



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:35 am GMT

PDB ID : 1XDV
Title : Experimentally Phased Structure of Human the Son of Sevenless protein at 4.1 Ang.
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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

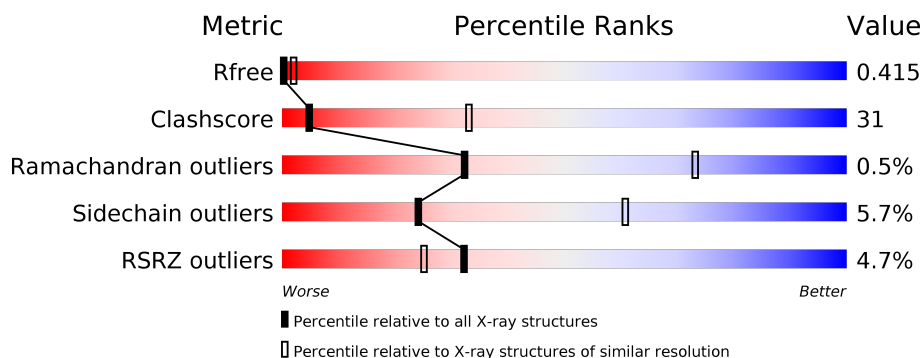
1 Overall quality at a glance

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}	100719	1153 (4.60-3.60)
Clashscore	112137	1002 (4.54-3.66)
Ramachandran outliers	110173	1000 (4.58-3.62)
Sidechain outliers	110143	1191 (4.60-3.60)
RSRZ outliers	101464	1165 (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 ≥ 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>4%</div> <div> <div></div> <div>59%</div> <div>28%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	847	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>29%</div> <div>•</div> <div>10%</div> </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.

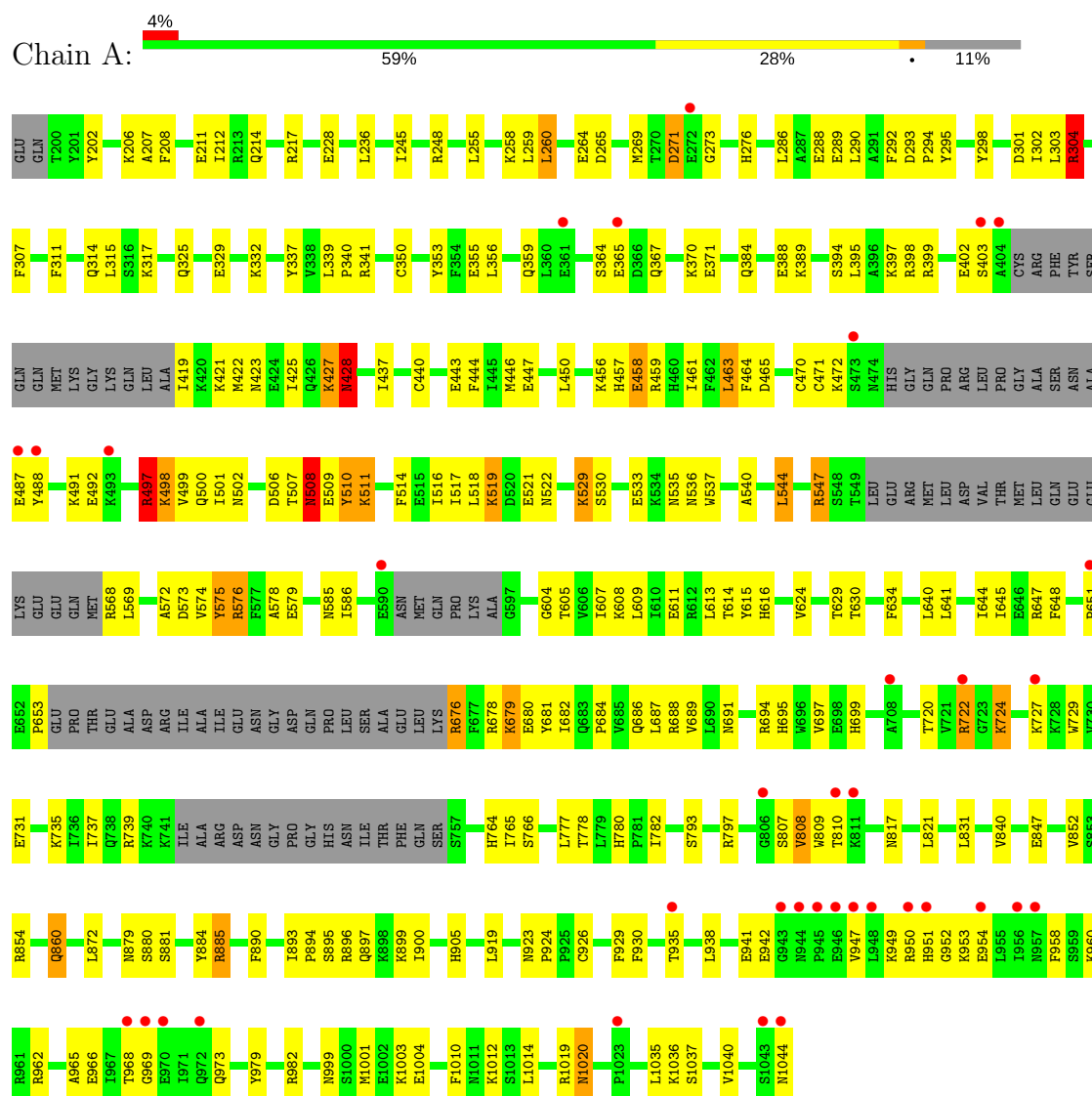
- Molecule 1 is a protein called Son of sevenless protein homolog 1.

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 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: Son of sevenless protein homolog 1



- Molecule 1: Son of sevenless protein homolog 1



T935	R797	R688	H612	B547	ARG	CYS	R301	GLU
L938	P801	V689	L613	SS46	LEU	ARG	I302	GLN
E941	S802	L690	T614	T549	PRO	PHE	L303	T200
E942	S805	N691	Y615	L550	GLY	TYR	R304	Y201
V947	V806	H695	H616	GLU	ALA	SER	R310	Y202
L948	S806	V696	A619	ARG	ASN	GLN	F311	K206
K949	V697	ASP	V624	MET	ALA	MET	Q314	A207
R950	V808	VAL	R625	LEU	E487	LYS	L315	F208
R950	W809	THR	T626	MET	R489	GLY	S316	E211
K953	T810	LEU	T629	LEU	L490	GLN	K317	I212
E954	N817	GLN	T630	GLN	K491	LEU	E213	E213
L955	L821	GLU	L640	GLU	E492	ALA	Q325	Q214
L956	L831	LYS	L644	LYS	K493	ALA	K332	R217
F958	L831	GLU	R647	GLU	F494	K421	E333	E218
S959	V840	GLN	P648	GLN	F495	M422	Q336	L219
R961	E847	MET	E649	MET	M496	N423	Y337	N220
R962	V852	R568	E650	R576	K497	E424	Y338	L221
K963	V853	L569	P651	F577	K498	I425	P340	K224
V964	S853	P652	P653	AS72	V499	Q426	R341	V225
A965	R854	GLU	GLU	D573	Q500	K427	L342	E228
T968	Q860	PRO	THR	D506	I501	N428	C350	K235
Y979	L872	ALA	ALA	N508	N502	G431	Y353	L236
R999	N879	ARG	ASP	F577	D503	I437	F354	N244
S1000	S880	ILE	ILE	E579	K504	G438	E355	L245
M1001	S881	ASP	ILE	E583	D505	Q439	L356	R248
K1003	Y884	GLY	ILE	E584	S516	C440	L357	E254
E1004	R885	PRO	ASN	N585	I517	F444	K358	L255
F1010	F890	GLY	GLY	T586	Y510	M445	E369	K258
M1011	I893	HIS	ASP	E589	K511	E447	E368	L260
K1012	P894	ASN	PRO	E590	E521	G448	E264	E264
L1014	S895	THR	ILE	ASN	S527	H457	E268	E268
R1019	R896	PHE	LEU	MET	A528	E458	E371	R269
M1020	Q897	GLN	SER	PRO	K529	R459	I377	E272
L1035	K898	SER	ALA	LYS	E532	H460	G386	H276
K1036	I900	LYS	GLU	ALA	E532	L461	K389	E288
V1040	H905	LYS	LYS	G597	N535	F463	L395	F292
N1044	A917	R676	R677	T600	N536	D465	R398	D293
	R918	R678	R679	L601	M537	C470	R399	P294
	L919	E680	E681	R602	M538	K472	I400	Y295
	R920	V681	V682	A603	A539	S473	S401	Y298
	C926	I682	I683	T605	L541	N474	E402	A299
	F929	V684	V685	V606	I542	HIS	A404	
	F930	P684	P685	I607	S543	GLY		
		V686	V687	R608	L544	GLN		
		L687	L688	E611	Y546	PRO		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	110.0	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , -10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.75	EDS
Total number of atoms	12516	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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	0.39	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:304:ARG:NE	1:A:307:PHE:HB2	1.54	1.21
1:A:1019:ARG:NH1	1:B:905:HIS:CD2	2.07	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:A:634:PHE:HB2	1:A:958:PHE:CZ	1.83	1.13
1:A:304:ARG:CZ	1:A:307:PHE:HB2	1.78	1.13
1:B:342:LEU:HD22	1:B:550:LEU:HD22	1.14	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:B:268:GLU:CD	1:B:619:ALA:HB1	1.57	1.07
1:A:269:MET:HE3	1:A:729:TRP:CZ2	1.62	1.07
1:A:885:ARG:HB3	1:B:884:TYR:CE2	1.89	1.06
1:B:341:ARG:HG2	1:B:539:ALA:HA	1.34	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:268:GLU:CD	1:B:619:ALA:HB3	1.72	1.04
1:B:602:LYS:HE2	1:B:948:LEU:HD12	1.31	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:304:ARG:CZ	1:A:307:PHE:CB	2.36	1.04
1:A:269:MET:HE3	1:A:729:TRP:CH2	1.92	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:A:884:TYR:HE2	1:B:885:ARG:HB3	1.16	1.00
1:A:935:THR:HG1	1:B:1004:GLU:CD	1.65	1.00
1:B:269:MET:CB	1:B:691:ASN:HD21	1.74	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:A:304:ARG:HH11	1:A:307:PHE:H	0.94	0.94
1:B:269:MET:HB3	1:B:691:ASN:OD1	1.64	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:A:629:THR:HG22	1:A:969:GLY:C	1.95	0.85
1:B:269:MET:CB	1:B:691:ASN:ND2	2.34	0.85
1:A:905:HIS:NE2	1:B:1014:LEU:CD1	2.40	0.85
1:A:881:SER:OG	1:B:881:SER:N	2.10	0.85
1:B:398:ARG:HG2	1:B:532:GLU:CD	1.97	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:499:VAL:CG1	1:B:517:ILE:HB	2.10	0.81
1:B:341:ARG:CZ	1:B:539:ALA:H	1.94	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:220:ASN:HB3	1:B:224:LYS:NZ	1.98	0.78
1:B:584:GLU:HG2	1:B:953:LYS:CG	2.14	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:496:MET:HA	1:B:498:LYS:NZ	1.99	0.77
1:B:342:LEU:CD2	1:B:550:LEU:HD22	2.06	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:A:1001:MET:HE3	1:B:810:THR:HG22	1.67	0.76
1:A:697:VAL:HG11	1:A:737:ILE:HG12	1.67	0.76
1:B:498:LYS:HE2	1:B:498:LYS:O	1.84	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: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:B:341:ARG:HG2	1:B:539:ALA:C	2.06	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:A:1003:LYS:HE3	1:B:929:PHE:CE1	2.21	0.74
1:B:342:LEU:CD2	1:B:550:LEU:CG	2.66	0.74
1:B:402:GLU:OE2	1:B:536:ASN:CA	2.34	0.74
1:B:402:GLU:OE2	1:B:535:ASN:C	2.26	0.74
1:B:584:GLU:CG	1:B:953:LYS:CD	2.57	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:GLU:O	1:B:955:LEU:CD2	2.35	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:A:314:GLN:NE2	1:A:317:LYS:HZ3	1.87	0.73
1:B:446:MET:HE1	1:B:537:TRP:HA	1.70	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:A:207:ALA:O	1:A:211:GLU:HG3	1.91	0.70
1:B:342:LEU:HD22	1:B:550:LEU:CD1	2.09	0.70
1:A:446:MET:HE1	1:A:537:TRP:HA	1.74	0.70
1:B:422:MET:CE	1:B:437:ILE:HG22	2.20	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:A:355:GLU:HG3	1:A:359:GLN:HE21	1.58	0.69
1:A:500:GLN:OE1	1:A:516:ILE:HG12	1.93	0.69
1:B:629:THR:HG22	1:B:805:VAL:HG21	1.74	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:629:THR:HG23	1:B:801:PRO:HB2	1.76	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:218:GLU:HG2	1:B:550:LEU:C	2.15	0.67
1:A:506:ASP:CG	1:A:508:ASN:HB3	2.13	0.67
1:B:337:TYR:CG	1:B:538:MET:HE1	2.29	0.67
1:B:679:LYS:HD2	1:B:679:LYS:O	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:A:276:HIS:HE1	1:A:365:GLU:H	1.42	0.67
1:B:547:ARG:NH1	1:B:547:ARG:HB3	2.09	0.67
1:A:840:VAL:HG13	1:A:1012:LYS:HB3	1.76	0.67
1:B:220:ASN:O	1:B:224:LYS:HG2	1.95	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:529:LYS:HE3	1:A:533:GLU:OE2	1.95	0.66
1:A:630:THR:HG23	1:A:969:GLY:HA3	1.62	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:A:1003:LYS:CE	1:B:929:PHE:HE1	2.08	0.66
1:B:341:ARG:HG3	1:B:403:SER:OG	1.95	0.66
1:A:947:VAL:HG11	1:A:954:GLU:HG3	1.76	0.66
1:B:602:LYS:CA	1:B:958:PHE:HB3	2.25	0.66
1:A:881:SER:HG	1:B:880:SER:C	1.98	0.66
1:A:1019:ARG:CZ	1:B:905:HIS:NE2	2.59	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:A:1003:LYS:HE3	1:B:929:PHE:CZ	2.30	0.65
1:B:614:THR:HG21	1:B:689:VAL:HG23	1.78	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:314:GLN:NE2	1:A:317:LYS:NZ	2.44	0.65
1:A:544:LEU:HA	1:A:547:ARG:NH1	2.11	0.65
1:A:547:ARG:HH11	1:A:547:ARG:HB2	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:929:PHE:HE1	1:B:1003:LYS:CE	2.10	0.65
1:B:793:SER:O	1:B:797:ARG:HG3	1.97	0.65
1:B:336:GLN:NE2	1:B:502:ASN:ND2	2.45	0.65
1:B:500:GLN:NE2	1:B:545:GLN:HB2	2.12	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:446:MET:HE3	1:B:537:TRP:CE3	2.32	0.64
1:B:629:THR:HG23	1:B:801:PRO:CB	2.28	0.64
1:A:630:THR:CB	1:A:969:GLY:HA3	2.20	0.64
1:B:614:THR:HG22	1:B:614:THR:O	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: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: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:459:ARG:HG2	1:A:459:ARG:HH11	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:444:PHE:HZ	1:A:447:GLU:HB2	1.62	0.63
1:A:614:THR:HG22	1:A:614:THR:O	1.98	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:A:419:ILE:HG13	1:A:422:MET:SD	2.39	0.63
1:B:630:THR:CB	1:B:805:VAL:CG1	2.75	0.63
1:B:568:ARG:C	1:B:569:LEU:HD22	2.18	0.63
1:A:402:GLU:CG	1:A:536:ASN:OD1	2.46	0.63
1:B:602:LYS:C	1:B:958:PHE:HB2	2.17	0.63
1:A:780:HIS:CE1	1:A:782:ILE:HD12	2.33	0.62
1:B:235:LYS:HD3	1:B:235:LYS:H	1.64	0.62
1:A:301:ASP:O	1:A:304:ARG:CG	2.46	0.62
1:A:568:ARG:C	1:A:569:LEU:HD22	2.18	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

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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:A:810:THR:HG22	1:B:1001:MET:CE	2.29	0.62
1:B:629:THR:O	1:B:805:VAL:HG21	1.99	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:547:ARG:NH1	1:A:547:ARG:HB2	2.16	0.61
1:A:905:HIS:CD2	1:B:1019:ARG:HH22	2.17	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:260:LEU:HD22	1:A:264:GLU:HG3	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:304:ARG:NE	1:A:304:ARG:H	1.98	0.60
1:A:367:GLN:O	1:A:371:GLU:HG2	2.01	0.60
1:A:840:VAL:CG1	1:A:1012:LYS:HB3	2.32	0.60
1:A:905:HIS:CE1	1:B:1014:LEU:CD1	2.73	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:456:LYS:H	1:B:456:LYS:HE3	1.67	0.59
1:B:630:THR:HG22	1:B:805:VAL:HG21	1.85	0.59
1:A:260:LEU:O	1:A:264:GLU:HG3	2.03	0.59
1:A:905:HIS:CD2	1:B:1019:ARG:NH2	2.70	0.59
1:B:428:ASN:ND2	1:B:487:GLU:N	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:LEU:HD13	1:B:905:HIS:NE2	2.18	0.59
1:B:272:GLU:HG3	1:B:625:ARG:NH2	2.17	0.58
1:A:575:TYR:HD2	1:A:651:PRO:HG2	1.69	0.58
1:B:644:ILE:HG23	1:B:689:VAL:HG13	1.85	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:258:LYS:HA	1:B:258:LYS:NZ	2.19	0.58
1:B:269:MET:HB3	1:B:691:ASN:CG	2.24	0.58
1:A:630:THR:CG2	1:A:969:GLY:CA	2.17	0.57
1:B:458:GLU:CD	1:B:458:GLU:O	2.42	0.57
1:B:269:MET:CB	1:B:691:ASN:OD1	2.45	0.57
1:A:428:ASN:ND2	1:A:487:GLU:N	2.51	0.57
1:B:456:LYS:H	1:B:456:LYS:CE	2.17	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:506:ASP:OD1	1:A:510:TYR:CE2	2.57	0.57
1:A:629:THR:O	1:A:969:GLY:HA2	2.04	0.57
1:A:498:LYS:HB2	1:A:517:ILE:O	2.04	0.57
1:A:271:ASP:CG	1:A:273:GLY:H	2.08	0.57
1:B:276:HIS:CE1	1:B:365:GLU:H	2.22	0.57
1:B:497:ARG:H	1:B:498:LYS:HD3	1.70	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:NH1	1:B:767:ARG:HB2	2.20	0.57
1:B:235:LYS:HD3	1:B:235:LYS:N	2.20	0.56
1:B:218:GLU:CG	1:B:550:LEU:C	2.74	0.56
1:A:1003:LYS:CE	1:B:929:PHE:CE1	2.84	0.56
1:A:419:ILE:HG13	1:A:422:MET:HB2	1.87	0.56
1:B:584:GLU:CD	1:B:953:LYS:HD2	2.25	0.56
1:A:269:MET:HE2	1:A:729:TRP:NE1	2.19	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: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:B:269:MET:CE	1:B:691:ASN:N	2.66	0.56
1:A:276:HIS:CE1	1:A:365:GLU:H	2.22	0.56
1:A:419:ILE:CG1	1:A:422:MET:HB2	2.36	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:A:314:GLN:HE22	1:A:317:LYS:NZ	2.04	0.56
1:B:506:ASP:CG	1:B:508:ASN:HB3	2.24	0.56
1:A:929:PHE:CZ	1:B:1003:LYS:HE3	2.40	0.56
1:A:421:LYS:HZ1	1:A:425:ILE:HD11	1.72	0.55
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: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:A:611:GLU:HA	1:A:647:ARG:NH1	2.22	0.55
1:B:235:LYS:NZ	1:B:235:LYS:HB2	2.21	0.55
1:A:629:THR:HG21	1:A:969:GLY:O	2.00	0.55
1:B:342:LEU:CD1	1:B:550:LEU:CD2	2.74	0.55
1:B:403:SER:OG	1:B:539:ALA:HB1	2.06	0.55
1:B:601:ILE:O	1:B:958:PHE:HD2	1.87	0.55
1:B:269:MET:CA	1:B:691:ASN:ND2	2.69	0.55
1:A:302:ILE:O	1:A:304:ARG:CZ	2.55	0.55
1:B:269:MET:HA	1:B:691:ASN:ND2	2.22	0.55
1:B:504:LYS:HA	1:B:504:LYS:HE3	1.89	0.55
1:B:547:ARG:O	1:B:547:ARG:HD2	2.06	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: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:947:VAL:HG11	1:B:954:GLU:CG	2.37	0.54
1:A:446:MET:HE2	1:A:463:LEU:HD12	1.89	0.54
1:A:499:VAL:CG2	1:A:517:ILE:HB	2.25	0.54
1:B:221:LEU:CD1	1:B:549:THR:OG1	2.54	0.54
1:B:629:THR:HG21	1:B:968:THR:HG21	1.89	0.54
1:B:630:THR:HG22	1:B:805:VAL:CG1	2.38	0.54
1:B:519:LYS:O	1:B:519:LYS:HD3	2.06	0.54
1:B:630:THR:HG22	1:B:805:VAL:HG22	1.88	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: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:217:ARG:NH2	1:B:548:SER:C	2.44	0.53
1:B:611:GLU:HA	1:B:647:ARG:NH1	2.22	0.53
1:A:511:LYS:O	1:A:511:LYS:HD2	2.09	0.53
1:A:402:GLU:HG3	1:A:536:ASN:OD1	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:498:LYS:HD2	1:B:518:LEU:HD13	1.89	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:A:498:LYS:CG	1:A:518:LEU:HD23	2.38	0.53
1:B:603:ALA:HA	1:B:956:ILE:HB	1.91	0.53
1:A:304:ARG:NH1	1:A:307:PHE:HB2	2.09	0.53
1:A:421:LYS:NZ	1:A:425:ILE:HD11	2.24	0.53
1:B:604:GLY:H	1:B:956:ILE:CG1	2.22	0.53
1:A:394:SER:O	1:A:398:ARG:HG2	2.09	0.53
1:A:947:VAL:HG11	1:A:954:GLU:CG	2.37	0.53
1:B:695:HIS:CD2	1:B:699:HIS:HD2	2.27	0.53
1:B:963:LYS:HZ2	1:B:963:LYS:HB3	1.73	0.53
1:B:245:ILE:HD11	1:B:314:GLN:HG2	1.91	0.53
1:B:500:GLN:CD	1:B:545:GLN:HB2	2.29	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: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: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: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: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:780:HIS:HE1	1:A:782:ILE:HD12	1.74	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:A:302:ILE:C	1:A:304:ARG:HH21	2.13	0.51
1:B:601:ILE:O	1:B:958:PHE:CG	2.63	0.51
1:B:890:PHE:HA	1:B:893:ILE:HD12	1.93	0.51
1:A:311:PHE:O	1:A:315:LEU:HD13	2.09	0.51
1:B:337:TYR:CD1	1:B:538:MET:HE2	2.42	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:780:HIS:HE1	1:A:782:ILE:CD1	2.24	0.50
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:727:LYS:O	1:A:731:GLU:HG3	2.12	0.50
1:B:602:LYS:CA	1:B:958:PHE:CB	2.89	0.50
1:A:890:PHE:HA	1:A:893:ILE:HD12	1.93	0.50
1:A:206:LYS:NZ	1:A:206:LYS:HB3	2.26	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: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:A:648:PHE:HE2	1:A:722:ARG:NH1	2.09	0.50
1:A:896:ARG:HG2	1:A:896:ARG:HH11	1.77	0.50
1:B:630:THR:HB	1:B:805:VAL:CG1	2.41	0.50
1:B:727:LYS:O	1:B:731:GLU:HG3	2.12	0.50
1:A:399:ARG:O	1:A:402:GLU:HB3	2.12	0.50
1:B:399:ARG:O	1:B: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:A:926:CYS:HA	1:A:979:TYR:OH	2.13	0.49
1:B:235:LYS:HZ3	1:B:235:LYS:HB2	1.77	0.49
1:B:496:MET:CA	1:B:498:LYS:HZ3	2.17	0.49
1:B:579:GLU:O	1:B:608:LYS:HE2	2.12	0.49
1:B:648:PHE:HE2	1:B:722:ARG:NH1	2.09	0.49
1:A:579:GLU:O	1:A:608:LYS:HE2	2.12	0.49
1:B:446:MET:CE	1:B:463:LEU:HD12	2.43	0.49
1:B:498:LYS:N	1:B:498:LYS:HD3	2.26	0.49
1:B:926:CYS:HA	1:B:979:TYR:OH	2.13	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:A:458:GLU:H	1:A:458:GLU:CD	2.16	0.49
1:A:720:THR:O	1:A:722:ARG:HD3	2.13	0.49
1:B:337:TYR:CD1	1:B:538:MET:CE	2.95	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: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
1:A:1003:LYS:HE2	1:B:929:PHE:HE1	1.76	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:499:VAL:HG23	1:B:545:GLN:HE22	1.79	0.48
1:B:269:MET:SD	1:B:687:LEU:HG	2.53	0.48
1:B:720:THR:O	1:B:722:ARG:HD3	2.13	0.48
1:A:808:VAL:HG11	1:A:817:ASN:HB3	1.95	0.48
1:B:603:ALA:C	1:B:956:ILE:HB	2.31	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: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:B:603:ALA:CA	1:B:956:ILE:CB	2.89	0.48
1:A:265:ASP:HB3	1:A:687:LEU:CD2	2.41	0.48
1:B:456:LYS:N	1:B:456:LYS:HE3	2.28	0.48
1:B:398:ARG:CG	1:B:532:GLU:CD	2.72	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:260:LEU:HD22	1:B:264:GLU:CG	2.44	0.48
1:B:498:LYS:HG2	1:B:517:ILE:O	2.14	0.48
1:B:496:MET:SD	1:B:498:LYS:NZ	2.86	0.48
1:A:423:ASN:O	1:A:427:LYS:HG3	2.14	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:B:543:SER:HA	1:B:550:LEU:HD12	1.96	0.48
1:B:586:ILE:HG13	1:B:608:LYS:HG2	1.94	0.47
1:B:963:LYS:NZ	1:B:963:LYS:HB3	2.28	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:500:GLN:C	1:A:501:ILE:HD12	2.35	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:B:941:GLU:HA	1:B:960:LYS:HE3	1.96	0.47
1:A:547:ARG:HH11	1:A:547:ARG:CB	2.27	0.47
1:A:576:ARG:HB3	1:A:578:ALA:H	1.78	0.47
1:B:506:ASP:OD2	1:B:510:TYR:CE2	2.67	0.47
1:B:575:TYR:O	1:B:576:ARG:HG2	2.14	0.47
1:B:735:LYS:HE3	1:B:739:ARG:HH21	1.79	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:310:ARG:HH21	1:B:310:ARG:HG2	1.79	0.47
1:B:499:VAL:HG11	1:B:517:ILE:HD12	1.97	0.47
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.80	0.47
1:A:304:ARG:HD2	1:A:307:PHE:N	2.30	0.47
1:A:314:GLN:HE21	1:A:317:LYS:HZ3	1.62	0.47
1:A:935:THR:CB	1:B:1004:GLU:OE2	2.58	0.47
1:B:457:HIS:NE2	1:B:459:ARG:NH1	2.63	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: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:B:421:LYS:O	1:B:425:ILE:HG13	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:530:SER:OG	1:A:533:GLU:HG3	2.15	0.46
1:A:446:MET:CE	1:A:540:ALA:HB3	2.45	0.46
1:A:676:ARG:HG2	1:A:676:ARG:HH11	1.79	0.46
1:A:507:THR:C	1:A:509:GLU:N	2.67	0.46
1:A:510:TYR:O	1:A:510:TYR:CD1	2.69	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:B:498:LYS:CG	1:B:517:ILE:O	2.64	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:A:398:ARG:CA	1:A:398:ARG:HH21	2.28	0.46
1:A:735:LYS:CE	1:A:739:ARG:HH21	2.28	0.46
1:B:457:HIS:CD2	1:B:472:LYS:HG3	2.51	0.46
1:B:269:MET:HE3	1:B:691:ASN:N	2.13	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:272:GLU:CG	1:B:625:ARG:NH2	2.79	0.46
1:B:507:THR:C	1:B:509:GLU:N	2.67	0.46
1:B:510:TYR:CD1	1:B:510:TYR:O	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:GLU:HA	1:A:228:GLU:OE1	2.15	0.45
1:A:458:GLU:HG2	1:A:458:GLU:O	2.17	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:605:THR:HG22	1:B:607:ILE:H	1.80	0.45
1:B:735:LYS:HD3	1:B:735:LYS:O	2.15	0.45
1:A:202:TYR:CE2	1:A:206:LYS:HD2	2.51	0.45
1:A:497:ARG:NH2	1:A:519:LYS:HB3	2.31	0.45
1:B:584:GLU:HG2	1:B:953:LYS:HG3	1.97	0.45
1:B:603:ALA:CB	1:B:955:LEU:C	2.62	0.45
1:A:629:THR:HG23	1:A:969:GLY:O	2.04	0.45
1:B:254:GLU:O	1:B:258:LYS:HG2	2.17	0.45
1:B:499:VAL:CG1	1:B:517:ILE:HD12	2.46	0.45
1:B:506:ASP:C	1:B:508:ASN:N	2.68	0.45
1:B:519:LYS:HD3	1:B:520:ASP:OD2	2.17	0.45
1:A:398:ARG:HB3	1:A:398:ARG:NH2	2.31	0.45
1:A:470:CYS:HB2	1:A:492:GLU:HB2	1.99	0.45
1:A:682:ILE:HG23	1:A:686:GLN:HE21	1.82	0.45
1:A:609:LEU:HD21	1:A:962:ARG:NH1	2.32	0.45
1:B:202:TYR:CD2	1:B:206:LYS:HD2	2.52	0.45
1:B:650:ILE:HA	1:B:651:PRO:HD3	1.82	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:767:ARG:HD3	1:B:767:ARG:N	2.31	0.45
1:A:389:LYS:HD3	1:A:389:LYS:O	2.16	0.45
1:B:421:LYS:NZ	1:B:425:ILE:HG13	2.32	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:O	1:A:574:VAL:HG12	2.17	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:B:547:ARG:HD2	1:B:547:ARG:C	2.37	0.44
1:A:456:LYS:HD3	1:A:456:LYS:O	2.18	0.44
1:A:609:LEU:HD21	1:A:962:ARG:HH11	1.82	0.44
1:A:885:ARG:HD2	1:B:884:TYR:CZ	2.52	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:A:847:GLU:HG2	1:A:1035:LEU:HD21	1.98	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:B:298:TYR:CE2	1:B:302:ILE:HG13	2.52	0.44
1:B:402:GLU:OE2	1:B:535:ASN:HB2	2.18	0.44
1:B:341:ARG:NH2	1:B:536:ASN:C	2.71	0.44
1:A:364:SER:HB3	1:A:370:LYS:HG3	1.99	0.44
1:A:500:GLN:HE22	1:A:516:ILE:HG12	1.82	0.44
1:A:722:ARG:N	1:A:722:ARG:HD3	2.33	0.44
1:B:457:HIS:NE2	1:B:472:LYS:HD2	2.33	0.44
1:B:498:LYS:CD	1:B:518:LEU:HD13	2.47	0.44
1:B:568:ARG:NH1	1:B:616:HIS:CE1	2.86	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:457:HIS:CD2	1:A:472:LYS:NZ	2.86	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:248:ARG:NE	1:A:248:ARG:HA	2.33	0.43
1:A:942:GLU:OE2	1:B:999:ASN:ND2	2.52	0.43
1:B:364:SER:HB3	1:B:370:LYS:HG3	1.99	0.43
1:B:682:ILE:HG23	1:B:686:GLN:HE21	1.82	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:358:LYS:HE2	1:B:358:LYS:HA	2.01	0.43
1:B:422:MET:HG2	1:B:464:PHE:HE2	1.83	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:872:LEU:HD12	1:A:929:PHE:CG	2.53	0.43
1:A:1010:PHE:HE2	1:B:905:HIS:HE1	1.66	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: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:208:PHE:CE1	1:B:353:TYR:HE1	2.37	0.43
1:B:722:ARG:N	1:B:722:ARG:HD3	2.33	0.43
1:A:339:LEU:N	1:A:340:PRO:HD2	2.34	0.43
1:A:422:MET:HG2	1:A:464:PHE:HE2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ASP:OD1	1:A:510:TYR:CD2	2.72	0.42
1:A:629:THR:CG2	1:A:969:GLY:C	2.67	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:402:GLU:CD	1:B:535:ASN:C	2.75	0.42
1:B:422:MET:HG2	1:B:464:PHE:CE2	2.54	0.42
1:A:1019:ARG:CZ	1:B:905:HIS:CG	2.99	0.42
1:A:271:ASP:OD2	1:A:273:GLY:N	2.51	0.42
1:A:422:MET:HG2	1:A:464:PHE:CE2	2.54	0.42
1:B:341:ARG:NH2	1:B:539:ALA:H	2.14	0.42
1:A:341:ARG:NH2	1:A:536:ASN:HA	2.34	0.42
1:A:292:PHE:HE2	1:A:353:TYR:CE2	2.36	0.42
1:A:419:ILE:O	1:A:419:ILE:HG12	2.19	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: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:A:325:GLN:HG3	1:A:332:LYS:HD2	2.02	0.42
1:A:395:LEU:HD22	1:A:395:LEU:N	2.35	0.42
1:B:516:ILE:HG22	1:B:518:LEU:HD22	2.01	0.42
1:A:764:HIS:CG	1:A:765:ILE:N	2.88	0.42
1:A:852:VAL:HG11	1:A:893:ILE:HD11	2.01	0.42
1:A:500:GLN:CD	1:A:516:ILE:HG12	2.38	0.42
1:A:764:HIS:CG	1:A:765:ILE:H	2.38	0.42
1:B:506:ASP:OD1	1:B:510:TYR:CG	2.73	0.42
1:B:852:VAL:HG11	1:B:893:ILE:HD11	2.01	0.42
1:B:603:ALA:HA	1:B:956:ILE:CB	2.48	0.42
1:A:572:ALA:O	1:A:573:ASP:HB3	2.20	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:B:395:LEU:HD22	1:B:395:LEU:N	2.35	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: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:A:879:ASN:CG	1:B:1010:PHE:CZ	2.93	0.41
1:B:572:ALA:O	1:B:573:ASP:HB3	2.20	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
1:B:780:HIS:HE1	1:B:782:ILE:CG1	2.33	0.41
1:B:630:THR:CG2	1:B:805:VAL:CG1	2.98	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:325:GLN:HG3	1:B:332:LYS:HD2	2.02	0.41
1:B:506:ASP:O	1:B:506:ASP:OD1	2.39	0.41
1:A:544:LEU:CA	1:A:547:ARG:HH12	2.26	0.41
1:B:465:ASP:HA	1:B:544:LEU:HD21	2.02	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:A:880:SER:CA	1:B:881:SER:HG	2.34	0.41
1:B:896:ARG:HG3	1:B:897:GLN:N	2.36	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:518:LEU:HB2	1:B:521:GLU:HB2	2.02	0.41
1:B:600:ILE:HG23	1:B:962:ARG:HH12	1.77	0.41
1:A:295:TYR:CD1	1:A:350:CYS:HB2	2.55	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: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: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:295:TYR:CD1	1:B:350:CYS:HB2	2.55	0.41
1:B:547:ARG:NH1	1:B:548:SER:N	2.64	0.41
1:B:640:LEU:HD13	1:B:696:TRP:CZ3	2.56	0.41
1:A:212:ILE:CG2	1:A:260:LEU:HG	2.51	0.40
1:B:244:ASN:HB3	1:B:310:ARG:CZ	2.50	0.40
1:B:371:GLU:HA	1:B:371:GLU:OE1	2.21	0.40
1:B:459:ARG:NE	1:B:492:GLU:OE1	2.54	0.40
1:A:585:ASN:HB3	1:A:608:LYS:HG2	2.02	0.40
1:B:421:LYS:HZ3	1:B:425:ILE:HG13	1.84	0.40
1:A:641:LEU:O	1:A:645:ILE:HG13	2.21	0.40
1:A:506:ASP:C	1:A:508:ASN:H	2.25	0.40
1:A:568:ARG:NH1	1:A:681:TYR:CD2	2.88	0.40
1:B:498:LYS:HB2	1:B:517:ILE:O	2.20	0.40
1:B:506:ASP:C	1:B:508:ASN:H	2.25	0.40
1:B:576:ARG:HD3	1:B:577:PHE:H	1.87	0.40
1:B:629:THR:HG23	1:B:801:PRO:HB3	1.99	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 [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	744/847 (88%)	709 (95%)	31 (4%)	4 (0%)	32	73
1	B	745/847 (88%)	710 (95%)	31 (4%)	4 (0%)	32	73
All	All	1489/1694 (88%)	1419 (95%)	62 (4%)	8 (0%)	32	73

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	698/773 (90%)	661 (95%)	37 (5%)	26	63
1	B	699/773 (90%)	656 (94%)	43 (6%)	21	58
All	All	1397/1546 (90%)	1317 (94%)	80 (6%)	24	61

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, 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	758/847 (89%)	0.22	36 (4%) 32 25	27, 27, 27, 27	0
1	B	759/847 (89%)	0.27	36 (4%) 32 25	27, 27, 27, 27	0
All	All	1517/1694 (89%)	0.24	72 (4%) 32 25	27, 27, 27, 27	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	496	MET	6.2
1	B	549	THR	5.3
1	B	498	LYS	5.3
1	A	969	GLY	4.7
1	B	497	ARG	4.6
1	B	495	PHE	4.3
1	B	571	SER	4.0
1	B	653	PRO	3.9
1	B	462	PHE	3.8
1	A	944	ASN	3.7
1	B	516	ILE	3.6
1	B	493	LYS	3.5
1	A	590	GLU	3.5
1	A	404	ALA	3.5
1	B	508	ASN	3.5
1	B	438	GLY	3.5
1	B	501	ILE	3.4
1	A	947	VAL	3.4
1	B	507	THR	3.3
1	A	956	ILE	3.3
1	B	439	GLN	3.3
1	B	550	LEU	3.3
1	A	945	PRO	3.2
1	A	951	HIS	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	811	LYS	3.1
1	A	810	THR	3.0
1	A	1044	ASN	3.0
1	A	968	THR	3.0
1	B	546	TYR	3.0
1	A	488	TYR	2.9
1	B	499	VAL	2.9
1	A	403	SER	2.8
1	A	957	ASN	2.8
1	A	954	GLU	2.8
1	A	651	PRO	2.8
1	A	970	GLU	2.8
1	A	946	GLU	2.7
1	A	272	GLU	2.7
1	A	722	ARG	2.7
1	B	456	LYS	2.7
1	B	420	LYS	2.6
1	B	515	GLU	2.6
1	A	806	GLY	2.6
1	A	1043	SER	2.5
1	B	520	ASP	2.5
1	B	950	ARG	2.5
1	B	492	GLU	2.4
1	B	948	LEU	2.4
1	A	1023	PRO	2.4
1	A	935	THR	2.4
1	A	972	GLN	2.3
1	B	570	PRO	2.3
1	B	490	LEU	2.3
1	A	487	GLU	2.3
1	A	950	ARG	2.2
1	B	542	ILE	2.2
1	B	401	SER	2.2
1	B	450	LEU	2.2
1	A	943	GLY	2.2
1	B	431	GLY	2.1
1	A	708	ALA	2.1
1	A	493	LYS	2.1
1	B	444	PHE	2.1
1	A	365	GLU	2.1
1	A	361	GLU	2.1
1	A	727	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	539	ALA	2.1
1	B	527	SER	2.1
1	A	473	SER	2.1
1	B	288	GLU	2.1
1	B	548	SER	2.0
1	A	948	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.