A:783:ILE:HG13	2.21	0.40
1:A:1176:ALA:O	1:A:1180:TYR:N	2.54	0.40
2:B:662:PHE:CG	2:B:727:LEU:HD12	2.56	0.40
2:B:763:GLU:CB	2:B:764:PRO:CD	2.87	0.40
1:A:169:TRP:N	1:A:169:TRP:CD1	2.90	0.40
1:A:372:VAL:HG22	1:A:432:ILE:HG23	2.02	0.40
1:A:375:TRP:HE3	1:A:378:VAL:HG21	1.83	0.40
1:A:938:THR:HG22	1:A:939:GLU:H	1.86	0.40
1:A:1160:VAL:O	1:A:1164:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:ILE:HB	2:B:359:SER:HB3	2.03	0.40
2:B:664:VAL:CG1	2:B:665:ASP:N	2.85	0.40
2:B:1241:GLU:OE2	2:B:1298:ARG:NH1	2.49	0.40
2:B:1344:LYS:HA	2:B:1344:LYS:HE3	2.03	0.40
1:A:357:ARG:HD3	1:A:1101:LYS:NZ	2.37	0.40
1:A:986:SER:HB3	1:A:1027:LEU:HD22	2.03	0.40
2:B:222:HIS:CB	2:B:251:ARG:HG2	2.51	0.40
2:B:478:HIS:O	2:B:482:GLY:HA3	2.21	0.40
2:B:605:ARG:HE	2:B:649:TRP:CD1	2.40	0.40
2:B:690:GLN:O	2:B:691:ASP:HB2	2.21	0.40
2:B:1116:LEU:HB2	2:B:1136:LEU:CD2	2.48	0.40
2:B:1233:PHE:CE1	2:B:1277:LEU:HG	2.56	0.40
1:A:338:PHE:CD2	1:A:417:HIS:HB3	2.57	0.40
1:A:384:GLU:O	1:A:388:ILE:HG13	2.22	0.40
1:A:662:PRO:C	1:A:664:ASP:N	2.80	0.40
1:A:1057:ASP:C	1:A:1059:ASP:H	2.29	0.40
1:A:1191:ILE:HG22	1:A:1196:GLU:HG3	2.03	0.40
2:B:636:LEU:HD12	2:B:636:LEU:C	2.45	0.40
2:B:810:LEU:HD21	2:B:958:LEU:HB2	2.04	0.40
2:B:970:LEU:HD23	2:B:1066:VAL:HG11	2.03	0.40
2:B:1286:TYR:N	2:B:1287:PRO:CD	2.85	0.40
2:B:1326:LEU:O	2:B:1330:GLN:HG3	2.22	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	1190/1308 (91%)	1108 (93%)	75 (6%)	7 (1%)	21	50
2	B	1120/1323 (85%)	1043 (93%)	75 (7%)	2 (0%)	43	71
All	All	2310/2631 (88%)	2151 (93%)	150 (6%)	9 (0%)	30	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
1	A	568	VAL
2	B	1285	SER
1	A	25	LYS
1	A	717	LEU
2	B	832	ASP
1	A	661	GLU
1	A	662	PRO
1	A	1071	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	1093/1188 (92%)	986 (90%)	107 (10%)	7	27
2	B	1030/1193 (86%)	938 (91%)	92 (9%)	9	31
All	All	2123/2381 (89%)	1924 (91%)	199 (9%)	8	29

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ASP
1	A	13	THR
1	A	19	GLU
1	A	33	LEU
1	A	46	LEU
1	A	57	SER
1	A	75	LEU
1	A	95	LEU
1	A	96	GLU
1	A	99	HIS
1	A	119	ASP
1	A	126	SER
1	A	160	LEU
1	A	171	GLN

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Mol	Chain	Res	Type
1	A	175	ILE
1	A	177	LEU
1	A	217	LEU
1	A	240	LEU
1	A	263	GLU
1	A	264	LEU
1	A	275	ILE
1	A	316	LEU
1	A	343	LEU
1	A	365	LEU
1	A	377	HIS
1	A	399	LEU
1	A	427	LEU
1	A	438	GLN
1	A	441	LEU
1	A	446	ASN
1	A	449	VAL
1	A	462	LEU
1	A	479	LYS
1	A	496	GLN
1	A	502	VAL
1	A	510	MET
1	A	529	LEU
1	A	542	LEU
1	A	556	GLN
1	A	560	SER
1	A	564	THR
1	A	571	HIS
1	A	587	ILE
1	A	597	GLN
1	A	599	ASP
1	A	604	LEU
1	A	612	LEU
1	A	621	SER
1	A	624	GLN
1	A	630	LEU
1	A	631	LYS
1	A	641	LEU
1	A	651	LEU
1	A	659	LEU
1	A	663	LEU
1	A	666	LEU

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Mol	Chain	Res	Type
1	A	697	LEU
1	A	730	GLN
1	A	754	GLU
1	A	766	LYS
1	A	768	GLU
1	A	775	THR
1	A	786	GLU
1	A	807	LYS
1	A	821	ILE
1	A	838	MET
1	A	839	HIS
1	A	846	LEU
1	A	864	GLN
1	A	881	LEU
1	A	908	LEU
1	A	919	LEU
1	A	928	GLN
1	A	940	GLU
1	A	949	GLN
1	A	964	ASN
1	A	965	LEU
1	A	973	PHE
1	A	980	LEU
1	A	981	LEU
1	A	982	ILE
1	A	995	THR
1	A	1001	GLN
1	A	1009	ILE
1	A	1011	LYS
1	A	1012	GLU
1	A	1015	GLN
1	A	1021	CYS
1	A	1024	LEU
1	A	1025	MET
1	A	1027	LEU
1	A	1037	SER
1	A	1062	ILE
1	A	1063	GLU
1	A	1160	VAL
1	A	1163	LEU
1	A	1170	ILE
1	A	1188	SER

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Mol	Chain	Res	Type
1	A	1199	VAL
1	A	1201	LEU
1	A	1206	LEU
1	A	1212	SER
1	A	1249	ILE
1	A	1252	LEU
1	A	1272	VAL
1	A	1275	MET
1	A	1284	ARG
2	B	56	THR
2	B	71	VAL
2	B	114	SER
2	B	128	PHE
2	B	136	LEU
2	B	138	LEU
2	B	161	GLU
2	B	178	LEU
2	B	183	ARG
2	B	203	VAL
2	B	276	PHE
2	B	280	VAL
2	B	287	VAL
2	B	298	GLU
2	B	305	VAL
2	B	378	LEU
2	B	416	ASP
2	B	429	ILE
2	B	436	LEU
2	B	439	THR
2	B	441	PHE
2	B	444	GLN
2	B	447	ARG
2	B	462	PHE
2	B	495	LEU
2	B	496	GLU
2	B	505	MET
2	B	522	MET
2	B	549	ILE
2	B	554	HIS
2	B	557	ILE
2	B	563	SER
2	B	565	VAL

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Mol	Chain	Res	Type
2	B	605	ARG
2	B	609	THR
2	B	636	LEU
2	B	640	ARG
2	B	650	VAL
2	B	686	GLU
2	B	687	TYR
2	B	695	ILE
2	B	704	GLU
2	B	727	LEU
2	B	737	CYS
2	B	753	LEU
2	B	762	LEU
2	B	763	GLU
2	B	776	ARG
2	B	778	LEU
2	B	785	LEU
2	B	800	GLN
2	B	802	SER
2	B	810	LEU
2	B	830	ILE
2	B	834	VAL
2	B	925	GLU
2	B	927	ASP
2	B	928	ILE
2	B	930	VAL
2	B	979	THR
2	B	1013	CYS
2	B	1019	THR
2	B	1021	MET
2	B	1070	LEU
2	B	1086	HIS
2	B	1097	LYS
2	B	1101	GLN
2	B	1120	HIS
2	B	1123	VAL
2	B	1135	LEU
2	B	1191	THR
2	B	1208	GLU
2	B	1223	THR
2	B	1225	THR
2	B	1228	THR

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Mol	Chain	Res	Type
2	B	1236	MET
2	B	1237	MET
2	B	1265	TYR
2	B	1266	TRP
2	B	1281	LYS
2	B	1284	ASP
2	B	1288	VAL
2	B	1289	LEU
2	B	1314	SER
2	B	1318	HIS
2	B	1344	LYS
2	B	1349	THR
2	B	1365	LEU
2	B	1379	ARG
2	B	1384	LEU
2	B	1387	LEU
2	B	1391	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	GLN
1	A	216	GLN
1	A	292	HIS
1	A	298	GLN
1	A	438	GLN
1	A	503	GLN
1	A	528	GLN
1	A	545	ASN
1	A	665	HIS
1	A	730	GLN
1	A	733	ASN
1	A	738	ASN
1	A	928	GLN
1	A	959	GLN
1	A	1001	GLN
2	B	110	ASN
2	B	157	GLN
2	B	193	GLN
2	B	207	HIS
2	B	221	GLN
2	B	236	ASN

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Mol	Chain	Res	Type
2	B	411	GLN
2	B	422	HIS
2	B	508	ASN
2	B	635	ASN
2	B	638	GLN
2	B	800	GLN
2	B	972	GLN
2	B	1003	HIS
2	B	1016	GLN
2	B	1029	HIS
2	B	1065	GLN
2	B	1086	HIS
2	B	1290	HIS
2	B	1330	GLN
2	B	1342	HIS
2	B	1354	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](#)

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 ⓘ

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	1206/1308 (92%)	-0.37	7 (0%) 85 75	48, 100, 204, 311	0
2	B	1146/1323 (86%)	-0.25	8 (0%) 84 73	74, 127, 192, 236	0
All	All	2352/2631 (89%)	-0.31	15 (0%) 85 75	48, 116, 198, 311	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	398	ILE	4.3
2	B	1029	HIS	3.4
2	B	1277	LEU	3.3
1	A	399	LEU	3.3
1	A	299	GLY	2.9
2	B	1266	TRP	2.8
1	A	401	GLY	2.7
2	B	765	GLY	2.6
1	A	301	PRO	2.4
2	B	1270	VAL	2.3
2	B	373	ALA	2.2
1	A	819	ASP	2.2
2	B	1191	THR	2.1
1	A	760	SER	2.0
2	B	221	GLN	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.