



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:28 PM GMT

PDB ID : 1XDV  
Title : Experimentally Phased Structure of Human the Son of Sevenless protein at 4.1 Å.  
Authors : Sondermann, H.; Soisson, S.M.; Boykevisch, S.; Yang, S.S.; Bar-Sagi, D.; Kuriyan, J.  
Deposited on : 2004-09-08  
Resolution : 4.10 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

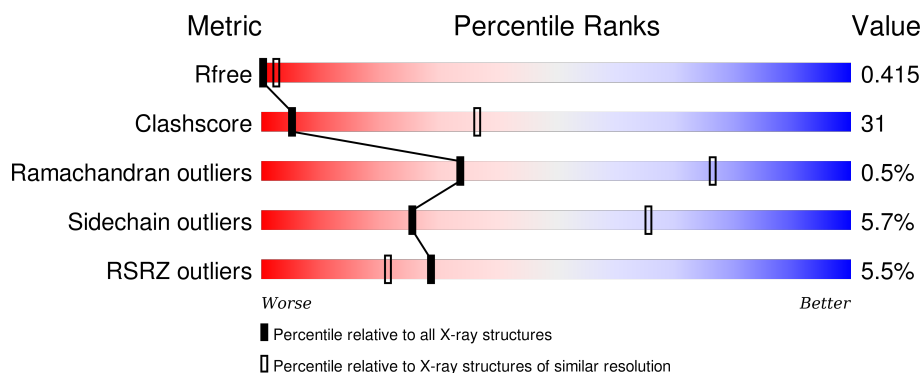
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.10 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))
$R_{free}$	91344	1018 (4.60-3.60)
Clashscore	102246	1117 (4.60-3.60)
Ramachandran outliers	100387	1063 (4.60-3.60)
Sidechain outliers	100360	1049 (4.60-3.60)
RSRZ outliers	91569	1022 (4.60-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	847	<div> <div>5%</div> <div>59%</div> <div>28%</div> <div>•</div> <div>11%</div> </div>
1	B	847	<div> <div>5%</div> <div>56%</div> <div>29%</div> <div>•</div> <div>10%</div> </div>

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12516 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.

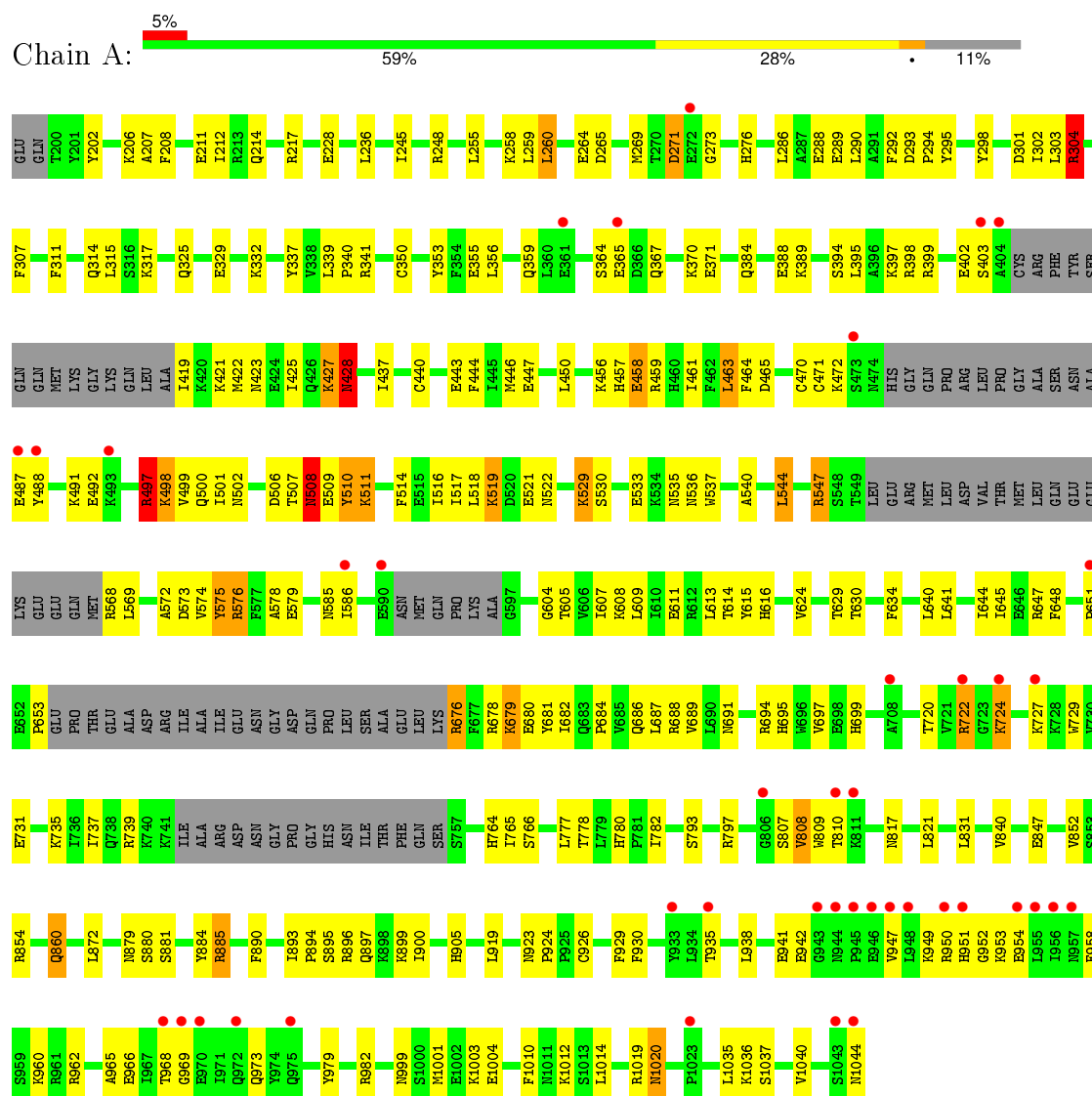
- Molecule 1 is a protein called Son of sevenless protein homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total	C	N	O	S	0	0	0
			6254	4009	1066	1151	28			
1	B	759	Total	C	N	O	S	0	0	0
			6262	4015	1067	1152	28			

### 3 Residue-property plots

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

- Molecule 1: Son of sevenless protein homolog 1



- Molecule 1: Son of sevenless protein homolog 1



F929	I782	V685	K608	L544	PRO	CYS	B301	GLU
F930	S793	Q686	E611	Q545	ARG	ARG	I302	GLN
T935	R797	R687	R612	Y546	LEU	PHE	L303	Y200
L938	R801	V689	L613	S548	GLY	TYR	R304	Y202
E941	S802	L690	T614	T549	ALA	GLN	R310	K206
E942	R806	N691	Y615	L550	SER	GLN	F311	A207
V947	R807	H695	H616	GLU	ASN	MET	Q314	F208
L948	S807	W696	A619	ARG	ALA	LYS	L315	E211
K949	W808	V697	V624	LEU	Y488	GLY	S316	I212
R950	W809	E698	R625	ASP	R489	LYS	K317	E213
H951	T810	H699	T626	THR	K491	LEU	Q325	Q214
G952	N817	Y702	T629	MET	E492	ALA	K332	R217
K953	T720	T721	T630	GLN	K493	K420	E333	E218
E954	R722	L640	L644	GLU	F495	M422	L219	N220
L955	G723	I644	I644	GLY	M496	N423	L221	L221
R957	K724	R647	R648	LYS	K497	E424	Y337	K224
F958	K727	F649	E649	GLU	R498	I425	Y338	V225
S959	E731	E649	L650	MET	V499	Q426	P340	K341
K960	E735	P670	P651	GLU	Q500	K427	R342	E228
R961	I736	E652	E652	LEU	I501	N428	C350	K235
R962	I737	P653	P653	L568	N502	G431	Y353	L236
G963	Q738	GLU	GLU	P670	D503	I437	F354	N244
A965	R739	THR	THR	V574	T507	G438	E355	L245
T968	K740	GLU	GLU	V575	N508	Q439	L356	R248
Y979	R741	ALA	ALA	A576	E509	F444	I357	E254
N999	ILE	ASP	ASP	F577	K511	I445	K358	L255
S1000	ARG	ASP	ILE	E579	F514	M446	S364	K258
M1001	ASN	ASN	ALA	E583	E515	E447	E385	L259
E1002	GLY	GLY	ILE	E584	I516	G448	D366	L260
K1003	PRO	PRO	GLU	N585	L517	T449	Q367	E264
E1004	GLY	GLY	ASN	I586	L518	L450	E368	E268
F1010	HIS	HIS	GLY	E589	K519	K456	D369	K269
M1011	ASN	ASN	ASP	E521	D520	H457	K370	E272
K1012	ILE	ILE	PRO	F526	E521	E458	E371	H276
S1013	THR	THR	LEU	S527	F526	R459	I377	E288
L1014	PHE	GLN	SER	A528	A528	H460	G386	F292
R1019	SER	SER	ALA	K529	K529	I461	K389	D293
M1020	S757	GLU	LEU	E532	E532	L463	L395	P294
L1035	H764	LYS	LYS	N535	N535	F464	L400	Y295
K1036	I765	R676	R676	N536	N536	D465	S401	Y298
V1040	S766	R677	R677	I600	I600	C470	S402	A299
Y1044	R767	R678	R678	1601	1601	K471	E402	R300
	L777	K679	K679	XG02	XG02	K472	S403	
	L778	E680	E681	A603	A603	S473	A404	
	T778	Y681	Y681	G604	G604	N474		
	L779	I682	I682	1605	1605	HIS		
	H780	Q683	Q683	1606	1606	GLY		
	P781	P684	P684	1607	1607	GLN		

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.03Å 124.71Å 245.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 4.10 49.19 – 4.10	Depositor EDS
% Data completeness (in resolution range)	91.0 (8.00-4.10) 94.5 (49.19-4.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.84 (at 4.14Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.433 , 0.449 0.403 , 0.415	Depositor DCC
$R_{free}$ test set	1584 reflections (9.85%)	DCC
Wilson B-factor (Å <sup>2</sup> )	110.0	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 18877 reflections	Xtriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	12516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.39	2/6390 (0.0%)	0.61	2/8615 (0.0%)
1	B	0.40	3/6398 (0.0%)	0.61	2/8626 (0.0%)
All	All	0.39	5/12788 (0.0%)	0.61	4/17241 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	269	MET	CG-SD	6.62	1.98	1.81
1	B	427	LYS	CA-C	-5.53	1.38	1.52
1	A	427	LYS	CA-C	-5.50	1.38	1.52
1	A	428	ASN	N-CA	-5.18	1.35	1.46
1	B	428	ASN	N-CA	-5.18	1.35	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	MET	CG-SD-CE	7.27	111.83	100.20
1	B	1020	ASN	N-CA-C	5.13	124.86	111.00
1	A	1020	ASN	N-CA-C	5.13	124.84	111.00
1	A	304	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	6254	0	6262	384	122
1	B	6262	0	6267	477	116
All	All	12516	0	12529	766	122

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 31.

All (766) 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:269:MET:CE	1:A:729:TRP:CZ2	1.75	1.68
1:A:1019:ARG:HH22	1:B:905:HIS:CE1	1.17	1.60
1:B:342:LEU:HD21	1:B:550:LEU:CD1	1.20	1.58
1:B:269:MET:CG	1:B:691:ASN:HD21	0.94	1.58
1:A:269:MET:HE2	1:A:729:TRP:CZ2	1.25	1.56
1:A:630:THR:HG22	1:A:969:GLY:CA	1.24	1.56
1:A:630:THR:CG2	1:A:969:GLY:HA3	1.26	1.54
1:B:602:LYS:HE2	1:B:948:LEU:CD1	1.36	1.51
1:B:268:GLU:CD	1:B:619:ALA:CB	1.78	1.48
1:A:905:HIS:CD2	1:B:1019:ARG:HH12	1.32	1.48
1:B:342:LEU:CD2	1:B:550:LEU:HD13	1.43	1.46
1:B:402:GLU:CG	1:B:536:ASN:HA	1.45	1.46
1:A:905:HIS:CE1	1:B:1019:ARG:HH22	1.32	1.44
1:A:304:ARG:NH2	1:A:399:ARG:NH1	1.63	1.44
1:B:342:LEU:CD2	1:B:550:LEU:CD1	1.97	1.43
1:A:1019:ARG:HH12	1:B:905:HIS:CD2	1.37	1.42
1:B:402:GLU:OE2	1:B:536:ASN:N	1.58	1.35
1:A:269:MET:CE	1:A:729:TRP:CE2	2.12	1.33
1:A:1019:ARG:NH2	1:B:905:HIS:CE1	1.96	1.29
1:B:268:GLU:OE2	1:B:619:ALA:CB	1.78	1.29
1:B:398:ARG:HG2	1:B:532:GLU:OE2	1.13	1.29
1:B:337:TYR:CB	1:B:538:MET:HE2	1.64	1.26
1:A:269:MET:CG	1:A:691:ASN:HD21	1.48	1.26
1:A:269:MET:HG2	1:A:691:ASN:ND2	1.52	1.25
1:B:630:THR:CA	1:B:805:VAL:HG11	1.66	1.24
1:B:217:ARG:NE	1:B:548:SER:O	1.68	1.24
1:A:905:HIS:CD2	1:B:1019:ARG:NH1	2.08	1.22
1:A:269:MET:HE2	1:A:729:TRP:CE2	1.71	1.21
1:A:1019:ARG:NH1	1:B:905:HIS:CD2	2.07	1.21
1:A:304:ARG:NE	1:A:307:PHE:HB2	1.54	1.21
1:A:935:THR:OG1	1:B:1004:GLU:OE2	1.60	1.20
1:A:905:HIS:CE1	1:B:1019:ARG:NH2	2.10	1.20

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:GLU:OE1	1:B:999:ASN:ND2	1.77	1.18
1:B:342:LEU:HD22	1:B:550:LEU:CD2	1.73	1.17
1:A:304:ARG:CD	1:A:307:PHE:HB2	1.75	1.16
1:B:584:GLU:HG2	1:B:953:LYS:CD	1.76	1.16
1:B:269:MET:HG2	1:B:691:ASN:ND2	1.41	1.14
1:B:342:LEU:HD22	1:B:550:LEU:HD22	1.14	1.13
1:A:304:ARG:CZ	1:A:307:PHE:HB2	1.78	1.13
1:A:634:PHE:HB2	1:A:958:PHE:CZ	1.83	1.13
1:B:268:GLU:OE2	1:B:619:ALA:HB1	0.95	1.13
1:B:342:LEU:HD13	1:B:550:LEU:HD21	1.26	1.12
1:B:402:GLU:HG2	1:B:536:ASN:HA	1.30	1.12
1:B:584:GLU:HG2	1:B:953:LYS:HD2	1.16	1.12
1:B:604:GLY:H	1:B:956:ILE:HB	1.01	1.11
1:A:884:TYR:CE2	1:B:885:ARG:HB3	1.85	1.11
1:B:402:GLU:CG	1:B:536:ASN:CA	2.14	1.10
1:A:629:THR:CG2	1:A:969:GLY:O	2.00	1.09
1:B:602:LYS:CE	1:B:948:LEU:HD11	1.83	1.09
1:B:341:ARG:HG2	1:B:539:ALA:CA	1.48	1.09
1:B:630:THR:HA	1:B:805:VAL:HG11	1.09	1.09
1:B:337:TYR:HB3	1:B:538:MET:HE2	1.10	1.08
1:B:341:ARG:CG	1:B:539:ALA:HA	1.81	1.07
1:B:602:LYS:CE	1:B:948:LEU:CD1	2.31	1.07
1:A:506:ASP:OD1	1:A:508:ASN:HB3	1.54	1.07
1:B:218:GLU:HG2	1:B:550:LEU:HA	1.32	1.07
1:A:269:MET:HE3	1:A:729:TRP:CZ2	1.62	1.07
1:B:268:GLU:CD	1:B:619:ALA:HB1	1.57	1.07
1:B:341:ARG:HG2	1:B:539:ALA:HA	1.34	1.06
1:A:885:ARG:HB3	1:B:884:TYR:CE2	1.89	1.06
1:B:604:GLY:N	1:B:956:ILE:HB	1.71	1.06
1:B:506:ASP:OD2	1:B:508:ASN:HB3	1.56	1.05
1:B:602:LYS:HE2	1:B:948:LEU:HD12	1.31	1.04
1:B:268:GLU:CD	1:B:619:ALA:HB3	1.72	1.04
1:B:217:ARG:CZ	1:B:548:SER:O	2.05	1.04
1:B:398:ARG:CG	1:B:532:GLU:OE2	2.06	1.04
1:A:269:MET:HE3	1:A:729:TRP:CH2	1.92	1.04
1:A:304:ARG:CZ	1:A:307:PHE:CB	2.36	1.04
1:A:938:LEU:HD21	1:B:999:ASN:HB2	1.41	1.03
1:A:905:HIS:ND1	1:B:1019:ARG:NH2	2.06	1.03
1:B:337:TYR:CG	1:B:538:MET:HE2	1.94	1.03
1:B:342:LEU:HD21	1:B:550:LEU:HD11	1.05	1.02
1:B:342:LEU:CD1	1:B:550:LEU:HD21	1.89	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:VAL:HG23	1:A:517:ILE:HB	1.39	1.02
1:B:217:ARG:NH2	1:B:548:SER:O	1.92	1.02
1:A:303:LEU:HA	1:A:304:ARG:HH21	1.24	1.01
1:A:905:HIS:CE1	1:B:1014:LEU:HD11	1.93	1.01
1:B:767:ARG:HH11	1:B:767:ARG:H	1.02	1.00
1:A:885:ARG:HB3	1:B:884:TYR:HE2	1.20	1.00
1:B:269:MET:CB	1:B:691:ASN:HD21	1.74	1.00
1:A:935:THR:HG1	1:B:1004:GLU:CD	1.65	1.00
1:A:884:TYR:HE2	1:B:885:ARG:HB3	1.16	1.00
1:B:584:GLU:CG	1:B:953:LYS:HD2	1.91	1.00
1:B:217:ARG:HH21	1:B:548:SER:C	1.65	1.00
1:B:602:LYS:HE2	1:B:948:LEU:HD11	1.04	0.99
1:B:341:ARG:CG	1:B:539:ALA:CA	2.17	0.97
1:B:337:TYR:CG	1:B:538:MET:CE	2.47	0.97
1:B:337:TYR:CB	1:B:538:MET:CE	2.43	0.97
1:B:422:MET:HE3	1:B:437:ILE:HG22	1.46	0.97
1:A:1004:GLU:OE2	1:B:935:THR:OG1	1.82	0.97
1:A:1019:ARG:NH2	1:B:905:HIS:ND1	2.03	0.96
1:B:604:GLY:H	1:B:956:ILE:CB	1.78	0.96
1:A:634:PHE:HB2	1:A:958:PHE:HZ	1.22	0.96
1:B:601:ILE:O	1:B:958:PHE:HB3	1.67	0.94
1:A:630:THR:HB	1:A:965:ALA:O	1.68	0.94
1:B:583:GLU:O	1:B:955:LEU:HD21	1.68	0.94
1:B:269:MET:HB3	1:B:691:ASN:OD1	1.64	0.94
1:A:304:ARG:HH11	1:A:307:PHE:H	0.94	0.94
1:A:337:TYR:OH	1:A:502:ASN:ND2	2.01	0.94
1:B:269:MET:HG2	1:B:691:ASN:HD21	0.77	0.93
1:A:999:ASN:ND2	1:B:942:GLU:OE1	1.99	0.93
1:B:342:LEU:CD2	1:B:550:LEU:CD2	2.47	0.93
1:A:269:MET:SD	1:A:687:LEU:HD11	2.09	0.93
1:A:269:MET:HG2	1:A:691:ASN:HD21	0.78	0.93
1:B:268:GLU:CD	1:B:619:ALA:HB2	1.88	0.93
1:B:499:VAL:HG12	1:B:517:ILE:HB	1.51	0.93
1:B:269:MET:CG	1:B:691:ASN:ND2	1.78	0.92
1:A:422:MET:HE3	1:A:437:ILE:HG22	1.50	0.92
1:A:1004:GLU:CD	1:B:935:THR:HG1	1.71	0.92
1:A:905:HIS:CG	1:B:1019:ARG:HH22	1.88	0.92
1:A:302:ILE:O	1:A:304:ARG:NH2	2.02	0.92
1:B:630:THR:HA	1:B:805:VAL:CG1	1.99	0.92
1:A:304:ARG:NH1	1:A:307:PHE:CB	2.31	0.91
1:A:301:ASP:O	1:A:304:ARG:HG3	1.70	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:THR:HG22	1:A:969:GLY:O	1.68	0.91
1:B:268:GLU:CG	1:B:619:ALA:HB2	1.99	0.91
1:B:342:LEU:HD21	1:B:550:LEU:HD13	0.99	0.91
1:B:496:MET:HA	1:B:498:LYS:HZ3	1.34	0.91
1:B:358:LYS:HE3	1:B:377:ILE:HD13	1.53	0.90
1:B:218:GLU:HG2	1:B:550:LEU:CA	2.01	0.90
1:B:630:THR:CB	1:B:805:VAL:HG11	2.03	0.89
1:A:304:ARG:NH1	1:A:307:PHE:HB3	1.88	0.88
1:B:337:TYR:HB3	1:B:538:MET:CE	2.00	0.88
1:A:304:ARG:HH11	1:A:307:PHE:N	1.71	0.88
1:A:935:THR:OG1	1:B:1004:GLU:CD	2.11	0.87
1:A:614:THR:HG23	1:A:688:ARG:HB2	1.56	0.87
1:B:268:GLU:OE1	1:B:619:ALA:HB3	1.72	0.87
1:A:1019:ARG:HH22	1:B:905:HIS:CG	1.92	0.87
1:A:881:SER:N	1:B:881:SER:OG	2.08	0.87
1:B:402:GLU:CD	1:B:536:ASN:N	2.29	0.86
1:A:269:MET:CE	1:A:687:LEU:HD11	2.05	0.85
1:B:614:THR:HG23	1:B:688:ARG:HB2	1.56	0.85
1:A:303:LEU:HA	1:A:304:ARG:NH2	1.90	0.85
1:B:269:MET:CB	1:B:691:ASN:ND2	2.34	0.85
1:A:629:THR:HG22	1:A:969:GLY:C	1.95	0.85
1:A:905:HIS:NE2	1:B:1014:LEU:CD1	2.40	0.85
1:B:398:ARG:HG2	1:B:532:GLU:CD	1.97	0.85
1:A:881:SER:OG	1:B:881:SER:N	2.10	0.85
1:A:1014:LEU:HD11	1:B:905:HIS:CE1	2.12	0.85
1:B:402:GLU:CD	1:B:536:ASN:CA	2.45	0.84
1:A:896:ARG:O	1:A:899:LYS:HG2	1.78	0.84
1:B:268:GLU:CG	1:B:619:ALA:CB	2.56	0.83
1:B:402:GLU:CD	1:B:536:ASN:HA	1.98	0.83
1:A:303:LEU:CA	1:A:304:ARG:HH21	1.91	0.83
1:A:1019:ARG:NH1	1:B:905:HIS:NE2	2.18	0.83
1:A:269:MET:HE2	1:A:729:TRP:HZ2	1.03	0.82
1:A:1019:ARG:NH2	1:B:905:HIS:CG	2.47	0.82
1:A:630:THR:HG22	1:A:969:GLY:N	1.93	0.82
1:A:905:HIS:CG	1:B:1019:ARG:NH2	2.47	0.82
1:A:304:ARG:NE	1:A:304:ARG:N	2.28	0.82
1:B:202:TYR:O	1:B:206:LYS:HG3	1.80	0.81
1:B:341:ARG:CZ	1:B:539:ALA:H	1.94	0.81
1:B:499:VAL:CG1	1:B:517:ILE:HB	2.10	0.81
1:B:366:ASP:OD2	1:B:368:GLU:HG2	1.79	0.81
1:B:767:ARG:HH11	1:B:767:ARG:N	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ARG:NH1	1:A:307:PHE:H	1.78	0.80
1:A:202:TYR:O	1:A:206:LYS:HG3	1.81	0.80
1:B:506:ASP:OD2	1:B:508:ASN:CB	2.29	0.79
1:A:938:LEU:HD21	1:B:999:ASN:CB	2.13	0.79
1:B:584:GLU:HG2	1:B:953:LYS:CG	2.14	0.78
1:B:220:ASN:HB3	1:B:224:LYS:NZ	1.98	0.78
1:B:498:LYS:HG3	1:B:518:LEU:HD13	1.63	0.78
1:A:269:MET:HE3	1:A:687:LEU:HD11	1.66	0.78
1:A:929:PHE:CE1	1:B:1003:LYS:HE3	2.19	0.78
1:A:304:ARG:CZ	1:A:307:PHE:HB3	2.12	0.78
1:A:905:HIS:NE2	1:B:1014:LEU:HD13	1.98	0.78
1:A:629:THR:OG1	1:A:973:GLN:OE1	2.00	0.77
1:A:341:ARG:NH2	1:A:536:ASN:OD1	2.17	0.77
1:A:519:LYS:HD3	1:A:519:LYS:H	1.50	0.77
1:B:268:GLU:HG2	1:B:619:ALA:HB2	1.65	0.77
1:B:342:LEU:CD2	1:B:550:LEU:HD22	2.06	0.77
1:B:496:MET:HA	1:B:498:LYS:NZ	1.99	0.77
1:A:1019:ARG:CZ	1:B:905:HIS:CD2	2.67	0.76
1:B:630:THR:HG22	1:B:805:VAL:CG2	2.15	0.76
1:B:498:LYS:O	1:B:498:LYS:HE2	1.84	0.76
1:A:697:VAL:HG11	1:A:737:ILE:HG12	1.67	0.76
1:A:1001:MET:HE3	1:B:810:THR:HG22	1.67	0.76
1:A:999:ASN:HB2	1:B:938:LEU:HD21	1.67	0.76
1:B:342:LEU:HD22	1:B:550:LEU:HD13	1.65	0.76
1:B:767:ARG:H	1:B:767:ARG:NH1	1.82	0.76
1:B:341:ARG:HG2	1:B:539:ALA:C	2.06	0.76
1:A:304:ARG:CD	1:A:307:PHE:CB	2.63	0.76
1:A:634:PHE:CB	1:A:958:PHE:CZ	2.68	0.76
1:A:1019:ARG:NH2	1:B:905:HIS:NE2	2.34	0.76
1:B:601:ILE:O	1:B:958:PHE:CD2	2.38	0.75
1:A:544:LEU:HA	1:A:547:ARG:HH12	1.50	0.75
1:B:697:VAL:HG11	1:B:737:ILE:HG12	1.67	0.75
1:A:1004:GLU:CD	1:B:935:THR:OG1	2.21	0.75
1:A:258:LYS:HE2	1:A:286:LEU:HD21	1.68	0.75
1:B:498:LYS:HG3	1:B:518:LEU:HA	1.69	0.74
1:B:342:LEU:HD13	1:B:550:LEU:CD2	2.11	0.74
1:B:342:LEU:CD2	1:B:550:LEU:CG	2.66	0.74
1:A:1003:LYS:HE3	1:B:929:PHE:CE1	2.21	0.74
1:B:402:GLU:OE2	1:B:536:ASN:CA	2.34	0.74
1:B:583:GLU:O	1:B:955:LEU:CD2	2.35	0.74
1:B:402:GLU:OE2	1:B:535:ASN:C	2.26	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:584:GLU:CG	1:B:953:LYS:CD	2.57	0.74
1:A:341:ARG:HH12	1:A:535:ASN:HB3	1.52	0.74
1:A:884:TYR:OH	1:B:885:ARG:HD2	1.87	0.73
1:B:342:LEU:HD22	1:B:550:LEU:CG	2.18	0.73
1:A:269:MET:HE1	1:A:729:TRP:CE2	2.19	0.73
1:B:446:MET:HE1	1:B:537:TRP:HA	1.70	0.73
1:A:314:GLN:NE2	1:A:317:LYS:HZ3	1.87	0.73
1:A:422:MET:CE	1:A:437:ILE:HG22	2.20	0.72
1:A:634:PHE:CB	1:A:958:PHE:HZ	2.01	0.72
1:A:905:HIS:NE2	1:B:1019:ARG:NH1	2.27	0.72
1:B:508:ASN:O	1:B:509:GLU:HG3	1.90	0.72
1:A:905:HIS:NE2	1:B:1014:LEU:HD11	2.04	0.72
1:A:1019:ARG:HH22	1:B:905:HIS:ND1	1.29	0.71
1:A:269:MET:O	1:A:694:ARG:NH1	2.23	0.71
1:B:244:ASN:HB3	1:B:310:ARG:NH2	2.06	0.71
1:B:300:ARG:O	1:B:304:ARG:HG3	1.90	0.71
1:B:207:ALA:O	1:B:211:GLU:HG3	1.91	0.71
1:B:221:LEU:HD13	1:B:549:THR:OG1	1.90	0.70
1:A:265:ASP:HB3	1:A:687:LEU:HD21	1.72	0.70
1:B:702:TYR:CE1	1:B:802:SER:OG	2.14	0.70
1:B:342:LEU:HD22	1:B:550:LEU:CD1	2.09	0.70
1:A:207:ALA:O	1:A:211:GLU:HG3	1.91	0.70
1:B:422:MET:CE	1:B:437:ILE:HG22	2.20	0.70
1:A:446:MET:HE1	1:A:537:TRP:HA	1.74	0.70
1:A:942:GLU:CD	1:B:999:ASN:ND2	2.44	0.70
1:A:879:ASN:HB3	1:B:1010:PHE:CZ	2.27	0.70
1:B:314:GLN:NE2	1:B:317:LYS:HZ3	1.90	0.70
1:A:905:HIS:CD2	1:B:1019:ARG:CZ	2.74	0.69
1:A:880:SER:C	1:B:881:SER:HG	1.95	0.69
1:B:421:LYS:HA	1:B:421:LYS:HE2	1.73	0.69
1:B:220:ASN:HB3	1:B:224:LYS:HZ1	1.56	0.69
1:A:604:GLY:O	1:A:962:ARG:NH2	2.26	0.69
1:A:304:ARG:HD3	1:A:307:PHE:HB2	1.69	0.69
1:B:629:THR:HG22	1:B:805:VAL:HG21	1.74	0.69
1:A:500:GLN:OE1	1:A:516:ILE:HG12	1.93	0.69
1:A:355:GLU:HG3	1:A:359:GLN:HE21	1.58	0.69
1:A:679:LYS:HD2	1:A:679:LYS:O	1.93	0.69
1:A:498:LYS:HG2	1:A:518:LEU:HA	1.75	0.68
1:B:947:VAL:HG11	1:B:954:GLU:HG3	1.76	0.68
1:A:498:LYS:HG2	1:A:518:LEU:HD23	1.75	0.68
1:B:355:GLU:HG3	1:B:359:GLN:HE21	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:ARG:HH22	1:B:905:HIS:CD2	2.11	0.68
1:A:446:MET:HE3	1:A:537:TRP:CE3	2.29	0.68
1:B:342:LEU:HD23	1:B:550:LEU:HD13	1.66	0.68
1:B:601:ILE:O	1:B:958:PHE:CB	2.41	0.68
1:B:602:LYS:HA	1:B:958:PHE:HB3	1.76	0.68
1:B:629:THR:HG23	1:B:801:PRO:HB2	1.76	0.68
1:B:218:GLU:HG2	1:B:550:LEU:C	2.15	0.67
1:B:337:TYR:CG	1:B:538:MET:HE1	2.29	0.67
1:A:506:ASP:CG	1:A:508:ASN:HB3	2.13	0.67
1:B:679:LYS:O	1:B:679:LYS:HD2	1.93	0.67
1:A:634:PHE:HB2	1:A:958:PHE:CE2	2.28	0.67
1:B:341:ARG:CZ	1:B:539:ALA:N	2.54	0.67
1:B:547:ARG:NH1	1:B:547:ARG:HB3	2.09	0.67
1:A:276:HIS:HE1	1:A:365:GLU:H	1.42	0.67
1:B:220:ASN:O	1:B:224:LYS:HG2	1.95	0.67
1:A:840:VAL:HG13	1:A:1012:LYS:HB3	1.76	0.67
1:A:1019:ARG:NH2	1:B:905:HIS:CD2	2.62	0.67
1:A:341:ARG:HG3	1:A:403:SER:OG	1.95	0.67
1:A:929:PHE:HE1	1:B:1003:LYS:HE3	1.59	0.67
1:A:609:LEU:CD2	1:A:962:ARG:NH1	2.58	0.66
1:A:630:THR:HG23	1:A:969:GLY:HA3	1.62	0.66
1:A:529:LYS:HE3	1:A:533:GLU:OE2	1.95	0.66
1:B:840:VAL:HG13	1:B:1012:LYS:HB3	1.76	0.66
1:B:276:HIS:HE1	1:B:365:GLU:H	1.42	0.66
1:B:341:ARG:HG3	1:B:403:SER:OG	1.95	0.66
1:A:1003:LYS:CE	1:B:929:PHE:HE1	2.08	0.66
1:B:602:LYS:CA	1:B:958:PHE:HB3	2.25	0.66
1:A:947:VAL:HG11	1:A:954:GLU:HG3	1.76	0.66
1:A:1019:ARG:CZ	1:B:905:HIS:NE2	2.59	0.66
1:A:881:SER:HG	1:B:880:SER:C	1.98	0.66
1:A:1014:LEU:CD1	1:B:905:HIS:NE2	2.59	0.65
1:A:506:ASP:OD1	1:A:508:ASN:CB	2.38	0.65
1:B:614:THR:HG21	1:B:689:VAL:HG23	1.78	0.65
1:A:1003:LYS:HE3	1:B:929:PHE:CZ	2.30	0.65
1:A:880:SER:C	1:B:881:SER:OG	2.34	0.65
1:B:314:GLN:NE2	1:B:317:LYS:NZ	2.44	0.65
1:A:885:ARG:HD2	1:B:884:TYR:OH	1.96	0.65
1:A:614:THR:HG21	1:A:689:VAL:HG23	1.77	0.65
1:A:544:LEU:HA	1:A:547:ARG:NH1	2.11	0.65
1:A:314:GLN:NE2	1:A:317:LYS:NZ	2.44	0.65
1:A:929:PHE:HE1	1:B:1003:LYS:CE	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ARG:HH11	1:A:547:ARG:HB2	1.62	0.65
1:B:793:SER:O	1:B:797:ARG:HG3	1.97	0.65
1:B:500:GLN:NE2	1:B:545:GLN:HB2	2.12	0.65
1:B:336:GLN:NE2	1:B:502:ASN:ND2	2.45	0.65
1:A:810:THR:HG22	1:B:1001:MET:HE3	1.77	0.64
1:B:589:GLU:OE1	1:B:959:SER:HB2	1.97	0.64
1:A:507:THR:C	1:A:509:GLU:H	1.99	0.64
1:A:793:SER:O	1:A:797:ARG:HG3	1.97	0.64
1:B:629:THR:HG23	1:B:801:PRO:CB	2.28	0.64
1:B:446:MET:HE3	1:B:537:TRP:CE3	2.32	0.64
1:A:630:THR:CB	1:A:969:GLY:HA3	2.20	0.64
1:B:614:THR:O	1:B:614:THR:HG22	1.98	0.64
1:B:500:GLN:OE1	1:B:545:GLN:HB2	1.98	0.64
1:B:444:PHE:HZ	1:B:447:GLU:HB2	1.62	0.64
1:B:602:LYS:O	1:B:956:ILE:O	2.13	0.64
1:B:603:ALA:CA	1:B:956:ILE:HB	2.27	0.64
1:A:303:LEU:CA	1:A:304:ARG:NH2	2.57	0.64
1:A:884:TYR:CE2	1:B:885:ARG:CB	2.73	0.64
1:A:459:ARG:HH11	1:A:459:ARG:HG2	1.63	0.64
1:B:507:THR:C	1:B:509:GLU:H	1.99	0.64
1:A:398:ARG:HH21	1:A:398:ARG:HA	1.62	0.63
1:A:614:THR:HG22	1:A:614:THR:O	1.98	0.63
1:A:444:PHE:HZ	1:A:447:GLU:HB2	1.62	0.63
1:A:905:HIS:HE1	1:B:1014:LEU:HD11	1.59	0.63
1:B:547:ARG:HH11	1:B:548:SER:N	1.97	0.63
1:B:780:HIS:CE1	1:B:782:ILE:HD12	2.34	0.63
1:B:214:GLN:HE22	1:B:550:LEU:C	2.00	0.63
1:A:1010:PHE:CZ	1:B:879:ASN:HB3	2.33	0.63
1:B:602:LYS:C	1:B:958:PHE:CB	2.66	0.63
1:A:269:MET:HB3	1:A:694:ARG:HH12	1.64	0.63
1:B:630:THR:CB	1:B:805:VAL:CG1	2.75	0.63
1:A:419:ILE:HG13	1:A:422:MET:SD	2.39	0.63
1:B:568:ARG:C	1:B:569:LEU:HD22	2.18	0.63
1:B:602:LYS:C	1:B:958:PHE:HB2	2.17	0.63
1:A:402:GLU:CG	1:A:536:ASN:OD1	2.46	0.63
1:B:235:LYS:H	1:B:235:LYS:HD3	1.64	0.62
1:A:780:HIS:CE1	1:A:782:ILE:HD12	2.33	0.62
1:A:301:ASP:O	1:A:304:ARG:CG	2.46	0.62
1:B:333:GLU:HG2	1:B:501:ILE:HG13	1.81	0.62
1:B:500:GLN:HE22	1:B:545:GLN:HB2	1.62	0.62
1:A:568:ARG:C	1:A:569:LEU:HD22	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:LEU:HD22	1:A:962:ARG:NH1	2.15	0.62
1:A:269:MET:HE3	1:A:687:LEU:CD1	2.28	0.62
1:B:459:ARG:HG2	1:B:459:ARG:HH11	1.63	0.62
1:B:629:THR:O	1:B:805:VAL:HG21	1.99	0.62
1:A:810:THR:HG22	1:B:1001:MET:CE	2.29	0.62
1:A:735:LYS:HD2	1:A:739:ARG:NH2	2.15	0.62
1:A:881:SER:OG	1:B:880:SER:C	2.37	0.61
1:B:450:LEU:HD12	1:B:461:ILE:HD12	1.83	0.61
1:B:342:LEU:CD2	1:B:550:LEU:HD11	1.94	0.61
1:B:367:GLN:O	1:B:371:GLU:HG2	2.01	0.61
1:A:905:HIS:CD2	1:B:1019:ARG:HH22	2.17	0.61
1:A:547:ARG:NH1	1:A:547:ARG:HB2	2.16	0.61
1:B:735:LYS:HD2	1:B:739:ARG:NH2	2.15	0.61
1:A:364:SER:HB3	1:A:370:LYS:HG2	1.82	0.61
1:B:260:LEU:HD22	1:B:264:GLU:HG3	1.83	0.61
1:B:341:ARG:HH12	1:B:535:ASN:HA	1.66	0.61
1:A:629:THR:HG21	1:A:973:GLN:HB2	1.83	0.60
1:A:364:SER:HB3	1:A:370:LYS:CG	2.32	0.60
1:A:450:LEU:HD12	1:A:461:ILE:HD12	1.83	0.60
1:B:777:LEU:HD23	1:B:854:ARG:HG3	1.83	0.60
1:A:260:LEU:HD22	1:A:264:GLU:HG3	1.83	0.60
1:A:905:HIS:CE1	1:B:1014:LEU:CD1	2.73	0.60
1:A:304:ARG:NE	1:A:304:ARG:H	1.98	0.60
1:A:840:VAL:CG1	1:A:1012:LYS:HB3	2.32	0.60
1:A:367:GLN:O	1:A:371:GLU:HG2	2.01	0.60
1:B:364:SER:HB3	1:B:370:LYS:CG	2.32	0.60
1:A:777:LEU:HD23	1:A:854:ARG:HG3	1.83	0.60
1:B:840:VAL:CG1	1:B:1012:LYS:HB3	2.32	0.60
1:B:917:ALA:HA	1:B:920:ARG:NH2	2.17	0.60
1:B:269:MET:CB	1:B:691:ASN:CG	2.69	0.59
1:A:885:ARG:CB	1:B:884:TYR:CE2	2.77	0.59
1:B:224:LYS:HG3	1:B:225:VAL:HG23	1.84	0.59
1:A:269:MET:HG2	1:A:691:ASN:CG	2.21	0.59
1:B:221:LEU:HD23	1:B:550:LEU:CD2	2.33	0.59
1:B:364:SER:HB3	1:B:370:LYS:HG2	1.83	0.59
1:A:1001:MET:CE	1:B:810:THR:HG22	2.32	0.59
1:B:630:THR:HG22	1:B:805:VAL:HG21	1.85	0.59
1:B:456:LYS:H	1:B:456:LYS:HE3	1.67	0.59
1:A:260:LEU:O	1:A:264:GLU:HG3	2.03	0.59
1:A:1014:LEU:HD13	1:B:905:HIS:NE2	2.18	0.59
1:A:905:HIS:CD2	1:B:1019:ARG:NH2	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ASN:ND2	1:B:487:GLU:N	2.51	0.59
1:B:272:GLU:HG3	1:B:625:ARG:NH2	2.17	0.58
1:B:644:ILE:HG23	1:B:689:VAL:HG13	1.85	0.58
1:A:575:TYR:HD2	1:A:651:PRO:HG2	1.69	0.58
1:A:629:THR:HG22	1:A:969:GLY:CA	2.33	0.58
1:B:575:TYR:HD2	1:B:651:PRO:HG2	1.69	0.58
1:B:260:LEU:O	1:B:264:GLU:HG3	2.03	0.58
1:A:644:ILE:HG23	1:A:689:VAL:HG13	1.85	0.58
1:B:269:MET:HB3	1:B:691:ASN:CG	2.24	0.58
1:B:258:LYS:NZ	1:B:258:LYS:HA	2.19	0.58
1:A:630:THR:CG2	1:A:969:GLY:CA	2.17	0.57
1:B:269:MET:CB	1:B:691:ASN:OD1	2.45	0.57
1:B:458:GLU:CD	1:B:458:GLU:O	2.42	0.57
1:B:456:LYS:H	1:B:456:LYS:CE	2.17	0.57
1:A:428:ASN:ND2	1:A:487:GLU:N	2.51	0.57
1:B:519:LYS:NZ	1:B:519:LYS:HB2	2.19	0.57
1:A:1014:LEU:HD11	1:B:905:HIS:NE2	2.19	0.57
1:A:629:THR:O	1:A:969:GLY:HA2	2.04	0.57
1:A:506:ASP:OD1	1:A:510:TYR:CE2	2.57	0.57
1:A:498:LYS:HB2	1:A:517:ILE:O	2.04	0.57
1:B:497:ARG:H	1:B:498:LYS:HD3	1.70	0.57
1:B:276:HIS:CE1	1:B:365:GLU:H	2.22	0.57
1:A:271:ASP:CG	1:A:273:GLY:H	2.08	0.57
1:A:905:HIS:NE2	1:B:1019:ARG:NH2	2.48	0.57
1:B:428:ASN:HD21	1:B:487:GLU:N	2.03	0.57
1:B:767:ARG:HB2	1:B:767:ARG:NH1	2.20	0.57
1:B:218:GLU:CG	1:B:550:LEU:C	2.74	0.56
1:B:235:LYS:HD3	1:B:235:LYS:N	2.20	0.56
1:A:269:MET:HE2	1:A:729:TRP:NE1	2.19	0.56
1:B:584:GLU:CD	1:B:953:LYS:HD2	2.25	0.56
1:A:419:ILE:HG13	1:A:422:MET:HB2	1.87	0.56
1:A:1003:LYS:CE	1:B:929:PHE:CE1	2.84	0.56
1:B:423:ASN:O	1:B:427:LYS:HD3	2.04	0.56
1:B:314:GLN:HE22	1:B:317:LYS:NZ	2.04	0.56
1:B:269:MET:CE	1:B:691:ASN:N	2.66	0.56
1:A:302:ILE:C	1:A:304:ARG:HE	2.09	0.56
1:A:456:LYS:HD2	1:A:457:HIS:CD2	2.39	0.56
1:A:860:GLN:HG3	1:A:900:ILE:HD13	1.87	0.56
1:A:419:ILE:CG1	1:A:422:MET:HB2	2.36	0.56
1:A:276:HIS:CE1	1:A:365:GLU:H	2.22	0.56
1:A:428:ASN:HD21	1:A:487:GLU:N	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ASP:CG	1:B:508:ASN:HB3	2.24	0.56
1:A:314:GLN:HE22	1:A:317:LYS:NZ	2.04	0.56
1:A:929:PHE:CZ	1:B:1003:LYS:HE3	2.40	0.56
1:B:221:LEU:HD23	1:B:550:LEU:HD23	1.88	0.55
1:B:602:LYS:CE	1:B:948:LEU:HD12	2.17	0.55
1:A:421:LYS:HZ1	1:A:425:ILE:HD11	1.72	0.55
1:B:860:GLN:HG3	1:B:900:ILE:HD13	1.87	0.55
1:A:507:THR:O	1:A:509:GLU:N	2.39	0.55
1:B:235:LYS:NZ	1:B:235:LYS:HB2	2.21	0.55
1:A:611:GLU:HA	1:A:647:ARG:NH1	2.22	0.55
1:B:342:LEU:CD1	1:B:550:LEU:CD2	2.74	0.55
1:A:629:THR:HG21	1:A:969:GLY:O	2.00	0.55
1:B:269:MET:CA	1:B:691:ASN:ND2	2.69	0.55
1:B:601:ILE:O	1:B:958:PHE:HD2	1.87	0.55
1:B:403:SER:OG	1:B:539:ALA:HB1	2.06	0.55
1:B:269:MET:HA	1:B:691:ASN:ND2	2.22	0.55
1:A:302:ILE:O	1:A:304:ARG:CZ	2.55	0.55
1:B:547:ARG:O	1:B:547:ARG:HD2	2.06	0.55
1:B:504:LYS:HA	1:B:504:LYS:HE3	1.89	0.55
1:A:269:MET:SD	1:A:687:LEU:HD21	2.47	0.54
1:A:999:ASN:ND2	1:B:942:GLU:CD	2.60	0.54
1:B:947:VAL:HG11	1:B:954:GLU:CG	2.37	0.54
1:A:766:SER:OG	1:A:778:THR:HB	2.07	0.54
1:B:766:SER:OG	1:B:778:THR:HB	2.08	0.54
1:B:221:LEU:CD1	1:B:549:THR:OG1	2.54	0.54
1:B:630:THR:HG22	1:B:805:VAL:CG1	2.38	0.54
1:B:629:THR:HG21	1:B:968:THR:HG21	1.89	0.54
1:A:499:VAL:CG2	1:A:517:ILE:HB	2.25	0.54
1:A:446:MET:HE2	1:A:463:LEU:HD12	1.89	0.54
1:B:630:THR:HG22	1:B:805:VAL:HG22	1.88	0.54
1:B:519:LYS:O	1:B:519:LYS:HD3	2.06	0.54
1:B:547:ARG:HH11	1:B:547:ARG:HB3	1.73	0.54
1:A:1036:LYS:HD3	1:A:1037:SER:O	2.08	0.54
1:B:272:GLU:HG3	1:B:625:ARG:HH22	1.71	0.54
1:B:217:ARG:NH2	1:B:548:SER:C	2.44	0.53
1:A:397:LYS:HB3	1:A:397:LYS:NZ	2.24	0.53
1:A:568:ARG:HG3	1:A:568:ARG:HH21	1.73	0.53
1:B:456:LYS:HG2	1:B:457:HIS:ND1	2.22	0.53
1:B:611:GLU:HA	1:B:647:ARG:NH1	2.22	0.53
1:A:402:GLU:HG3	1:A:536:ASN:OD1	2.07	0.53
1:B:498:LYS:HD2	1:B:518:LEU:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:LYS:O	1:A:511:LYS:HD2	2.09	0.53
1:B:498:LYS:CG	1:B:518:LEU:HD13	2.33	0.53
1:A:269:MET:CG	1:A:691:ASN:ND2	2.33	0.53
1:B:603:ALA:HA	1:B:956:ILE:HB	1.91	0.53
1:A:498:LYS:CG	1:A:518:LEU:HD23	2.38	0.53
1:A:304:ARG:NH1	1:A:307:PHE:HB2	2.09	0.53
1:B:604:GLY:H	1:B:956:ILE:CG1	2.22	0.53
1:A:421:LYS:NZ	1:A:425:ILE:HD11	2.24	0.53
1:A:947:VAL:HG11	1:A:954:GLU:CG	2.37	0.53
1:A:394:SER:O	1:A:398:ARG:HG2	2.09	0.53
1:B:963:LYS:HZ2	1:B:963:LYS:HB3	1.73	0.53
1:B:695:HIS:CD2	1:B:699:HIS:HD2	2.27	0.53
1:B:500:GLN:CD	1:B:545:GLN:HB2	2.29	0.53
1:B:245:ILE:HD11	1:B:314:GLN:HG2	1.91	0.53
1:A:269:MET:CE	1:A:729:TRP:NE1	2.68	0.52
1:A:653:PRO:HD3	1:A:678:ARG:NH1	2.24	0.52
1:A:304:ARG:NH2	1:A:399:ARG:HH11	1.92	0.52
1:A:245:ILE:HD11	1:A:314:GLN:HG2	1.91	0.52
1:B:1036:LYS:NZ	1:B:1036:LYS:HB2	2.23	0.52
1:B:653:PRO:HD3	1:B:678:ARG:NH1	2.24	0.52
1:B:568:ARG:HG3	1:B:568:ARG:HH21	1.73	0.52
1:B:568:ARG:O	1:B:569:LEU:HD13	2.09	0.52
1:B:258:LYS:HA	1:B:258:LYS:HZ2	1.74	0.52
1:B:449:THR:HG23	1:B:458:GLU:OE1	2.09	0.52
1:A:905:HIS:NE2	1:B:1019:ARG:CZ	2.72	0.52
1:B:311:PHE:O	1:B:315:LEU:HD13	2.09	0.52
1:A:519:LYS:CD	1:A:519:LYS:H	2.22	0.52
1:A:518:LEU:HB2	1:A:521:GLU:HB2	1.91	0.52
1:A:684:PRO:O	1:A:688:ARG:HG2	2.10	0.52
1:A:780:HIS:HE1	1:A:782:ILE:HD12	1.74	0.52
1:A:568:ARG:O	1:A:569:LEU:HD13	2.09	0.52
1:A:695:HIS:CD2	1:A:699:HIS:HD2	2.27	0.52
1:A:630:THR:HG22	1:A:969:GLY:C	2.19	0.51
1:B:547:ARG:HH11	1:B:547:ARG:C	2.13	0.51
1:B:511:LYS:O	1:B:511:LYS:HD2	2.09	0.51
1:B:601:ILE:O	1:B:958:PHE:CG	2.63	0.51
1:A:302:ILE:C	1:A:304:ARG:HH21	2.13	0.51
1:B:890:PHE:HA	1:B:893:ILE:HD12	1.93	0.51
1:B:337:TYR:CD1	1:B:538:MET:HE2	2.42	0.51
1:A:311:PHE:O	1:A:315:LEU:HD13	2.09	0.51
1:B:601:ILE:C	1:B:958:PHE:HB3	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:PRO:O	1:B:688:ARG:HG2	2.10	0.51
1:A:884:TYR:CZ	1:B:885:ARG:HD2	2.45	0.50
1:B:507:THR:O	1:B:509:GLU:N	2.40	0.50
1:A:780:HIS:HE1	1:A:782:ILE:CD1	2.24	0.50
1:B:602:LYS:CA	1:B:958:PHE:CB	2.89	0.50
1:A:727:LYS:O	1:A:731:GLU:HG3	2.12	0.50
1:A:890:PHE:HA	1:A:893:ILE:HD12	1.93	0.50
1:A:304:ARG:CZ	1:A:304:ARG:N	2.74	0.50
1:A:304:ARG:HD3	1:A:307:PHE:CB	2.36	0.50
1:A:206:LYS:NZ	1:A:206:LYS:HB3	2.26	0.50
1:B:446:MET:HE2	1:B:463:LEU:HD12	1.94	0.50
1:B:896:ARG:HH11	1:B:896:ARG:HG2	1.77	0.50
1:B:630:THR:HB	1:B:805:VAL:CG1	2.41	0.50
1:A:896:ARG:HG2	1:A:896:ARG:HH11	1.77	0.50
1:B:727:LYS:O	1:B:731:GLU:HG3	2.12	0.50
1:A:648:PHE:HE2	1:A:722:ARG:NH1	2.09	0.50
1:B:399:ARG:O	1:B:402:GLU:HB3	2.12	0.50
1:A:399:ARG:O	1:A:402:GLU:HB3	2.12	0.50
1:B:780:HIS:HE1	1:B:782:ILE:HD12	1.74	0.50
1:A:905:HIS:HE1	1:B:1010:PHE:HE2	1.60	0.50
1:B:780:HIS:HE1	1:B:782:ILE:CD1	2.24	0.50
1:A:999:ASN:CB	1:B:938:LEU:HD21	2.38	0.49
1:B:496:MET:CA	1:B:498:LYS:HZ3	2.17	0.49
1:B:235:LYS:HZ3	1:B:235:LYS:HB2	1.77	0.49
1:B:648:PHE:HE2	1:B:722:ARG:NH1	2.09	0.49
1:A:926:CYS:HA	1:A:979:TYR:OH	2.13	0.49
1:B:579:GLU:O	1:B:608:LYS:HE2	2.12	0.49
1:B:498:LYS:N	1:B:498:LYS:HD3	2.26	0.49
1:B:446:MET:CE	1:B:463:LEU:HD12	2.43	0.49
1:B:926:CYS:HA	1:B:979:TYR:OH	2.13	0.49
1:A:579:GLU:O	1:A:608:LYS:HE2	2.12	0.49
1:A:500:GLN:HE22	1:A:516:ILE:CG1	2.25	0.49
1:A:304:ARG:H	1:A:304:ARG:HE	1.60	0.49
1:B:337:TYR:CD1	1:B:538:MET:CE	2.95	0.49
1:A:720:THR:O	1:A:722:ARG:HD3	2.13	0.49
1:A:458:GLU:CD	1:A:458:GLU:H	2.16	0.49
1:B:268:GLU:OE1	1:B:619:ALA:CB	2.34	0.49
1:B:808:VAL:HG11	1:B:817:ASN:HB3	1.95	0.49
1:A:1003:LYS:HE2	1:B:929:PHE:HE1	1.76	0.49
1:A:446:MET:CE	1:A:463:LEU:HD12	2.42	0.49
1:A:613:LEU:HD11	1:A:624:VAL:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:MET:HE3	1:A:729:TRP:CE2	2.15	0.48
1:B:269:MET:SD	1:B:687:LEU:HG	2.53	0.48
1:B:499:VAL:HG23	1:B:545:GLN:HE22	1.79	0.48
1:B:720:THR:O	1:B:722:ARG:HD3	2.13	0.48
1:B:603:ALA:C	1:B:956:ILE:HB	2.31	0.48
1:A:808:VAL:HG11	1:A:817:ASN:HB3	1.95	0.48
1:A:575:TYR:O	1:A:576:ARG:HG2	2.14	0.48
1:A:586:ILE:HG13	1:A:608:LYS:HG2	1.94	0.48
1:B:613:LEU:HD11	1:B:624:VAL:HA	1.94	0.48
1:B:603:ALA:CA	1:B:956:ILE:CB	2.89	0.48
1:A:303:LEU:C	1:A:304:ARG:NH2	2.66	0.48
1:B:202:TYR:CE2	1:B:206:LYS:HD2	2.48	0.48
1:A:265:ASP:HB3	1:A:687:LEU:CD2	2.41	0.48
1:B:398:ARG:CG	1:B:532:GLU:CD	2.72	0.48
1:B:456:LYS:N	1:B:456:LYS:HE3	2.28	0.48
1:A:568:ARG:HH12	1:A:616:HIS:CE1	2.32	0.48
1:B:576:ARG:HB3	1:B:578:ALA:H	1.78	0.48
1:B:498:LYS:HG2	1:B:517:ILE:O	2.14	0.48
1:B:260:LEU:HD22	1:B:264:GLU:CG	2.44	0.48
1:B:496:MET:SD	1:B:498:LYS:NZ	2.86	0.48
1:B:543:SER:HA	1:B:550:LEU:HD12	1.96	0.48
1:A:443:GLU:HG2	1:A:444:PHE:N	2.29	0.48
1:A:735:LYS:HE3	1:A:739:ARG:HH21	1.79	0.48
1:A:423:ASN:O	1:A:427:LYS:HG3	2.14	0.48
1:B:963:LYS:NZ	1:B:963:LYS:HB3	2.28	0.47
1:B:586:ILE:HG13	1:B:608:LYS:HG2	1.94	0.47
1:A:941:GLU:HA	1:A:960:LYS:HE3	1.96	0.47
1:B:402:GLU:OE2	1:B:536:ASN:CG	2.53	0.47
1:B:500:GLN:C	1:B:501:ILE:HD12	2.35	0.47
1:B:676:ARG:HG2	1:B:676:ARG:HH11	1.79	0.47
1:A:269:MET:HG3	1:A:691:ASN:HD21	1.61	0.47
1:B:584:GLU:CG	1:B:953:LYS:CE	2.92	0.47
1:A:500:GLN:C	1:A:501:ILE:HD12	2.35	0.47
1:B:941:GLU:HA	1:B:960:LYS:HE3	1.96	0.47
1:B:506:ASP:OD2	1:B:510:TYR:CE2	2.67	0.47
1:A:547:ARG:HH11	1:A:547:ARG:CB	2.27	0.47
1:B:735:LYS:HE3	1:B:739:ARG:HH21	1.79	0.47
1:A:576:ARG:HB3	1:A:578:ALA:H	1.78	0.47
1:B:575:TYR:O	1:B:576:ARG:HG2	2.14	0.47
1:A:735:LYS:O	1:A:735:LYS:HD3	2.15	0.47
1:A:519:LYS:HD3	1:A:519:LYS:N	2.25	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:499:VAL:HG11	1:B:517:ILE:HD12	1.97	0.47
1:B:310:ARG:HH21	1:B:310:ARG:HG2	1.79	0.47
1:A:304:ARG:HD2	1:A:307:PHE:N	2.30	0.47
1:A:935:THR:CB	1:B:1004:GLU:OE2	2.58	0.47
1:A:314:GLN:HE21	1:A:317:LYS:HZ3	1.62	0.47
1:B:457:HIS:NE2	1:B:459:ARG:NH1	2.63	0.47
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.80	0.47
1:A:260:LEU:HD22	1:A:264:GLU:CG	2.44	0.47
1:B:807:SER:HA	1:B:809:TRP:CZ3	2.50	0.47
1:B:626:THR:HG23	1:B:965:ALA:HB2	1.96	0.47
1:B:446:MET:CE	1:B:540:ALA:HB3	2.45	0.47
1:B:568:ARG:HH12	1:B:616:HIS:CE1	2.32	0.47
1:A:630:THR:HG21	1:A:966:GLU:O	2.15	0.46
1:B:421:LYS:O	1:B:425:ILE:HG13	2.15	0.46
1:A:421:LYS:O	1:A:425:ILE:HG13	2.15	0.46
1:B:228:GLU:HA	1:B:228:GLU:OE1	2.15	0.46
1:A:1014:LEU:HD11	1:B:905:HIS:HE1	1.75	0.46
1:A:202:TYR:CD2	1:A:206:LYS:HD2	2.50	0.46
1:A:446:MET:CE	1:A:540:ALA:HB3	2.45	0.46
1:A:530:SER:OG	1:A:533:GLU:HG3	2.15	0.46
1:A:676:ARG:HG2	1:A:676:ARG:HH11	1.79	0.46
1:A:630:THR:O	1:A:965:ALA:HB1	2.14	0.46
1:A:905:HIS:CG	1:B:1019:ARG:CZ	2.98	0.46
1:A:510:TYR:O	1:A:510:TYR:CD1	2.69	0.46
1:B:498:LYS:CG	1:B:517:ILE:O	2.64	0.46
1:A:507:THR:C	1:A:509:GLU:N	2.67	0.46
1:A:605:THR:HG22	1:A:607:ILE:H	1.80	0.46
1:A:506:ASP:OD2	1:A:506:ASP:O	2.33	0.46
1:B:735:LYS:CE	1:B:739:ARG:HH21	2.28	0.46
1:B:269:MET:HE3	1:B:691:ASN:N	2.13	0.46
1:A:398:ARG:CA	1:A:398:ARG:HH21	2.28	0.46
1:B:457:HIS:CD2	1:B:472:LYS:HG3	2.51	0.46
1:A:735:LYS:CE	1:A:739:ARG:HH21	2.28	0.46
1:A:519:LYS:O	1:A:521:GLU:HG2	2.16	0.46
1:A:807:SER:HA	1:A:809:TRP:CZ3	2.50	0.46
1:A:258:LYS:HE2	1:A:286:LEU:CD2	2.40	0.46
1:A:879:ASN:CB	1:B:1010:PHE:CZ	2.98	0.46
1:B:217:ARG:HG3	1:B:217:ARG:HH11	1.80	0.46
1:B:507:THR:C	1:B:509:GLU:N	2.67	0.46
1:B:510:TYR:O	1:B:510:TYR:CD1	2.69	0.46
1:B:272:GLU:CG	1:B:625:ARG:NH2	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:GLU:HG2	1:A:458:GLU:O	2.17	0.45
1:A:228:GLU:HA	1:A:228:GLU:OE1	2.15	0.45
1:B:341:ARG:HG3	1:B:539:ALA:HB1	1.07	0.45
1:B:847:GLU:HG2	1:B:1035:LEU:HD21	1.98	0.45
1:A:269:MET:SD	1:A:687:LEU:CD1	2.95	0.45
1:A:500:GLN:NE2	1:A:516:ILE:HG12	2.32	0.45
1:B:735:LYS:HD3	1:B:735:LYS:O	2.15	0.45
1:B:605:THR:HG22	1:B:607:ILE:H	1.80	0.45
1:B:603:ALA:CB	1:B:955:LEU:C	2.62	0.45
1:B:584:GLU:HG2	1:B:953:LYS:HG3	1.97	0.45
1:A:497:ARG:NH2	1:A:519:LYS:HB3	2.31	0.45
1:A:202:TYR:CE2	1:A:206:LYS:HD2	2.51	0.45
1:A:629:THR:HG23	1:A:969:GLY:O	2.04	0.45
1:B:506:ASP:C	1:B:508:ASN:N	2.68	0.45
1:B:499:VAL:CG1	1:B:517:ILE:HD12	2.46	0.45
1:B:254:GLU:O	1:B:258:LYS:HG2	2.17	0.45
1:B:519:LYS:HD3	1:B:520:ASP:OD2	2.17	0.45
1:A:470:CYS:HB2	1:A:492:GLU:HB2	1.99	0.45
1:A:398:ARG:HB3	1:A:398:ARG:NH2	2.31	0.45
1:B:202:TYR:CD2	1:B:206:LYS:HD2	2.52	0.45
1:A:609:LEU:HD21	1:A:962:ARG:NH1	2.32	0.45
1:B:650:ILE:HA	1:B:651:PRO:HD3	1.82	0.45
1:A:682:ILE:HG23	1:A:686:GLN:HE21	1.82	0.45
1:B:767:ARG:N	1:B:767:ARG:HD3	2.31	0.45
1:A:929:PHE:CE1	1:B:1003:LYS:CE	2.89	0.45
1:B:314:GLN:HE21	1:B:317:LYS:HZ3	1.64	0.45
1:B:421:LYS:NZ	1:B:425:ILE:HG13	2.32	0.45
1:A:389:LYS:HD3	1:A:389:LYS:O	2.16	0.45
1:A:471:CYS:HB3	1:A:488:TYR:HB3	2.00	0.44
1:B:471:CYS:HB3	1:B:488:TYR:HB3	1.99	0.44
1:B:574:VAL:O	1:B:574:VAL:HG12	2.17	0.44
1:A:574:VAL:HG12	1:A:574:VAL:O	2.17	0.44
1:B:547:ARG:HD2	1:B:547:ARG:C	2.37	0.44
1:A:506:ASP:C	1:A:508:ASN:N	2.68	0.44
1:A:724:LYS:NZ	1:A:727:LYS:NZ	2.65	0.44
1:A:885:ARG:HD2	1:B:884:TYR:CZ	2.52	0.44
1:A:609:LEU:HD21	1:A:962:ARG:HH11	1.82	0.44
1:A:456:LYS:O	1:A:456:LYS:HD3	2.18	0.44
1:B:724:LYS:NZ	1:B:727:LYS:NZ	2.65	0.44
1:A:568:ARG:NH1	1:A:616:HIS:CE1	2.86	0.44
1:B:676:ARG:HD3	1:B:676:ARG:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:LEU:O	1:A:317:LYS:NZ	2.51	0.44
1:B:402:GLU:OE2	1:B:535:ASN:HB2	2.18	0.44
1:A:394:SER:HA	1:A:397:LYS:HZ2	1.83	0.44
1:A:676:ARG:HD3	1:A:676:ARG:N	2.33	0.44
1:A:847:GLU:HG2	1:A:1035:LEU:HD21	1.98	0.44
1:B:298:TYR:CE2	1:B:302:ILE:HG13	2.52	0.44
1:B:341:ARG:NH2	1:B:536:ASN:C	2.71	0.44
1:B:498:LYS:CD	1:B:518:LEU:HD13	2.47	0.44
1:A:500:GLN:HE22	1:A:516:ILE:HG12	1.82	0.44
1:B:568:ARG:NH1	1:B:616:HIS:CE1	2.86	0.44
1:B:457:HIS:NE2	1:B:472:LYS:HD2	2.33	0.44
1:A:364:SER:HB3	1:A:370:LYS:HG3	1.99	0.44
1:A:722:ARG:N	1:A:722:ARG:HD3	2.33	0.44
1:B:519:LYS:O	1:B:520:ASP:CG	2.56	0.43
1:A:298:TYR:CE2	1:A:302:ILE:HG13	2.52	0.43
1:A:609:LEU:CD2	1:A:962:ARG:HH11	2.31	0.43
1:B:470:CYS:HB2	1:B:492:GLU:HB2	1.99	0.43
1:A:457:HIS:CD2	1:A:472:LYS:NZ	2.86	0.43
1:A:942:GLU:OE2	1:B:999:ASN:ND2	2.52	0.43
1:B:872:LEU:HD12	1:B:929:PHE:CG	2.53	0.43
1:B:947:VAL:HG12	1:B:949:LYS:HZ2	1.83	0.43
1:B:364:SER:HB3	1:B:370:LYS:HG3	1.99	0.43
1:A:248:ARG:NE	1:A:248:ARG:HA	2.33	0.43
1:B:682:ILE:HG23	1:B:686:GLN:HE21	1.82	0.43
1:B:422:MET:HG2	1:B:464:PHE:HE2	1.83	0.43
1:B:358:LYS:HA	1:B:358:LYS:HE2	2.01	0.43
1:A:459:ARG:HG2	1:A:459:ARG:NH1	2.32	0.43
1:A:647:ARG:HD2	1:A:647:ARG:HA	1.92	0.43
1:B:248:ARG:NE	1:B:248:ARG:HA	2.33	0.43
1:A:1010:PHE:HE2	1:B:905:HIS:HE1	1.66	0.43
1:A:872:LEU:HD12	1:A:929:PHE:CG	2.53	0.43
1:B:236:LEU:O	1:B:317:LYS:NZ	2.51	0.43
1:B:292:PHE:HE2	1:B:353:TYR:CE2	2.36	0.43
1:B:722:ARG:N	1:B:722:ARG:HD3	2.33	0.43
1:B:208:PHE:CE1	1:B:353:TYR:HE1	2.37	0.43
1:A:293:ASP:N	1:A:294:PRO:CD	2.82	0.43
1:A:208:PHE:CE1	1:A:353:TYR:HE1	2.37	0.43
1:B:221:LEU:HD22	1:B:549:THR:C	2.31	0.43
1:B:500:GLN:OE1	1:B:541:LEU:O	2.37	0.43
1:A:422:MET:HG2	1:A:464:PHE:HE2	1.83	0.43
1:A:339:LEU:N	1:A:340:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:ARG:CZ	1:B:905:HIS:CG	2.99	0.42
1:A:629:THR:CG2	1:A:969:GLY:C	2.67	0.42
1:B:402:GLU:CD	1:B:535:ASN:C	2.75	0.42
1:A:506:ASP:OD1	1:A:510:TYR:CD2	2.72	0.42
1:B:422:MET:HG2	1:B:464:PHE:CE2	2.54	0.42
1:B:293:ASP:N	1:B:294:PRO:CD	2.82	0.42
1:B:339:LEU:N	1:B:340:PRO:HD2	2.34	0.42
1:B:341:ARG:NH2	1:B:539:ALA:H	2.14	0.42
1:A:422:MET:HG2	1:A:464:PHE:CE2	2.54	0.42
1:A:271:ASP:OD2	1:A:273:GLY:N	2.51	0.42
1:A:341:ARG:NH2	1:A:536:ASN:HA	2.34	0.42
1:B:337:TYR:C	1:B:542:ILE:HG13	2.39	0.42
1:B:630:THR:CG2	1:B:805:VAL:HG11	2.49	0.42
1:A:419:ILE:O	1:A:419:ILE:HG12	2.19	0.42
1:A:292:PHE:HE2	1:A:353:TYR:CE2	2.36	0.42
1:A:500:GLN:NE2	1:A:514:PHE:HD1	2.18	0.42
1:A:777:LEU:HA	1:A:854:ARG:NH1	2.35	0.42
1:B:516:ILE:HG22	1:B:518:LEU:HD22	2.01	0.42
1:A:395:LEU:HD22	1:A:395:LEU:N	2.35	0.42
1:A:325:GLN:HG3	1:A:332:LYS:HD2	2.02	0.42
1:A:852:VAL:HG11	1:A:893:ILE:HD11	2.01	0.42
1:A:764:HIS:CG	1:A:765:ILE:N	2.88	0.42
1:B:603:ALA:HA	1:B:956:ILE:CB	2.48	0.42
1:B:506:ASP:OD1	1:B:510:TYR:CG	2.73	0.42
1:A:500:GLN:CD	1:A:516:ILE:HG12	2.38	0.42
1:B:852:VAL:HG11	1:B:893:ILE:HD11	2.01	0.42
1:A:764:HIS:CG	1:A:765:ILE:H	2.38	0.42
1:A:935:THR:OG1	1:B:1004:GLU:CG	2.68	0.42
1:B:777:LEU:HA	1:B:854:ARG:NH1	2.34	0.42
1:A:572:ALA:O	1:A:573:ASP:HB3	2.20	0.42
1:B:585:ASN:HB3	1:B:608:LYS:HG2	2.02	0.42
1:B:764:HIS:CG	1:B:765:ILE:N	2.88	0.42
1:B:395:LEU:HD22	1:B:395:LEU:N	2.35	0.42
1:A:879:ASN:CG	1:B:1010:PHE:CZ	2.93	0.41
1:A:304:ARG:CZ	1:A:399:ARG:NH1	2.65	0.41
1:A:465:ASP:HA	1:A:544:LEU:HD21	2.02	0.41
1:B:572:ALA:O	1:B:573:ASP:HB3	2.20	0.41
1:B:630:THR:CG2	1:B:805:VAL:CG1	2.98	0.41
1:B:780:HIS:HE1	1:B:782:ILE:CG1	2.33	0.41
1:A:780:HIS:HE1	1:A:782:ILE:CG1	2.33	0.41
1:B:420:LYS:O	1:B:424:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:896:ARG:HG3	1:A:897:GLN:N	2.36	0.41
1:B:506:ASP:O	1:B:506:ASP:OD1	2.39	0.41
1:B:325:GLN:HG3	1:B:332:LYS:HD2	2.02	0.41
1:A:880:SER:CA	1:B:881:SER:HG	2.34	0.41
1:A:544:LEU:CA	1:A:547:ARG:HH12	2.26	0.41
1:B:446:MET:HE2	1:B:540:ALA:HB3	2.01	0.41
1:B:852:VAL:CG1	1:B:893:ILE:HD11	2.51	0.41
1:B:896:ARG:HG3	1:B:897:GLN:N	2.36	0.41
1:B:465:ASP:HA	1:B:544:LEU:HD21	2.02	0.41
1:B:518:LEU:HB2	1:B:521:GLU:HB2	2.02	0.41
1:A:459:ARG:NE	1:A:492:GLU:OE1	2.54	0.41
1:A:852:VAL:CG1	1:A:893:ILE:HD11	2.50	0.41
1:B:600:ILE:HG23	1:B:962:ARG:HH12	1.77	0.41
1:A:371:GLU:HA	1:A:371:GLU:OE1	2.21	0.41
1:B:519:LYS:HZ2	1:B:519:LYS:HB2	1.86	0.41
1:A:295:TYR:CD1	1:A:350:CYS:HB2	2.55	0.41
1:A:389:LYS:HD3	1:A:389:LYS:C	2.41	0.41
1:A:923:ASN:HA	1:A:924:PRO:HD2	1.85	0.41
1:A:630:THR:HG22	1:A:969:GLY:HA3	0.52	0.41
1:B:547:ARG:NH1	1:B:548:SER:N	2.64	0.41
1:A:1004:GLU:CG	1:B:935:THR:OG1	2.68	0.41
1:B:212:ILE:CG2	1:B:260:LEU:HG	2.51	0.41
1:B:640:LEU:HD13	1:B:696:TRP:CZ3	2.56	0.41
1:B:295:TYR:CD1	1:B:350:CYS:HB2	2.55	0.41
1:B:244:ASN:HB3	1:B:310:ARG:CZ	2.50	0.40
1:B:459:ARG:NE	1:B:492:GLU:OE1	2.54	0.40
1:B:371:GLU:HA	1:B:371:GLU:OE1	2.21	0.40
1:A:212:ILE:CG2	1:A:260:LEU:HG	2.51	0.40
1:B:421:LYS:HZ3	1:B:425:ILE:HG13	1.84	0.40
1:A:585:ASN:HB3	1:A:608:LYS:HG2	2.02	0.40
1:A:641:LEU:O	1:A:645:ILE:HG13	2.21	0.40
1:B:629:THR:HG23	1:B:801:PRO:HB3	1.99	0.40
1:A:506:ASP:C	1:A:508:ASN:H	2.25	0.40
1:B:506:ASP:C	1:B:508:ASN:H	2.25	0.40
1:B:498:LYS:HB2	1:B:517:ILE:O	2.20	0.40
1:A:568:ARG:NH1	1:A:681:TYR:CD2	2.88	0.40
1:B:576:ARG:HD3	1:B:577:PHE:H	1.87	0.40

All (122) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ASP:OD2	1:B:300:ARG:NE[2_765]	0.38	1.82
1:A:894:PRO:C	1:B:575:TYR:OH[3_755]	0.54	1.66
1:A:949:LYS:CA	1:B:573:ASP:OD2[1_655]	0.56	1.64
1:A:953:LYS:CA	1:B:574:VAL:CG2[1_655]	0.66	1.54
1:A:953:LYS:N	1:B:574:VAL:CA[1_655]	0.67	1.53
1:A:953:LYS:CG	1:B:574:VAL:CG1[1_655]	0.72	1.48
1:A:949:LYS:CB	1:B:573:ASP:CG[1_655]	0.74	1.46
1:A:895:SER:N	1:B:575:TYR:CZ[3_755]	0.75	1.45
1:A:575:TYR:CE2	1:B:895:SER:O[3_845]	0.76	1.44
1:A:521:GLU:OE2	1:B:727:LYS:NZ[3_855]	0.84	1.36
1:A:953:LYS:CA	1:B:574:VAL:CB[1_655]	0.97	1.23
1:A:952:GLY:CA	1:B:575:TYR:N[1_655]	0.98	1.22
1:A:953:LYS:C	1:B:574:VAL:CG2[1_655]	0.98	1.22
1:A:952:GLY:C	1:B:574:VAL:CA[1_655]	1.06	1.14
1:A:575:TYR:OH	1:B:898:LYS:N[3_845]	1.12	1.08
1:A:953:LYS:N	1:B:574:VAL:CB[1_655]	1.12	1.08
1:A:288:GLU:O	1:B:389:LYS:NZ[2_765]	1.17	1.03
1:A:575:TYR:CE1	1:B:898:LYS:C[3_845]	1.17	1.03
1:A:575:TYR:OH	1:B:897:GLN:C[3_845]	1.18	1.02
1:A:651:PRO:CB	1:B:899:LYS:NZ[3_845]	1.18	1.02
1:A:952:GLY:C	1:B:574:VAL:N[1_655]	1.18	1.02
1:A:949:LYS:CB	1:B:573:ASP:OD2[1_655]	1.20	1.00
1:A:575:TYR:CE1	1:B:898:LYS:CA[3_845]	1.22	0.98
1:A:293:ASP:CG	1:B:300:ARG:NE[2_765]	1.23	0.97
1:A:953:LYS:CB	1:B:574:VAL:CG1[1_655]	1.25	0.95
1:A:895:SER:N	1:B:575:TYR:CE1[3_755]	1.30	0.90
1:A:895:SER:OG	1:B:575:TYR:CD1[3_755]	1.30	0.90
1:A:521:GLU:OE2	1:B:727:LYS:CE[3_855]	1.31	0.89
1:A:293:ASP:OD2	1:B:300:ARG:CZ[2_765]	1.32	0.88
1:A:894:PRO:CA	1:B:575:TYR:OH[3_755]	1.36	0.84
1:A:894:PRO:C	1:B:575:TYR:CZ[3_755]	1.42	0.78
1:A:288:GLU:C	1:B:389:LYS:NZ[2_765]	1.42	0.78
1:A:517:ILE:CG2	1:A:1044:ASN:ND2[1_655]	1.43	0.77
1:A:895:SER:N	1:B:575:TYR:OH[3_755]	1.45	0.75
1:A:952:GLY:CA	1:B:574:VAL:C[1_655]	1.46	0.74
1:A:951:HIS:O	1:B:574:VAL:O[1_655]	1.49	0.71
1:A:651:PRO:CG	1:B:899:LYS:NZ[3_845]	1.50	0.70
1:A:575:TYR:CE1	1:B:899:LYS:N[3_845]	1.53	0.67
1:A:575:TYR:CZ	1:B:898:LYS:N[3_845]	1.54	0.66
1:A:894:PRO:O	1:B:575:TYR:OH[3_755]	1.54	0.66
1:A:575:TYR:CD2	1:B:895:SER:O[3_845]	1.55	0.65
1:A:953:LYS:CD	1:B:574:VAL:CG1[1_655]	1.57	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:LYS:C	1:B:573:ASP:OD2[1_655]	1.58	0.62
1:A:953:LYS:N	1:B:574:VAL:N[1_655]	1.62	0.58
1:A:949:LYS:CB	1:B:573:ASP:OD1[1_655]	1.62	0.58
1:A:952:GLY:C	1:B:574:VAL:C[1_655]	1.63	0.57
1:A:952:GLY:CA	1:B:574:VAL:N[1_655]	1.65	0.55
1:A:575:TYR:CE1	1:B:898:LYS:CB[3_845]	1.65	0.55
1:A:521:GLU:CD	1:B:727:LYS:NZ[3_855]	1.72	0.48
1:A:895:SER:OG	1:B:575:TYR:CG[3_755]	1.73	0.47
1:A:521:GLU:CA	1:B:724:LYS:NZ[3_855]	1.73	0.47
1:A:575:TYR:CD2	1:B:899:LYS:CD[3_845]	1.73	0.47
1:A:575:TYR:CG	1:B:899:LYS:CD[3_845]	1.73	0.47
1:A:575:TYR:CZ	1:B:899:LYS:N[3_845]	1.74	0.46
1:A:288:GLU:O	1:B:389:LYS:CE[2_765]	1.74	0.46
1:A:949:LYS:CA	1:B:573:ASP:CG[1_655]	1.74	0.46
1:A:949:LYS:CB	1:B:573:ASP:CB[1_655]	1.74	0.46
1:A:575:TYR:CD2	1:B:899:LYS:CE[3_845]	1.77	0.43
1:A:521:GLU:OE2	1:B:727:LYS:CD[3_855]	1.77	0.43
1:A:575:TYR:OH	1:B:897:GLN:CA[3_845]	1.79	0.41
1:A:952:GLY:C	1:B:574:VAL:CB[1_655]	1.80	0.40
1:A:954:GLU:N	1:B:574:VAL:CG2[1_655]	1.80	0.40
1:A:951:HIS:O	1:B:574:VAL:C[1_655]	1.80	0.40
1:A:293:ASP:OD2	1:B:300:ARG:CD[2_765]	1.80	0.40
1:A:289:GLU:N	1:B:389:LYS:NZ[2_765]	1.80	0.40
1:A:575:TYR:CZ	1:B:895:SER:O[3_845]	1.81	0.39
1:A:651:PRO:CG	1:B:899:LYS:CE[3_845]	1.83	0.37
1:A:952:GLY:CA	1:B:574:VAL:CA[1_655]	1.83	0.37
1:A:952:GLY:N	1:B:575:TYR:N[1_655]	1.84	0.36
1:A:952:GLY:N	1:B:573:ASP:O[1_655]	1.86	0.34
1:A:953:LYS:N	1:B:574:VAL:CG2[1_655]	1.87	0.33
1:A:953:LYS:CB	1:B:574:VAL:CB[1_655]	1.87	0.33
1:A:575:TYR:CB	1:B:899:LYS:CD[3_845]	1.88	0.32
1:A:949:LYS:CG	1:B:573:ASP:CB[1_655]	1.89	0.31
1:A:953:LYS:CA	1:B:574:VAL:CG1[1_655]	1.90	0.30
1:A:575:TYR:CE2	1:B:895:SER:C[3_845]	1.90	0.30
1:A:293:ASP:CG	1:B:300:ARG:CZ[2_765]	1.91	0.29
1:A:952:GLY:N	1:B:574:VAL:C[1_655]	1.92	0.28
1:A:575:TYR:OH	1:B:897:GLN:N[3_845]	1.93	0.27
1:A:575:TYR:CE1	1:B:898:LYS:N[3_845]	1.94	0.26
1:A:895:SER:N	1:B:575:TYR:CE2[3_755]	1.94	0.26
1:A:894:PRO:CA	1:B:575:TYR:CZ[3_755]	1.96	0.24
1:A:575:TYR:CD1	1:B:898:LYS:CB[3_845]	1.96	0.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:LYS:CB	1:B:574:VAL:CG2[1_655]	1.97	0.23
1:A:895:SER:CA	1:B:575:TYR:CE1[3_755]	1.97	0.23
1:A:949:LYS:CD	1:B:573:ASP:CB[1_655]	1.98	0.22
1:A:949:LYS:N	1:B:573:ASP:OD2[1_655]	1.99	0.21
1:A:289:GLU:OE1	1:B:389:LYS:CG[2_765]	1.99	0.21
1:A:522:ASN:N	1:B:724:LYS:CD[3_855]	1.99	0.21
1:A:329:GLU:CG	1:A:982:ARG:NE[1_655]	2.01	0.19
1:A:289:GLU:CA	1:B:389:LYS:NZ[2_765]	2.02	0.18
1:A:575:TYR:CD1	1:B:898:LYS:C[3_845]	2.03	0.17
1:A:575:TYR:CZ	1:B:898:LYS:CA[3_845]	2.03	0.17
1:A:290:LEU:CD1	1:B:386:GLY:O[2_765]	2.03	0.17
1:A:953:LYS:O	1:B:574:VAL:CG2[1_655]	2.04	0.16
1:A:952:GLY:O	1:B:574:VAL:N[1_655]	2.04	0.16
1:A:950:ARG:NH1	1:B:579:GLU:OE2[1_655]	2.05	0.15
1:A:951:HIS:C	1:B:574:VAL:C[1_655]	2.05	0.15
1:A:952:GLY:CA	1:B:573:ASP:C[1_655]	2.08	0.12
1:A:388:GLU:OE1	1:A:507:THR:O[4_466]	2.09	0.11
1:A:949:LYS:CG	1:B:573:ASP:CG[1_655]	2.09	0.11
1:A:894:PRO:CB	1:B:575:TYR:OH[3_755]	2.09	0.11
1:A:491:LYS:NZ	1:B:288:GLU:OE1[3_855]	2.10	0.10
1:A:293:ASP:OD2	1:B:300:ARG:NH2[2_765]	2.10	0.10
1:A:953:LYS:CA	1:B:574:VAL:CA[1_655]	2.10	0.10
1:A:952:GLY:C	1:B:575:TYR:N[1_655]	2.12	0.08
1:A:894:PRO:C	1:B:575:TYR:CE1[3_755]	2.12	0.08
1:A:575:TYR:CD1	1:B:899:LYS:N[3_845]	2.13	0.07
1:A:952:GLY:N	1:B:574:VAL:CA[1_655]	2.14	0.06
1:A:521:GLU:CD	1:B:724:LYS:NZ[3_855]	2.14	0.06
1:A:953:LYS:N	1:B:574:VAL:C[1_655]	2.15	0.05
1:A:329:GLU:CG	1:A:982:ARG:CZ[1_655]	2.15	0.05
1:A:651:PRO:CB	1:B:899:LYS:CE[3_845]	2.15	0.05
1:A:289:GLU:OE1	1:B:389:LYS:CD[2_765]	2.16	0.04
1:A:329:GLU:CG	1:A:982:ARG:CD[1_655]	2.16	0.04
1:A:952:GLY:O	1:B:574:VAL:CB[1_655]	2.16	0.04
1:A:895:SER:CA	1:B:575:TYR:CZ[3_755]	2.16	0.04
1:A:293:ASP:OD1	1:B:300:ARG:CZ[2_765]	2.17	0.03
1:A:384:GLN:NE2	1:A:509:GLU:CD[4_466]	2.17	0.03
1:A:575:TYR:CZ	1:B:898:LYS:C[3_845]	2.18	0.02
1:A:895:SER:OG	1:B:575:TYR:CE1[3_755]	2.19	0.01
1:A:293:ASP:CG	1:B:300:ARG:CD[2_765]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	744/847 (88%)	709 (95%)	31 (4%)	4 (0%)	34	76
1	B	745/847 (88%)	710 (95%)	31 (4%)	4 (0%)	34	76
All	All	1489/1694 (88%)	1419 (95%)	62 (4%)	8 (0%)	34	76

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1020	ASN
1	B	1020	ASN
1	A	497	ARG
1	A	508	ASN
1	B	497	ARG
1	B	508	ASN
1	A	440	CYS
1	B	440	CYS

### 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	698/773 (90%)	661 (95%)	37 (5%)	28	67
1	B	699/773 (90%)	656 (94%)	43 (6%)	23	63
All	All	1397/1546 (90%)	1317 (94%)	80 (6%)	25	65

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	255	LEU
1	A	259	LEU
1	A	260	LEU
1	A	271	ASP
1	A	304	ARG
1	A	356	LEU
1	A	428	ASN
1	A	458	GLU
1	A	463	LEU
1	A	497	ARG
1	A	498	LYS
1	A	508	ASN
1	A	510	TYR
1	A	511	LYS
1	A	519	LYS
1	A	529	LYS
1	A	544	LEU
1	A	547	ARG
1	A	575	TYR
1	A	576	ARG
1	A	615	TYR
1	A	640	LEU
1	A	676	ARG
1	A	679	LYS
1	A	680	GLU
1	A	722	ARG
1	A	724	LYS
1	A	808	VAL
1	A	821	LEU
1	A	831	LEU
1	A	860	GLN
1	A	885	ARG
1	A	919	LEU
1	A	930	PHE
1	A	968	THR
1	A	1040	VAL
1	B	214	GLN
1	B	235	LYS
1	B	255	LEU
1	B	258	LYS
1	B	259	LEU
1	B	260	LEU

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Mol	Chain	Res	Type
1	B	269	MET
1	B	356	LEU
1	B	389	LYS
1	B	421	LYS
1	B	428	ASN
1	B	456	LYS
1	B	463	LEU
1	B	498	LYS
1	B	504	LYS
1	B	509	GLU
1	B	510	TYR
1	B	511	LYS
1	B	519	LYS
1	B	529	LYS
1	B	544	LEU
1	B	547	ARG
1	B	575	TYR
1	B	576	ARG
1	B	615	TYR
1	B	640	LEU
1	B	676	ARG
1	B	679	LYS
1	B	680	GLU
1	B	722	ARG
1	B	724	LYS
1	B	767	ARG
1	B	808	VAL
1	B	821	LEU
1	B	831	LEU
1	B	860	GLN
1	B	885	ARG
1	B	899	LYS
1	B	919	LEU
1	B	930	PHE
1	B	968	THR
1	B	1036	LYS
1	B	1040	VAL

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

Mol	Chain	Res	Type
1	A	240	ASN

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Mol	Chain	Res	Type
1	A	244	ASN
1	A	276	HIS
1	A	314	GLN
1	A	359	GLN
1	A	375	GLN
1	A	428	ASN
1	A	457	HIS
1	A	500	GLN
1	A	508	ASN
1	A	585	ASN
1	A	683	GLN
1	A	691	ASN
1	A	695	HIS
1	A	699	HIS
1	A	866	ASN
1	A	888	HIS
1	A	936	ASN
1	B	214	GLN
1	B	240	ASN
1	B	244	ASN
1	B	276	HIS
1	B	314	GLN
1	B	336	GLN
1	B	359	GLN
1	B	375	GLN
1	B	428	ASN
1	B	508	ASN
1	B	585	ASN
1	B	683	GLN
1	B	691	ASN
1	B	695	HIS
1	B	699	HIS
1	B	770	HIS
1	B	866	ASN
1	B	888	HIS
1	B	936	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 carbohydrates 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	758/847 (89%)	0.28	41 (5%) 29 22	27, 27, 27, 27	0
1	B	759/847 (89%)	0.32	43 (5%) 27 20	27, 27, 27, 27	0
All	All	1517/1694 (89%)	0.30	84 (5%) 29 21	27, 27, 27, 27	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	MET	6.5
1	B	549	THR	5.6
1	B	498	LYS	5.4
1	A	969	GLY	5.0
1	B	497	ARG	4.7
1	B	495	PHE	4.5
1	B	571	SER	4.2
1	B	462	PHE	4.0
1	B	653	PRO	4.0
1	B	516	ILE	3.8
1	A	404	ALA	3.8
1	A	944	ASN	3.8
1	B	438	GLY	3.7
1	A	590	GLU	3.7
1	B	501	ILE	3.7
1	A	947	VAL	3.6
1	B	493	LYS	3.6
1	B	507	THR	3.6
1	B	508	ASN	3.6
1	A	956	ILE	3.5
1	B	550	LEU	3.5
1	B	439	GLN	3.4
1	A	945	PRO	3.3
1	A	951	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	546	TYR	3.3
1	A	810	THR	3.3
1	A	488	TYR	3.3
1	A	968	THR	3.2
1	A	811	LYS	3.1
1	A	1044	ASN	3.1
1	B	499	VAL	3.1
1	A	403	SER	3.0
1	A	954	GLU	2.9
1	A	957	ASN	2.9
1	A	970	GLU	2.9
1	A	946	GLU	2.9
1	A	272	GLU	2.8
1	A	651	PRO	2.8
1	A	722	ARG	2.8
1	B	456	LYS	2.7
1	A	806	GLY	2.7
1	B	515	GLU	2.7
1	B	948	LEU	2.6
1	A	1043	SER	2.6
1	B	420	LYS	2.6
1	B	520	ASP	2.6
1	B	492	GLU	2.6
1	B	950	ARG	2.6
1	A	935	THR	2.6
1	B	490	LEU	2.5
1	A	972	GLN	2.5
1	A	1023	PRO	2.5
1	B	570	PRO	2.4
1	B	542	ILE	2.4
1	B	450	LEU	2.4
1	A	487	GLU	2.4
1	A	708	ALA	2.4
1	A	950	ARG	2.3
1	A	943	GLY	2.3
1	B	539	ALA	2.3
1	B	401	SER	2.3
1	B	431	GLY	2.3
1	B	444	PHE	2.3
1	A	365	GLU	2.2
1	A	361	GLU	2.2
1	B	404	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	948	LEU	2.2
1	B	527	SER	2.2
1	B	288	GLU	2.2
1	A	473	SER	2.2
1	A	493	LYS	2.2
1	A	727	LYS	2.2
1	A	586	ILE	2.1
1	B	955	LEU	2.1
1	B	951	HIS	2.1
1	B	548	SER	2.1
1	A	933	TYR	2.1
1	B	526	PHE	2.0
1	B	443	GLU	2.0
1	A	975	GLN	2.0
1	B	403	SER	2.0
1	B	514	PHE	2.0
1	A	955	LEU	2.0
1	A	724	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.